libatomprobe

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Namespace Documentation

5.1 AtomProbe Namespace Reference

Classes

- class AbundanceData

  Class to load abundance information for natural isotopes.
- struct ATO_ENTRY
- class AxisCompare

  Functor allowing for sorting of points in 3D.
- struct BACKGROUND_PARAMS
- class BodyCentredCubicGen
- class BoundCube

  Helper class to define a bounding cube.
- class ComparePairFirst
- class ComparePairFirstReverse
- class ComparePairSecond
- class CrystalGen
- class EPOS_ENTRY
- class FaceCentredCubicGen
- struct FLATTENED_RANGE

  Structure that allows for the multirange data to be mapped into.
- class GnomonicProjection
- class IonHit

  This is a data holding class for POS file ions, from.
- struct IONHIT

  Record as stored in a .POS file.
- struct ISOTOPE_ENTRY
- class K3DNodeApprox

  Node Class for storing point.
- class K3DNodeExact

  Node Class for storing point.
- class K3DTreeApprox

  3D specific KD tree
- class K3DTreeExact

  3D specific KD tree

- class LibVersion

  Class to hold the library version data.
- class LINE
- class LinearFeedbackShiftReg

  This class implements a Linear Feedback Shift Register (in software)
- class MassTool

  Class that brute-force solves the knapsack problem.
- class Mesh

  Simple mesh class for storing and manipulating meshes consisting of 2 and 3D simplexes (triangles or tetrahedra)
- class MILLER_TRIPLET
- class ModifiedFocusSphericProjection
- class MultiRange

  Data storage and retrieval class for "ranging" a spectra, where overlapping ranges are permitted.
- struct OVERLAP_PROBLEM_SETTINGS
- class Point3D

  A 3D point data class storage.
- struct Point3f

  Data storage structure for points.
- class ProgressBar
- struct Quaternion

  Data storage structure for quaternions.
- class RandNumGen
- struct RANGE_MOLECULE
- class RangeFile

  Data storage and retrieval class for various range files.
- class ReconstructionSphereOnCone
- class RGBf

  Data holder for colour as float.
- struct SIMPLE_SPECIES
- class SimpleCubicGen
- struct SINGLE_HIT

  Single 3DAP hit event.
- class SphericPlaneProjection
- struct SphericProjectionParams
- class StereographicProjection
- class TETRAHEDRON
- struct THREEDAP_DATA

  experimental setup data
- struct THREEDAP_EXPERIMENT

  Data structure that contains the experiment information present in a 3Dap file.
- class TRIANGLE
- struct TriangleWithIndexedVertices
- class TriangleWithVertexNorm
- struct VOLTAGE_DATA

  Voltage data structure – these updates occur periodically during the experiment.
- class Voxels

  Template class that stores 3D voxel data.
- class Weight

  Placeholder class for containing input weights for MassTool.
- struct ZECH_ROOT

Typedefs

- typedef struct AtomProbe::ATO_ENTRY ATO_ENTRY
- typedef struct AtomProbe::IONHIT IONHIT

  Record as stored in a .POS file.

Enumerations

- enum { HULL_SURFREDUCE_NEGATIVE_SCALE_FACT =1, HULL_ERR_USER_ABORT, HULL_ERR_NO_MEM }
- enum PointDir { POINTDIR_TOGETHER =0, POINTDIR_IN_COMMON, POINTDIR_APART }
- enum { BOUND_CLIP =1, BOUND_HOLD, BOUND_DERIV_HOLD, BOUND_MIRROR, BOUND_ZERO, BOUND_ENUM_END }

  Boundary clipping mode.
- enum { VOX_INTERP_NONE, VOX_INTERP_LINEAR, VOX_INTERP_ENUM_END }
- enum { ADJ_ALL, ADJ_PLUS }
- enum { VOXELS_BAD_FILE_READ =1, VOXELS_BAD_FILE_OPEN, VOXELS_BAD_FILE_SIZE, VOXELS_OUT_OF_MEMORY }
- enum { CLIP_NONE =0, CLIP_LOWER_SOUTH_WEST, CLIP_UPPER_NORTH_EAST }

  Clipping direction constants.
- enum { VOXEL_ABORT_ERR, VOXEL_MEMORY_ERR, VOXEL_BOUNDS_INVALID_ERR }
- enum { PROP_PARSE_ERR = 1, PROP_BAD_ATT }
- enum { RECORDREAD_ERR_GET_FILESIZE =1, RECORDREAD_ERR_FILESIZE_MODULO, RECORDREAD_ERR_FILE_OPEN, RECORDREAD_ERR_NOMEM, RECORDREAD_BAD_FILEREAD, RECORDREAD_ERR_CHUNKOFFSET, RECORDREAD_BAD_RECORD }
- enum { ATO_OPEN_FAIL =1, ATO_EMPTY_FAIL, ATO_SIZE_ERR, ATO_VERSIONCHECK_ERR, ATO_MEM_ERR, ATO_BAD_ENDIAN_DETECT, ATO_ENUM_END }
- enum { TEXT_ERR_FILE_OPEN =1, TEXT_ERR_FILE_NUM_FIELDS, TEXT_ERR_FILE_FORMAT }
- enum { OPSREADER_FORMAT_CLINE_ERR =1, OPSREADER_FORMAT_DETECTORLINE_ERR, OPSREADER_FORMAT_LINE_DASH_ERR, OPSREADER_FORMAT_LINE_VOLTAGE_ERR, OPSREADER_FORMAT_LINE_VOLTAGE_NOBETA, OPSREADER_FORMAT_LINE_VOLTAGE_DATA_ERR, OPSREADER_FORMAT_LINE_VOLTAGE_DATACOUNT_ERR, OPSREADER_FORMAT_LINETYPE_ERR, OPSREADER_FORMAT_CHANNELS_ERR, OPSREADER_CHANNELS_DATA_ERR, OPSREADER_FORMAT_SLINE_EVENTCOUNT_ERR, OPSREADER_FORMAT_SLINE_EVENTDATA_ERR, OPSREADER_FORMAT_SLINE_FORMAT_ERR, OPSREADER_FORMAT_SLINE_PREFIX_ERR, OPSREADER_FORMAT_DUPLICATE_SYSDATA, OPSREADER_FORMAT_DUPLICATE_DETECTORSIZE, OPSREADER_FORMAT_TRAILING_DASH_ERR, OPSREADER_FORMAT_DOUBLEDASH, OPSREADER_OPEN_ERR, OPSREADER_READ_ERR, OPSREADER_ABORT_ERR, OPSREADER_ENUM_END }

  Error codes for OPS file loading.
- enum { MULTIRANGE_FORMAT_XML }
- enum { RANGE_FORMAT_ORNL, RANGE_FORMAT_DBL_ORNL, RANGE_FORMAT_ENV, RANGE_FORMAT_RRNG, RANGE_FORMAT_END_OF_ENUM }

- enum {
  RANGE_ERR_FORMAT =1, RANGE_ERR_FORMAT_HEADER, RANGE_ERR_EMPTY, RANGE_ERR_↩
  FORMAT_LONGNAME,
  RANGE_ERR_FORMAT_SHORTNAME, RANGE_ERR_FORMAT_COLOUR, RANGE_ERR_FORMAT_↩
  TABLESEPARATOR, RANGE_ERR_FORMAT_MASS_PAIR,
  RANGE_ERR_FORMAT_TABLE_ENTRY, PARSE_RANGE_FORMAT_GENERIC_FAIL, RANGE_ERR_↩
  DATA_TOO_MANY_USELESS_RANGES, RANGE_ERR_DATA_FLIPPED,
  RANGE_ERR_DATA_INCONSISTENT, RANGE_ERR_DATA_NOMAPPED_IONNAME, RANGE_ERR_↩
  OPEN, RANGE_ERR_FORMAT_RANGETABLE,
  RANGE_ERR_FORMAT_TABLEHEADER_NUMIONS, RANGE_ERR_NONUNIQUE_POLYATOMIC, RA↩
  NGE_ERR_TOO_LARGE, RANGE_ERR_DASHHEADER,
  RANGE_ERR_IONBLOCK_CONTENT, RANGE_ERR_NUMIONS, RANGE_ERR_NUMIONS_DUPLICA↩
  TED, RANGE_ERR_TOO_MANYIONS,
  RANGE_ERR_ION_BLOCK_NOT_PRESENT, RANGE_ERR_DUPLICATE_NUMRANGES, RANGE_ER↩
  R_NUMRANGE_PARSE, RANGE_ERR_RRNG_IONS_TOOSHORT,
  RANGE_ERR_RRNG_COLON_SEPARATOR, RANGE_ERR_BADCOLOUR, RANGE_ERR_ION_NOT_↩
  MAPPED, RANGE_ERR_BADSTART,
  RANGE_ERR_BADEND, RANGE_ERR_NAME_EMPTY, RANGE_ERR_BAD_LINE_RANGEBLOCK, RA↩
  NGE_ERR_MISSING_IONBLOCK,
  RANGE_ERR_NO_RANGES, RANGE_ERR_NO_BASIC_IONS, RANGE_ERR_MISMATCHED_NUMRA↩
  NGES, RANGE_ERR_RANGEBLOCK_FORMAT,
  RANGE_ERR_BAD_MULTIPLICITY, RANGE_ERR_FORMAT_EMPTY_RANGEROW, RANGE_ERR_FI↩
  LESIZE, RANGE_ERR_ENUM_END }
- enum {
  COMPPARSE_BAD_INPUT_FORMAT =1, COMPPARSE_BAD_COMP_VALUE, COMPPARSE_BAD_B↩
  AL_USAGE, COMPPARSE_BAD_SYMBOL,
  COMPPARSE_DUPLICATE_SYMBOL, COMPPARSE_BAD_TOTAL_COMP }

  composition parsing error messages
- enum { CRYSTAL_BAD_UNIT_CELL, CRYSTAL_ENUM_END }
- enum { LATTICE_FCC, LATTICE_BCC, LATTICE_HCP, LATTICE_END_OF_ENUM }
- enum { ELEMENT_TRIANGLE =1, ELEMENT_TETRAHEDRON =2, ELEMENT_LINE =4 }
- enum { EVOLUTION_MODE_SHANKANGLE }
- enum { BACK_FIT_MODE_CONST_TOF, BACK_FIT_MODE_ENUM_END }

  Background fitting modes.
- enum {
  POS_ALLOC_FAIL =1, POS_OPEN_FAIL, POS_SIZE_MODULUS_ERR, POS_SIZE_EMPTY_ERR,
  POS_READ_FAIL, POS_NAN_LOAD_ERROR, POS_FILE_ENUM_END }
- enum { TAPSIM_FILE_FORMAT_FAIL =1, TAPSIM_OPEN_FAIL }
- enum {
  MULTIRANGE_ERR_NO_PARSER =1, MULTIRANGE_ERR_NO_XML_DOC, MULTIRANGE_ERR_NO↩
  _XML_CONTEXT, MULTIRANGE_ERR_NO_NODEPTR,
  MULTIRANGE_NOT_VALID_ROOTNODE, MULTIRANGE_ERR_NO_CONTENT, MULTIRANGE_ERR_↩
  NO_TIMESTAMP, MULTIRANGE_ERR_NO_MOLECULES,
  MULTIRANGE_ERR_NO_MOLECULE_ENTRIES, MULTIRANGE_ERR_MOL_MISSING_ENTRY, MULT↩
  IRANGE_ERR_MOL_MISSING_NAME, MULTIRANGE_ERR_MOL_MISSING_COMPONENTS,
  MULTIRANGE_ERR_BAD_RANGE, MULTIRANGE_ERR_BAD_RANGES, MULTIRANGE_ERR_MOL_↩
  MISSING_COLOUR, MULTIRANGE_ERR_MOL_BAD_COLOUR,
  MULTIRANGE_ERR_NO_RANGES, MULTIRANGE_ERR_BAD_GROUP, MULTIRANGE_ERR_SELF_I↩
  NCONSISTENT, MULTIRANGE_ERR_RANGE_NOPARENT,
  MULTIRANGE_ERR_ENUM_END }
- enum {
  MESH_LOAD_UNSPECIFIED_ERROR =1, MESH_LOAD_BAD_NODECOUNT, MESH_LOAD_BAD_EL↩
  EMENTCOUNT, MESH_LOAD_IS_INSANE,
  MESH_LOAD_ENUM_END }

Functions

- unsigned int generate1DAxialDistHist (const std::vector< Point3D > &pointList, K3DTreeExact &tree, const Point3D &axisDir, float distMax, std::vector< unsigned int > &histogram)

  Generate a 1D axial distribution function,.
- unsigned int generate1DAxialDistHistSweep (const std::vector< Point3D > &pointList, K3DTreeExact &tree, float distMax, float dTheta, float dPhi, ProgressBar &prog, std::vector< std::vector< std::vector< unsigned int > > > &histogram)

  Generate a series of 1D distribution functions, one per pixel in a 2D grid of spherical coordinate directions.
- void computeIonDistAdjacency (const MultiRange &mrf, const AbundanceData &abundance, const OVERLAP_PROBLEM_SETTINGS &settings, gsl_matrix *&m, gsl_vector *&vOwnership, gsl_vector *&vMass)

  Calculate the adjacency matrix for the ions in a multirange.
- unsigned int GetReducedHullPts (const std::vector< IonHit > &points, float reductionDim, unsigned int *progress, bool(*callback)(bool), std::vector< IonHit > &pointResult)

  Obtain a set of points that are a subset of points the convex hull that are at least "reductionDim" away from the hull itself.
- unsigned int computeConvexHull (const std::vector< IonHit > &data, unsigned int *progress, bool(*callback)(bool), std::vector< Point3D > &curHull, bool freeHull)

  Obtain the convex hull of a set of ions.
- void filterPeakNeedBiggerObs (const AbundanceData &massTable, const std::vector< float > &peakData, float tolerance, size_t solutionCharge, std::vector< std::vector< ISOTOPE_ENTRY > > &solutions)
- void filterBySolutionPPM (const AbundanceData &massTable, float minPpm, std::vector< std::vector< ISOTOPE_ENTRY > > &solutions)

  Use the maximum possible PPM for each isotopic combination to filter possible solutions.
- std::vector< float > maxExplainedFraction (const std::vector< std::pair< float, float > > &massData, float peakMass, float massWidth, const std::vector< std::vector< ISOTOPE_ENTRY > > &solutions, const AbundanceData &massTable, float massDistTol, unsigned int solutionCharge)

  Compute the fraction of the data that has been explained, using the natural abundance information, and intensity data.
- bool correlationHistogram (const std::vector< EPOS_ENTRY > &eposIons, std::vector< std::vector< unsigned int > > &histogram, float stepMass, float endMass, bool lowerTriangular=false)

  Generates an ion "correlation histogram" from a vector of EPOS ions. The input vector MUST
- bool accumulateCorrelationHistogram (const std::vector< EPOS_ENTRY > &eposIons, std::vector< std::vector< unsigned int > > &histogram, float stepMass, float endMass, bool lowerTriangular=true)

  Increments a correlation histogram, as per correlationHistogram,.
- template<class T >
  void linearHistogram (const std::vector< T > &data, T start, T end, T step, std::vector< T > &histVals)
- void marchingCubes (const Voxels< float > &v, float isoValue, std::vector< TriangleWithVertexNorm > &tVec)
- void checkMassRangingCorrectness (const RangeFile &rng, AbundanceData &massTable, float massTolerance, unsigned int maxChargeState, unsigned int maxComponents, std::vector< bool > &badRanges)

  Ensure that each mass given spans a peak that should exist.
- void computeRotationMatrix (const Point3D &ur1, const Point3D &ur2, const Point3D &r1, const Point3D &r2, gsl_matrix *m)
- void setHardAssert (bool enabled)

  Do assertions cause a straight up crash (enabled), or write a mesage to stderr (disabled)? By default, hard crash.
- void askAssert (const char *, unsigned int)

  Either abort program, or ask the user what to do for an assertion. depending on hardAssert setting.
- void computeComposition (const std::vector< unsigned int > &countData, std::vector< float > &compositionData)
- void convertEPOStoPos (const std::vector< EPOS_ENTRY > &eposEntry, std::vector< IonHit > &posFile)

  Convert an incoming entry of EPOS files to pos, and the append this to the pos vector given.
- unsigned int estimateRank (const gsl_matrix *m, float tolerance=sqrt(std::numeric_limits< float >::epsilon()))

  Estimate the rank of the given matrix.

- bool solveLeastSquares (gsl_matrix *m, gsl_vector *b, gsl_vector *&x)

  Use an SVD based least-squares solver to solve Mx=b (for x).
- template<class T >
  T weightedMean (const std::vector< T > &values, const std::vector< T > &weight)
- template<typename T >
  void meanAndStdev (const std::vector< T > &f, float &meanVal, float &stdevVal, bool normalCorrection=true)
- unsigned int vectorPointDir (const Point3D &pA, const Point3D &pB, const Point3D &vC, const Point3D &vD)

  Check which way vectors attached to two 3D points "point",.
- float distanceToSegment (const Point3D &fA, const Point3D &fB, const Point3D &p)
- float signedDistanceToFacet (const Point3D &fA, const Point3D &fB, const Point3D &fC, const Point3D &normal, const Point3D &p)

  Find the distance between a point, and a triangular facet – may be positive or negative.
- float distanceToFacet (const Point3D &fA, const Point3D &fB, const Point3D &fC, const Point3D &normal, const Point3D &p)
- float dotProduct (float a1, float a2, float a3, float b1, float b2, float b3)

  Inline func for calculating a(dot)b.
- double det3by3 (const double *ptArray)
- double pyramidVol (const Point3D *planarPts, const Point3D &apex)
- bool triIsDegenerate (const Point3D &fA, const Point3D &fB, const Point3D &fC)
- void quat_rot (Point3D &p, const Point3D &r, float angle)

  Rotate a point around a given rotation axis by a specified angle.
- void quat_rot (Point3f *point, const Point3f *rotVec, float angle)

  Rotate a point around a given vector, with specified angle.
- void quat_rot_array (Point3f *point, unsigned int n, const Point3f *rotVec, float angle)

  Rotate each point in array of size n around a given vector, with specified angle.
- void quat_rot_array (Point3D *point, unsigned int n, const Point3f *rotVec, float angle)

  Rotate each point in array of size n around a given vector, with specified angle.
- void quat_get_rot_quat (const Point3f *rotVec, float angle, Quaternion *rotQuat)

  Compute the quaternion for specified rotation.
- void quat_rot_apply_quat (Point3f *point, const Quaternion *rotQuat)

  Use previously generated quats from quat_get_rot_quats to rotate a point.
- void applyQuaternionRotation (std::vector< Point3D > &pts, const Quaternion &q)

  Apply the given quaternion rotation to the input points.
- template<class T >
  bool tolEqual (const T &a, const T &b, const T &f)
- template<class T >
  void selectElements (const std::vector< T > &in, const std::vector< unsigned int > &indices, std::vector< T > &out)
- template<class T >
  void transposeVector (std::vector< std::vector< T > > &v)
- template<class T >
  void vectorMultiErase (std::vector< T > &vec, const std::vector< bool > &wantKill)
- void sampleIons (const std::vector< IonHit > &ions, float sampleFactor, std::vector< IonHit > &sampled, bool strongRandom=true)
- template<class T >
  size_t randomSelect (std::vector< T > &result, const std::vector< T > &source, size_t num, gsl_rng *rng)
- template<class T >
  void randomIndices (std::vector< T > &res, size_t num, size_t nMax, gsl_rng *rng)
- template<class T1 , class T2 >
  bool stream_cast (T1 &result, const T2 &obj)

  Template function to cast and object to another by the stringstream.
- template<class T >
  void strAppend (std::string s, const T &a)
- void genColString (unsigned char r, unsigned char g, unsigned char b, unsigned char a, std::string &s)

- void genColString (unsigned char r, unsigned char g, unsigned char b, std::string &s)
- bool parseColString (const std::string &str, unsigned char &r, unsigned char &g, unsigned char &b, unsigned char &a)

  Parse a colour string containing rgb[a]; hex for with leading #.
- std::string digitString (unsigned int thisDigit, unsigned int maxDigit)

  Generate a string with leading digits up to maxDigit (eg, if maxDigit is 424, and thisDigit is 1.
- std::string stripWhite (const std::string &str)

  Strip whitespace, (eg tab,space) from either side of a string.
- std::string stripChars (const std::string &Str, const char *chars)
- std::string lowercase (std::string s)

  Return a lowercase version for a given string.
- std::string uppercase (std::string s)

  Return a uppercase version for a given string.
- void stripZeroEntries (std::vector< std::string > &s)
- void splitStrsRef (const char *cpStr, const char delim, std::vector< std::string > &v)

  Split string references using a single delimiter.
- void splitStrsRef (const char *cpStr, const char *delim, std::vector< std::string > &v)

  Split string references using any of a given string of delimiters.
- std::string onlyFilename (const std::string &path)

  Return only the filename component.
- std::string onlyDir (const std::string &path)

  Return only the directory name component of the full path.
- std::string convertFileStringToNative (const std::string &s)

  Convert a path format into a native path from unix format.
- std::string convertFileStringToCanonical (const std::string &s)

  Convert a path format into a unix path from native format.
- std::string tabs (unsigned int nTabs)
- std::string stlWStrToStlStr (const std::wstring &s)
- std::wstring stlStrToStlWStr (const std::string &s)
- void nullifyMarker (char *buffer, char marker)
- template<class T , class U >
  void castVoxels (const Voxels< T > &src, Voxels< U > &dest)

  Convert one type of voxel into another by assignment operator.
- template<class T , class U >
  void sumVoxels (const Voxels< T > &src, U &counter)

  Use one counting type to sum counts in a voxel of given type.
- unsigned int XMLHelpNextType (xmlNodePtr &node, int)
- unsigned int XMLHelpFwdToElem (xmlNodePtr &node, const char *nodeName)
- unsigned int XMLHelpFwdNotElem (xmlNodePtr &node, const char *nodeName)
- unsigned int XMLHelpFwdToList (xmlNodePtr &node, const std::vector< std::string > &nodeList)
- std::string XMLHelpGetText (xmlNodePtr &node)
- void XMLFreeDoc (void *data)

  Free a xmlDoc pointer. For use in conjunction with std::unique_ptr for auto-deallocation.
- template<class T >
  unsigned int XMLHelpGetProp (T &prop, xmlNodePtr node, std::string propName)
- template<class T >
  bool XMLGetNextElemAttrib (xmlNodePtr &nodePtr, T &v, const char *nodeName, const char *attrib)

  Grab the specified attribute from the next element, then stream_cast() it into the passed-in object. Returns true on success, false on error.
- const char * getRecordReadErrString (unsigned int errCode)
- const char * getAtoErrString (unsigned int errCode)
- unsigned int loadPosFile (std::vector< IonHit > &posIons, const char *posFile)

Load a pos file directly into a single ion list.

- unsigned int loadPosFile (std::vector< IonHit > &posIons, const char *posFile, unsigned int nSamplesMax)

  As per loadPosFile, but with an additional setting for the maximum number of ions to load.
- const char * getPosFileErrString (unsigned int errMesg)
- unsigned int savePosFile (const std::vector< Point3D > &points, float mass, const char *name, bool append=false)

  Save a vector of Point3Ds into a pos file, using a fixed mass, return nonzero on error.
- unsigned int savePosFile (const std::vector< IonHit > &data, const char *name, bool append=false)

  Save a vector of IonHits into a "pos" file, return nonzero on error.
- unsigned int saveTapsimBin (std::ostream &f, std::vector< IonHit > &posIons)

  Write a tapsim file from a bunch of IonHits.
- size_t loadEposFile (std::vector< EPOS_ENTRY > &outData, const char *filename)

  Load an entire "EPOS" File.
- size_t chunkLoadEposFile (std::vector< EPOS_ENTRY > &outData, const char *filename, unsigned int chunkSize, unsigned int chunkOffset, unsigned int &nEntriesLeft)

  Load an "EPOS" file, with a maximum chunk size.
- unsigned int loadTextData (const char *cpFilename, std::vector< std::vector< float > > &dataVec, std::vector< std::string > &headerVec, const char *delim, bool allowNan=true)

  Load a CSV, TSV or similar text file. Assumes "C" Locale for input (ie "." as decimal separator).
- unsigned int readPosapOps (const char *file, THREEDAP_EXPERIMENT &data, unsigned int &badLine, unsigned int &progress, std::atomic< bool > &wantAbort, unsigned int nDelayLines=2, bool strictMode=false)

  Function to read POSAP "OPS" files.
- unsigned int loadATOFile (const char *fileName, std::vector< ATO_ENTRY > &ions, unsigned int forceEndian=0)

  Load a LAWATAP "ATO" file.
- bool operator< (const SIMPLE_SPECIES &a, const SIMPLE_SPECIES &b)
- unsigned int parseCompositionData (const std::vector< std::string > &s, const AbundanceData &atomTable, std::map< unsigned int, double > &atomData)

  Convert atomic string label data, in the form "Fe 0.81" to fraction map.
- void convertMolToMass (const AbundanceData &atomTable, const std::map< unsigned int, double > &compositionMols, std::map< unsigned int, double > &compositionMass)

  Convert the given composition from molar fraction data to mass fraction.
- void convertMassToMol (const AbundanceData &atomTable, const std::map< unsigned int, double > &compositionMass, std::map< unsigned int, double > &compositionMols)

  Convert the given composition from mass fraction data to molar fraction.
- void findOverlaps (const AbundanceData &natData, const RangeFile &rng, float massDelta, unsigned int maxCharge, std::vector< std::pair< size_t, size_t > > &overlapIdx, std::vector< std::pair< float, float > > &overlapMasses)

  Find the overlaps stemming from a given rangefile.
- void findOverlaps (const AbundanceData &natData, const std::vector< std::string > &ions, float massDelta, unsigned int maxCharge, std::vector< std::pair< size_t, size_t > > &overlapIdx, std::vector< std::pair< float, float > > &overlapMasses)

  As per findOverlaps(...Rangefile ...) , but uses a vector of ions instead.
- void findOverlapsFromSpectra (const std::vector< std::vector< std::pair< float, float > > > &massDistributions, float massDelta, const std::set< unsigned int > &skipIDs, std::vector< std::pair< size_t, size_t > > &overlapIdx, std::vector< std::pair< float, float > > &overlapMasses)

  Find overlaps in the given mass distributions, as per findOverlaps(...Rangefile...)
- void gsl_matrix_mult (const gsl_matrix *a, const gsl_matrix *b, gsl_matrix *&res)
- bool reconstructTest ()
- unsigned int doFitBackground (const std::vector< float > &massData, BACKGROUND_PARAMS &params)

  Perform a background fit, assuming constant TOF noise, from 0->inf time.
- std::string getFitErrorMsg (unsigned int errCode)

- void createMassBackground (float massStart, float massEnd, unsigned int nBinsMass, float tofBackIntensity, std::vector< float > &histogram)

  Build a histogram of the background counts.
- void findPeaks (const std::vector< float > &x0, std::vector< unsigned int > &peakInds, float sel, bool autoSel=true, bool includeEndpoints=true)

  Simple peak-finding algorithm.
- void poissonConfidenceObservation (float counts, float alpha, float &lBound, float &uBound)

  Obtain poisson confidence limits for the mean of a poisson distribution.
- bool numericalEstimatePoissRatioConf (float lambda1, float lambda2, float alpha, unsigned int nTrials, gsl_rng *r, float &lBound, float &uBound)

  Brute-force poisson ratio confidence estimator. Returns the confidence interval in the estimate of the mean, at the given rates.
- bool numericalEstimateGaussRatioConf (float mu1, float mu2, float var1, float var2, float alpha, unsigned int nTrials, gsl_rng *r, float &lBound, float &uBound)

  Brute-force guassian ratio confidence estimator.
- bool numericalEstimateSkellamConf (float lambda1, float lambda2, float alpha, unsigned int nTrials, gsl_rng *r, float &lBound, float &uBound)

  Brute-force the confidence bounds of a skellam distribution.
- bool zechConfidenceLimits (float lambdaBack, unsigned int observation, float alpha, float &estimate)

  Provides a best estimate for true signal when true signal, background.
- bool rangeOverlaps (const pair< float, float > &r1, const pair< float, float > &r2)
- void computeRangeAdjacency (const MultiRange &mrf, const OVERLAP_PROBLEM_SETTINGS &settings, gsl_matrix *&m)
- void freeConvexHull ()
- unsigned int doHull (unsigned int bufferSize, double *buffer, vector< Point3D > &resHull, Point3D &midPoint, bool freeHullOnExit)
- unsigned int countIntensityEvents (const vector< pair< float, float > > &data, float minV, float maxV)
- void buildFrequencyTable (const vector< ISOTOPE_ENTRY > &solutionVec, vector< size_t > &solutionElements, vector< size_t > &solutionFrequency)
- vector< float > maxExplainedFraction (const vector< pair< float, float > > &intensityData, float peakMass, float massWidth, const vector< vector< ISOTOPE_ENTRY > > &solutions, const AbundanceData &massTable, float massDistTol, unsigned int solutionCharge)
- bool incrementCorrelationHist (const std::vector< EPOS_ENTRY > &eposIons, std::vector< std::vector< unsigned int > > &histogram, float stepMass, float endMass)
- template<class T >
  void removeElements (const std::vector< size_t > &elems, std::vector< T > &vec)
- bool pairContains (const pair< float, float > &p, float m)
- RANGE_MOLECULE getRangeMolecule (const AbundanceData &massTable, const RangeFile &rng, unsigned int rangeId)
- float nullBackground (float rangeStart, float rangeEnd)
- bool leastSquaresDeconvolve (const MultiRange &rangeData, const AbundanceData &abundance, const float massTol, const vector< IonHit > &hits, float(*backgroundEstimator)(float, float), vector< pair< unsigned int, float > > &decomposedHits)
- bool getHardAssert ()
- char * myStrDup (const char *s)
- void pushLocale (const char *newLocale, int type)
- void popLocale ()
- bool getFilesize (const char *fname, size_t &size)
- void gsl_print_matrix (const gsl_matrix *m)
- void gsl_print_vector (const gsl_vector *v)
- float gsl_determinant (const gsl_matrix *m)
- bool isNotDirectory (const char *filename)
- int fpeek (FILE *stream)
- void quat_mult_no_second_a (Quaternion *result, const Quaternion *q1, const Quaternion *q2)
- void quat_pointmult (Point3f *result, const Quaternion *q1, const Quaternion *q2)

- void quat_invert (Quaternion *quat)
- void ucharToHexStr (unsigned char c, std::string &s)
- void hexStrToUChar (const std::string &s, unsigned char &c)
- void incrementDataDistanceWeight (const Point3D &p, Voxels< float > &v)
- void countDataDistanceWeight (const vector< Point3D > &pts, Voxels< float > &v)
- string XMLHelpGetText (xmlNodePtr node)
- template<class T >
  unsigned int fixedRecordReader (const char *filename, bool(*recordReader)(const char *bufRead, const char *destBuf), size_t recordSize, std::vector< T > &outputData)
- template<class T >
  unsigned int fixedRecordChunkReader (const char *filename, bool(*recordReader)(const char *bufRead, const char *destBuf), size_t recordSize, std::vector< T > &outputData, unsigned int chunkSize, unsigned int chunkOffset, unsigned int &nEntriesLeft)
- unsigned int loadTapsimBinFile (vector< IonHit > &posIons, const char *posfile)
- bool readEposRecord (const char *src, const char *dest)
- bool strhas (const char *cpTest, const char *cpPossible)
- template<class T >
  void linkIdentifiers (vector< T > &link)
- bool pairOverlaps (float aStart, float aEnd, float bStart, float bEnd)
- string rangeToStr (const pair< float, float > &rng)
- bool matchComposedName (const std::map< string, size_t > &composedNames, const vector< pair< string, size_t > > &namesToFind, size_t &matchOffset)
- void findOverlapsFromSpectra (const vector< vector< pair< float, float > > > &massDistributions, float massDelta, const set< unsigned int > &skipIDs, vector< pair< size_t, size_t > > &overlapIdx, vector< pair< float, float > > &overlapMasses)
- void findOverlaps (const AbundanceData &natData, const RangeFile &rng, float massDelta, unsigned int maxCharge, vector< pair< size_t, size_t > > &overlapIdx, vector< pair< float, float > > &overlapMasses)
- void findOverlaps (const AbundanceData &natData, const vector< string > &ionNames, float massDelta, unsigned int maxCharge, vector< pair< size_t, size_t > > &overlapIdx, vector< pair< float, float > > &overlapMasses)
- int gcd (int a, int b)
- std::ostream & operator<< (std::ostream &stream, const BoundCube &b)
- std::ostream & operator<< (std::ostream &stream, const IonHit &ion)
- bool antiRotateMatch (const unsigned int *a, const unsigned int *b, size_t n)
- bool rotateMatch (const unsigned int *a, const unsigned int *b, size_t n, bool directionForwards=true)
- float signVal (unsigned int val)
- size_t findMaxLessThanOrEq (const vector< std::pair< size_t, size_t > > &v, size_t value)
- float Determinant (float **a, int n)
- float fourDeterminant (const Point3D &a, const Point3D &b, const Point3D &c, const Point3D &d)
- unsigned int edgeIdx (unsigned int i, unsigned int j)
- int intersect_RayTriangle (const Point3D &rayStart, const Point3D &rayEnd, Point3D *tri, Point3D &I)
- void findNearVerticies (float tolerance, const vector< Point3D > &ptVec, vector< std::pair< size_t, vector< size_t > > > &clusterList)
- void findNearVerticies (float tolerance, const vector< Point3D > &ptVec, std::list< std::pair< size_t, vector< size_t > > > &clusterList)
- std::ostream & operator<< (std::ostream &stream, const Point3D &pt)
- double SphericProjectionEqn (double eta, void *p)
- template<class T >
  bool andersonDarlingStatistic (std::vector< T > vals, float &meanV, float &stdevVal, float &statistic, size_t &undefCount, bool computeMeanAndStdev=true)
- void makeHistogram (const vector< float > &data, float start, float end, float step, vector< float > &histVals)
- void diff (const vector< float > &in, vector< float > &out)
- template<class T , class T2 >
  std::iterator_traits< T >::value_type kahansum (T begin, T end, T2 other)
- double zechRoot (double sigGuess, void *params)
- template<class T >
  void cumTrapezoid (const vector< T > &x, const vector< T > &vals, vector< T > &res)
- double gauss_ratio_pdf (double x, double muX, double muY, double varX, double varY)

Variables

- LibVersion libVersion
- RandNumGen randGen
- const char * RECORDREAD_ERR_STRINGS [ ]
- const char * ATO_ERR_STRINGS [ ]

  Human readable error messages for use with ATO reader return values.
- const char * OPS_ENUM_ERRSTRINGS [ ]
- const unsigned int NUM_ELEMENTS =119
- const size_t EPOS_RECORD_SIZE = 11*4
- const unsigned int ELEM_SINGLE_NODE_POINT =15
- const unsigned int ELEM_TWO_NODE_LINE =1
- const unsigned int ELEM_THREE_NODE_TRIANGLE =2
- const unsigned int ELEM_FOUR_NODE_TETRAHEDRON =4
- const char * MESH_LOAD_ERRS [ ]
- bool qhullInited =false
- const unsigned int HULL_GRAB_SIZE =4096
- int aiCubeEdgeFlags [256]
- int a2iTriangleConnectionTable [256][16]
- const unsigned int VERTEX_OFFSET [8][3]
- int edgeRemap [12]
- bool hardAssert =true
- const size_t maximumLinearTable [ ]
- const char MULTIRANGE_FORMAT_VERSION [ ] = "0.0.1"
- const size_t MAX_LINE_SIZE = 16536
- const size_t MAX_RANGEFILE_SIZE = 50*1024*1024
- const char * RANGE_EXTS [ ]
- const char * elementList [ ]
- const char * ABUNDANCE_ERROR [ ]
- const size_t PROGRESS_REDUCE =500

5.1.1 Typedef Documentation

5.1.1.1 ATO_ENTRY

```
typedef struct AtomProbe::ATO_ENTRY AtomProbe::ATO_ENTRY
```

5.1.1.2 IONHIT

```
typedef struct AtomProbe::IONHIT AtomProbe::IONHIT
```

Record as stored in a .POS file.

5.1.2 Enumeration Type Documentation

5.1.2.1 anonymous enum

```
anonymous enum
```

Enumerator

HULL_SURFREDUCE_NEGATIVE_SCALE_FACT	
HULL_ERR_USER_ABORT	
HULL_ERR_NO_MEM	

Definition at line 11 of file convexHull.h.

5.1.2.2 anonymous enum

`anonymous enum`

Enumerator

ATO_OPEN_FAIL	
ATO_EMPTY_FAIL	
ATO_SIZE_ERR	
ATO_VERSIONCHECK_ERR	
ATO_MEM_ERR	
ATO_BAD_ENDIAN_DETECT	
ATO_ENUM_END	

Definition at line 49 of file dataFiles.h.

5.1.2.3 anonymous enum

`anonymous enum`

Enumerator

TEXT_ERR_FILE_OPEN	
TEXT_ERR_FILE_NUM_FIELDS	
TEXT_ERR_FILE_FORMAT	

Definition at line 60 of file dataFiles.h.

5.1.2.4 anonymous enum

`anonymous enum`

Error codes for OPS file loading.

Enumerator

OPSREADER_FORMAT_CLINE_ERR	
OPSREADER_FORMAT_DETECTORLINE_ERR	
OPSREADER_FORMAT_LINE_DASH_ERR	
OPSREADER_FORMAT_LINE_VOLTAGE_ERR	
OPSREADER_FORMAT_LINE_VOLTAGE_NOBETA	
OPSREADER_FORMAT_LINE_VOLTAGE_DATA_ERR	
OPSREADER_FORMAT_LINE_VOLTAGE_DATACOUNT_ERR	
OPSREADER_FORMAT_LINETYPE_ERR	
OPSREADER_FORMAT_CHANNELS_ERR	
OPSREADER_CHANNELS_DATA_ERR	
OPSREADER_FORMAT_SLINE_EVENTCOUNT_ERR	
OPSREADER_FORMAT_SLINE_EVENTDATA_ERR	
OPSREADER_FORMAT_SLINE_FORMAT_ERR	
OPSREADER_FORMAT_SLINE_PREFIX_ERR	
OPSREADER_FORMAT_DUPLICATE_SYSDATA	
OPSREADER_FORMAT_DUPLICATE_DETECTORSIZE	
OPSREADER_FORMAT_TRAILING_DASH_ERR	
OPSREADER_FORMAT_DOUBLEDASH	
OPSREADER_OPEN_ERR	
OPSREADER_READ_ERR	
OPSREADER_ABORT_ERR	
OPSREADER_ENUM_END	

Definition at line 168 of file dataFiles.h.

5.1.2.5 anonymous enum

```
anonymous enum
```

Enumerator

MULTIRANGE_FORMAT_XML	

Definition at line 57 of file multiRange.h.

5.1.2.6 anonymous enum

```
anonymous enum
```

Enumerator

RANGE_FORMAT_ORNL	
RANGE_FORMAT_DBL_ORNL	

Enumerator

RANGE_FORMAT_ENV	
RANGE_FORMAT_RRNG	
RANGE_FORMAT_END_OF_ENUM	

Definition at line 36 of file ranges.h.

5.1.2.7 anonymous enum

```
anonymous enum
```

Enumerator

RANGE_ERR_FORMAT	
RANGE_ERR_FORMAT_HEADER	
RANGE_ERR_EMPTY	
RANGE_ERR_FORMAT_LONGNAME	
RANGE_ERR_FORMAT_SHORTNAME	
RANGE_ERR_FORMAT_COLOUR	
RANGE_ERR_FORMAT_TABLESEPARATOR	
RANGE_ERR_FORMAT_MASS_PAIR	
RANGE_ERR_FORMAT_TABLE_ENTRY	
PARSE_RANGE_FORMAT_GENERIC_FAIL	
RANGE_ERR_DATA_TOO_MANY_USELESS_RANGES	
RANGE_ERR_DATA_FLIPPED	
RANGE_ERR_DATA_INCONSISTENT	
RANGE_ERR_DATA_NOMAPPED_IONNAME	
RANGE_ERR_OPEN	
RANGE_ERR_FORMAT_RANGETABLE	
RANGE_ERR_FORMAT_TABLEHEADER_NUMIONS	
RANGE_ERR_NONUNIQUE_POLYATOMIC	
RANGE_ERR_TOO_LARGE	
RANGE_ERR_DASHHEADER	
RANGE_ERR_IONBLOCK_CONTENT	
RANGE_ERR_NUMIONS	
RANGE_ERR_NUMIONS_DUPLICATED	
RANGE_ERR_TOO_MANYIONS	
RANGE_ERR_ION_BLOCK_NOT_PRESENT	
RANGE_ERR_DUPLICATE_NUMRANGES	
RANGE_ERR_NUMRANGE_PARSE	
RANGE_ERR_RRNG_IONS_TOOSHORT	
RANGE_ERR_RRNG_COLON_SEPARATOR	
RANGE_ERR_BADCOLOUR	
RANGE_ERR_ION_NOT_MAPPED	
RANGE_ERR_BADSTART	
RANGE_ERR_BADEND	
RANGE_ERR_NAME_EMPTY	

Enumerator

RANGE_ERR_BAD_LINE_RANGEBLOCK	
RANGE_ERR_MISSING_IONBLOCK	
RANGE_ERR_NO_RANGES	
RANGE_ERR_NO_BASIC_IONS	
RANGE_ERR_MISMATCHED_NUMRANGES	
RANGE_ERR_RANGEBLOCK_FORMAT	
RANGE_ERR_BAD_MULTIPLICITY	
RANGE_ERR_FORMAT_EMPTY_RANGEROW	
RANGE_ERR_FILESIZE	
RANGE_ERR_ENUM_END	

Definition at line 43 of file ranges.h.

5.1.2.8 anonymous enum

`anonymous enum`

composition parsing error messages

Enumerator

COMPPARSE_BAD_INPUT_FORMAT	
COMPPARSE_BAD_COMP_VALUE	
COMPPARSE_BAD_BAL_USAGE	
COMPPARSE_BAD_SYMBOL	
COMPPARSE_DUPLICATE_SYMBOL	
COMPPARSE_BAD_TOTAL_COMP	

Definition at line 10 of file massconvert.h.

5.1.2.9 anonymous enum

`anonymous enum`

Enumerator

CRYSTAL_BAD_UNIT_CELL	
CRYSTAL_ENUM_END	

Definition at line 80 of file generate.h.

5.1.2.10 anonymous enum

```
anonymous enum
```

Enumerator

LATTICE_FCC	
LATTICE_BCC	
LATTICE_HCP	
LATTICE_END_OF_ENUM	

Definition at line 11 of file millerIndex.h.

5.1.2.11 anonymous enum

```
anonymous enum
```

Boundary clipping mode.

These constants defines the behaviour of the routines when presented with a boundary value problem, such as in convolution.

Enumerator

BOUND_CLIP	
BOUND_HOLD	
BOUND_DERIV_HOLD	
BOUND_MIRROR	
BOUND_ZERO	
BOUND_ENUM_END	

Definition at line 46 of file voxels.h.

5.1.2.12 anonymous enum

```
anonymous enum
```

Enumerator

ELEMENT_TRIANGLE	
ELEMENT_TETRAHEDRON	
ELEMENT_LINE	

Definition at line 44 of file mesh.h.

5.1.2.13 anonymous enum

```
anonymous enum
```

Enumerator

EVOLUTION_MODE_SHANKANGLE	

Definition at line 29 of file reconstruction-simple.h.

5.1.2.14 anonymous enum

```
anonymous enum
```

Background fitting modes.

Enumerator

BACK_FIT_MODE_CONST_TOF	
BACK_FIT_MODE_ENUM_END	

Definition at line 22 of file processing.h.

5.1.2.15 anonymous enum

```
anonymous enum
```

Enumerator

POS_ALLOC_FAIL	
POS_OPEN_FAIL	
POS_SIZE_MODULUS_ERR	
POS_SIZE_EMPTY_ERR	
POS_READ_FAIL	
POS_NAN_LOAD_ERROR	
POS_FILE_ENUM_END	

Definition at line 53 of file dataFiles.cpp.

5.1.2.16 anonymous enum

```
anonymous enum
```

Enumerator

TAPSIM_FILE_FORMAT_FAIL	
TAPSIM_OPEN_FAIL	

Definition at line 65 of file dataFiles.cpp.

5.1.2.17 anonymous enum

```
anonymous enum
```

Enumerator

MULTIRANGE_ERR_NO_PARSER	
MULTIRANGE_ERR_NO_XML_DOC	
MULTIRANGE_ERR_NO_XML_CONTEXT	
MULTIRANGE_ERR_NO_NODEPTR	
MULTIRANGE_NOT_VALID_ROOTNODE	
MULTIRANGE_ERR_NO_CONTENT	
MULTIRANGE_ERR_NO_TIMESTAMP	
MULTIRANGE_ERR_NO_MOLECULES	
MULTIRANGE_ERR_NO_MOLECULE_ENTRIES	
MULTIRANGE_ERR_MOL_MISSING_ENTRY	
MULTIRANGE_ERR_MOL_MISSING_NAME	
MULTIRANGE_ERR_MOL_MISSING_COMPONENTS	
MULTIRANGE_ERR_BAD_RANGE	
MULTIRANGE_ERR_BAD_RANGES	
MULTIRANGE_ERR_MOL_MISSING_COLOUR	
MULTIRANGE_ERR_MOL_BAD_COLOUR	
MULTIRANGE_ERR_NO_RANGES	
MULTIRANGE_ERR_BAD_GROUP	
MULTIRANGE_ERR_SELF_INCONSISTENT	
MULTIRANGE_ERR_RANGE_NOPARENT	
MULTIRANGE_ERR_ENUM_END	

Definition at line 48 of file multiRange.cpp.

5.1.2.18 anonymous enum

```
anonymous enum
```

Enumerator

MESH_LOAD_UNSPECIFIED_ERROR	

Enumerator

MESH_LOAD_BAD_NODECOUNT	
MESH_LOAD_BAD_ELEMENTCOUNT	
MESH_LOAD_IS_INSANE	
MESH_LOAD_ENUM_END	

Definition at line 44 of file mesh.cpp.

5.1.2.19 anonymous enum

`anonymous enum`

Enumerator

VOX_INTERP_NONE	
VOX_INTERP_LINEAR	
VOX_INTERP_ENUM_END	

Definition at line 56 of file voxels.h.

5.1.2.20 anonymous enum

`anonymous enum`

Enumerator

ADJ_ALL	
ADJ_PLUS	

Definition at line 63 of file voxels.h.

5.1.2.21 anonymous enum

`anonymous enum`

Enumerator

VOXELS_BAD_FILE_READ	
VOXELS_BAD_FILE_OPEN	
VOXELS_BAD_FILE_SIZE	
VOXELS_OUT_OF_MEMORY	

Definition at line 69 of file voxels.h.

5.1.2.22 anonymous enum

```
anonymous enum
```

Clipping direction constants.

Controls the clipping direction when performing clipping operations

Enumerator

CLIP_NONE	
CLIP_LOWER_SOUTH_WEST	
CLIP_UPPER_NORTH_EAST	

Definition at line 80 of file voxels.h.

5.1.2.23 anonymous enum

```
anonymous enum
```

Enumerator

VOXEL_ABORT_ERR	
VOXEL_MEMORY_ERR	
VOXEL_BOUNDS_INVALID_ERR	

Definition at line 87 of file voxels.h.

5.1.2.24 anonymous enum

```
anonymous enum
```

Enumerator

PROP_PARSE_ERR	
PROP_BAD_ATT	

Definition at line 36 of file XMLHelper.h.

5.1.2.25 anonymous enum

```
anonymous enum
```

Enumerator

RECORDREAD_ERR_GET_FILESIZE	
RECORDREAD_ERR_FILESIZE_MODULO	
RECORDREAD_ERR_FILE_OPEN	
RECORDREAD_ERR_NOMEM	
RECORDREAD_BAD_FILEREAD	
RECORDREAD_ERR_CHUNKOFFSET	
RECORDREAD_BAD_RECORD	

Definition at line 34 of file dataFiles.h.

5.1.2.26 PointDir

```
enum AtomProbe::PointDir
```

Enumerator

POINTDIR_TOGETHER	
POINTDIR_IN_COMMON	
POINTDIR_APART	

Definition at line 16 of file misc.h.

5.1.3 Function Documentation

5.1.3.1 accumulateCorrelationHistogram()

```
bool AtomProbe::accumulateCorrelationHistogram (
            const std::vector< EPOS_ENTRY > & eposIons,
            std::vector< std::vector< unsigned int > > & histogram,
            float stepMass,
            float endMass,
            bool lowerTriangular = true )
```

Increments a correlation histogram, as per correlationHistogram,.

For input parameters, see correlationHistogram(...). This version will have lower peak memory input, as eposIons can be chunked.

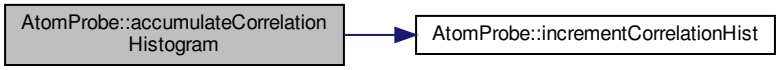
- The input histogram must be zero sized, or have the correct size when used. If zero sized, it will be resized and zeroed appropriately to contents
- The default here is that the lower triangular is true, unlike in correlationHistogram(...) so when performing the final accumulation, you may wish to set this to false, to ensure that histogram_ij = histogram_ji.
- Do not change endMass or stepMass between calls on the same histogram

Definition at line 119 of file histogram.cpp.

References incrementCorrelationHist().

Referenced by main().

Here is the call graph for this function:



5.1.3.2 andersonDarlingStatistic()

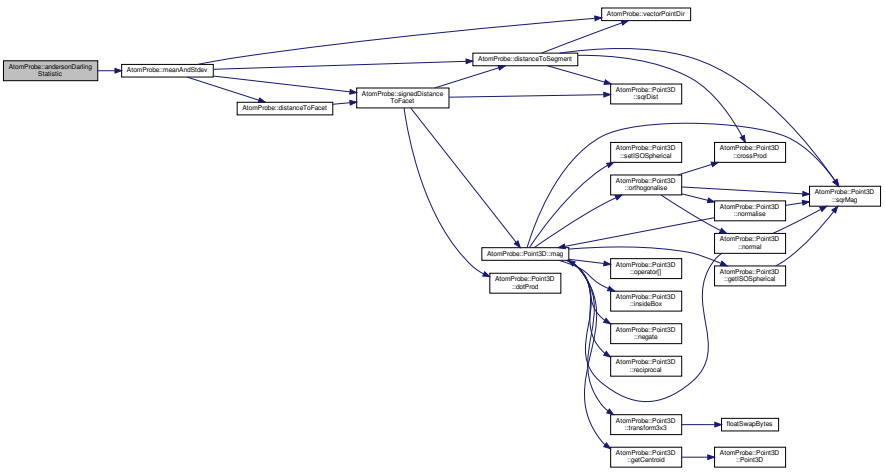
```
template<class T >
bool AtomProbe::andersonDarlingStatistic (
             std::vector< T > vals,
             float & meanV,
             float & stdevVal,
             float & statistic,
             size_t & undefCount,
             bool computeMeanAndStdev = true )
```

Definition at line 35 of file processing.cpp.

References meanAndStdev().

Referenced by doFitBackground().

Here is the call graph for this function:



5.1.3.3 antiRotateMatch()

```
bool AtomProbe::antiRotateMatch (
            const unsigned int * a,
            const unsigned int * b,
            size_t n )
```

Definition at line 63 of file mesh.cpp.

Referenced by AtomProbe::TRIANGLE::edgesMismatch().

5.1.3.4 applyQuaternionRotation()

```
void AtomProbe::applyQuaternionRotation (
            std::vector< Point3D > & pts,
            const Quaternion & q )
```

Apply the given quaternion rotation to the input points.

Rotation is in-place

5.1.3.5 askAssert()

```
void AtomProbe::askAssert (
            const char * filename,
            unsigned int lineNumber )
```

Either abort program, or ask the user what to do for an assertion. depending on hardAssert setting.

Definition at line 35 of file aptAssert.cpp.

5.1.3.6 buildFrequencyTable()

```
void AtomProbe::buildFrequencyTable (
            const vector< ISOTOPE_ENTRY > & solutionVec,
            vector< size_t > & solutionElements,
            vector< size_t > & solutionFrequency )
```

Definition at line 35 of file filter.cpp.

References ASSERT.

Referenced by filterPeakNeedBiggerObs(), and maxExplainedFraction().

5.1.3.7 castVoxels()

```
template<class T , class U >
void AtomProbe::castVoxels (
            const Voxels< T > & src,
            Voxels< U > & dest )
```

Convert one type of voxel into another by assignment operator.

Definition at line 383 of file voxels.h.

5.1.3.8 checkMassRangingCorrectness()

```
void AtomProbe::checkMassRangingCorrectness (
            const RangeFile & rng,
            AbundanceData & massTable,
            float massTolerance,
            unsigned int maxChargeState,
            unsigned int maxComponents,
            std::vector< bool > & badRanges )
```

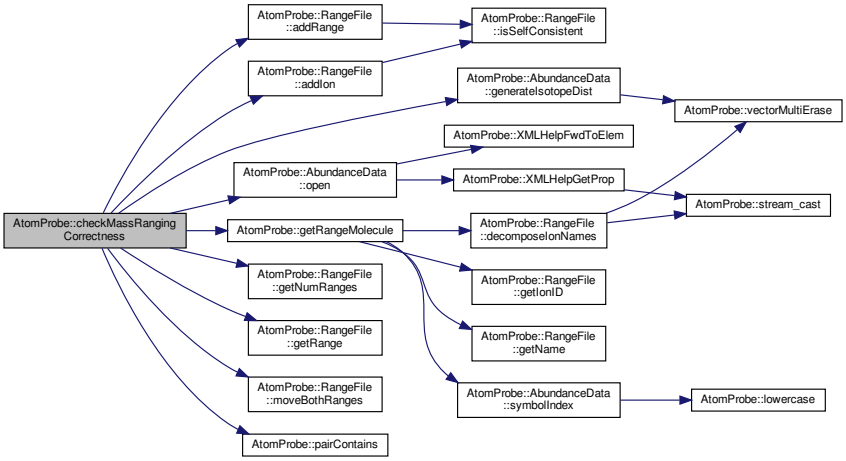
Ensure that each mass given spans a peak that should exist.

Each entry in badRanges is true if an inconsistent range is detected. There will be one entry per range in the parent rangefile Some ranges may be skipped if they cannot be understood maxComponents will skip checks for ions with more than this many atoms in the ionic molecule. Eg H2 would not be checked if maxComponents=1

Definition at line 101 of file rangeCheck.cpp.

References AtomProbe::RangeFile::addIon(), AtomProbe::RangeFile::addRange(), AtomProbe::RGBf::blue, AtomProbe::RANGE_MOLECULE::components, AtomProbe::AbundanceData::generateIsotopeDist(), AtomProbe::RangeFile::getNumRanges(), AtomProbe::RangeFile::getRange(), getRangeMolecule(), AtomProbe::RGBf::green, AtomProbe::RANGE_MOLECULE::isOK, AtomProbe::RangeFile::moveBothRanges(), AtomProbe::AbundanceData::open(), pairContains(), AtomProbe::RGBf::red, and TEST.

Here is the call graph for this function:



5.1.3.9 chunkLoadEposFile()

```
size_t AtomProbe::chunkLoadEposFile (
            std::vector< EPOS_ENTRY > & outData,
            const char * filename,
            unsigned int chunkSize,
            unsigned int chunkOffset,
            unsigned int & nEntriesLeft )
```

Load an "EPOS" file, with a maximum chunk size.

This is useful to avoid out-of-memory situations when working with large datasets If the file has fewer EPOS entries left than the chunk size, only the remaining entries will be read. Increment chunkOffset to seek to the next part of the file The file will be re-opened each time, so larger chunk sizes will increase speed at the cost of memory.

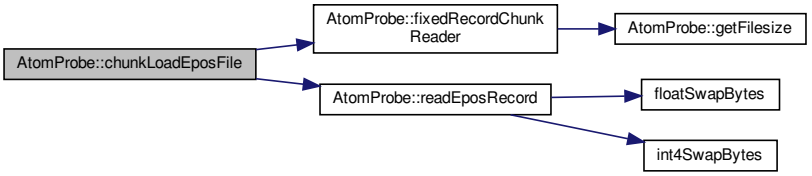
outData : the output to write the epos data to filename : the name of the EPOS formatted file to open chunkSize : the maximum number of entries to read in one go chunkOffset : the position (in chunks) of the file to start reading from, the caller must increment this to prevent the same section being re-read nEntriesLeft : returns the number of entries left in the file, The return value is nonzero on error, and is part of the RECORDREAD_ERR enum

Definition at line 757 of file dataFiles.cpp.

References EPOS_RECORD_SIZE, fixedRecordChunkReader(), and readEposRecord().

Referenced by getAtoErrString(), and main().

Here is the call graph for this function:



5.1.3.10 computeComposition()

```
void AtomProbe::computeComposition (
            const std::vector< unsigned int > & countData,
            std::vector< float > & compositionData )
```

Definition at line 13 of file composition.cpp.

Referenced by main().

5.1.3.11 computeConvexHull()

```
unsigned int AtomProbe::computeConvexHull (
            const std::vector< IonHit > & data,
            unsigned int * progress,
            bool(*)(bool) callback,
            std::vector< Point3D > & curHull,
            bool freeHull )
```

Obtain the convex hull of a set of ions.

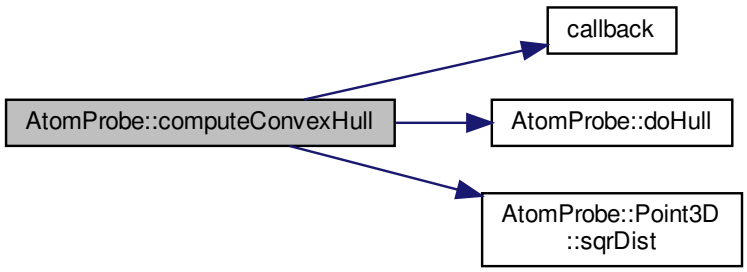
An existing set of points on the convex hull, "curHull", can be given as a starting set, optionally. For the last call to this routine , set "freeHull" to true. Returns 0 on success, nonzero on error, with error codes in above enum

Definition at line 149 of file convexHull.cpp.

References callback(), doHull(), HULL_ERR_NO_MEM, HULL_ERR_USER_ABORT, PROGRESS_REDUCE, and AtomProbe::Point3D::sqrDist().

Referenced by GetReducedHullPts().

Here is the call graph for this function:



5.1.3.12 computeIonDistAdjacency()

```
void AtomProbe::computeIonDistAdjacency (
            const MultiRange & mrf,
            const AbundanceData & abundance,
            const OVERLAP_PROBLEM_SETTINGS & settings,
            gsl_matrix *& m,
            gsl_vector *& vOwnership,
            gsl_vector *& vMass )
```

Calculate the adjacency matrix for the ions in a multirange.

Uses tolerance and other data in settings. Range data is NOT used. Vectors and matrices should not be allocated, but must be freed using gsl_matrix_free and gsl_vector_free after use. Return values are a 0/1 adjacency matrix,

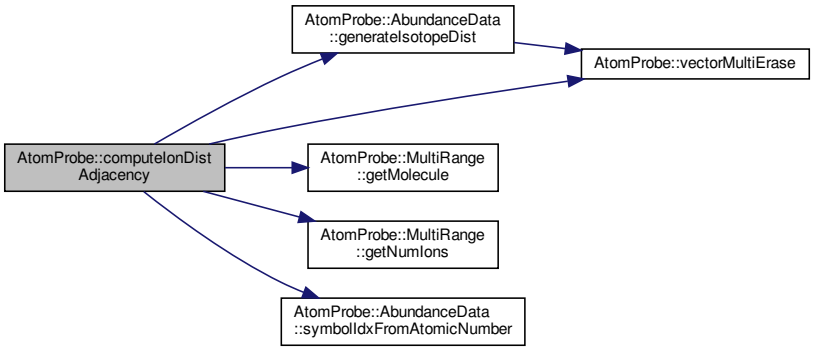
and two vectors, one describing the owner index of each ion and the other the mass. return matrix will be square, and vectors will have same size as matrix

Definition at line 40 of file componentAnalysis.cpp.

References ASSERT, AtomProbe::AbundanceData::generateIsotopeDist(), AtomProbe::MultiRange::getMolecule(), AtomProbe::MultiRange::getNumIons(), AtomProbe::OVERLAP_PROBLEM_SETTINGS::intensityTolerance, AtomProbe::OVERLAP_PROBLEM_SETTINGS::massTolerance, AtomProbe::OVERLAP_PROBLEM_SETTI↩NGS::maxDefaultCharge, AtomProbe::AbundanceData::symbolIdxFromAtomicNumber(), and vectorMultiErase().

Referenced by computeRangeAdjacency().

Here is the call graph for this function:



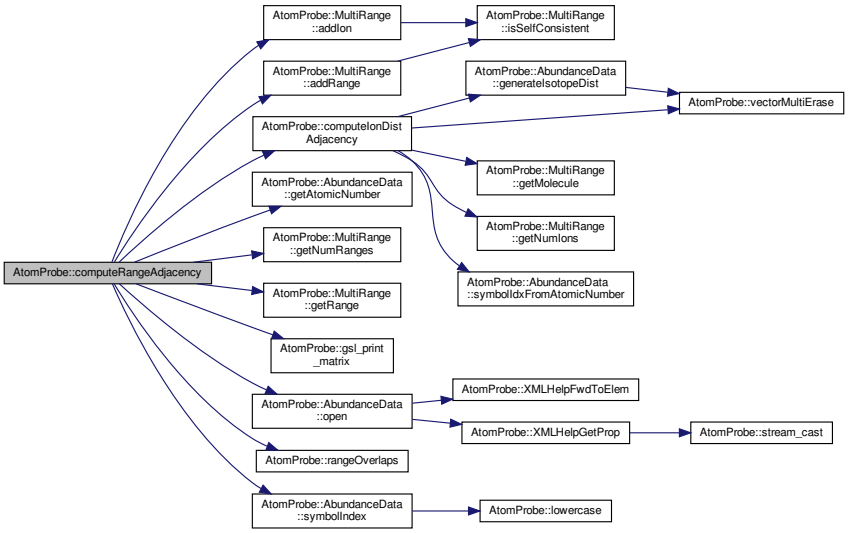
5.1.3.13 computeRangeAdjacency()

```
void AtomProbe::computeRangeAdjacency (
            const MultiRange & mrf,
            const OVERLAP_PROBLEM_SETTINGS & settings,
            gsl_matrix *& m )
```

Definition at line 172 of file componentAnalysis.cpp.

References AtomProbe::MultiRange::addIon(), AtomProbe::MultiRange::addRange(), ASSERT, AtomProbe::S↩IMPLE_SPECIES::atomicNumber, AtomProbe::RGBf::blue, computeIonDistAdjacency(), AtomProbe::SIMPLE↩_SPECIES::count, AtomProbe::AbundanceData::getAtomicNumber(), AtomProbe::MultiRange::getNumRanges(), AtomProbe::MultiRange::getRange(), AtomProbe::RGBf::green, gsl_print_matrix(), AtomProbe::OVERLAP_PRO↩BLEM_SETTINGS::massTolerance, AtomProbe::OVERLAP_PROBLEM_SETTINGS::maxDefaultCharge, Atom↩Probe::AbundanceData::open(), rangeOverlaps(), AtomProbe::RGBf::red, AtomProbe::AbundanceData::symbol↩Index(), TEST, and WARN.

Here is the call graph for this function:



5.1.3.14 computeRotationMatrix()

```
void AtomProbe::computeRotationMatrix (
            const Point3D & ur1,
            const Point3D & ur2,
            const Point3D & r1,
            const Point3D & r2,
            gsl_matrix * m )
```

Given two orthogonal and normal basis vectors, r1 and r2, and two matching rotated vectors ur1 and ur2, compute the rotation matrix that will transform between them.

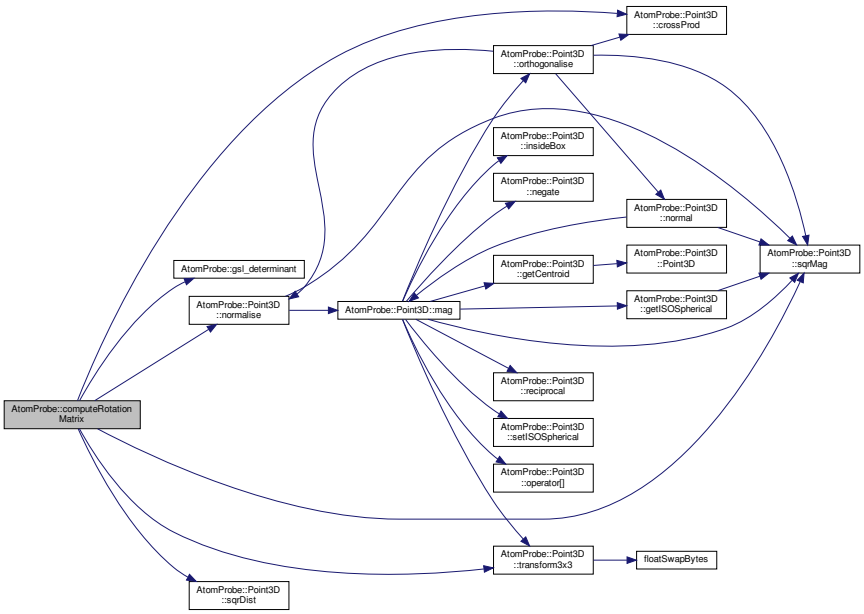
i.e. r = M∗ur, vector pairs (ur1,ur2) and (r1,r2) should be orthogonal and normalised matrix m must be pre-allocated as a 3x3 matrix, using e.g gsl_matrix_alloc(3,3)

Definition at line 12 of file rotations.cpp.

References ASSERT, AtomProbe::Point3D::crossProd(), gsl_determinant(), AtomProbe::Point3D::normalise(), AtomProbe::Point3D::sqrDist(), AtomProbe::Point3D::sqrMag(), TEST, and AtomProbe::Point3D::transform3x3().

Referenced by main().

Here is the call graph for this function:



5.1.3.15 convertEPOStoPos()

```
void AtomProbe::convertEPOStoPos (
            const std::vector< EPOS_ENTRY > & eposEntry,
            std::vector< IonHit > & posFile )
```

Convert an incoming entry of EPOS files to pos, and the append this to the pos vector given.

Definition at line 29 of file convert.cpp.

5.1.3.16 convertFileStringToCanonical()

```
std::string AtomProbe::convertFileStringToCanonical (
            const std::string & s )
```

Convert a path format into a unix path from native format.

Referenced by strAppend().

5.1.3.17 convertFileStringToNative()

```
std::string AtomProbe::convertFileStringToNative (
            const std::string & s )
```

Convert a path format into a native path from unix format.

Referenced by strAppend().

5.1.3.18 convertMassToMol()

```
void AtomProbe::convertMassToMol (
            const AbundanceData & atomTable,
            const std::map< unsigned int, double > & compositionMass,
            std::map< unsigned int, double > & compositionMols )
```

Convert the given composition from mass fraction data to molar fraction.

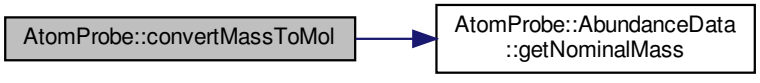
inputs are: compositionMass - relative mass fractions (this will be normalised automatically) massValues - weights of the masses input compositionMols - output results

Definition at line 74 of file massconvert.cpp.

References AtomProbe::AbundanceData::getNominalMass().

Referenced by parseCompositionData().

Here is the call graph for this function:



5.1.3.19 convertMolToMass()

```
void AtomProbe::convertMolToMass (
            const AbundanceData & atomTable,
            const std::map< unsigned int, double > & compositionMols,
            std::map< unsigned int, double > & compositionMass )
```

Convert the given composition from molar fraction data to mass fraction.

Inputs are:

- atomTable - the natural abundance table, to provide weights
- compositionMols : relative molar fractions (this will be normalised automatically). First entry in map is ion index in abundance table. Second is relative fraction.

Outputs are:

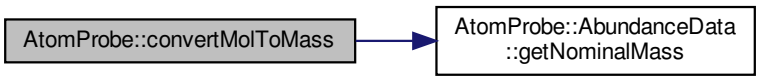
- compositionMass : output results, as mass fractions First entry is the position in the abundance table, second is relative fraction

Definition at line 41 of file massconvert.cpp.

References ASSERT, and AtomProbe::AbundanceData::getNominalMass().

Referenced by parseCompositionData().

Here is the call graph for this function:



5.1.3.20 correlationHistogram()

```
bool AtomProbe::correlationHistogram (
            const std::vector< EPOS_ENTRY > & eposIons,
            std::vector< std::vector< unsigned int > > & histogram,
            float stepMass,
            float endMass,
            bool lowerTriangular = false )
```

Generates an ion "correlation histogram" from a vector of EPOS ions. The input vector *MUST*

The nature of the plot is described in the following paper (Saxey et al, 2011): DOI : 10.1016/j.ultramic.2010.11.021, see e.g, Figure 3a.

The histogram will be allocated for you - do not pre-allocate

As the plot is symmetric around the m1=m2 line, the lowerTriangular setting controls if mirroring of the calculation is done. Setting this to true will ensure that only the lower half of the data field is calculated (faster).

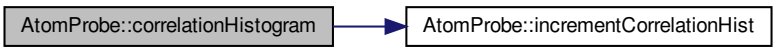
StepMass > 0 EndMass > 0

in both cases, the histogram will use the full rectangular memory space (arrays will not be ragged)

Definition at line 85 of file histogram.cpp.

References incrementCorrelationHist().

Here is the call graph for this function:



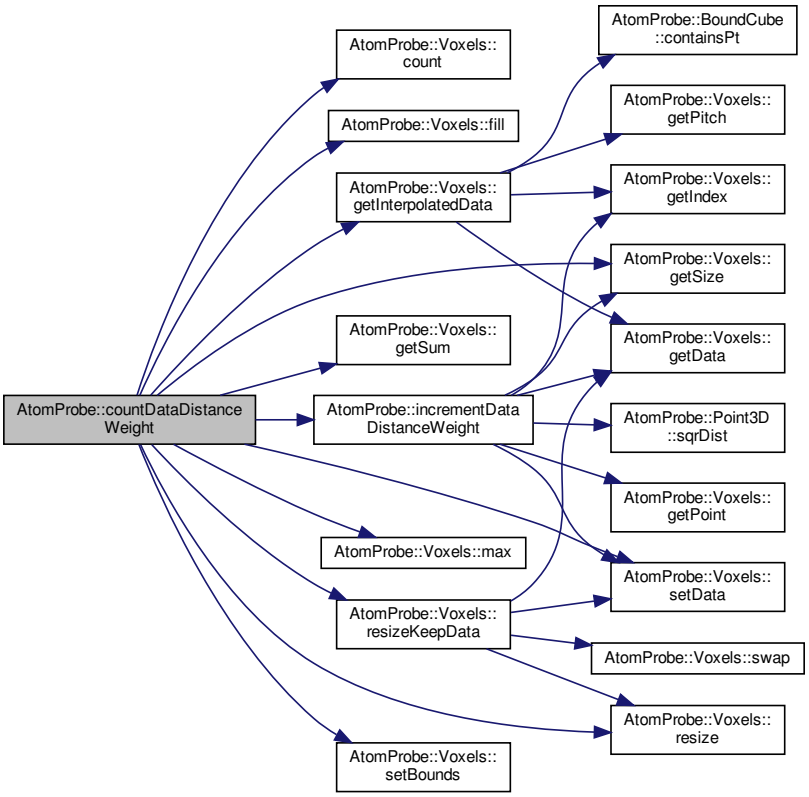
5.1.3.21 countDataDistanceWeight()

```
void AtomProbe::countDataDistanceWeight (
            const vector< Point3D > & pts,
            Voxels< float > & v )
```

Definition at line 120 of file voxels.cpp.

References ASSERT, AtomProbe::Voxels< T >::count(), AtomProbe::Voxels< T >::fill(), AtomProbe::Voxels< T >::getInterpolatedData(), AtomProbe::Voxels< T >::getSize(), AtomProbe::Voxels< T >::getSum(), incrementDataDistanceWeight(), AtomProbe::Voxels< T >::max(), AtomProbe::Voxels< T >::resize(), AtomProbe::Voxels< T >::resizeKeepData(), AtomProbe::Voxels< T >::setBounds(), AtomProbe::Voxels< T >::setData(), and TEST.

Here is the call graph for this function:



5.1.3.22 countIntensityEvents()

```
unsigned int AtomProbe::countIntensityEvents (
            const vector< pair< float, float > > & data,
            float minV,
            float maxV )
```

Definition at line 21 of file filter.cpp.

Referenced by maxExplainedFraction().

5.1.3.23 createMassBackground()

```
void AtomProbe::createMassBackground (
            float massStart,
            float massEnd,
            unsigned int nBinsMass,
            float tofBackIntensity,
            std::vector< float > & histogram )
```

Build a histogram of the background counts.

- Inputs : Start and end mass for background window, and bin count
- tofBackIntensity is the intensity level per unit time (proportional to sqrt mass) in the background, as obtained by doFitBackground.

Note : You may need to divide by bin width, depending on your application

Definition at line 208 of file processing.cpp.

Referenced by findPeaks().

5.1.3.24 cumTrapezoid()

```
template<class T >
void AtomProbe::cumTrapezoid (
             const vector< T > & x,
             const vector< T > & vals,
             vector< T > & res )
```

Definition at line 449 of file confidence.cpp.

References ASSERT, and kahansum().

Here is the call graph for this function:

5.1.3.25 det3by3()

```
double AtomProbe::det3by3 (
             const double * ptArray )
```

Definition at line 205 of file misc.cpp.

Referenced by dotProduct(), and pyramidVol().

5.1.3.26 Determinant()

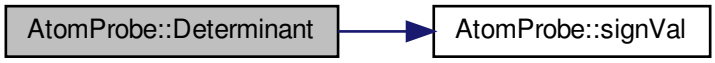
```
float AtomProbe::Determinant (
            float ** a,
            int n )
```

Definition at line 172 of file mesh.cpp.

References ASSERT, and signVal().

Referenced by fourDeterminant().

Here is the call graph for this function:



5.1.3.27 diff()

```
void AtomProbe::diff (
            const vector< float > & in,
            vector< float > & out )
```

Definition at line 233 of file processing.cpp.

Referenced by findPeaks().

5.1.3.28 digitString()

```
std::string AtomProbe::digitString (
            unsigned int thisDigit,
            unsigned int maxDigit )
```

Generate a string with leading digits up to maxDigit (eg, if maxDigit is 424, and thisDigit is 1.

Definition at line 115 of file stringFuncs.cpp.

References stream_cast().

Referenced by strAppend().

Here is the call graph for this function:

5.1.3.29 distanceToFacet()

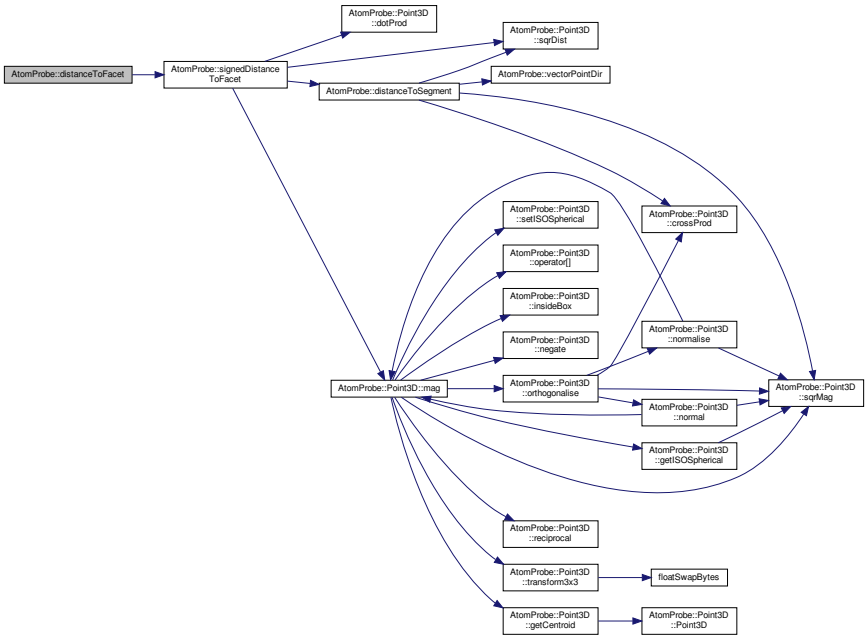
```
float AtomProbe::distanceToFacet (
            const Point3D & fA,
            const Point3D & fB,
            const Point3D & fC,
            const Point3D & normal,
            const Point3D & p )
```

Definition at line 199 of file misc.cpp.

References signedDistanceToFacet().

Referenced by GetReducedHullPts(), and meanAndStdev().

Here is the call graph for this function:



5.1.3.30 distanceToSegment()

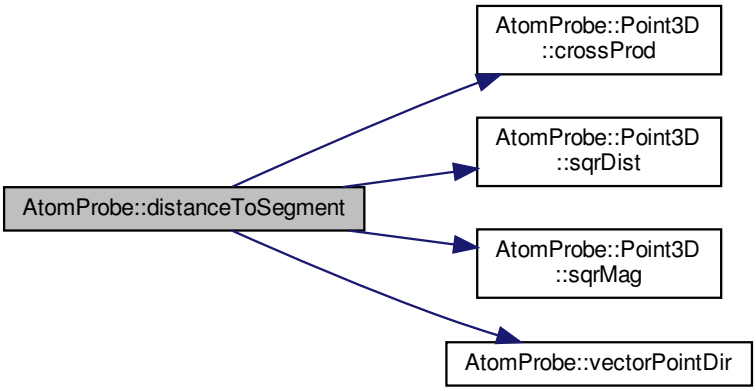
```
float AtomProbe::distanceToSegment (
            const Point3D & fA,
            const Point3D & fB,
            const Point3D & p )
```

Definition at line 105 of file misc.cpp.

References AtomProbe::Point3D::crossProd(), POINTDIR_TOGETHER, AtomProbe::Point3D::sqrDist(), AtomProbe::Point3D::sqrMag(), and vectorPointDir().

Referenced by meanAndStdev(), and signedDistanceToFacet().

Here is the call graph for this function:



5.1.3.31 doFitBackground()

```
unsigned int AtomProbe::doFitBackground (
            const std::vector< float > & massData,
            BACKGROUND_PARAMS & params )
```

Perform a background fit, assuming constant TOF noise, from 0->inf time.

- Background params has the input and output data for the fit.

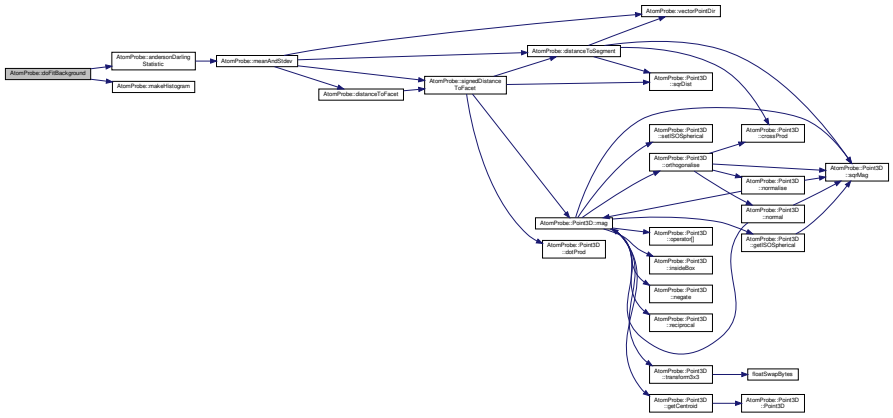
dataIn requires raw mass data, not histogram counts.

- returns zero on success, nonzero on error Return value is stored in params.intensity, as counts/bin. Use createMassBackground to re-generate the histogram

Definition at line 144 of file processing.cpp.

References andersonDarlingStatistic(), ASSERT, AtomProbe::BACKGROUND_PARAMS::binWidth, AtomProbe::BACKGROUND_PARAMS::FIT_FAIL_AVG_COUNTS, AtomProbe::BACKGROUND_PARAMS::FIT_FAIL_DATA_NON_GAUSSIAN, AtomProbe::BACKGROUND_PARAMS::FIT_FAIL_INSUFF_DATA, AtomProbe::BACKGROUND_PARAMS::FIT_FAIL_MIN_REQ_BINS, AtomProbe::BACKGROUND_PARAMS::intensity, makeHistogram(), AtomProbe::BACKGROUND_PARAMS::massEnd, AtomProbe::BACKGROUND_PARAMS::massStart, and AtomProbe::BACKGROUND_PARAMS::stdev.

Here is the call graph for this function:



5.1.3.32 doHull()

```
unsigned int AtomProbe::doHull (
            unsigned int bufferSize,
            double * buffer,
            vector< Point3D > & resHull,
            Point3D & midPoint,
            bool freeHullOnExit )
```

Definition at line 53 of file convexHull.cpp.

References HULL_ERR_NO_MEM.

Referenced by computeConvexHull().

5.1.3.33 dotProduct()

```
float AtomProbe::dotProduct (
            float a1,
            float a2,
            float a3,
            float b1,
            float b2,
            float b3 )  [inline]
```

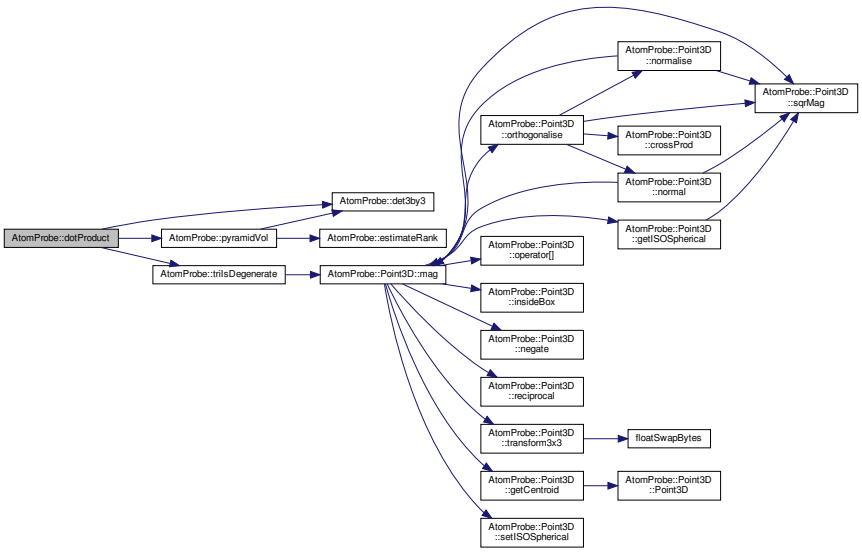
Inline func for calculating a(dot)b.

Definition at line 107 of file misc.h.

References det3by3(), pyramidVol(), and triIsDegenerate().

Referenced by GetReducedHullPts().

Here is the call graph for this function:



5.1.3.34 edgeIdx()

```
unsigned int AtomProbe::edgeIdx (
            unsigned int i,
            unsigned int j )
```

Definition at line 249 of file mesh.cpp.

References ASSERT.

5.1.3.35 estimateRank()

```
unsigned int AtomProbe::estimateRank (
            const gsl_matrix * m,
            float tolerance = sqrt(std::numeric_limits<float>::epsilon()) )
```

Estimate the rank of the given matrix.

Definition at line 7 of file misc.cpp.

Referenced by leastSquaresDeconvolve(), and pyramidVol().

5.1.3.36 filterBySolutionPPM()

```
void AtomProbe::filterBySolutionPPM (
            const AbundanceData & massTable,
            float minPpm,
            std::vector< std::vector< ISOTOPE_ENTRY > > & solutions )
```

Use the maximum possible PPM for each isotopic combination to filter possible solutions.

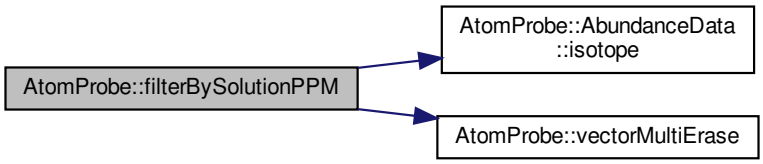
For example, 17^O:17^O:17^O in a naturally abundant mix has a maximum possible concentration of 5e-11 at. fraction. Isotope group tolerance is used to group the abundance distribution of nearby isotopes

massTable - a table of natural abundances minPpm - Minimum PPM below which to discard solutions solutions - list of solutions, which will be culled.

Definition at line 68 of file filter.cpp.

References AtomProbe::ISOTOPE_ENTRY::abundance, AtomProbe::AbundanceData::isotope(), and vectorMulti↩Erase().

Here is the call graph for this function:



5.1.3.37 filterPeakNeedBiggerObs()

```
void AtomProbe::filterPeakNeedBiggerObs (
            const AbundanceData & massTable,
            const std::vector< float > & peakData,
            float tolerance,
            size_t solutionCharge,
            std::vector< std::vector< ISOTOPE_ENTRY > > & solutions )
```

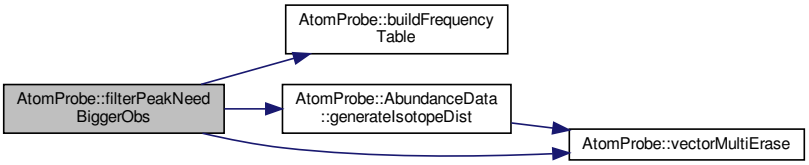
Remove peaks for which an experimental set of observed peaks do not show a peak at a position which is expected from the peak distribution for this element. Only works with single-atom peaks

- Solutions are the input solutions,
- peakData is a list of peak mass positions
- tolerance is the error allowed to fit a peak (+/-)
- solutionCharge - charge state for the input isotope entries

Definition at line 104 of file filter.cpp.

References ASSERT, buildFrequencyTable(), AtomProbe::AbundanceData::generateIsotopeDist(), and vector↩ MultiErase().

Here is the call graph for this function:



5.1.3.38 findMaxLessThanOrEq()

```
size_t AtomProbe::findMaxLessThanOrEq (
            const vector< std::pair< size_t, size_t > > & v,
            size_t value )
```

Definition at line 155 of file mesh.cpp.

References ASSERT.

5.1.3.39 findNearVerticies() [1/2]

```
void AtomProbe::findNearVerticies (
            float tolerance,
            const vector< Point3D > & ptVec,
            vector< std::pair< size_t, vector< size_t > > > & clusterList )
```

Definition at line 365 of file mesh.cpp.

References ASSERT.

Referenced by AtomProbe::Mesh::mergeDuplicateVertices(), and AtomProbe::Mesh::setTriangleMesh().

5.1.3.40 findNearVerticies() [2/2]

```
void AtomProbe::findNearVerticies (
            float tolerance,
            const vector< Point3D > & ptVec,
            std::list< std::pair< size_t, vector< size_t > > > & clusterList )
```

Definition at line 404 of file mesh.cpp.

References ASSERT.

5.1.3.41 findOverlaps() [1/4]

```
void AtomProbe::findOverlaps (
            const AbundanceData & natData,
            const RangeFile & rng,
            float massDelta,
            unsigned int maxCharge,
            std::vector< std::pair< size_t, size_t > > & overlapIdx,
            std::vector< std::pair< float, float > > & overlapMasses )
```

Find the overlaps stemming from a given rangefile.

An overlap is defined as "natural abundances within +-massDelta at same mass to charge"

- Species not in the rangefile will not be marked as overlapping
- FIXME: The output index is abused at this time, the range's index is actually given by dividing the output by the mass to charge. The charge state is given by modulo (massToCharge) +1
- The range mass information in the rangefile is not used - it is abused as an ion list

Inputs are:

- rng: The rangefile to use. The species in the rangefile are used to compute the overlaps
- massDelta: tolerance in amu,
- maxCharge: the maximum charge that species can be estimated to have

Outputs are:

- overlapIdx: the range indices of the overlapping species (ion index in rangefile)
- overlapMasses: the masses of the overlapping species, which should be within +-massDelta of one another

Note that ion's names will be decomposed, so Fe2H will be considered an Fe-Fe-H molecule

Referenced by findOverlaps(), and main().

5.1.3.42 findOverlaps() [2/4]

```
void AtomProbe::findOverlaps (
            const AbundanceData & natData,
            const std::vector< std::string > & ions,
            float massDelta,
            unsigned int maxCharge,
            std::vector< std::pair< size_t, size_t > > & overlapIdx,
            std::vector< std::pair< float, float > > & overlapMasses )
```

As per findOverlaps(...Rangefile ...) , but uses a vector of ions instead.

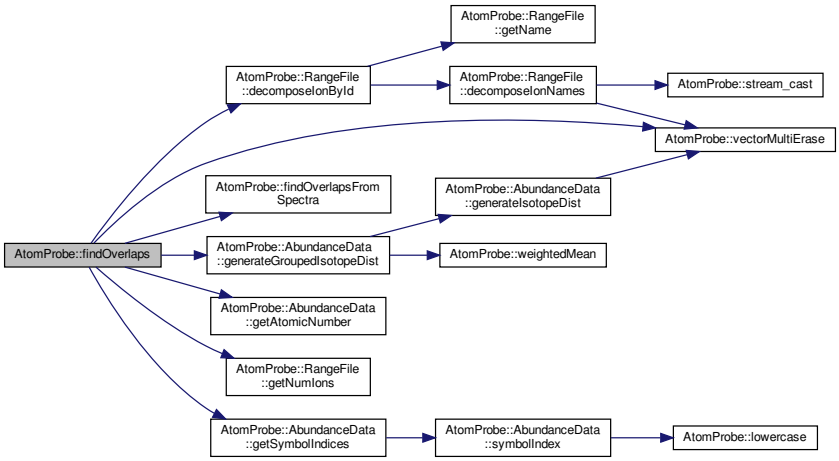
5.1.3.43 findOverlaps() [3/4]

```
void AtomProbe::findOverlaps (
            const AbundanceData & natData,
            const RangeFile & rng,
            float massDelta,
            unsigned int maxCharge,
            vector< pair< size_t, size_t > > & overlapIdx,
            vector< pair< float, float > > & overlapMasses )
```

Definition at line 78 of file overlaps.cpp.

References ASSERT, AtomProbe::RangeFile::decomposeIonById(), findOverlapsFromSpectra(), AtomProbe::↩
AbundanceData::generateGroupedIsotopeDist(), AtomProbe::AbundanceData::getAtomicNumber(), AtomProbe↩
::RangeFile::getNumIons(), AtomProbe::AbundanceData::getSymbolIndices(), and vectorMultiErase().

Here is the call graph for this function:



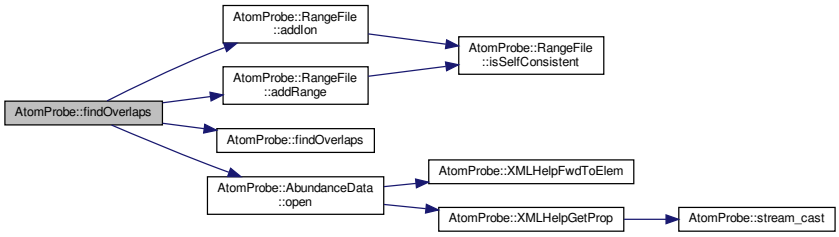
5.1.3.44 findOverlaps() [4/4]

```
void AtomProbe::findOverlaps (
            const AbundanceData & natData,
            const vector< string > & ionNames,
            float massDelta,
            unsigned int maxCharge,
            vector< pair< size_t, size_t > > & overlapIdx,
            vector< pair< float, float > > & overlapMasses )
```

Definition at line 202 of file overlaps.cpp.

References AtomProbe::RangeFile::addIon(), AtomProbe::RangeFile::addRange(), AtomProbe::RGBf::blue, findOverlaps(), AtomProbe::RGBf::green, AtomProbe::AbundanceData::open(), AtomProbe::RGBf::red, and TEST.

Here is the call graph for this function:



5.1.3.45 findOverlapsFromSpectra() [1/2]

```
void AtomProbe::findOverlapsFromSpectra (
            const vector< vector< pair< float, float > > > & massDistributions,
            float massDelta,
            const set< unsigned int > & skipIDs,
            vector< pair< size_t, size_t > > & overlapIdx,
            vector< pair< float, float > > & overlapMasses )
```

Definition at line 30 of file overlaps.cpp.

References EQ_TOLV.

5.1.3.46 findOverlapsFromSpectra() [2/2]

```
void AtomProbe::findOverlapsFromSpectra (
            const std::vector< std::vector< std::pair< float, float > > > & massDistributions,
            float massDelta,
            const std::set< unsigned int > & skipIDs,
            std::vector< std::pair< size_t, size_t > > & overlapIdx,
            std::vector< std::pair< float, float > > & overlapMasses )
```

Find overlaps in the given mass distributions, as per findOverlaps(...Rangefile...)

Referenced by findOverlaps().

5.1.3.47 findPeaks()

```
void AtomProbe::findPeaks (
            const std::vector< float > & x0,
            std::vector< unsigned int > & peakInds,
            float sel,
            bool autoSel = true,
            bool includeEndpoints = true )
```

Simple peak-finding algorithm.

Adapted from Nathaniel Yoder's: https://uk.mathworks.com/matlabcentral/fileexchange/25500-peakfind
which is BSD licenced.

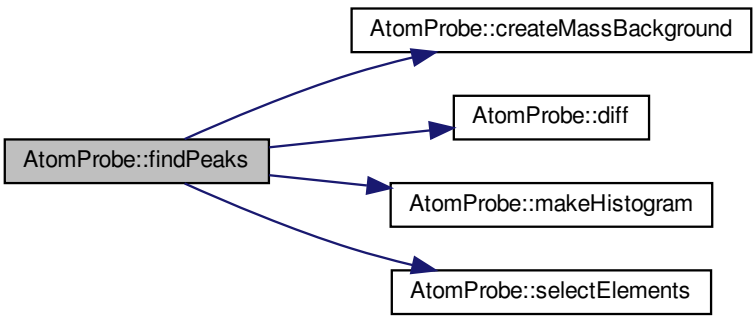
The performance of this function may or may not be suitable for your application, and your histogram may require pre-processing to optimise false postive/false-negative performance

- x0 : input mass histogram, must be > 2 elements
- sel : Selectivity for peaks - larger is more selective
- autosel : whether to determine sel automatically, or not
- includeEndpoints : allow edge values to be peaks

Definition at line 252 of file processing.cpp.

References ASSERT, createMassBackground(), diff(), makeHistogram(), NUM_IONS, and selectElements().

Here is the call graph for this function:



5.1.3.48 fixedRecordChunkReader()

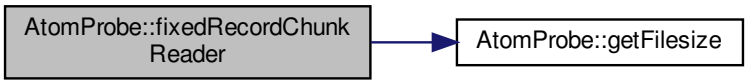
```
template<class T >
unsigned int AtomProbe::fixedRecordChunkReader (
            const char * filename,
            bool(*)(const char *bufRead, const char *destBuf) recordReader,
            size_t recordSize,
            std::vector< T > & outputData,
            unsigned int chunkSize,
            unsigned int chunkOffset,
            unsigned int & nEntriesLeft )
```

Definition at line 144 of file dataFiles.cpp.

References getFilesize(), RECORDREAD_BAD_FILEREAD, RECORDREAD_BAD_RECORD, RECORDREAD_↩ ERR_CHUNKOFFSET, RECORDREAD_ERR_FILE_OPEN, RECORDREAD_ERR_FILESIZE_MODULO, REC↩ ORDREAD_ERR_GET_FILESIZE, and RECORDREAD_ERR_NOMEM.

Referenced by chunkLoadEposFile().

Here is the call graph for this function:



5.1.3.49 fixedRecordReader()

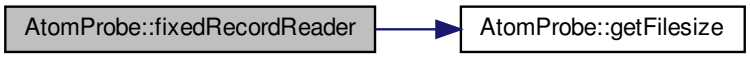
```
template<class T >
unsigned int AtomProbe::fixedRecordReader (
            const char * filename,
            bool(*)(const char *bufRead, const char *destBuf) recordReader,
            size_t recordSize,
            std::vector< T > & outputData )
```

Definition at line 93 of file dataFiles.cpp.

References getFilesize(), RECORDREAD_BAD_FILEREAD, RECORDREAD_BAD_RECORD, RECORDREAD_↩ ERR_FILE_OPEN, RECORDREAD_ERR_FILESIZE_MODULO, RECORDREAD_ERR_GET_FILESIZE, and R↩ ECORDREAD_ERR_NOMEM.

Referenced by loadEposFile().

Here is the call graph for this function:



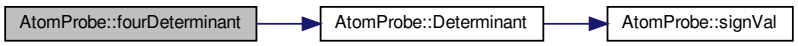
5.1.3.50 fourDeterminant()

```
float AtomProbe::fourDeterminant (
            const Point3D & a,
            const Point3D & b,
            const Point3D & c,
            const Point3D & d )
```

Definition at line 212 of file mesh.cpp.

References Determinant().

Here is the call graph for this function:



5.1.3.51 fpeek()

```
int AtomProbe::fpeek (
            FILE * stream )  [inline]
```

Definition at line 69 of file helpFuncs.h.

Referenced by AtomProbe::RangeFile::rangeTypeString().

5.1.3.52 freeConvexHull()

```
void AtomProbe::freeConvexHull ( )
```

Definition at line 47 of file convexHull.cpp.

Referenced by GetReducedHullPts().

5.1.3.53 gauss_ratio_pdf()

```
double AtomProbe::gauss_ratio_pdf (
            double x,
            double muX,
            double muY,
            double varX,
            double varY )
```

Definition at line 471 of file confidence.cpp.

References M_PI.

5.1.3.54 gcd()

```
int AtomProbe::gcd (
            int a,
            int b )
```

Definition at line 12 of file millerIndex.cpp.

Referenced by AtomProbe::MILLER_TRIPLET::simplify().

5.1.3.55 genColString() [1/2]

```
void AtomProbe::genColString (
            unsigned char r,
            unsigned char g,
            unsigned char b,
            unsigned char a,
            std::string & s )
```

Referenced by strAppend(), AtomProbe::RGBf::toHex(), and AtomProbe::RangeFile::write().

5.1.3.56 genColString() [2/2]

```
void AtomProbe::genColString (
            unsigned char r,
            unsigned char g,
            unsigned char b,
            std::string & s )
```

Definition at line 308 of file stringFuncs.cpp.

References ucharToHexStr().

Here is the call graph for this function:

5.1.3.57 generate1DAxialDistHist()

```
unsigned int AtomProbe::generate1DAxialDistHist (
            const std::vector< Point3D > & pointList,
            K3DTreeExact & tree,
            const Point3D & axisDir,
            float distMax,
            std::vector< unsigned int > & histogram )
```

Generate a 1D axial distribution function,.

This generates a histogram of point-point distances, from the points in the point list to the points in the tree, within a specified radius of the source point.

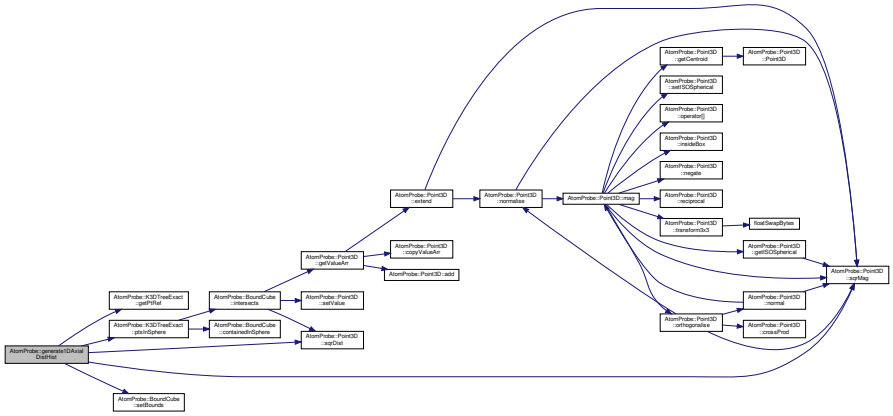
This is variously called a 1D "Spatial Distribution Map (SDM)" "Atom Vicinity" or similar

- pointList : the source points for the distribution function
- tree : a pre-generated KD tree with the target points
- distMax : radius of the points around which to search
- histogram : a vector with the number of bins that are required for output. Does not need to be zero filled

Definition at line 22 of file axialdf.cpp.

References ASSERT, AtomProbe::K3DTreeExact::getPtRef(), AtomProbe::K3DTreeExact::ptsInSphere(), AtomProbe::BoundCube::setBounds(), AtomProbe::Point3D::sqrDist(), and AtomProbe::Point3D::sqrMag().

Here is the call graph for this function:



5.1.3.58 generate1DAxialDistHistSweep()

```
unsigned int AtomProbe::generate1DAxialDistHistSweep (
            const std::vector< Point3D > & pointList,
            K3DTreeExact & tree,
            float distMax,
            float dTheta,
            float dPhi,
            ProgressBar & prog,
            std::vector< std::vector< std::vector< unsigned int > > > & histogram )
```

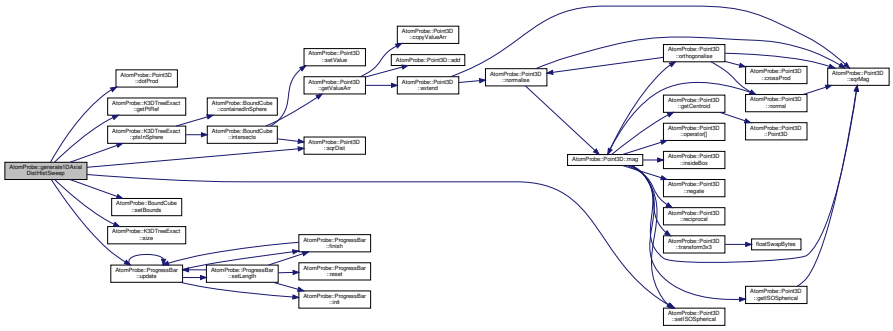
Generate a series of 1D distribution functions, one per pixel in a 2D grid of spherical coordinate directions.

Using a stepped spherical coordinates in equal delta-Theta, delta-Phi increments pointList : the source points from which to search tree : K3D Tree of target points distMax : maximum distance around which to search dTheta : step size in theta (radiians). dPhi : step size in phi (radiians) prog : Progress bar histogram : resultant data as a 2D vector, one bin per angular entry. Each vector will have the same size. The inner most vector contains the analysis data, over +-distMax

Definition at line 116 of file axialdf.cpp.

References ASSERT, AtomProbe::Point3D::dotProd(), AtomProbe::K3DTreeExact::getPtRef(), M_PI, AtomProbe::K3DTreeExact::ptsInSphere(), AtomProbe::BoundCube::setBounds(), AtomProbe::Point3D::setISOSpherical(), AtomProbe::K3DTreeExact::size(), AtomProbe::Point3D::sqrDist(), and AtomProbe::ProgressBar::update().

Here is the call graph for this function:



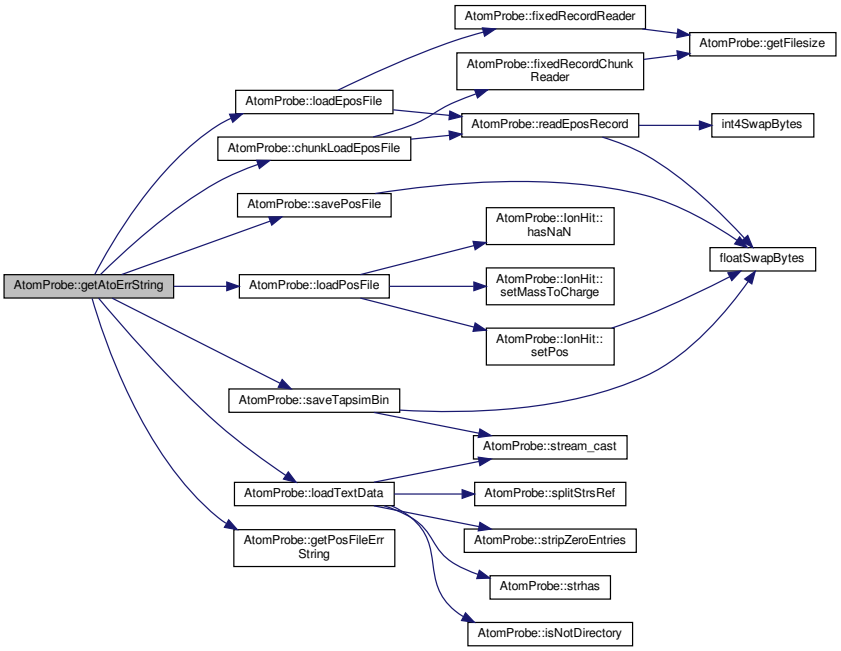
5.1.3.59 getAtoErrString()

```
const char* AtomProbe::getAtoErrString (
            unsigned int errCode )  [inline]
```

Definition at line 82 of file dataFiles.h.

References chunkLoadEposFile(), getPosFileErrString(), loadEposFile(), loadPosFile(), loadTextData(), AtomProbe::ATO_ENTRY::mass, savePosFile(), and saveTapsimBin().

Here is the call graph for this function:



5.1.3.60 getFilesize()

```
bool AtomProbe::getFilesize (
            const char * fname,
            size_t & size )
```

Definition at line 107 of file helpFuncs.cpp.

Referenced by fixedRecordChunkReader(), fixedRecordReader(), AtomProbe::RangeFile::openFormat(), AtomProbe::ComparePairFirstReverse::operator()(), and readPosapOps().

5.1.3.61 getFitErrorMsg()

```
string AtomProbe::getFitErrorMsg (
            unsigned int errCode )
```

Obtain a human readable error, which has arison when using doFitBackground Input is the error code from doFitBackground

Definition at line 130 of file processing.cpp.

References ASSERT, and AtomProbe::BACKGROUND_PARAMS::FIT_FAIL_END.

5.1.3.62 getHardAssert()

```
bool AtomProbe::getHardAssert ( )
```

Definition at line 25 of file aptAssert.cpp.

References hardAssert.

5.1.3.63 getPosFileErrString()

```
const char * AtomProbe::getPosFileErrString (
            unsigned int errMesg )
```

Definition at line 238 of file dataFiles.cpp.

References ARRAYSIZE, and POS_FILE_ENUM_END.

Referenced by getAtoErrString(), and main().

5.1.3.64 getRangeMolecule()

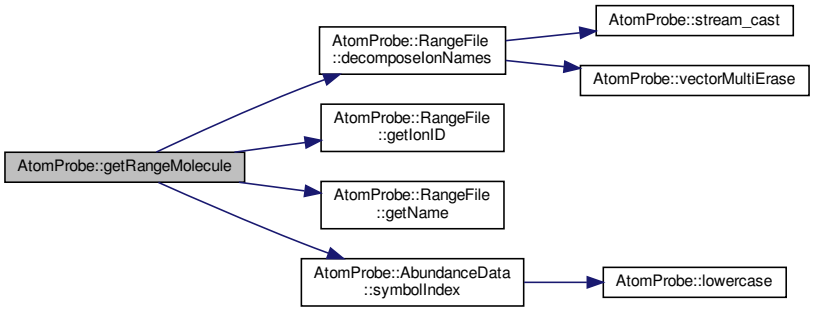
```
RANGE_MOLECULE AtomProbe::getRangeMolecule (
            const AbundanceData & massTable,
            const RangeFile & rng,
            unsigned int rangeId )
```

Definition at line 55 of file rangeCheck.cpp.

References AtomProbe::RANGE_MOLECULE::components, AtomProbe::RangeFile::decomposeIonNames(), AtomProbe::RangeFile::getIonID(), AtomProbe::RangeFile::getName(), AtomProbe::RANGE_MOLECULE::isOK, AtomProbe::RANGE_MOLECULE::name, and AtomProbe::AbundanceData::symbolIndex().

Referenced by checkMassRangingCorrectness().

Here is the call graph for this function:



5.1.3.65 getRecordReadErrString()

```
const char* AtomProbe::getRecordReadErrString (
            unsigned int errCode )  [inline]
```

Definition at line 46 of file dataFiles.h.

5.1.3.66 GetReducedHullPts()

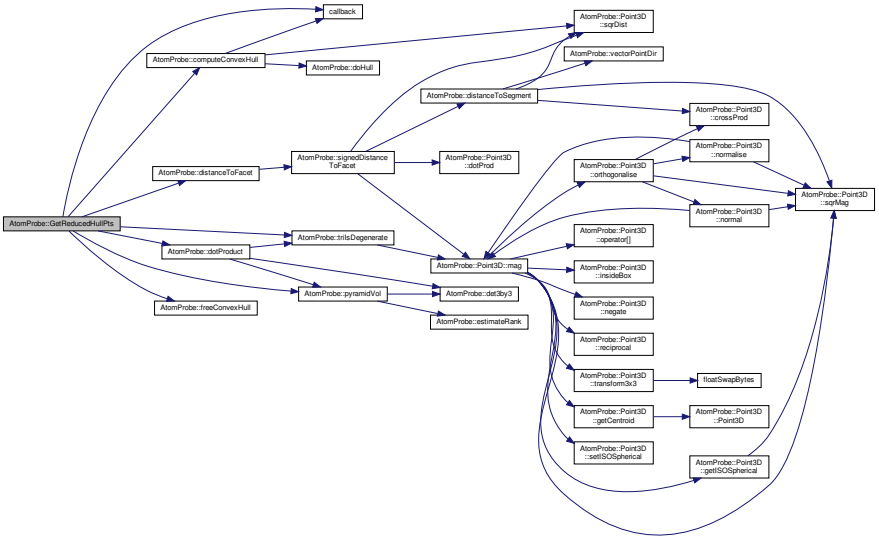
```
unsigned int AtomProbe::GetReducedHullPts (
            const std::vector< IonHit > & points,
            float reductionDim,
            unsigned int * progress,
            bool(*)(bool) callback,
            std::vector< IonHit > & pointResult )
```

Obtain a set of points that are a subset of points the convex hull that are at least "reductionDim" away from the hull itself.

Definition at line 289 of file convexHull.cpp.

References ASSERT, callback(), computeConvexHull(), distanceToFacet(), dotProduct(), freeConvexHull(), HULL↩ _SURFREDUCE_NEGATIVE_SCALE_FACT, NUM_IONS, pyramidVol(), SCALE, and triIsDegenerate().

Here is the call graph for this function:



5.1.3.67 gsl_determinant()

```
float AtomProbe::gsl_determinant (
            const gsl_matrix * m )
```

Definition at line 143 of file helpFuncs.cpp.

References ASSERT.

Referenced by computeRotationMatrix(), and AtomProbe::ComparePairFirstReverse::operator()().

5.1.3.68 gsl_matrix_mult()

```
void AtomProbe::gsl_matrix_mult (
            const gsl_matrix * a,
            const gsl_matrix * b,
            gsl_matrix *& res )
```

Definition at line 40 of file point3D.cpp.

Referenced by main().

5.1.3.69 gsl_print_matrix()

```
void AtomProbe::gsl_print_matrix (
            const gsl_matrix * m )
```

Definition at line 122 of file helpFuncs.cpp.

Referenced by computeRangeAdjacency(), and AtomProbe::ComparePairFirstReverse::operator()().

5.1.3.70 gsl_print_vector()

```
void AtomProbe::gsl_print_vector (
            const gsl_vector * v )
```

Definition at line 134 of file helpFuncs.cpp.

Referenced by AtomProbe::ComparePairFirstReverse::operator()().

5.1.3.71 hexStrToUChar()

```
void AtomProbe::hexStrToUChar (
            const std::string & s,
            unsigned char & c )
```

Definition at line 92 of file stringFuncs.cpp.

References ASSERT.

Referenced by parseColString().

5.1.3.72 incrementCorrelationHist()

```
bool AtomProbe::incrementCorrelationHist (
            const std::vector< EPOS_ENTRY > & eposIons,
            std::vector< std::vector< unsigned int > > & histogram,
            float stepMass,
            float endMass )
```

Definition at line 29 of file histogram.cpp.

Referenced by accumulateCorrelationHistogram(), and correlationHistogram().

5.1.3.73 incrementDataDistanceWeight()

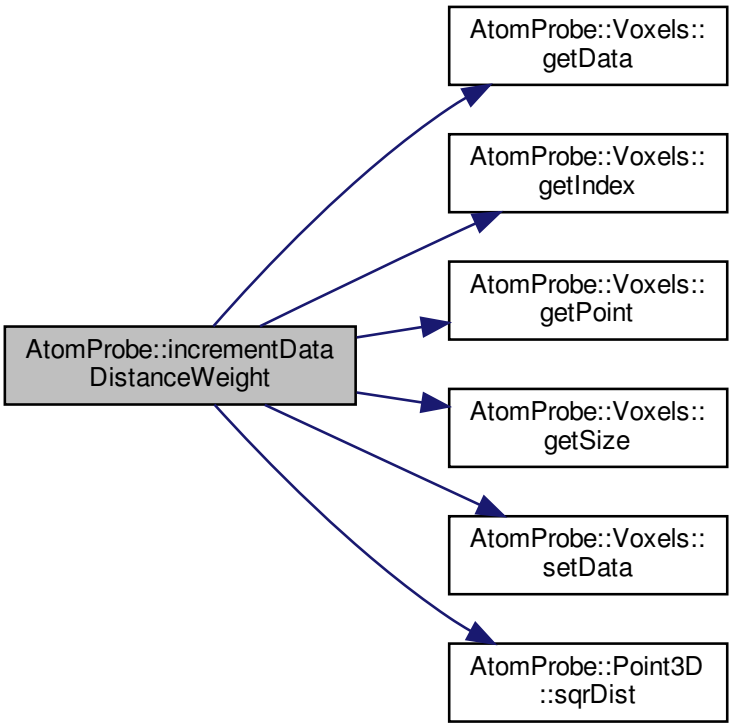
```
void AtomProbe::incrementDataDistanceWeight (
            const Point3D & p,
            Voxels< float > & v )
```

Definition at line 33 of file voxels.cpp.

References AtomProbe::Voxels< T >::getData(), AtomProbe::Voxels< T >::getIndex(), AtomProbe::Voxels< T >::getPoint(), AtomProbe::Voxels< T >::getSize(), AtomProbe::Voxels< T >::setData(), and AtomProbe::Point3D::sqrDist().

Referenced by countDataDistanceWeight().

Here is the call graph for this function:



5.1.3.74 intersect_RayTriangle()

```
int AtomProbe::intersect_RayTriangle (
            const Point3D & rayStart,
            const Point3D & rayEnd,
```

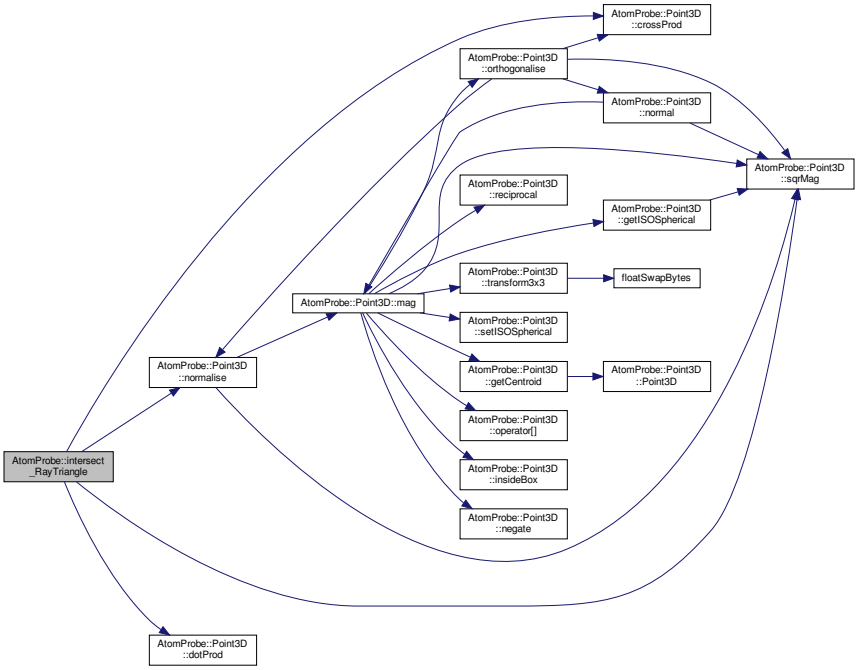
```
            Point3D * tri,
            Point3D & I )
```

Definition at line 280 of file mesh.cpp.

References AtomProbe::Point3D::crossProd(), AtomProbe::Point3D::dotProd(), AtomProbe::Point3D::normalise(), and AtomProbe::Point3D::sqrMag().

Referenced by AtomProbe::Mesh::pointsInside().

Here is the call graph for this function:



5.1.3.75 isNotDirectory()

```
bool AtomProbe::isNotDirectory (
            const char * filename )
```

Definition at line 170 of file helpFuncs.cpp.

Referenced by AtomProbe::RangeFile::detectFileType(), loadTextData(), and AtomProbe::ComparePairFirst↩ Reverse::operator()().

5.1.3.76 kahansum()

```
template<class T , class T2 >
std::iterator_traits<T>::value_type AtomProbe::kahansum (
            T begin,
            T end,
            T2 other )
```

Definition at line 34 of file confidence.cpp.

Referenced by cumTrapezoid().

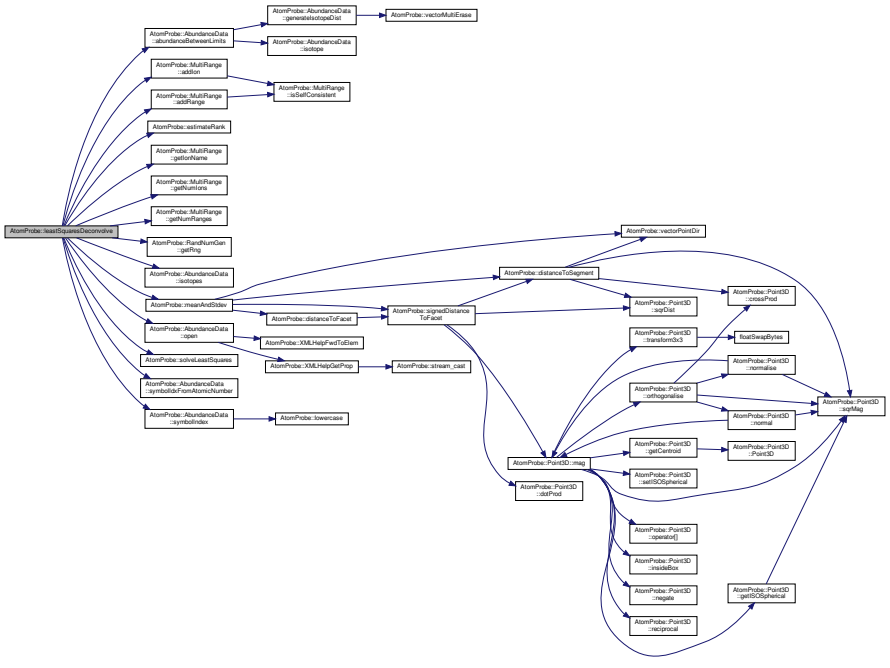
5.1.3.77 leastSquaresDeconvolve()

```
bool AtomProbe::leastSquaresDeconvolve (
            const MultiRange & rangeData,
            const AbundanceData & abundance,
            const float massTol,
            const vector< IonHit > & hits,
            float(*)(float, float) backgroundEstimator,
            vector< pair< unsigned int, float > > & decomposedHits )
```

Definition at line 32 of file deconvolution.cpp.

References AtomProbe::AbundanceData::abundanceBetweenLimits(), AtomProbe::MultiRange::addIon(), AtomProbe::MultiRange::addRange(), ASSERT, AtomProbe::SIMPLE_SPECIES::atomicNumber, AtomProbe::RGBf::blue, AtomProbe::SIMPLE_SPECIES::count, estimateRank(), AtomProbe::MultiRange::getIonName(), AtomProbe::MultiRange::getNumIons(), AtomProbe::MultiRange::getNumRanges(), AtomProbe::RandNumGen::getRng(), AtomProbe::RGBf::green, AtomProbe::AbundanceData::isotopes(), meanAndStdev(), AtomProbe::AbundanceData::open(), randGen, AtomProbe::RGBf::red, solveLeastSquares(), AtomProbe::AbundanceData::symbolIdxFromAtomicNumber(), AtomProbe::AbundanceData::symbolIndex(), and WARN.

Here is the call graph for this function:



5.1.3.78 linearHistogram()

```
template<class T >
void AtomProbe::linearHistogram (
            const std::vector< T > & data,
            T start,
            T end,
            T step,
            std::vector< T > & histVals )
```

Make a linearly spaced histogram with the given spacings Takes a vector of floats as input,

Parameters

data	

Definition at line 75 of file histogram.h.

References ASSERT.

Referenced by main().

5.1.3.79 linkIdentifiers()

```
template<class T >
void AtomProbe::linkIdentifiers (
            vector< T > & link )
```

Definition at line 88 of file multiRange.cpp.

Referenced by AtomProbe::MultiRange::splitOverlapping().

5.1.3.80 loadATOFile()

```
unsigned int AtomProbe::loadATOFile (
            const char * fileName,
            std::vector< ATO_ENTRY > & ions,
            unsigned int forceEndian = 0 )
```

Load a LAWATAP "ATO" file.

ATO files contain a mix of experiment and analysis data, including voltage, positioning and reconstructed data. There are specific algorithm generated data (eg clustering) which are not loaded in structures in this library to reduce memory consumption. Returns 0 on success, nonzero on error

- Filename : the name of the data file to read
- ions : the returned entries from the file

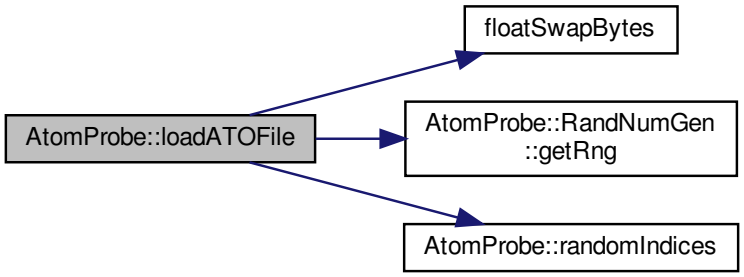
- forceEndian : if nonzero, this wil force the use of either little-endian reading (1), or big-endian(2). If zero, the routine will try to automatically determine endianness from the file contents.

Returned code if nonzero can be converted to human readable form using ATO_ERR_STRINGS. Note if calling from outside C++, use getAtoErrString(...) to return the error string

Definition at line 1204 of file dataFiles.cpp.

References ASSERT, ATO_EMPTY_FAIL, ATO_MEM_ERR, ATO_OPEN_FAIL, ATO_SIZE_ERR, ATO_VERSI↩ ONCHECK_ERR, floatSwapBytes(), AtomProbe::RandNumGen::getRng(), randGen, and randomIndices().

Here is the call graph for this function:



5.1.3.81 loadEposFile()

```
size_t AtomProbe::loadEposFile (
            std::vector< EPOS_ENTRY > & outData,
            const char * filename )
```

Load an entire "EPOS" File.

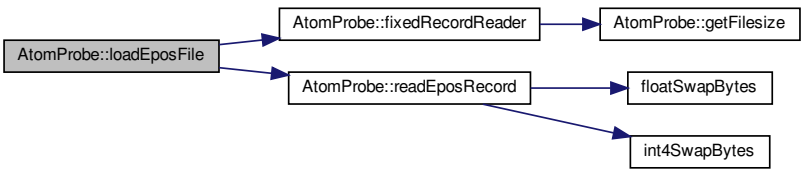
Epos files are very large and unwieldy. Ensure that you really want to do this, as it is possible you will run out of memory. Consider using the "chunkLoadEposFile" to process your data if possible. The file contains x,y,z,m-to-c,tof(uncorrected?). The return value is nonzero on error, and is part of the RECORDREAD_ERR enum

Definition at line 748 of file dataFiles.cpp.

References EPOS_RECORD_SIZE, fixedRecordReader(), and readEposRecord().

Referenced by getAtoErrString(), and main().

Here is the call graph for this function:



5.1.3.82 loadPosFile() [1/2]

```
unsigned int AtomProbe::loadPosFile (
            std::vector< IonHit > & posIons,
            const char * posFile )
```

Load a pos file directly into a single ion list.

Load a pos file from a file. Returns nonzero on exit.

Pos files are fixed record size files, with data stored as 4byte big endian floating point. (IEEE 754?). Data is stored as x,y,z,mass/charge.

Currently loads entire file in one gulp. This is bad from the point of view of gigabyte size pos files generated by laser atom probes.. Returns 0 on ok, nonzero on success.

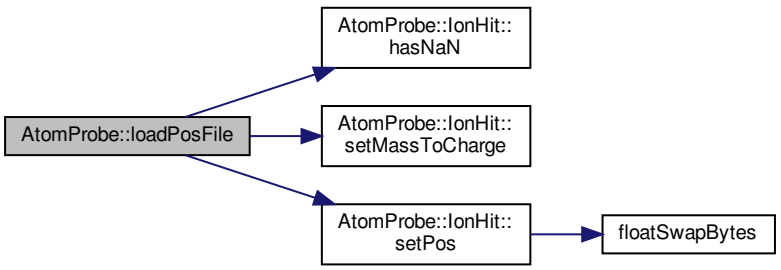
arguments : posfile | path to pos-formatted file posIons | will return any ions that are loaded from the dataset. Behaviour for loading into * a non-empty vector is undefined Return code can be decoded with getPosFileErrString

Definition at line 256 of file dataFiles.cpp.

References ASSERT, AtomProbe::IonHit::hasNaN(), AtomProbe::IONHIT::massToCharge, AtomProbe::IONHIT↩ ::pos, POS_ALLOC_FAIL, POS_NAN_LOAD_ERROR, POS_OPEN_FAIL, POS_READ_FAIL, POS_SIZE_EMP↩ TY_ERR, POS_SIZE_MODULUS_ERR, AtomProbe::IonHit::setMassToCharge(), and AtomProbe::IonHit::setPos().

Referenced by getAtoErrString(), loadPosFile(), and main().

Here is the call graph for this function:



5.1.3.83 loadPosFile() [2/2]

```
unsigned int AtomProbe::loadPosFile (
            std::vector< IonHit > & posIons,
            const char * posFile,
            unsigned int nSamplesMax )
```

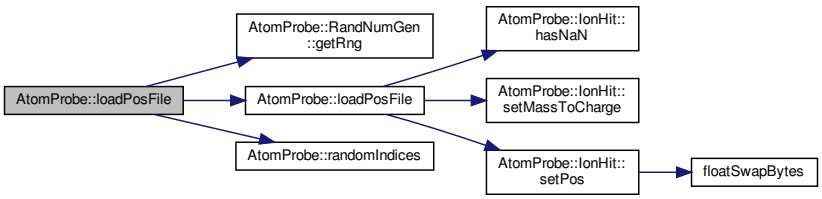
As per loadPosFile, but with an additional setting for the maximum number of ions to load.

Ions will be randomly sampled to form nSamples. This will be likely much slower than loading a full file, depending on the size of nSamples. The samples are not guaranteed to be the same for each load. Speed will be nlogn in nSamplesMax, o(1) in posIons.

Definition at line 364 of file dataFiles.cpp.

References AtomProbe::RandNumGen::getRng(), loadPosFile(), AtomProbe::IONHIT::massToCharge, AtomProbe::IONHIT::pos, POS_ALLOC_FAIL, POS_NAN_LOAD_ERROR, POS_OPEN_FAIL, POS_READ_FAIL, POS_SIZE_EMPTY_ERR, POS_SIZE_MODULUS_ERR, randGen, and randomIndices().

Here is the call graph for this function:



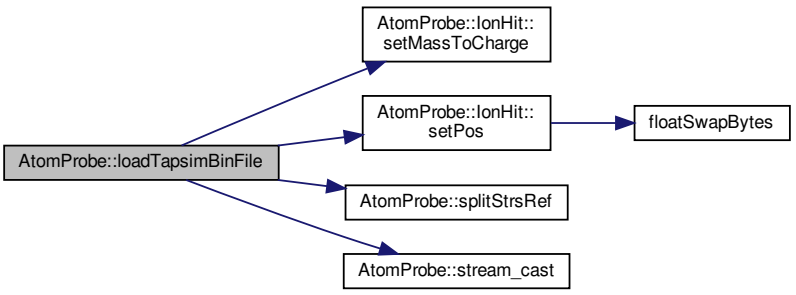
5.1.3.84 loadTapsimBinFile()

```
unsigned int AtomProbe::loadTapsimBinFile (
            vector< IonHit > & posIons,
            const char * posfile )
```

Definition at line 538 of file dataFiles.cpp.

References AtomProbe::IonHit::setMassToCharge(), AtomProbe::IonHit::setPos(), splitStrsRef(), stream_cast(), TAPSIM_FILE_FORMAT_FAIL, and TAPSIM_OPEN_FAIL.

Here is the call graph for this function:



5.1.3.85 loadTextData()

```
unsigned int AtomProbe::loadTextData (
            const char * cpFilename,
            std::vector< std::vector< float > > & dataVec,
            std::vector< std::string > & headerVec,
            const char * delim,
            bool allowNan = true )
```

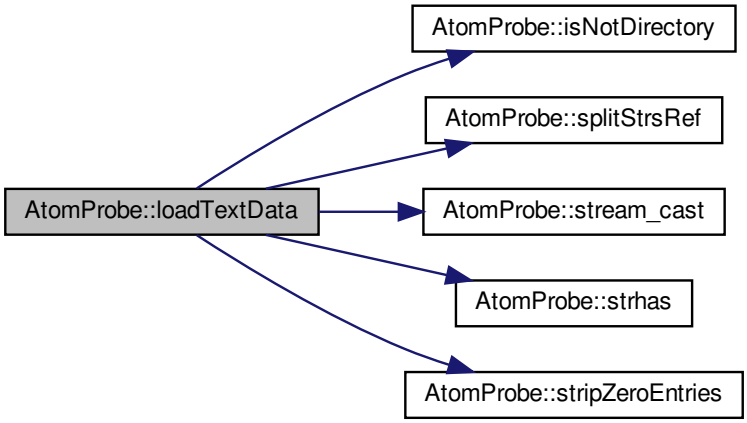
Load a CSV, TSV or similar text file. Assumes "C" Locale for input (ie "." as decimal separator).

Definition at line 1496 of file dataFiles.cpp.

References isNotDirectory(), splitStrsRef(), stream_cast(), strhas(), stripZeroEntries(), TEXT_ERR_FILE_FORMAT, TEXT_ERR_FILE_NUM_FIELDS, and TEXT_ERR_FILE_OPEN.

Referenced by getAtoErrString(), and main().

Here is the call graph for this function:



5.1.3.86 lowercase()

```
std::string AtomProbe::lowercase (
            std::string s )
```

Return a lowercase version for a given string.

Definition at line 176 of file stringFuncs.cpp.

Referenced by AtomProbe::RangeFile::detectFileType(), main(), parseCompositionData(), AtomProbe::Range↩File::rangeTypeString(), strAppend(), and AtomProbe::AbundanceData::symbolIndex().

5.1.3.87 makeHistogram()

```
void AtomProbe::makeHistogram (
            const vector< float > & data,
            float start,
            float end,
            float step,
            vector< float > & histVals )
```

Definition at line 110 of file processing.cpp.

References ASSERT.

Referenced by doFitBackground(), and findPeaks().

5.1.3.88 marchingCubes()

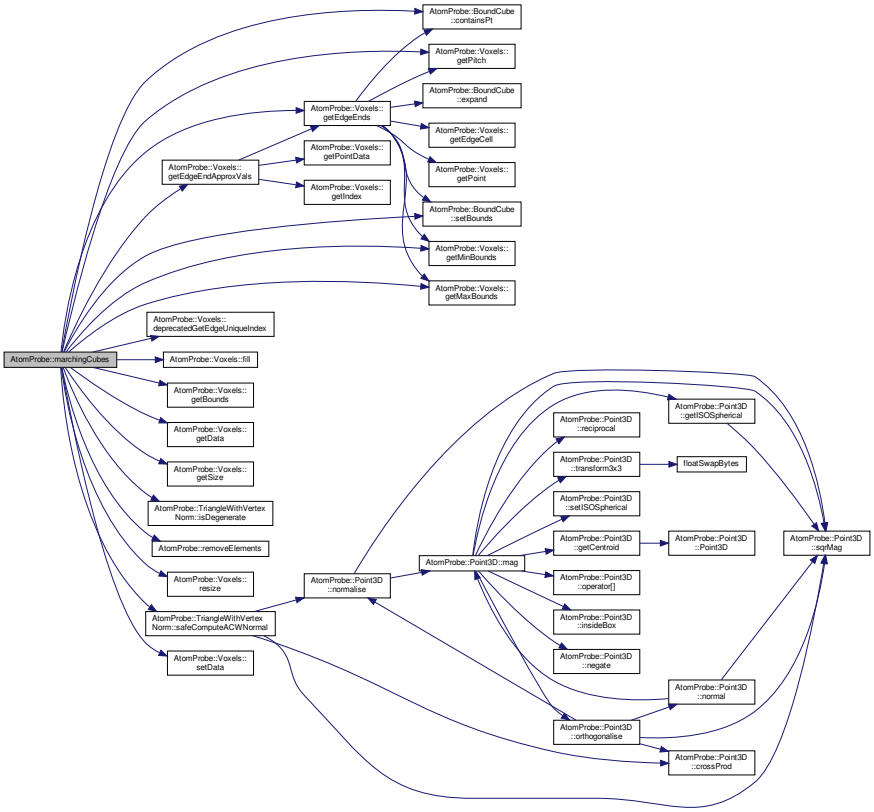
```
void AtomProbe::marchingCubes (
            const Voxels< float > & v,
            float isoValue,
            std::vector< TriangleWithVertexNorm > & tVec )
```

Definition at line 494 of file isoSurface.cpp.

References ASSERT, AtomProbe::BoundCube::containsPt(), AtomProbe::Voxels< T >::deprecatedGetEdgeUniqueIndex(), AtomProbe::Voxels< T >::fill(), AtomProbe::Voxels< T >::getBounds(), AtomProbe::Voxels< T >::getData(), AtomProbe::Voxels< T >::getEdgeEndApproxVals(), AtomProbe::Voxels< T >::getEdgeEnds(), AtomProbe::Voxels< T >::getMaxBounds(), AtomProbe::Voxels< T >::getMinBounds(), AtomProbe::Voxels< T >::getPitch(), AtomProbe::Voxels< T >::getSize(), AtomProbe::TriangleWithVertexNorm::isDegenerate(), AtomProbe::TriangleWithVertexNorm::normal, AtomProbe::TriangleWithVertexNorm::p, AtomProbe::TriangleWithIndexedVertices::p, AtomProbe::TRIANGLE::p, AtomProbe::TRIANGLE::physGroup, removeElements(), AtomProbe::Voxels< T >::resize(), AtomProbe::TriangleWithVertexNorm::safeComputeACWNormal(), AtomProbe::BoundCube::setBounds(), AtomProbe::Voxels< T >::setData(), and TEST.

Referenced by main().

Here is the call graph for this function:



5.1.3.89 matchComposedName()

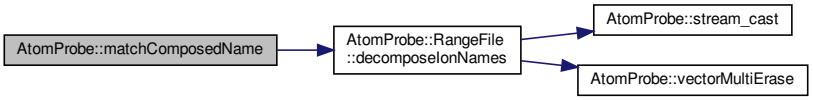
```
bool AtomProbe::matchComposedName (
            const std::map< string, size_t > & composedNames,
            const vector< pair< string, size_t > > & namesToFind,
            size_t & matchOffset )
```

Definition at line 253 of file ranges.cpp.

References AtomProbe::RangeFile::decomposeIonNames().

Referenced by AtomProbe::RangeFile::open().

Here is the call graph for this function:



5.1.3.90 maxExplainedFraction() [1/2]

```
std::vector<float> AtomProbe::maxExplainedFraction (
            const std::vector< std::pair< float, float > > & massData,
            float peakMass,
            float massWidth,
            const std::vector< std::vector< ISOTOPE_ENTRY > > & solutions,
            const AbundanceData & massTable,
            float massDistTol,
            unsigned int solutionCharge )
```

Compute the fraction of the data that has been explained, using the natural abundance information, and intensity data.

Specifically, this returns the maximum possible fraction of this peak that is explained by the isotopic fingerprint for a given solution set, and the count data given. This is returned as a vector with a value for each proposed solution Note the solutions do not need to sum to 1

massData - list of location and intensities for peaks in dataset peakMass - peak we wish to query. Must be present (within tolerance) in peak list (massData) massWidth - tolerance width (+-) when locating peaks solutions - list of candidate solutions we want to find the explained fraction for massDistTol - tolerance to use when checking for peaks in mass distribution solutionCharge - charge state to apply to isotope distribuion

Referenced by maxExplainedFraction().

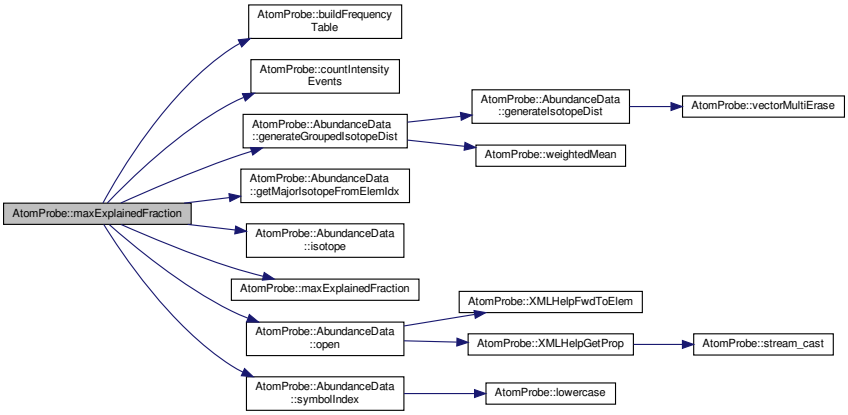
5.1.3.91 maxExplainedFraction() [2/2]

```
vector<float> AtomProbe::maxExplainedFraction (
            const vector< pair< float, float > > & intensityData,
            float peakMass,
            float massWidth,
            const vector< vector< ISOTOPE_ENTRY > > & solutions,
            const AbundanceData & massTable,
            float massDistTol,
            unsigned int solutionCharge )
```

Definition at line 206 of file filter.cpp.

References ASSERT, buildFrequencyTable(), countIntensityEvents(), AtomProbe::AbundanceData::generate↩GroupedIsotopeDist(), AtomProbe::AbundanceData::getMajorIsotopeFromElemIdx(), AtomProbe::Abundance↩Data::isotope(), AtomProbe::ISOTOPE_ENTRY::mass, maxExplainedFraction(), AtomProbe::AbundanceData↩::open(), AtomProbe::AbundanceData::symbolIndex(), and TEST.

Here is the call graph for this function:



5.1.3.92 meanAndStdev()

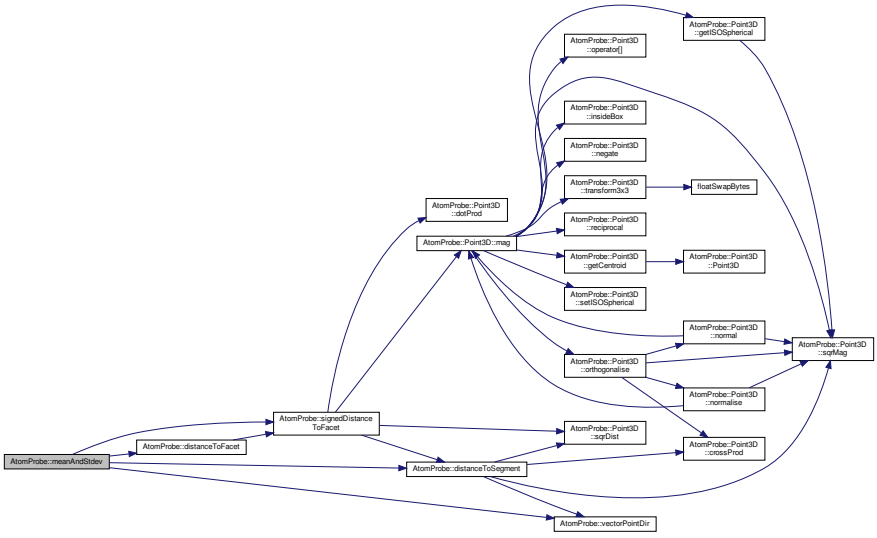
```
template<typename T >
void AtomProbe::meanAndStdev (
            const std::vector< T > & f,
            float & meanVal,
            float & stdevVal,
            bool normalCorrection = true )
```

Definition at line 55 of file misc.h.

References distanceToFacet(), distanceToSegment(), signedDistanceToFacet(), and vectorPointDir().

Referenced by andersonDarlingStatistic(), and leastSquaresDeconvolve().

Here is the call graph for this function:



5.1.3.93 myStrDup()

```
char* AtomProbe::myStrDup (
            const char * s )
```

Definition at line 39 of file helpFuncs.cpp.

Referenced by pushLocale().

5.1.3.94 nullBackground()

```
float AtomProbe::nullBackground (
            float rangeStart,
            float rangeEnd )
```

Definition at line 26 of file deconvolution.cpp.

5.1.3.95 nullifyMarker()

```
void AtomProbe::nullifyMarker (
            char * buffer,
            char marker )
```

Definition at line 55 of file stringFuncs.cpp.

Referenced by AtomProbe::RangeFile::rangeTypeString(), and stlStrToStlWStr().

5.1.3.96 numericalEstimateGaussRatioConf()

```
bool AtomProbe::numericalEstimateGaussRatioConf (
            float mu1,
            float mu2,
            float var1,
            float var2,
            float alpha,
            unsigned int nTrials,
            gsl_rng * r,
            float & lBound,
            float & uBound )
```

Brute-force guassian ratio confidence estimator.

Performs monte-carlo trials to determine the distribution of Z=X/Y. where X∼Gaussian(L1), Y∼max(Gaussian(L2),1)

Biased, as it enforces 1, in the denominator of L1/L2 (ie L2=0 has p=0) returns false if either bound could not be computed

- mu1 : Mean 1 (must be +ve)
- mu2 : Mean 2 (must be +ve)
- var1 : Variance 1 (must be +ve)
- var2 : Variance 2 (must be +ve)
- alpha : confidence interval in distribution
- nTrials : number of computations of Z.
- lBound : returned lower bound at confidence alpha
- uBound : returned upper bound at confidence alpha

Note that the estimator seems to biased to the number of trials, and needs to be improved.

Definition at line 260 of file confidence.cpp.

References ASSERT.

Referenced by poissonConfidenceObservation().

5.1.3.97 numericalEstimatePoissRatioConf()

```
bool AtomProbe::numericalEstimatePoissRatioConf (
             float lambda1,
             float lambda2,
             float alpha,
             unsigned int nTrials,
             gsl_rng * r,
             float & lBound,
             float & uBound )
```

Brute-force poisson ratio confidence estimator. Returns the confidence interval in the estimate of the mean, at the given rates.

Performs monte-carlo trials to determine the distribution of Z=X/Y. where X∼Poisson(L1), Y∼Poisson(L2) Biased, as it enforces 1, in the denominator of L1/L2 (ie L2=0 has p=0) returns false if either bound could not be computed

- lambda1 : Poisson rate 1 (must be +ve)
- lambda2 : Poisson rate 2 (must be +ve)
- alpha : confidence interval in distribution
- nTrials : number of computations of Z.
- lBound : returned lower bound at confidence alpha. This is interpolated, so is a real number
- uBound : returned upper bound at confidence alpha. This is interpolated, so is a real number.

Note that the estimator seems to slightly biased to the number of trials, and needs to be improved.

Definition at line 53 of file confidence.cpp.

References ASSERT.

Referenced by poissonConfidenceObservation().

5.1.3.98 numericalEstimateSkellamConf()

```
bool AtomProbe::numericalEstimateSkellamConf (
            float lambda1,
            float lambda2,
            float alpha,
            unsigned int nTrials,
            gsl_rng * r,
            float & lBound,
            float & uBound )
```

Brute-force the confidence bounds of a skellam distribution.

Performs monte-carlo trials to determine Z = X - Y, where X, Y are poisson (Lambda1, Lambda2).

- Lambda1 : poisson rate for X
- Lambda2: poisson rate for Y
- alpha : confidence bound
- nTrials : number of computations of Z.
- lBound : returned lower bound at confidence alpha. This is interpolated, so is a real number
- uBound : returned upper bound at confidence alpha. This is interpolated, so is a real number

Definition at line 158 of file confidence.cpp.

References ASSERT.

Referenced by poissonConfidenceObservation().

5.1.3.99 onlyDir()

```
std::string AtomProbe::onlyDir (
            const std::string & path )
```

Return only the directory name component of the full path.

Definition at line 44 of file stringFuncs.cpp.

Referenced by strAppend().

5.1.3.100 onlyFilename()

```
std::string AtomProbe::onlyFilename (
            const std::string & path )
```

Return only the filename component.

Definition at line 33 of file stringFuncs.cpp.

Referenced by strAppend().

5.1.3.101 operator<()

```
bool AtomProbe::operator< (
            const SIMPLE_SPECIES & a,
            const SIMPLE_SPECIES & b )
```

Definition at line 117 of file multiRange.cpp.

References AtomProbe::SIMPLE_SPECIES::atomicNumber, and AtomProbe::SIMPLE_SPECIES::count.

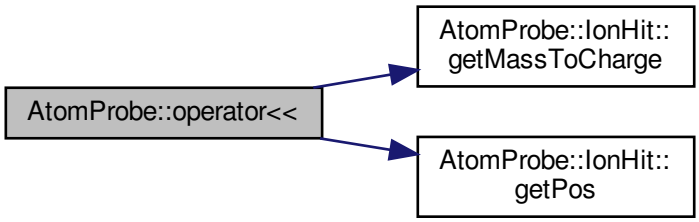
5.1.3.102 operator<<() [1/3]

```
std::ostream& AtomProbe::operator<< (
            std::ostream & stream,
            const IonHit & ion )
```

Definition at line 181 of file ionhit.cpp.

References AtomProbe::IonHit::getMassToCharge(), and AtomProbe::IonHit::getPos().

Here is the call graph for this function:



5.1.3.103 operator<<() [2/3]

```
std::ostream& AtomProbe::operator<< (
            std::ostream & stream,
            const Point3D & pt )
```

Definition at line 425 of file point3D.cpp.

5.1.3.104 operator<<() [3/3]

```
std::ostream& AtomProbe::operator<< (
            std::ostream & stream,
            const BoundCube & b )
```

Definition at line 563 of file boundcube.cpp.

5.1.3.105 pairContains()

```
bool AtomProbe::pairContains (
            const pair< float, float > & p,
            float m )
```

Definition at line 46 of file rangeCheck.cpp.

References ASSERT.

Referenced by checkMassRangingCorrectness().

5.1.3.106 pairOverlaps()

```
bool AtomProbe::pairOverlaps (
            float aStart,
            float aEnd,
            float bStart,
            float bEnd )
```

Definition at line 122 of file multiRange.cpp.

References ASSERT.

Referenced by AtomProbe::MultiRange::splitOverlapping().

5.1.3.107 parseColString()

```
bool AtomProbe::parseColString (
            const std::string & str,
            unsigned char & r,
            unsigned char & g,
            unsigned char & b,
            unsigned char & a )
```

Parse a colour string containing rgb[a]; hex for with leading #.

Definition at line 269 of file stringFuncs.cpp.

References hexStrToUChar().

Referenced by AtomProbe::RGBf::fromHex(), AtomProbe::MultiRange::open(), AtomProbe::RangeFile::rangeTypeString(), and strAppend().

Here is the call graph for this function:

5.1.3.108 parseCompositionData()

```
unsigned int AtomProbe::parseCompositionData (
            const std::vector< std::string > & s,
            const AbundanceData & atomTable,
            std::map< unsigned int, double > & atomData )
```

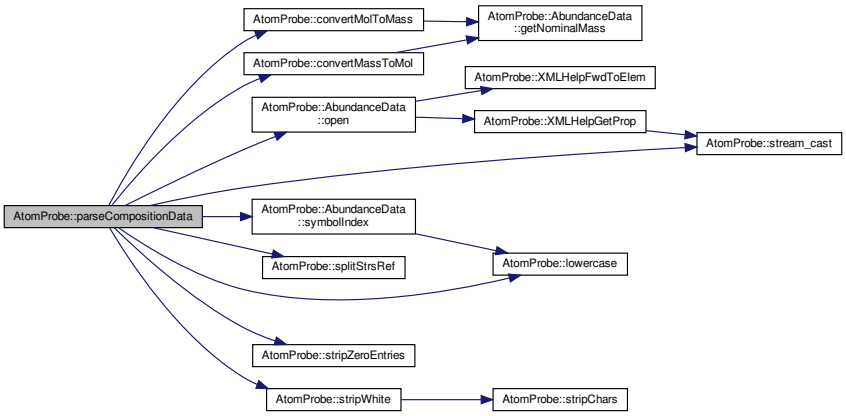
Convert atomic string label data, in the form "Fe 0.81" to fraction map.

The input type (mol/mass) is not relevant for this function, but should be in fraction the label "bal" can be used in place of a composition value exactly once to provide "balance" mass to sum to 1 returns 0 on success, nonzero on error (see COMPPARSE enum)

Definition at line 100 of file massconvert.cpp.

References COMPPARSE_BAD_BAL_USAGE, COMPPARSE_BAD_COMP_VALUE, COMPPARSE_BAD_INPUT_FORMAT, COMPPARSE_BAD_SYMBOL, COMPPARSE_BAD_TOTAL_COMP, COMPPARSE_DUPLICATE_SYMBOL, convertMassToMol(), convertMolToMass(), lowercase(), AtomProbe::AbundanceData::open(), splitStrsRef(), stream_cast(), stripWhite(), stripZeroEntries(), AtomProbe::AbundanceData::symbolIndex(), and TEST.

Here is the call graph for this function:



5.1.3.109 poissonConfidenceObservation()

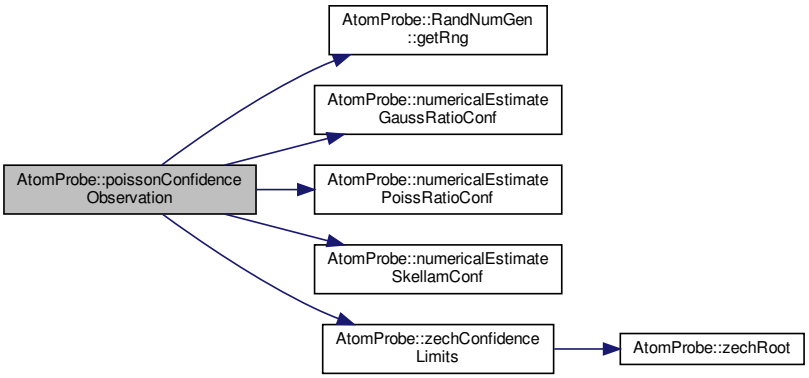
```
void AtomProbe::poissonConfidenceObservation (
            float counts,
            float alpha,
            float & lBound,
            float & uBound )
```

Obtain poisson confidence limits for the mean of a poisson distribution.

Definition at line 496 of file confidence.cpp.

References ASSERT, AtomProbe::RandNumGen::getRng(), numericalEstimateGaussRatioConf(), numerical↩ EstimatePoissRatioConf(), numericalEstimateSkellamConf(), randGen, TEST, and zechConfidenceLimits().

Here is the call graph for this function:



5.1.3.110 popLocale()

```
void AtomProbe::popLocale ( )
```

Definition at line 96 of file helpFuncs.cpp.

Referenced by AtomProbe::RangeFile::openFormat().

5.1.3.111 pushLocale()

```
void AtomProbe::pushLocale (
            const char * newLocale,
            int type )
```

Definition at line 62 of file helpFuncs.cpp.

References ASSERT, and myStrDup().

Referenced by AtomProbe::RangeFile::openFormat().

Here is the call graph for this function:

5.1.3.112 pyramidVol()

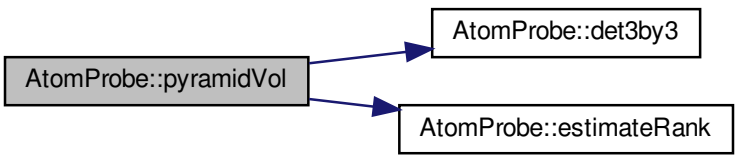
```
double AtomProbe::pyramidVol (
            const Point3D * planarPts,
            const Point3D & apex )
```

Definition at line 239 of file misc.cpp.

References ASSERT, det3by3(), and estimateRank().

Referenced by dotProduct(), and GetReducedHullPts().

Here is the call graph for this function:



5.1.3.113 quat_get_rot_quat()

```
void AtomProbe::quat_get_rot_quat (
            const Point3f * rotVec,
            float angle,
            Quaternion * rotQuat )
```

Compute the quaternion for specified rotation.

angle is in radians. pass to quat_rot_apply_quat to compute rotation

Definition at line 184 of file quat.cpp.

References AtomProbe::Quaternion::a, ASSERT, AtomProbe::Quaternion::b, AtomProbe::Quaternion::c, AtomProbe::Quaternion::d, AtomProbe::Point3f::fx, AtomProbe::Point3f::fy, and AtomProbe::Point3f::fz.

Referenced by AtomProbe::Mesh::rotate().

5.1.3.114 quat_invert()

```
void AtomProbe::quat_invert (
            Quaternion * quat )
```

Definition at line 219 of file quat.cpp.

References AtomProbe::Quaternion::b, AtomProbe::Quaternion::c, and AtomProbe::Quaternion::d.

5.1.3.115 quat_mult_no_second_a()

```
void AtomProbe::quat_mult_no_second_a (
            Quaternion * result,
            const Quaternion * q1,
            const Quaternion * q2 )
```

Definition at line 39 of file quat.cpp.

References AtomProbe::Quaternion::a, AtomProbe::Quaternion::b, AtomProbe::Quaternion::c, and AtomProbe::Quaternion::d.

Referenced by quat_rot(), quat_rot_apply_quat(), and quat_rot_array().

5.1.3.116 quat_pointmult()

```
void AtomProbe::quat_pointmult (
            Point3f * result,
            const Quaternion * q1,
            const Quaternion * q2 )
```

Definition at line 50 of file quat.cpp.

References AtomProbe::Quaternion::a, AtomProbe::Quaternion::b, AtomProbe::Quaternion::c, AtomProbe::Quaternion::d, AtomProbe::Point3f::fx, AtomProbe::Point3f::fy, and AtomProbe::Point3f::fz.

Referenced by quat_rot(), quat_rot_apply_quat(), and quat_rot_array().

5.1.3.117 quat_rot() [1/2]

```
void AtomProbe::quat_rot (
            Point3D & p,
            const Point3D & r,
            float angle )
```

Rotate a point around a given rotation axis by a specified angle.

This is not efficient for large numbers of points, as this will recompute the quaternion each time

Definition at line 59 of file quat.cpp.

References AtomProbe::Point3f::fx, AtomProbe::Point3f::fy, and AtomProbe::Point3f::fz.

5.1.3.118 quat_rot() [2/2]

```
void AtomProbe::quat_rot (
            Point3f * point,
            const Point3f * rotVec,
            float angle )
```

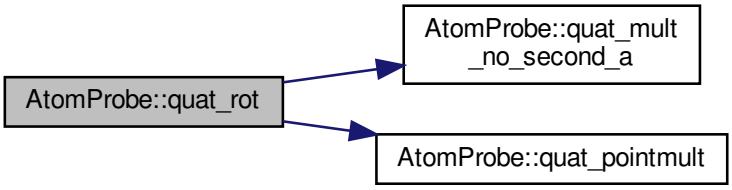
Rotate a point around a given vector, with specified angle.

This is not efficient for large numbers of points, as this will recompute the quaternion each time. angle (radians) is anti-clockwise as viewed from positive side of vector (right-handed)

Definition at line 77 of file quat.cpp.

References AtomProbe::Quaternion::a, ASSERT, AtomProbe::Quaternion::b, AtomProbe::Quaternion::c, AtomProbe::Quaternion::d, AtomProbe::Point3f::fx, AtomProbe::Point3f::fy, AtomProbe::Point3f::fz, quat_mult_no_second_a(), and quat_pointmult().

Here is the call graph for this function:



5.1.3.119 quat_rot_apply_quat()

```
void AtomProbe::quat_rot_apply_quat (
            Point3f * point,
            const Quaternion * rotQuat )
```

Use previously generated quats from quat_get_rot_quats to rotate a point.

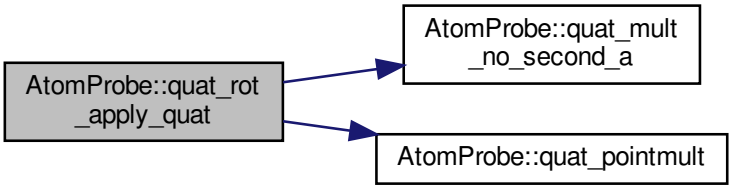
Rotation is in-place, on single point

Definition at line 206 of file quat.cpp.

References AtomProbe::Quaternion::b, AtomProbe::Quaternion::c, AtomProbe::Quaternion::d, AtomProbe::↩
Point3f::fx, AtomProbe::Point3f::fy, AtomProbe::Point3f::fz, quat_mult_no_second_a(), and quat_pointmult().

Referenced by AtomProbe::Mesh::rotate().

Here is the call graph for this function:



5.1.3.120 quat_rot_array() [1/2]

```
void AtomProbe::quat_rot_array (
            Point3f * point,
            unsigned int n,
            const Point3f * rotVec,
            float angle )
```

Rotate each point in array of size n around a given vector, with specified angle.

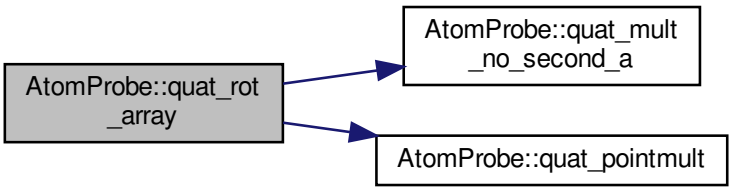
rotVec is the rotation, angle is the anti-clockwise angle as viewed from positive side of vector (right-handed) rotation of points is in-place

Definition at line 139 of file quat.cpp.

References AtomProbe::Quaternion::a, ASSERT, AtomProbe::Quaternion::b, AtomProbe::Quaternion::c, AtomProbe::Quaternion::d, AtomProbe::Point3f::fx, AtomProbe::Point3f::fy, AtomProbe::Point3f::fz, quat_mult_no_second_a(), and quat_pointmult().

Referenced by quat_rot_array().

Here is the call graph for this function:



5.1.3.121 quat_rot_array() [2/2]

```
void AtomProbe::quat_rot_array (
            Point3D * point,
            unsigned int n,
            const Point3f * rotVec,
            float angle )
```

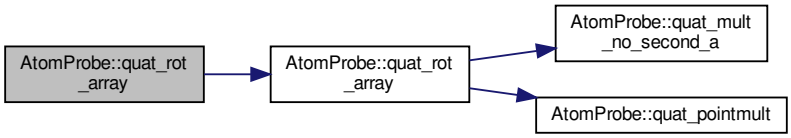
Rotate each point in array of size n around a given vector, with specified angle.

rotVec is the rotation, angle is the anti-clockwise angle as viewed from positive side of vector (right-handed). rotation of points is in-place

Definition at line 115 of file quat.cpp.

References AtomProbe::Point3f::fx, AtomProbe::Point3f::fy, AtomProbe::Point3f::fz, and quat_rot_array().

Here is the call graph for this function:



5.1.3.122 randomIndices()

```
template<class T >
void AtomProbe::randomIndices (
             std::vector< T > & res,
             size_t num,
             size_t nMax,
             gsl_rng * rng )
```

Definition at line 113 of file sampling.h.

Referenced by loadATOFile(), and loadPosFile().

5.1.3.123 randomSelect()

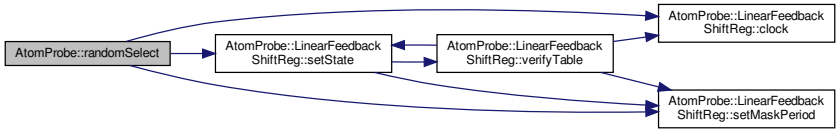
```
template<class T >
size_t AtomProbe::randomSelect (
             std::vector< T > & result,
             const std::vector< T > & source,
             size_t num,
             gsl_rng * rng )
```

Definition at line 40 of file sampling.h.

References AtomProbe::LinearFeedbackShiftReg::clock(), AtomProbe::LinearFeedbackShiftReg::setMaskPeriod(), and AtomProbe::LinearFeedbackShiftReg::setState().

Referenced by sampleIons().

Here is the call graph for this function:



5.1.3.124 rangeOverlaps()

```
bool AtomProbe::rangeOverlaps (
            const pair< float, float > & r1,
            const pair< float, float > & r2 )
```

Definition at line 150 of file componentAnalysis.cpp.

Referenced by computeRangeAdjacency().

5.1.3.125 rangeToStr()

```
string AtomProbe::rangeToStr (
            const pair< float, float > & rng )
```

Definition at line 85 of file ranges.cpp.

References stream_cast().

Referenced by AtomProbe::RangeFile::isSelfConsistent().

Here is the call graph for this function:

5.1.3.126 readEposRecord()

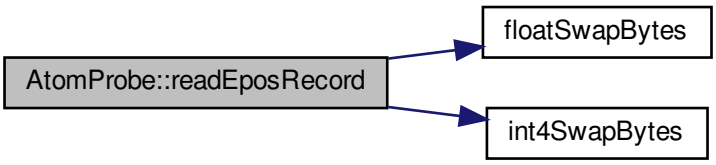
```
bool AtomProbe::readEposRecord (
            const char * src,
            const char * dest )
```

Definition at line 703 of file dataFiles.cpp.

References AtomProbe::EPOS_ENTRY::deltaPulse, floatSwapBytes(), AtomProbe::EPOS_ENTRY::hitMultiplicity, int4SwapBytes(), AtomProbe::EPOS_ENTRY::massToCharge, AtomProbe::EPOS_ENTRY::timeOfFlight, AtomProbe::EPOS_ENTRY::voltDC, AtomProbe::EPOS_ENTRY::voltPulse, AtomProbe::EPOS_ENTRY::x, AtomProbe::EPOS_ENTRY::xDetector, AtomProbe::EPOS_ENTRY::y, AtomProbe::EPOS_ENTRY::yDetector, and AtomProbe::EPOS_ENTRY::z.

Referenced by chunkLoadEposFile(), and loadEposFile().

Here is the call graph for this function:



5.1.3.127 readPosapOps()

```
unsigned int AtomProbe::readPosapOps (
            const char * file,
            THREEDAP_EXPERIMENT & data,
            unsigned int & badLine,
            unsigned int & progress,
            std::atomic< bool > & wantAbort,
            unsigned int nDelayLines = 2,
            bool strictMode = false )
```

Function to read POSAP "OPS" files.

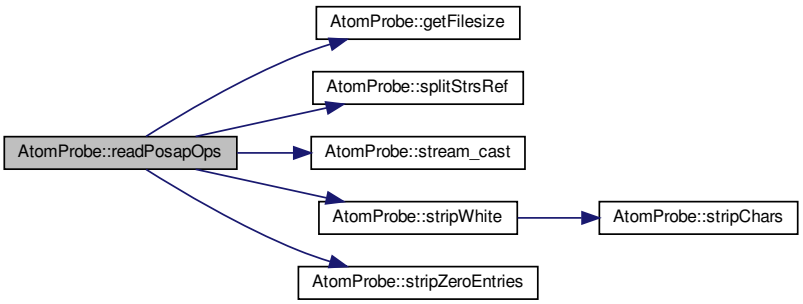
OPS files contain data on voltage, positioned hits and time of flights as well as some instrument parameters. This format is not standardised, so variants may exist

- badLine returns the line on which an error was encountered.
- progress gives a 0-100% progress value (counted in file size). Can be used to multithread monitor progress
- nDelayLines - The number of delay lines in the system. Usually 2, possibly 3.
- strictMode - enable to throw errors in cases where files appear to be badly formatted TODO: Can we work out how to obtain nDelayLines from parsing the file?

Definition at line 797 of file dataFiles.cpp.

References AtomProbe::THREEDAP_DATA::alpha, ARRAYSIZE, ASSERT, AtomProbe::VOLTAGE_DATA::beta, AtomProbe::THREEDAP_DATA::beta, AtomProbe::THREEDAP_DATA::detectorChannels, AtomProbe::THREE↩DAP_DATA::detectorRadius, AtomProbe::THREEDAP_EXPERIMENT::eventData, AtomProbe::THREEDAP_EX↩PERIMENT::eventPulseNumber, AtomProbe::THREEDAP_DATA::flightPath, getFilesize(), AtomProbe::VOLTA↩GE_DATA::nextHitGroupOffset, OPSREADER_ABORT_ERR, OPSREADER_CHANNELS_DATA_ERR, OPSR↩EADER_ENUM_END, OPSREADER_FORMAT_CHANNELS_ERR, OPSREADER_FORMAT_CLINE_ERR, O↩PSREADER_FORMAT_DETECTORLINE_ERR, OPSREADER_FORMAT_DOUBLEDASH, OPSREADER_FO↩RMAT_DUPLICATE_DETECTORSIZE, OPSREADER_FORMAT_DUPLICATE_SYSDATA, OPSREADER_FOR↩MAT_LINE_DASH_ERR, OPSREADER_FORMAT_LINE_VOLTAGE_DATA_ERR, OPSREADER_FORMAT_L↩INE_VOLTAGE_DATACOUNT_ERR, OPSREADER_FORMAT_LINE_VOLTAGE_NOBETA, OPSREADER_FO↩RMAT_LINETYPE_ERR, OPSREADER_FORMAT_SLINE_EVENTCOUNT_ERR, OPSREADER_FORMAT_SL↩INE_EVENTDATA_ERR, OPSREADER_FORMAT_SLINE_FORMAT_ERR, OPSREADER_FORMAT_SLINE_↩PREFIX_ERR, OPSREADER_FORMAT_TRAILING_DASH_ERR, OPSREADER_OPEN_ERR, OPSREADER_↩READ_ERR, AtomProbe::THREEDAP_EXPERIMENT::params, AtomProbe::VOLTAGE_DATA::pulseVolt, split↩StrsRef(), stream_cast(), stripWhite(), stripZeroEntries(), AtomProbe::SINGLE_HIT::tof, AtomProbe::THREEDAP↩_DATA::tZero, AtomProbe::VOLTAGE_DATA::voltage, and AtomProbe::THREEDAP_EXPERIMENT::voltageData.

Here is the call graph for this function:



5.1.3.128 reconstructTest()

```
bool AtomProbe::reconstructTest ( )
```

Referenced by AtomProbe::ReconstructionSphereOnCone::reconstruct(), and runTests().

5.1.3.129 removeElements()

```
template<class T >
void AtomProbe::removeElements (
            const std::vector< size_t > & elems,
            std::vector< T > & vec )
```

Definition at line 64 of file isoSurface.cpp.

References ASSERT.

Referenced by marchingCubes().

5.1.3.130 rotateMatch()

```
bool AtomProbe::rotateMatch (
            const unsigned int * a,
            const unsigned int * b,
            size_t n,
            bool directionForwards = true )
```

Definition at line 100 of file mesh.cpp.

Referenced by AtomProbe::TRIANGLE::edgesMismatch().

5.1.3.131 sampleIons()

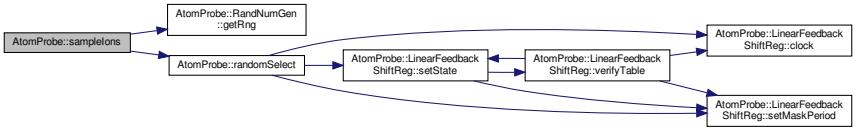
```
void AtomProbe::sampleIons (
            const std::vector< IonHit > & ions,
            float sampleFactor,
            std::vector< IonHit > & sampled,
            bool strongRandom = true )
```

Definition at line 30 of file sampling.cpp.

References AtomProbe::RandNumGen::getRng(), randGen, randomSelect(), and TEST.

Referenced by main().

Here is the call graph for this function:



5.1.3.132 savePosFile() [1/2]

```
unsigned int AtomProbe::savePosFile (
            const std::vector< Point3D > & points,
            float mass,
            const char * name,
            bool append = false )
```

Save a vector of Point3Ds into a pos file, using a fixed mass, return nonzero on error.

Create an pos file from a vector of points, and a given mass.

A nonzero return code can be decoded with getPosFileErrString, which will provide a human readable error message

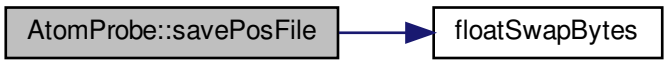
- if append is true, the the file will be appended to.

Definition at line 499 of file dataFiles.cpp.

References floatSwapBytes().

Referenced by getAtoErrString(), main(), and AtomProbe::ReconstructionSphereOnCone::reconstruct().

Here is the call graph for this function:



5.1.3.133 savePosFile() [2/2]

```
unsigned int AtomProbe::savePosFile (
            const std::vector< IonHit > & data,
            const char * name,
            bool append = false )
```

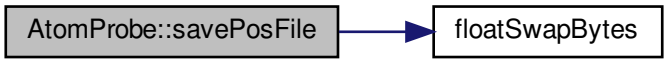
Save a vector of IonHits into a "pos" file, return nonzero on error.

Create an pos file from a vector of IonHits.

Definition at line 463 of file dataFiles.cpp.

References floatSwapBytes().

Here is the call graph for this function:



5.1.3.134 saveTapsimBin()

```
unsigned int AtomProbe::saveTapsimBin (
            std::ostream & f,
            std::vector< IonHit > & posIons )
```

Write a tapsim file from a bunch of IonHits.

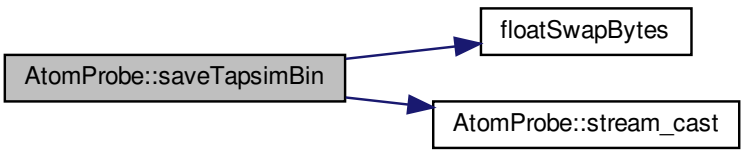
Note: there is some data loss here. Tapsim data basically writes a short header and then the ion data is little endian stored, not big-endian. Finally, m/c data is written as short, hence data loss

Definition at line 667 of file dataFiles.cpp.

References ASSERT, floatSwapBytes(), and stream_cast().

Referenced by getAtoErrString().

Here is the call graph for this function:



5.1.3.135 selectElements()

```
template<class T >
void AtomProbe::selectElements (
            const std::vector< T > & in,
            const std::vector< unsigned int > & indices,
            std::vector< T > & out )
```

Definition at line 60 of file misc.h.

Referenced by findPeaks().

5.1.3.136 setHardAssert()

```
void AtomProbe::setHardAssert (
            bool enabled )
```

Do assertions cause a straight up crash (enabled), or write a mesage to stderr (disabled)? By default, hard crash.

Definition at line 30 of file aptAssert.cpp.

5.1.3.137 signedDistanceToFacet()

```
float AtomProbe::signedDistanceToFacet (
            const Point3D & fA,
            const Point3D & fB,
            const Point3D & fC,
            const Point3D & normal,
            const Point3D & p )
```

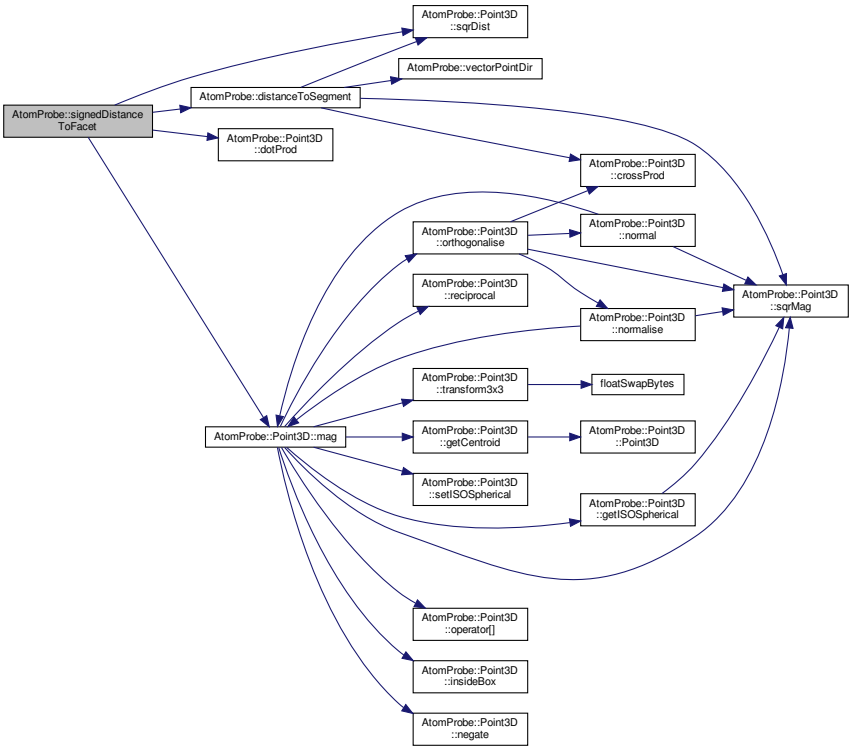
Find the distance between a point, and a triangular facet – may be positive or negative.

Definition at line 121 of file misc.cpp.

References ASSERT, distanceToSegment(), AtomProbe::Point3D::dotProd(), AtomProbe::Point3D::mag(), and AtomProbe::Point3D::sqrDist().

Referenced by distanceToFacet(), AtomProbe::Mesh::getNearestTri(), and meanAndStdev().

Here is the call graph for this function:



5.1.3.138 signVal()

```
float AtomProbe::signVal (
            unsigned int val )
```

Definition at line 147 of file mesh.cpp.

Referenced by Determinant().

5.1.3.139 solveLeastSquares()

```
bool AtomProbe::solveLeastSquares (
            gsl_matrix * m,
            gsl_vector * b,
            gsl_vector *& x )
```

Use an SVD based least-squares solver to solve Mx=b (for x).

Definition at line 43 of file misc.cpp.

Referenced by leastSquaresDeconvolve().

5.1.3.140 SphericProjectionEqn()

```
double AtomProbe::SphericProjectionEqn (
            double eta,
            void * p )
```

Definition at line 25 of file projection.cpp.

References AtomProbe::SphericProjectionParams::focusDist, and AtomProbe::SphericProjectionParams::theta.

Referenced by AtomProbe::StereographicProjection::thetaToEta(), and AtomProbe::ModifiedFocusSpheric↩ Projection::thetaToEta().

5.1.3.141 splitStrsRef() [1/2]

```
void AtomProbe::splitStrsRef (
            const char * cpStr,
            const char delim,
            std::vector< std::string > & v )
```

Split string references using a single delimiter.

Definition at line 187 of file stringFuncs.cpp.

Referenced by AtomProbe::RangeFile::detectFileType(), AtomProbe::Mesh::loadGmshMesh(), loadTapsimBin↩ File(), loadTextData(), main(), AtomProbe::Point3D::parse(), parseCompositionData(), AtomProbe::RangeFile↩ ::rangeTypeString(), readPosapOps(), and strAppend().

5.1.3.142 splitStrsRef() [2/2]

```
void AtomProbe::splitStrsRef (
            const char * cpStr,
            const char * delim,
            std::vector< std::string > & v )
```

Split string references using any of a given string of delimiters.

Definition at line 221 of file stringFuncs.cpp.

5.1.3.143 stlStrToStlWStr()

```
std::wstring AtomProbe::stlStrToStlWStr (
            const std::string & s )  [inline]
```

Definition at line 115 of file stringFuncs.h.

References nullifyMarker().

Here is the call graph for this function:

5.1.3.144 stlWStrToStlStr()

```
std::string AtomProbe::stlWStrToStlStr (
            const std::wstring & s )  [inline]
```

Definition at line 108 of file stringFuncs.h.

5.1.3.145 strAppend()

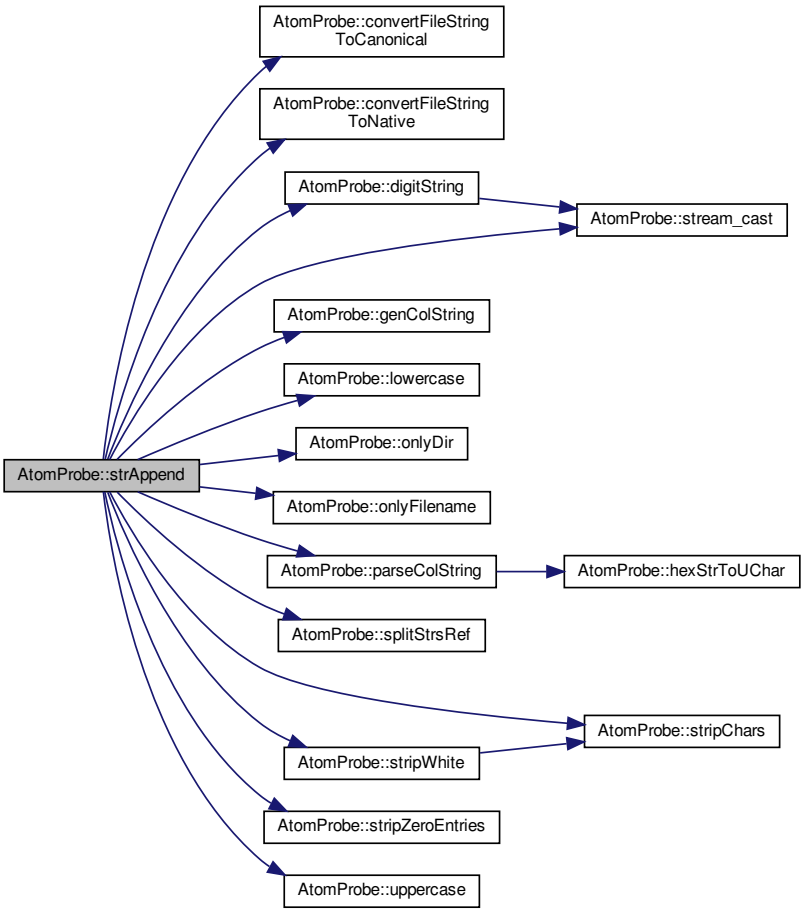
```
template<class T >
void AtomProbe::strAppend (
            std::string s,
            const T & a )
```

Definition at line 41 of file stringFuncs.h.

References convertFileStringToCanonical(), convertFileStringToNative(), digitString(), genColString(), lowercase(), onlyDir(), onlyFilename(), parseColString(), splitStrsRef(), stream_cast(), stripChars(), stripWhite(), stripZero↩Entries(), and uppercase().

Referenced by AtomProbe::RangeFile::isSelfConsistent().

Here is the call graph for this function:



5.1.3.146 stream_cast()

```
template<class T1 , class T2 >
bool AtomProbe::stream_cast (
            T1 & result,
            const T2 & obj )
```

Template function to cast and object to another by the stringstream.

Definition at line 32 of file stringFuncs.h.

Referenced by AtomProbe::RangeFile::decomposeIonNames(), AtomProbe::RangeFile::detectFileType(), digitString(), AtomProbe::LibVersion::getVersionStr(), AtomProbe::Mesh::loadGmshMesh(), loadTapsimBinFile(), loadTextData(), main(), AtomProbe::MultiRange::open(), AtomProbe::RangeFile::open(), AtomProbe::Point3D::parse(), parseCompositionData(), rangeToStr(), AtomProbe::RangeFile::rangeTypeString(), readPosapOps(), saveTapsimBin(), strAppend(), XMLGetNextElemAttrib(), and XMLHelpGetProp().

5.1.3.147 strhas()

```
bool AtomProbe::strhas (
            const char * cpTest,
            const char * cpPossible )
```

Definition at line 1477 of file dataFiles.cpp.

Referenced by loadTextData().

5.1.3.148 stripChars()

```
std::string AtomProbe::stripChars (
            const std::string & Str,
            const char * chars )
```

Definition at line 137 of file stringFuncs.cpp.

Referenced by AtomProbe::RangeFile::rangeTypeString(), strAppend(), and stripWhite().

5.1.3.149 stripWhite()

```
std::string AtomProbe::stripWhite (
            const std::string & str )
```

Strip whitespace, (eg tab,space) from either side of a string.

Definition at line 132 of file stringFuncs.cpp.

References stripChars().

Referenced by AtomProbe::RangeFile::detectFileType(), AtomProbe::Point3D::parse(), parseCompositionData(), AtomProbe::RangeFile::rangeTypeString(), readPosapOps(), and strAppend().

Here is the call graph for this function:

5.1.3.150 stripZeroEntries()

```
void AtomProbe::stripZeroEntries (
            std::vector< std::string > & s )
```

Definition at line 155 of file stringFuncs.cpp.

Referenced by AtomProbe::RangeFile::detectFileType(), loadTextData(), main(), parseCompositionData(), AtomProbe::RangeFile::rangeTypeString(), readPosapOps(), and strAppend().

5.1.3.151 sumVoxels()

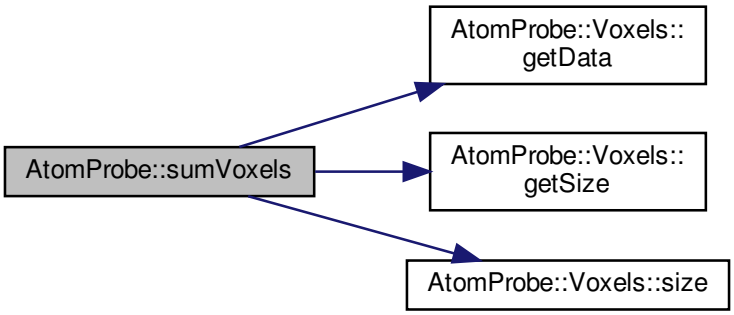
```
template<class T , class U >
void AtomProbe::sumVoxels (
            const Voxels< T > & src,
            U & counter )
```

Use one counting type to sum counts in a voxel of given type.

Definition at line 391 of file voxels.h.

References AtomProbe::Voxels< T >::getData(), AtomProbe::Voxels< T >::getSize(), and AtomProbe::Voxels< T >::size().

Here is the call graph for this function:



5.1.3.152 tabs()

```
std::string AtomProbe::tabs (
            unsigned int nTabs )  [inline]
```

Definition at line 99 of file stringFuncs.h.

Referenced by AtomProbe::MultiRange::write().

5.1.3.153 tolEqual()

```
template<class T >
bool AtomProbe::tolEqual (
            const T & a,
            const T & b,
            const T & f )
```

Definition at line 53 of file misc.h.

Referenced by AtomProbe::ModifiedFocusSphericProjection::scaleUp().

5.1.3.154 transposeVector()

```
template<class T >
void AtomProbe::transposeVector (
            std::vector< std::vector< T > > & v )
```

Definition at line 72 of file misc.h.

Referenced by main().

5.1.3.155 triIsDegenerate()

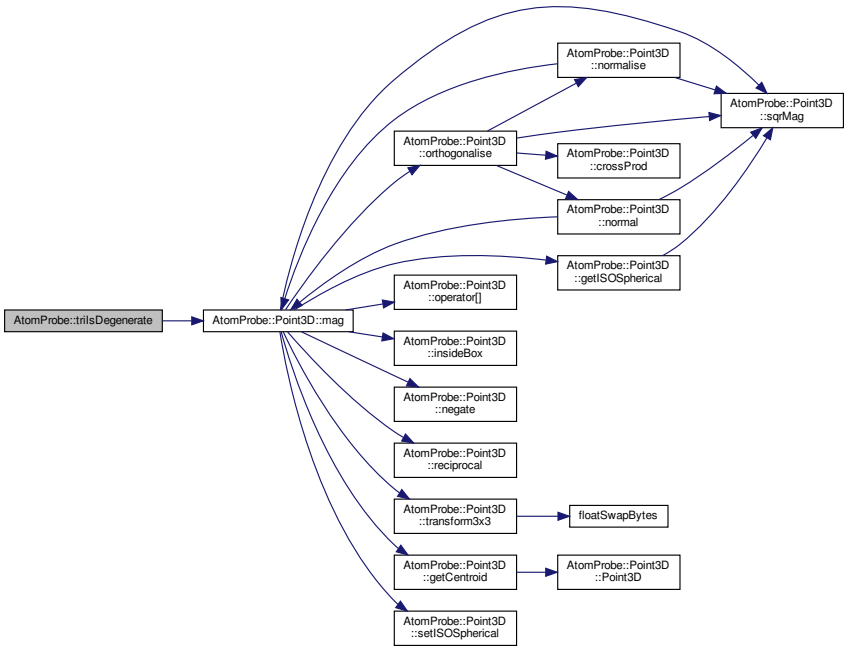
```
bool AtomProbe::triIsDegenerate (
            const Point3D & fA,
            const Point3D & fB,
            const Point3D & fC )
```

Definition at line 215 of file misc.cpp.

References AtomProbe::Point3D::mag().

Referenced by dotProduct(), and GetReducedHullPts().

Here is the call graph for this function:



5.1.3.156 ucharToHexStr()

```
void AtomProbe::ucharToHexStr (
            unsigned char c,
            std::string & s )
```

Definition at line 68 of file stringFuncs.cpp.

Referenced by genColString().

5.1.3.157 uppercase()

```
std::string AtomProbe::uppercase (
            std::string s )
```

Return a uppercase version for a given string.

Referenced by strAppend().

5.1.3.158 vectorMultiErase()

```
template<class T >
void AtomProbe::vectorMultiErase (
            std::vector< T > & vec,
            const std::vector< bool > & wantKill )
```

Definition at line 102 of file misc.h.

Referenced by computeIonDistAdjacency(), AtomProbe::RangeFile::decomposeIonNames(), AtomProbe::RangeFile::eraseIon(), filterBySolutionPPM(), filterPeakNeedBiggerObs(), findOverlaps(), AtomProbe::AbundanceData::generateIsotopeDist(), AtomProbe::RangeFile::makeSelfConsistent(), and FixedStack< T >::~FixedStack().

5.1.3.159 vectorPointDir()

```
unsigned int AtomProbe::vectorPointDir (
            const Point3D & pA,
            const Point3D & pB,
            const Point3D & vC,
            const Point3D & vD )
```

Check which way vectors attached to two 3D points "point",.

Two vectors may point "together", /__\ "apart" __/ or "In common" /__/ or __\

Definition at line 76 of file misc.cpp.

References ASSERT, POINTDIR_APART, POINTDIR_IN_COMMON, and POINTDIR_TOGETHER.

Referenced by distanceToSegment(), and meanAndStdev().

5.1.3.160 weightedMean()

```
template<class T >
T AtomProbe::weightedMean (
            const std::vector< T > & values,
            const std::vector< T > & weight )
```

Definition at line 31 of file misc.h.

Referenced by AtomProbe::AbundanceData::generateGroupedIsotopeDist().

5.1.3.161 XMLFreeDoc()

```
void AtomProbe::XMLFreeDoc (
            void * data )
```

Free a xmlDoc pointer. For use in conjunction with std::unique_ptr for auto-deallocation.

Definition at line 23 of file XMLHelper.cpp.

Referenced by AtomProbe::MultiRange::open().

5.1.3.162 XMLGetNextElemAttrib()

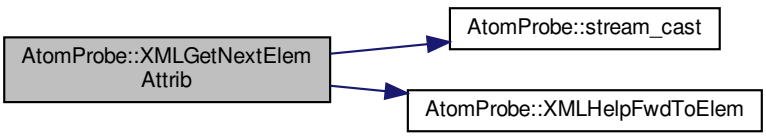
```
template<class T >
bool AtomProbe::XMLGetNextElemAttrib (
            xmlNodePtr & nodePtr,
            T & v,
            const char * nodeName,
            const char * attrib )
```

Grab the specified attribute from the next element, then stream_cast() it into the passed-in object. Returns true on success, false on error.

Definition at line 112 of file XMLHelper.h.

References stream_cast(), and XMLHelpFwdToElem().

Here is the call graph for this function:



5.1.3.163 XMLHelpFwdNotElem()

```
unsigned int AtomProbe::XMLHelpFwdNotElem (
            xmlNodePtr & node,
            const char * nodeName )
```

Definition at line 53 of file XMLHelper.cpp.

5.1.3.164 XMLHelpFwdToElem()

```
unsigned int AtomProbe::XMLHelpFwdToElem (
            xmlNodePtr & node,
            const char * nodeName )
```

Definition at line 41 of file XMLHelper.cpp.

Referenced by AtomProbe::AbundanceData::open(), AtomProbe::MultiRange::open(), and XMLGetNextElem↩Attrib().

5.1.3.165 XMLHelpFwdToList()

```
unsigned int AtomProbe::XMLHelpFwdToList (
            xmlNodePtr & node,
            const std::vector< std::string > & nodeList )
```

5.1.3.166 XMLHelpGetProp()

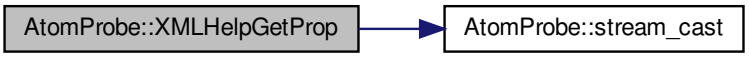
```
template<class T >
unsigned int AtomProbe::XMLHelpGetProp (
            T & prop,
            xmlNodePtr node,
            std::string propName )
```

Definition at line 87 of file XMLHelper.h.

References PROP_BAD_ATT, PROP_PARSE_ERR, and stream_cast().

Referenced by AtomProbe::AbundanceData::open(), and AtomProbe::MultiRange::open().

Here is the call graph for this function:



5.1.3.167 XMLHelpGetText() [1/2]

```
string AtomProbe::XMLHelpGetText (
            xmlNodePtr node )
```

Definition at line 64 of file XMLHelper.cpp.

References XMLHelpNextType().

Here is the call graph for this function:

5.1.3.168 XMLHelpGetText() [2/2]

```
std::string AtomProbe::XMLHelpGetText (
            xmlNodePtr & node )
```

5.1.3.169 XMLHelpNextType()

```
unsigned int AtomProbe::XMLHelpNextType (
            xmlNodePtr & node,
            int nodeType )
```

Definition at line 28 of file XMLHelper.cpp.

Referenced by XMLHelpGetText().

5.1.3.170 zechConfidenceLimits()

```
bool AtomProbe::zechConfidenceLimits (
            float lambdaBack,
            unsigned int observation,
            float alpha,
            float & estimate )
```

Provides a best estimate for true signal when true signal, background.

Nuclear Instruments and Methods in Physics Research A, 1989 608-610 "Upper limits in Experiments with Background or Measurement Errors" This is numerically unstable for large counts A similar problem is tackled by Bityukov, arxiv:hep-ex/0108020v1 Equation 3.5, but is less numerically stable

lambdaBack : background rate observation : Observed signal+background alpha : confidence parameter, (0,1) estimate : estimate for signal at confidence bound, specified by alpha Returns true if calculation succeeds, false otherwise. Note :this involves a root-finding approach, so may be slow

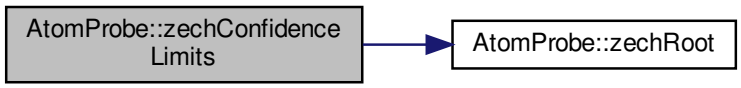
NOTE: may not be numerically stable for high lambdaback/observation, or lambdaback>>observation. This may cause GSL to error out.

Definition at line 391 of file confidence.cpp.

References AtomProbe::ZECH_ROOT::alpha, ASSERT, AtomProbe::ZECH_ROOT::lambdaBack, AtomProbe::ZECH_ROOT::observation, and zechRoot().

Referenced by poissonConfidenceObservation(), and zechCorrect().

Here is the call graph for this function:



5.1.3.171 zechRoot()

```
double AtomProbe::zechRoot (
            double sigGuess,
            void * params )
```

Definition at line 371 of file confidence.cpp.

References AtomProbe::ZECH_ROOT::alpha, AtomProbe::ZECH_ROOT::lambdaBack, and AtomProbe::ZECH_ROOT::observation.

Referenced by zechConfidenceLimits().

5.1.4 Variable Documentation

5.1.4.1 a2iTriangleConnectionTable

```
int AtomProbe::a2iTriangleConnectionTable[256][16]
```

Definition at line 194 of file isoSurface.cpp.

5.1.4.2 ABUNDANCE_ERROR

```
const char* AtomProbe::ABUNDANCE_ERROR[]
```

Initial value:

```
= { "Unable to read abundance data (opening file)",
                "Unable to create XML reader.",
                "Bad property found in XML file",
                "XML document did not match expected layout (DTD validation)",
                "Unable to find required node during parse",
                "Root node missing, expect <atomic-mass-table>!",
                "Found incorrect root node. Expected <atomic-mass-table>"
}
```

Definition at line 49 of file abundance.cpp.

5.1.4.3 aiCubeEdgeFlags

```
int AtomProbe::aiCubeEdgeFlags[256]
```

Initial value:

```
=
{
        0x000, 0x109, 0x203, 0x30a, 0x406, 0x50f, 0x605, 0x70c, 0x80c, 0x905, 0xa0f, 0xb06, 0xc0a, 0xd03,
      0xe09, 0xf00,
        0x190, 0x099, 0x393, 0x29a, 0x596, 0x49f, 0x795, 0x69c, 0x99c, 0x895, 0xb9f, 0xa96, 0xd9a, 0xc93,
      0xf99, 0xe90,
        0x230, 0x339, 0x033, 0x13a, 0x636, 0x73f, 0x435, 0x53c, 0xa3c, 0xb35, 0x83f, 0x936, 0xe3a, 0xf33,
      0xc39, 0xd30,
        0x3a0, 0x2a9, 0x1a3, 0x0aa, 0x7a6, 0x6af, 0x5a5, 0x4ac, 0xbac, 0xaa5, 0x9af, 0x8a6, 0xfaa, 0xea3,
      0xda9, 0xca0,
        0x460, 0x569, 0x663, 0x76a, 0x066, 0x16f, 0x265, 0x36c, 0xc6c, 0xd65, 0xe6f, 0xf66, 0x86a, 0x963,
      0xa69, 0xb60,
        0x5f0, 0x4f9, 0x7f3, 0x6fa, 0x1f6, 0x0ff, 0x3f5, 0x2fc, 0xdfc, 0xcf5, 0xfff, 0xef6, 0x9fa, 0x8f3,
      0xbf9, 0xaf0,
        0x650, 0x759, 0x453, 0x55a, 0x256, 0x35f, 0x055, 0x15c, 0xe5c, 0xf55, 0xc5f, 0xd56, 0xa5a, 0xb53,
      0x859, 0x950,
        0x7c0, 0x6c9, 0x5c3, 0x4ca, 0x3c6, 0x2cf, 0x1c5, 0x0cc, 0xfcc, 0xec5, 0xdcf, 0xcc6, 0xbca, 0xac3,
      0x9c9, 0x8c0,
        0x8c0, 0x9c9, 0xac3, 0xbca, 0xcc6, 0xdcf, 0xec5, 0xfcc, 0x0cc, 0x1c5, 0x2cf, 0x3c6, 0x4ca, 0x5c3,
      0x6c9, 0x7c0,
        0x950, 0x859, 0xb53, 0xa5a, 0xd56, 0xc5f, 0xf55, 0xe5c, 0x15c, 0x055, 0x35f, 0x256, 0x55a, 0x453,
      0x759, 0x650,
        0xaf0, 0xbf9, 0x8f3, 0x9fa, 0xef6, 0xfff, 0xcf5, 0xdfc, 0x2fc, 0x3f5, 0x0ff, 0x1f6, 0x6fa, 0x7f3,
      0x4f9, 0x5f0,
        0xb60, 0xa69, 0x963, 0x86a, 0xf66, 0xe6f, 0xd65, 0xc6c, 0x36c, 0x265, 0x16f, 0x066, 0x76a, 0x663,
      0x569, 0x460,
        0xca0, 0xda9, 0xea3, 0xfaa, 0x8a6, 0x9af, 0xaa5, 0xbac, 0x4ac, 0x5a5, 0x6af, 0x7a6, 0x0aa, 0x1a3,
      0x2a9, 0x3a0,
        0xd30, 0xc39, 0xf33, 0xe3a, 0x936, 0x83f, 0xb35, 0xa3c, 0x53c, 0x435, 0x73f, 0x636, 0x13a, 0x033,
      0x339, 0x230,
        0xe90, 0xf99, 0xc93, 0xd9a, 0xa96, 0xb9f, 0x895, 0x99c, 0x69c, 0x795, 0x49f, 0x596, 0x29a, 0x393,
      0x099, 0x190,
        0xf00, 0xe09, 0xd03, 0xc0a, 0xb06, 0xa0f, 0x905, 0x80c, 0x70c, 0x605, 0x50f, 0x406, 0x30a, 0x203,
      0x109, 0x000
}
```

Definition at line 166 of file isoSurface.cpp.

5.1.4.4 ATO_ERR_STRINGS

```
const char * AtomProbe::ATO_ERR_STRINGS
```

Initial value:

```
= { "",
                "Error opening file",
                "File is empty",
                "Filesize does not match expected format",
                "File version number not <4, as expected",
                "Unable to allocate memory to store data",
                "Unable to detect endian-ness in file"
                }
```

Human readable error messages for use with ATO reader return values.

Definition at line 73 of file dataFiles.cpp.

5.1.4.5 edgeRemap

```
int AtomProbe::edgeRemap[12]
```

Initial value:

```
={ 0,6,1,4,
              2,7,3,5,
              8,10,11,9}
```

Definition at line 488 of file isoSurface.cpp.

5.1.4.6 ELEM_FOUR_NODE_TETRAHEDRON

```
const unsigned int AtomProbe::ELEM_FOUR_NODE_TETRAHEDRON =4
```

Definition at line 38 of file mesh.h.

Referenced by AtomProbe::Mesh::loadGmshMesh(), and AtomProbe::Mesh::saveGmshMesh().

5.1.4.7 ELEM_SINGLE_NODE_POINT

```
const unsigned int AtomProbe::ELEM_SINGLE_NODE_POINT =15
```

Definition at line 35 of file mesh.h.

Referenced by AtomProbe::Mesh::loadGmshMesh(), and AtomProbe::Mesh::saveGmshMesh().

5.1.4.8 ELEM_THREE_NODE_TRIANGLE

```
const unsigned int AtomProbe::ELEM_THREE_NODE_TRIANGLE =2
```

Definition at line 37 of file mesh.h.

Referenced by AtomProbe::Mesh::loadGmshMesh(), and AtomProbe::Mesh::saveGmshMesh().

5.1.4.9 ELEM_TWO_NODE_LINE

```
const unsigned int AtomProbe::ELEM_TWO_NODE_LINE =1
```

Definition at line 36 of file mesh.h.

Referenced by AtomProbe::Mesh::loadGmshMesh(), and AtomProbe::Mesh::saveGmshMesh().

5.1.4.10 elementList

```
const char* AtomProbe::elementList[]
```

Initial value:

```
= {
"H", "He", "Li", "Be",  "B", "C", "N",  "O",  "F", "Ne",

"Na", "Mg", "Al", "Si", "P", "S", "Cl", "Ar",

"K", "Ca", "Sc","Ti",  "V", "Cr",  "Mn", "Fe",  "Co", "Ni",
   "Cu",  "Zn", "Ga", "Ge", "As", "Se",  "Br", "Kr",

"Rb", "Sr", "Y", "Zr", "Nb", "Mo", "Tc", "Ru", "Rh", "Pd",
   "Ag",  "Cd", "In", "Sn", "Sb", "Te",  "I", "Xe",

"Cs",  "Ba", "La",  "Ce", "Pr",  "Nd", "Pm", "Sm",  "Eu", "Gd",
    "Tb",  "Dy",  "Ho", "Er",  "Tm", "Yb", "Lu",  "Hf", "Ta",
    "W",  "Re", "Os",  "Ir", "Pt", "Au", "Hg",  "Tl", "Pb",
     "Bi",  "Po", "At", "Rn",

"Fr", "Ra",  "Ac", "Th",  "Pa", "U",  "Np", "Pu",  "Am", "Cm",
    "Bk", "Cf",  "Es", "Fm",  "Md",  "No",  "Lr",  "Rf",  "Db",
    "Sg",  "Bh",  "Hs",  "Mt",  "Ds",  "Rg",  "Cn",  "Uut",  "Fl",
     "Uup",  "Lv",  "Uus", "Uuo", ""
}
```

Definition at line 62 of file ranges.cpp.

5.1.4.11 EPOS_RECORD_SIZE

```
const size_t AtomProbe::EPOS_RECORD_SIZE = 11*4
```

Definition at line 139 of file ionHit.h.

Referenced by chunkLoadEposFile(), and loadEposFile().

5.1.4.12 hardAssert

```
bool AtomProbe::hardAssert =true
```

Definition at line 23 of file aptAssert.cpp.

Referenced by getHardAssert().

5.1.4.13 HULL_GRAB_SIZE

```
const unsigned int AtomProbe::HULL_GRAB_SIZE =4096
```

Definition at line 42 of file convexHull.cpp.

5.1.4.14 libVersion

```
LibVersion AtomProbe::libVersion
```

Definition at line 28 of file atomprobe.cpp.

Referenced by AtomProbe::RandNumGen::getRng().

5.1.4.15 MAX_LINE_SIZE

```
const size_t AtomProbe::MAX_LINE_SIZE = 16536
```

Definition at line 50 of file ranges.cpp.

Referenced by AtomProbe::RangeFile::open(), and AtomProbe::RangeFile::rangeTypeString().

5.1.4.16 MAX_RANGEFILE_SIZE

```
const size_t AtomProbe::MAX_RANGEFILE_SIZE = 50*1024*1024
```

Definition at line 52 of file ranges.cpp.

5.1.4.17 maximumLinearTable

```
const size_t AtomProbe::maximumLinearTable[]
```

Definition at line 22 of file lfsr.cpp.

Referenced by AtomProbe::LinearFeedbackShiftReg::verifyTable().

5.1.4.18 MESH_LOAD_ERRS

```
const char * AtomProbe::MESH_LOAD_ERRS
```

Initial value:

```
= {  "",
    "Missing error message. This is a bug, please report it",
    "Node count was different to number of present nodes",
    "Element count was less than number of present elements",
    "Mesh loaded, but failed to pass sanity checks"
}
```

Definition at line 53 of file mesh.cpp.

5.1.4.19 MULTIRANGE_FORMAT_VERSION

```
const char AtomProbe::MULTIRANGE_FORMAT_VERSION[] = "0.0.1"
```

Definition at line 46 of file multiRange.cpp.

5.1.4.20 NUM_ELEMENTS

```
const unsigned int AtomProbe::NUM_ELEMENTS =119
```

Definition at line 34 of file ranges.h.

5.1.4.21 OPS_ENUM_ERRSTRINGS

```
const char * AtomProbe::OPS_ENUM_ERRSTRINGS
```

Initial value:

```
=
{
    "",
        "\"C\" line (exp. parameters) not in expected format",
    "\"I\"  line (Detector parameters) not in expected format",
    "\"-\" line (Time-of-flights) not in expected format",
    "\"V\" line (voltage data) not in expected format",
    "Error interpreting \"V\" line (voltage data) data",
    "Missing beta value from \"V\" line - needs to be in voltage, or in system header (\"C\" line",
    "Incorrect number of \"V\" line (voltage data) data entries",
    "Unknown linetype in data file",
    "\"P\" line (detector channels) not in expected format",
    "Unable to interpret channels line",
    "Incorrect number of events in \"S\" (hit position) line",
    "Unable to interpret event data on \"S\" (hit position) line",
    "Unable to parse \"S\" (hit position) line event count (eg 8 in S8 ...)",
    "\"S\" (hit position) line data not preceded by TOF data, as it should have been",
    "Duplicate system data/experiment setup (\"C\") entry found -- there can only be one",
    "Duplicate detector (\"I\") data entry found -- there can only be one",
    "Trailing \"-\" line found -- should have be followed by a \"S\" line, but wasn't.",
    "Duplicate\"-\" line found -- should have be followed by a \"S\" line, but wasn't.",
    "Unable to open file",
    "unable to read file, after opening",
    "Abort requested"
}
```

Definition at line 768 of file dataFiles.cpp.

5.1.4.22 PROGRESS_REDUCE

```
const size_t AtomProbe::PROGRESS_REDUCE =500
```

Definition at line 61 of file mesh.cpp.

Referenced by AtomProbe::K3DTreeExact::build(), computeConvexHull(), and AtomProbe::Mesh::pointsInside().

5.1.4.23 qhullInited

```
bool AtomProbe::qhullInited =false
```

Definition at line 39 of file convexHull.cpp.

5.1.4.24 randGen

```
RandNumGen AtomProbe::randGen
```

Definition at line 29 of file atomprobe.cpp.

Referenced by AtomProbe::RandNumGen::getRng(), leastSquaresDeconvolve(), loadATOFile(), loadPosFile(), main(), poissonConfidenceObservation(), and sampleIons().

5.1.4.25 RANGE_EXTS

```
const char* AtomProbe::RANGE_EXTS[]
```

Initial value:

```
= { "rng",
              "env",
              "rng",
              "rrng",
                ""}
```

Definition at line 54 of file ranges.cpp.

5.1.4.26 RECORDREAD_ERR_STRINGS

```
const char * AtomProbe::RECORDREAD_ERR_STRINGS
```

Initial value:

```
= { "",
                    "Unable to determine filesize",
                    "Filesize indicates that file contains a non-integer number of entries",
                    "Unable to open file",
                    "Unable to allocate memory for reading file contents",
                    "Unable to perform read  operation on file",
                    "Read past end of file requested",
                    "Entry in file appears to be invalid",
    }
```

Definition at line 82 of file dataFiles.cpp.

Referenced by main().

5.1.4.27 VERTEX_OFFSET

```
const unsigned int AtomProbe::VERTEX_OFFSET[8][3]
```

Initial value:

```
=
{
        {0, 0, 0},{1, 0, 0},{1, 1, 0},{0, 1, 0},
        {0, 0, 1},{1, 0, 1},{1, 1, 1},{0, 1, 1}
}
```

Definition at line 462 of file isoSurface.cpp.

Chapter 6

Class Documentation

6.1 AtomProbe::AbundanceData Class Reference

Class to load abundance information for natural isotopes.

`#include <abundance.h>`

Public Member Functions

- size_t open (const char *file, bool strict=false)
  Attempt to open the abundance data file, return 0 on success, nonzero on failure.
- size_t numIsotopes () const
  Return the number of isotopes in the loaded table.
- size_t numElements () const
  Return the number of elements in the loaded table.
- size_t symbolIndex (const char *symbol, bool caseSensitive=true) const
  Return the element's position in table, starting from 0.
- void getSymbolIndices (const std::vector< std::string > &symbols, std::vector< size_t > &indices) const
  Return a vector of symbol indices.
- void getSymbolIndices (const std::vector< std::pair< std::string, size_t > > &symbols, std::vector< std::pair< size_t, unsigned int > > &indices) const
  Obtain the symbol indicies for a string,payload type. Resultant pair has first item in index, second is payload.
- std::string elementName (size_t elemIdx) const
  Obtain the name of an element from its index.
- size_t symbolIdxFromAtomicNumber (size_t atomicNumber) const
  Return the symbol index (offset in vector) for the given atomic number, -1 if it cannot be found.
- std::string elementNames (size_t start, size_t end, char separator=',') const
  Obtain a delimited list of element names, using the (optional) supplied separator, over the specified [start,end) range.
- void isotopeIndex (size_t elem, float mass, size_t &isotopeIdx) const
  Obtain the atom ID (first) and the isotope value(second).
- void isotopeIndex (size_t elem, float mass, float tolerance, size_t &isotopeIdx) const
  Return the first matching element in the table which has a given tolerance to the specified match.
- unsigned int getAtomicNumber (size_t elemIdx) const
  Obtain the atomic number for the given element, by element index.
- const std::vector< ISOTOPE_ENTRY > & isotopes (size_t offset) const

Return the isotope at a given position in the table. Offset must exist.

- void generateIsotopeDist (const std::vector< size_t > &elementIdx, const std::vector< size_t > &frequency, std::vector< std::pair< float, float > > &massDist) const

  Compute the mass-probability distribution for the grouped set of ions.

- void generateGroupedIsotopeDist (const std::vector< size_t > &elementIdx, const std::vector< size_t > &frequency, std::vector< std::pair< float, float > > &massDist, float massTolerance) const

  As per generateIsotopeDist, however, this convenience groups the distribution to limit the effect of minute mass changes.

- void generateSingleAtomDist (size_t atomIdx, unsigned int repeatCount, std::vector< std::pair< float, float > > &massDist) const

  Obtain the mass distribution from a single isotope that repeats. Output is not grouped.

- float abundanceBetweenLimits (const std::vector< size_t > &elemIdx, const std::vector< size_t > &frequency, float massStart, float massEnd) const

  Obtain the fractional abundance between two limits for the given species [start,end)

- const ISOTOPE_ENTRY & isotope (size_t elementIdx, size_t isotopeIdx) const

  Obtain a reference to a particular isotope, using the element's index in the table, and the isotope index.

- size_t getMajorIsotopeFromElemIdx (size_t elementIdx) const

  Obtain the most prominent isotope's index from the element index.

- float getNominalMass (size_t elementIdx) const

  Obtain the isotope weighted mass for the given element.

- size_t getNearestCharge (const std::vector< std::pair< size_t, size_t > > &molecule, float targetMass, size_t maxCharge) const

  Obtain the closest charge state for the given mass and species group.

Static Public Member Functions

- static const char * getErrorText (size_t errorCode)

  Obtain a human-readable error message from the open( ) call.

6.1.1 Detailed Description

Class to load abundance information for natural isotopes.

Definition at line 54 of file abundance.h.

6.1.2 Member Function Documentation

6.1.2.1 abundanceBetweenLimits()

```
float AtomProbe::AbundanceData::abundanceBetweenLimits (
            const std::vector< size_t > & elemIdx,
            const std::vector< size_t > & frequency,
            float massStart,
            float massEnd ) const
```

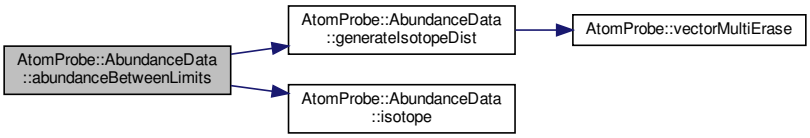
Obtain the fractional abundance between two limits for the given species [start,end)

Definition at line 455 of file abundance.cpp.

References ASSERT, generateIsotopeDist(), and isotope().

Referenced by AtomProbe::leastSquaresDeconvolve().

Here is the call graph for this function:



6.1.2.2 elementName()

```
std::string AtomProbe::AbundanceData::elementName (
            size_t elemIdx ) const  [inline]
```

Obtain the name of an element from its index.

Definition at line 107 of file abundance.h.

References AtomProbe::ISOTOPE_ENTRY::atomicNumber, and AtomProbe::ISOTOPE_ENTRY::mass.

Referenced by elementNames().

6.1.2.3 elementNames()

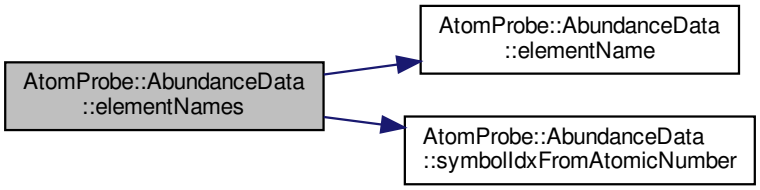
```
std::string AtomProbe::AbundanceData::elementNames (
            size_t start,
            size_t end,
            char separator = ',' ) const
```

Obtain a delimited list of element names, using the (optional) supplied separator, over the specified [start,end) range.

Definition at line 585 of file abundance.cpp.

References ASSERT, elementName(), and symbolIdxFromAtomicNumber().

Here is the call graph for this function:



6.1.2.4 generateGroupedIsotopeDist()

```
void AtomProbe::AbundanceData::generateGroupedIsotopeDist (
            const std::vector< size_t > & elementIdx,
            const std::vector< size_t > & frequency,
            std::vector< std::pair< float, float > > & massDist,
            float massTolerance ) const
```

As per generateIsotopeDist, however, this convenience groups the distribution to limit the effect of minute mass changes.

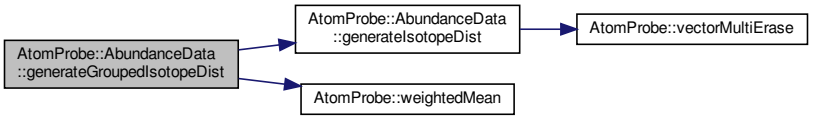
This groups the masses of nearby isotope combinations together. This is desirable due to species, such as Mo2, which have isotopes within <0.001 amu of one another. The mass centres are computed using a weighted average, and the intensities are summed

Definition at line 387 of file abundance.cpp.

References generateIsotopeDist(), and AtomProbe::weightedMean().

Referenced by AtomProbe::findOverlaps(), getMassDistributions(), getNearestCharge(), and AtomProbe::max↩ ExplainedFraction().

Here is the call graph for this function:



6.1.2.5 generateIsotopeDist()

```
void AtomProbe::AbundanceData::generateIsotopeDist (
            const std::vector< size_t > & elementIdx,
            const std::vector< size_t > & frequency,
            std::vector< std::pair< float, float > > & massDist ) const
```

Compute the mass-probability distribution for the grouped set of ions.

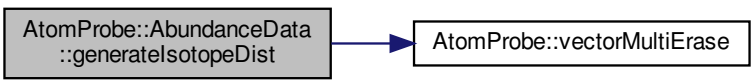
E.g., for C2, this would be elementIdx = elementIdx("C"), and frequency 2. This would return probabilities for each unique mass {C-12 C-12},{C-12 C-13} and {C-13 C-13}.... note an internal "grouping" tolerance is used to group-together very close masses. This may be smaller than what is needed for your application, so if you wish to obtain a more specific distribution use "generateGroupedIsotopeDist"

Definition at line 277 of file abundance.cpp.

References ASSERT, and AtomProbe::vectorMultiErase().

Referenced by abundanceBetweenLimits(), AtomProbe::checkMassRangingCorrectness(), AtomProbe::compute↩IonDistAdjacency(), AtomProbe::filterPeakNeedBiggerObs(), generateGroupedIsotopeDist(), getNearestCharge(), and AtomProbe::RangeFile::guessChargeState().

Here is the call graph for this function:



6.1.2.6 generateSingleAtomDist()

```
void AtomProbe::AbundanceData::generateSingleAtomDist (
            size_t atomIdx,
            unsigned int repeatCount,
            std::vector< std::pair< float, float > > & massDist ) const
```

Obtain the mass distribution from a single isotope that repeats. Output is not grouped.

Definition at line 509 of file abundance.cpp.

Referenced by AtomProbe::MultiRange::copyDataFromRange().

6.1.2.7 getAtomicNumber()

```
unsigned int AtomProbe::AbundanceData::getAtomicNumber (
            size_t elemIdx ) const
```

Obtain the atomic number for the given element, by element index.

Definition at line 495 of file abundance.cpp.

References ASSERT.

Referenced by AtomProbe::computeRangeAdjacency(), AtomProbe::findOverlaps(), and AtomProbe::MultiRange↩ ::MultiRange().

6.1.2.8 getErrorText()

```
const char * AtomProbe::AbundanceData::getErrorText (
            size_t errorCode )  [static]
```

Obtain a human-readable error message from the open( ) call.

Definition at line 59 of file abundance.cpp.

References ASSERT.

6.1.2.9 getMajorIsotopeFromElemIdx()

```
size_t AtomProbe::AbundanceData::getMajorIsotopeFromElemIdx (
            size_t elementIdx ) const
```

Obtain the most prominent isotope's index from the element index.

Definition at line 474 of file abundance.cpp.

References ASSERT.

Referenced by AtomProbe::maxExplainedFraction().

6.1.2.10 getNearestCharge()

```
size_t AtomProbe::AbundanceData::getNearestCharge (
            const std::vector< std::pair< size_t, size_t > > & molecule,
            float targetMass,
            size_t maxCharge ) const
```

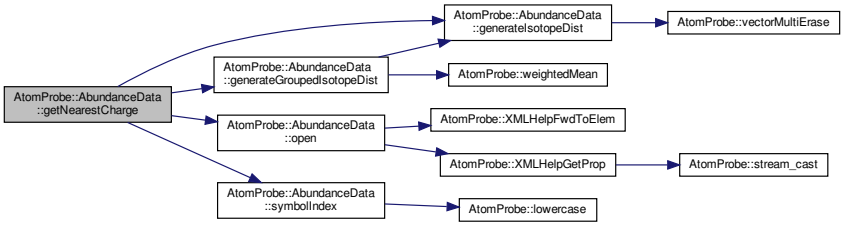
Obtain the closest charge state for the given mass and species group.

In the "molecule" parameter, the pair is <element index, count>, the target mass is given in Da, and the maximum charge is the maximum the function will search for

Definition at line 634 of file abundance.cpp.

References ASSERT, generateGroupedIsotopeDist(), generateIsotopeDist(), open(), symbolIndex(), and TEST.

Here is the call graph for this function:



6.1.2.11 getNominalMass()

```
float AtomProbe::AbundanceData::getNominalMass (
            size_t elementIdx ) const
```

Obtain the isotope weighted mass for the given element.

Definition at line 618 of file abundance.cpp.

Referenced by AtomProbe::convertMassToMol(), and AtomProbe::convertMolToMass().

6.1.2.12 getSymbolIndices() [1/2]

```
void AtomProbe::AbundanceData::getSymbolIndices (
            const std::vector< std::string > & symbols,
            std::vector< size_t > & indices ) const
```

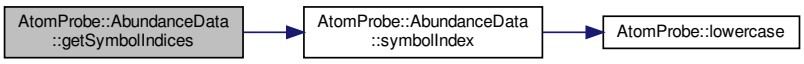
Return a vector of symbol indices.

Definition at line 551 of file abundance.cpp.

References symbolIndex().

Referenced by AtomProbe::MultiRange::copyDataFromRange(), AtomProbe::findOverlaps(), getMassDistributions(), and AtomProbe::MultiRange::MultiRange().

Here is the call graph for this function:



6.1.2.13 getSymbolIndices() [2/2]

```
void AtomProbe::AbundanceData::getSymbolIndices (
            const std::vector< std::pair< std::string, size_t > > & symbols,
            std::vector< std::pair< size_t, unsigned int > > & indices ) const
```

Obtain the symbol indicies for a string,payload type. Resultant pair has first item in index, second is payload.

6.1.2.14 isotope()

```
const ISOTOPE_ENTRY & AtomProbe::AbundanceData::isotope (
            size_t elementIdx,
            size_t isotopeIdx ) const
```

Obtain a reference to a particular isotope, using the element's index in the table, and the isotope index.

Definition at line 271 of file abundance.cpp.

References ASSERT.

Referenced by abundanceBetweenLimits(), AtomProbe::MultiRange::copyDataFromRange(), AtomProbe::filterBy↩SolutionPPM(), and AtomProbe::maxExplainedFraction().

6.1.2.15 isotopeIndex() [1/2]

```
void AtomProbe::AbundanceData::isotopeIndex (
            size_t elem,
            float mass,
            size_t & isotopeIdx ) const
```

Obtain the atom ID (first) and the isotope value(second).

The mass and element ID must match exactly NOTE: The element and isotope indices are *NOT* its isotopic number it is the offset to that isotope int the abundance table

Definition at line 238 of file abundance.cpp.

References ASSERT.

6.1.2.16 isotopeIndex() [2/2]

```
void AtomProbe::AbundanceData::isotopeIndex (
            size_t elem,
            float mass,
            float tolerance,
            size_t & isotopeIdx ) const
```

Return the first matching element in the table which has a given tolerance to the specified match.

Definition at line 254 of file abundance.cpp.

References ASSERT.

6.1.2.17 isotopes()

```
const std::vector< ISOTOPE_ENTRY > & AtomProbe::AbundanceData::isotopes (
            size_t offset ) const
```

Return the isotope at a given position in the table. Offset *must* exist.

Definition at line 613 of file abundance.cpp.

References ASSERT.

Referenced by AtomProbe::leastSquaresDeconvolve().

6.1.2.18 numElements()

```
size_t AtomProbe::AbundanceData::numElements ( ) const
```

Return the number of elements in the loaded table.

Definition at line 74 of file abundance.cpp.

6.1.2.19 numIsotopes()

```
size_t AtomProbe::AbundanceData::numIsotopes ( ) const
```

Return the number of isotopes in the loaded table.

Definition at line 65 of file abundance.cpp.

6.1.2.20 open()

```
size_t AtomProbe::AbundanceData::open (
            const char * file,
            bool strict = false )
```

Attempt to open the abundance data file, return 0 on success, nonzero on failure.

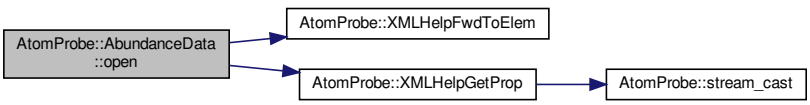
If nonzero, a human readable message can be obtained from getErrorText(...)

Definition at line 79 of file abundance.cpp.

References AtomProbe::ISOTOPE_ENTRY::abundance, AtomProbe::ISOTOPE_ENTRY::abundanceError, AtomProbe::ISOTOPE_ENTRY::atomicNumber, AtomProbe::ISOTOPE_ENTRY::mass, AtomProbe::ISOTOPE_ENTRY::massError, AtomProbe::ISOTOPE_ENTRY::massNumber, AtomProbe::ISOTOPE_ENTRY::symbol, AtomProbe::XMLHelpFwdToElem(), and AtomProbe::XMLHelpGetProp().

Referenced by AtomProbe::checkMassRangingCorrectness(), AtomProbe::computeRangeAdjacency(), AtomProbe::findOverlaps(), getNearestCharge(), AtomProbe::RangeFile::guessChargeState(), AtomProbe::leastSquaresDeconvolve(), main(), AtomProbe::maxExplainedFraction(), AtomProbe::parseCompositionData(), and runTests().

Here is the call graph for this function:



6.1.2.21 symbolIdxFromAtomicNumber()

```
size_t AtomProbe::AbundanceData::symbolIdxFromAtomicNumber (
            size_t atomicNumber ) const
```

Return the symbol index (offset in vector) for the given atomic number, -1 if it cannot be found.

Definition at line 601 of file abundance.cpp.

Referenced by AtomProbe::computeIonDistAdjacency(), elementNames(), and AtomProbe::leastSquaresDeconvolve().

6.1.2.22 symbolIndex()

```
size_t AtomProbe::AbundanceData::symbolIndex (
            const char * symbol,
            bool caseSensitive = true ) const
```

Return the element's position in table, starting from 0.

Notes

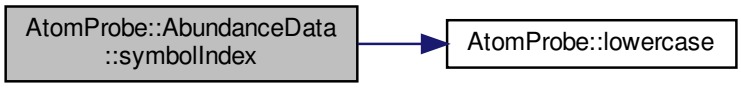
- Input is case insensitive.
- returns (unsigned) -1 if the symbol cannot be found

Definition at line 214 of file abundance.cpp.

References ASSERT, and AtomProbe::lowercase().

Referenced by AtomProbe::computeRangeAdjacency(), AtomProbe::MultiRange::copyDataFromRange(), getNearestCharge(), AtomProbe::getRangeMolecule(), getSymbolIndices(), AtomProbe::RangeFile::guessChargeState(), AtomProbe::leastSquaresDeconvolve(), AtomProbe::maxExplainedFraction(), and AtomProbe::parseCompositionData().

Here is the call graph for this function:



The documentation for this class was generated from the following files:

- include/atomprobe/isotopes/abundance.h
- src/isotopes/abundance.cpp

6.2 AtomProbe::ATO_ENTRY Struct Reference

`#include <dataFiles.h>`

Public Attributes

- float x
- float y
- float z
- float mass
- float approxPulse
- float voltage
- float tof
- float detectorX
- float detectorY
- float pulseVoltage

6.2.1 Detailed Description

Definition at line 67 of file dataFiles.h.

6.2.2 Member Data Documentation

6.2.2.1 approxPulse

`float AtomProbe::ATO_ENTRY::approxPulse`

Definition at line 72 of file dataFiles.h.

6.2.2.2 detectorX

`float AtomProbe::ATO_ENTRY::detectorX`

Definition at line 75 of file dataFiles.h.

6.2.2.3 detectorY

`float AtomProbe::ATO_ENTRY::detectorY`

Definition at line 75 of file dataFiles.h.

6.2.2.4 mass

```
float AtomProbe::ATO_ENTRY::mass
```

Definition at line 70 of file dataFiles.h.

Referenced by AtomProbe::getAtoErrString().

6.2.2.5 pulseVoltage

```
float AtomProbe::ATO_ENTRY::pulseVoltage
```

Definition at line 76 of file dataFiles.h.

6.2.2.6 tof

```
float AtomProbe::ATO_ENTRY::tof
```

Definition at line 74 of file dataFiles.h.

6.2.2.7 voltage

```
float AtomProbe::ATO_ENTRY::voltage
```

Definition at line 73 of file dataFiles.h.

6.2.2.8 x

```
float AtomProbe::ATO_ENTRY::x
```

Definition at line 69 of file dataFiles.h.

6.2.2.9 y

```
float AtomProbe::ATO_ENTRY::y
```

Definition at line 69 of file dataFiles.h.

6.2.2.10 z

```
float AtomProbe::ATO_ENTRY::z
```

Definition at line 69 of file dataFiles.h.

The documentation for this struct was generated from the following file:

- include/atomprobe/io/dataFiles.h

6.3 AtomProbe::AxisCompare Class Reference

Functor allowing for sorting of points in 3D.

```
#include <K3DTree-approx.h>
```

Public Member Functions

- AxisCompare ()
- void setAxis (unsigned int Axis)
- bool operator() (const Point3D &p1, const Point3D &p2) const

6.3.1 Detailed Description

Functor allowing for sorting of points in 3D.

Used by KD Tree to sort points based around which splitting axis is being used once the axis is set, points will be ranked based upon their relative value in that axis only

Definition at line 41 of file K3DTree-approx.h.

6.3.2 Constructor & Destructor Documentation

6.3.2.1 AxisCompare()

```
AtomProbe::AxisCompare::AxisCompare ( )
```

Definition at line 40 of file K3DTree-approx.cpp.

6.3.3 Member Function Documentation

6.3.3.1 operator()()

```
bool AtomProbe::AxisCompare::operator() (
            const Point3D & p1,
            const Point3D & p2 ) const  [inline]
```

Definition at line 48 of file K3DTree-approx.h.

6.3.3.2 setAxis()

```
void AtomProbe::AxisCompare::setAxis (
            unsigned int Axis )
```

Definition at line 44 of file K3DTree-approx.cpp.

Referenced by AtomProbe::K3DTreeApprox::buildByRef().

The documentation for this class was generated from the following files:

- include/atomprobe/algorithm/K3DTree-approx.h
- src/algorithm/K3DTree-approx.cpp

6.4 AxisCompareExact Class Reference

Functor allowing for sorting of points in 3D.

Public Member Functions

- void setAxis (unsigned int Axis)
- bool operator() (const std::pair< Point3D, size_t > &p1, const std::pair< Point3D, size_t > &p2) const

6.4.1 Detailed Description

Functor allowing for sorting of points in 3D.

Used by KD Tree to sort points based around which splitting axis is being used once the axis is set, points will be ranked based upon their relative value in that axis only

Definition at line 45 of file K3DTree-exact.cpp.

6.4.2 Member Function Documentation

6.4.2.1 operator()()

```
bool AxisCompareExact::operator() (
            const std::pair< Point3D, size_t > & p1,
            const std::pair< Point3D, size_t > & p2 ) const  [inline]
```

Definition at line 51 of file K3DTree-exact.cpp.

6.4.2.2 setAxis()

```
void AxisCompareExact::setAxis (
            unsigned int Axis )  [inline]
```

Definition at line 50 of file K3DTree-exact.cpp.

Referenced by AtomProbe::K3DTreeExact::build().

The documentation for this class was generated from the following file:

- src/algorithm/K3DTree-exact.cpp

6.5 AtomProbe::BACKGROUND_PARAMS Struct Reference

```
#include <processing.h>
```

Public Types

- enum {
  FIT_FAIL_MIN_REQ_BINS =1, FIT_FAIL_AVG_COUNTS, FIT_FAIL_INSUFF_DATA, FIT_FAIL_DATA_N↩
  ON_GAUSSIAN,
  FIT_FAIL_END }

Public Attributes

- unsigned int mode
- float massStart
- float massEnd
- float binWidth
- float intensity
- float stdev

6.5.1 Detailed Description

Definition at line 28 of file processing.h.

6.5.2 Member Enumeration Documentation

6.5.2.1 anonymous enum

```
anonymous enum
```

Enumerator

FIT_FAIL_MIN_REQ_BINS	
FIT_FAIL_AVG_COUNTS	
FIT_FAIL_INSUFF_DATA	
FIT_FAIL_DATA_NON_GAUSSIAN	
FIT_FAIL_END	

Definition at line 30 of file processing.h.

6.5.3 Member Data Documentation

6.5.3.1 binWidth

```
float AtomProbe::BACKGROUND_PARAMS::binWidth
```

Definition at line 43 of file processing.h.

Referenced by AtomProbe::doFitBackground().

6.5.3.2 intensity

```
float AtomProbe::BACKGROUND_PARAMS::intensity
```

Definition at line 46 of file processing.h.

Referenced by AtomProbe::doFitBackground().

6.5.3.3 massEnd

```
float AtomProbe::BACKGROUND_PARAMS::massEnd
```

Definition at line 41 of file processing.h.

Referenced by AtomProbe::doFitBackground().

6.5.3.4 massStart

```
float AtomProbe::BACKGROUND_PARAMS::massStart
```

Definition at line 41 of file processing.h.

Referenced by AtomProbe::doFitBackground().

6.5.3.5 mode

```
unsigned int AtomProbe::BACKGROUND_PARAMS::mode
```

Definition at line 39 of file processing.h.

6.5.3.6 stdev

```
float AtomProbe::BACKGROUND_PARAMS::stdev
```

Definition at line 46 of file processing.h.

Referenced by AtomProbe::doFitBackground().

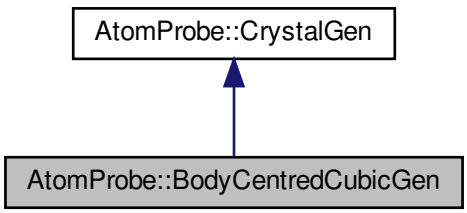
The documentation for this struct was generated from the following file:

- include/atomprobe/spectrum/processing.h

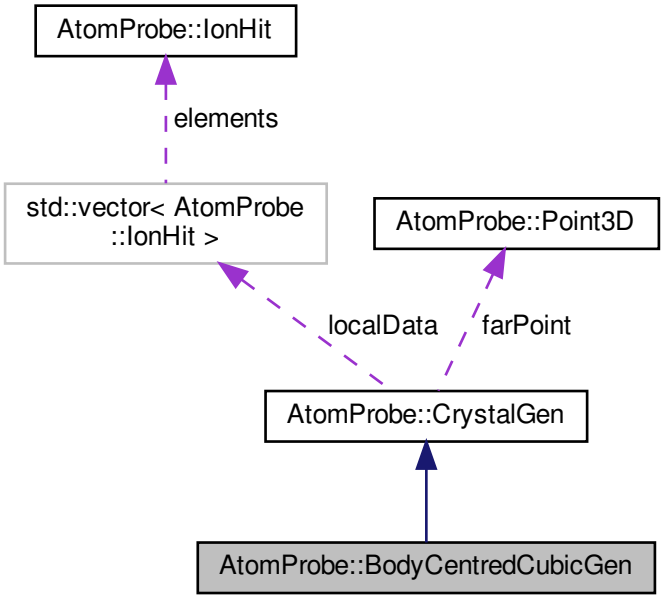
6.6 AtomProbe::BodyCentredCubicGen Class Reference

```
#include <generate.h>
```

Inheritance diagram for AtomProbe::BodyCentredCubicGen:



Collaboration diagram for AtomProbe::BodyCentredCubicGen:



Public Member Functions

- BodyCentredCubicGen (float latticeSpacing, float mToCCentre, const float mToCCorner, const Point3D &p)
- unsigned int generateLattice ()

Additional Inherited Members

6.6.1 Detailed Description

Definition at line 66 of file generate.h.

6.6.2 Constructor & Destructor Documentation

6.6.2.1 BodyCentredCubicGen()

```
AtomProbe::BodyCentredCubicGen::BodyCentredCubicGen (
            float latticeSpacing,
            float mToCCentre,
            const float mToCCorner,
            const Point3D & p )
```

Definition at line 223 of file generate.cpp.

References AtomProbe::CrystalGen::farPoint.

6.6.3 Member Function Documentation

6.6.3.1 generateLattice()

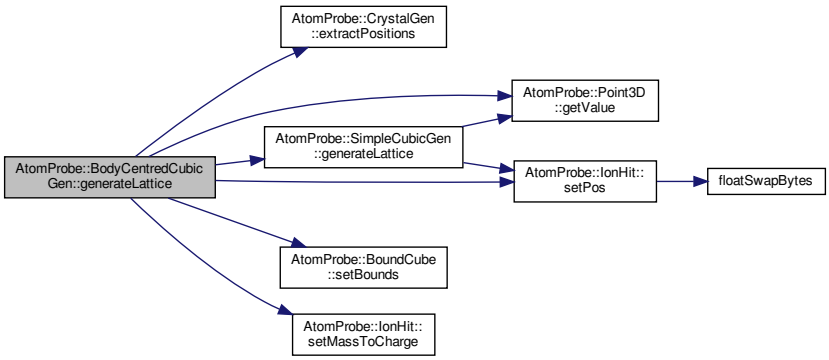
```
unsigned int AtomProbe::BodyCentredCubicGen::generateLattice ( )  [virtual]
```

Implements AtomProbe::CrystalGen.

Definition at line 232 of file generate.cpp.

References AtomProbe::CRYSTAL_BAD_UNIT_CELL, AtomProbe::CrystalGen::extractPositions(), AtomProbe::CrystalGen::farPoint, AtomProbe::SimpleCubicGen::generateLattice(), AtomProbe::Point3D::getValue(), AtomProbe::CrystalGen::localData, AtomProbe::BoundCube::setBounds(), AtomProbe::IonHit::setMassToCharge(), AtomProbe::IonHit::setPos(), and TEST.

Here is the call graph for this function:



The documentation for this class was generated from the following files:

- include/atomprobe/latticeplanes/generate.h
- src/lattice/generate.cpp

6.7 AtomProbe::BoundCube Class Reference

Helper class to define a bounding cube.

```
#include <boundcube.h>
```

Public Member Functions

- BoundCube ()
- BoundCube (const std::vector< Point3D > &pts)
- BoundCube (const std::vector< IonHit > &pts)
- BoundCube (const Point3D &p1, const Point3D &p2)
- bool operator== (const BoundCube &other) const
- void setBounds (float xMin, float yMin, float zMin, float xMax, float yMax, float zMax)

  Set the bounds by passing in minima and maxima of each dimension.
- void setBound (unsigned int bound, unsigned int minMax, float value)

  Set an individual bound.
- void setBounds (const BoundCube &b)

  Set the bounding cube to be the same as a different cube.
- void setBounds (const Point3D *ptArray, unsigned int nPoints)

  Obtain bounds from an array of Point3Ds.
- void setBounds (const Point3D &p, const Point3D &q)

  Use two points to set bounds – does not need to be high,low. This is worked out.
- void setBounds (const std::vector< Point3D > &ptArray)

  Obtain bounds from an array of Point3Ds.
- void setBounds (const std::vector< IonHit > &ptArray)

  Obtain bounds from an array of IonHits.
- void setBounds (const Point3D &p, float radius)

  Set the bounds using a single point and radius.
- void setInverseLimits ()

  Set the cube to be "inside out" at the limits of numeric results;.
- float getBound (unsigned int bound, unsigned int minMax) const

  Return the bound on the given dimension.
- Point3D getCentroid () const

  Return the centroid.
- void getBounds (Point3D &low, Point3D &high) const

  Get the bounds of the cube as two points, the lower left (minimum bound) and upper right corner (max bound)
- Point3D min () const
- Point3D max () const
- float getSize (unsigned int dim) const

  Return the size of the side parallel to the given dimension.
- bool isFlat () const

  Returns true if any bound is of null thickness.
- bool intersects (const Point3D &pt, float sqrRad) const

  Checks if a point intersects a sphere of centre Pt, radius^2 sqrRad.
- bool intersects (const BoundCube &b) const

  Check to see if this box intersects another.
- bool contains (const BoundCube &b) const

  Does this bounding box entirely contain another.
- bool containsPt (const Point3D &pt) const

  Check to see if the point is contained in, or part of the walls of the cube.
- bool containedInSphere (const Point3D &origin, float radius) const

  Returns true if this box is contained by the sphere, represented by the origin+radius.
- BoundCube makeUnion (const BoundCube &b) const

  Create the box containing a union of two bounding cubes.
- BoundCube makeIntersection (const BoundCube &b) const

  Create the box which is the intersection of two bounding cubes this is either null, or a box.

- float getMaxDistanceToBox (const Point3D &pt) const

  Returns maximum distance to box corners (which is an upper bound on max box distance).
- float getLargestDim () const

  Get the largest dimension of the bound cube.
- float getVolume () const

  Obtain the volume of the cube.
- void setLimits ()

  Set min-max bounds to fp min/max.
- unsigned int segmentTriple (unsigned int dim, float slice) const

  Return a triplet to indicate a spatial partition value lies in.
- BoundCube operator= (const BoundCube &)
- void expand (const BoundCube &b)

  Expand (as needed) volume such that the argument bounding cube is enclosed by this one.
- void expand (const Point3D &p)

  Expand such that point is contained in this volume. Existing volume must be valid.
- void expand (float f)

  Expand the bounding cube by this value in each dimension (upper and lower)

Friends

- class K3DTreeExact
- class K3DTreeApprox
- std::ostream & operator<< (std::ostream &stream, const BoundCube &b)

6.7.1 Detailed Description

Helper class to define a bounding cube.

Definition at line 29 of file boundcube.h.

6.7.2 Constructor & Destructor Documentation

6.7.2.1 BoundCube() [1/4]

```
AtomProbe::BoundCube::BoundCube ( )  [inline]
```

Definition at line 39 of file boundcube.h.

Referenced by BoundCube().

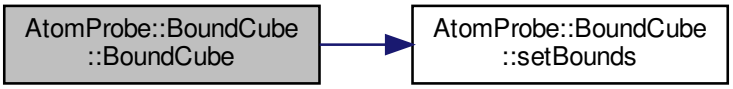
6.7.2.2 BoundCube() [2/4]

```
AtomProbe::BoundCube::BoundCube (
            const std::vector< Point3D > & pts )  [inline]
```

Definition at line 46 of file boundcube.h.

References setBounds().

Here is the call graph for this function:



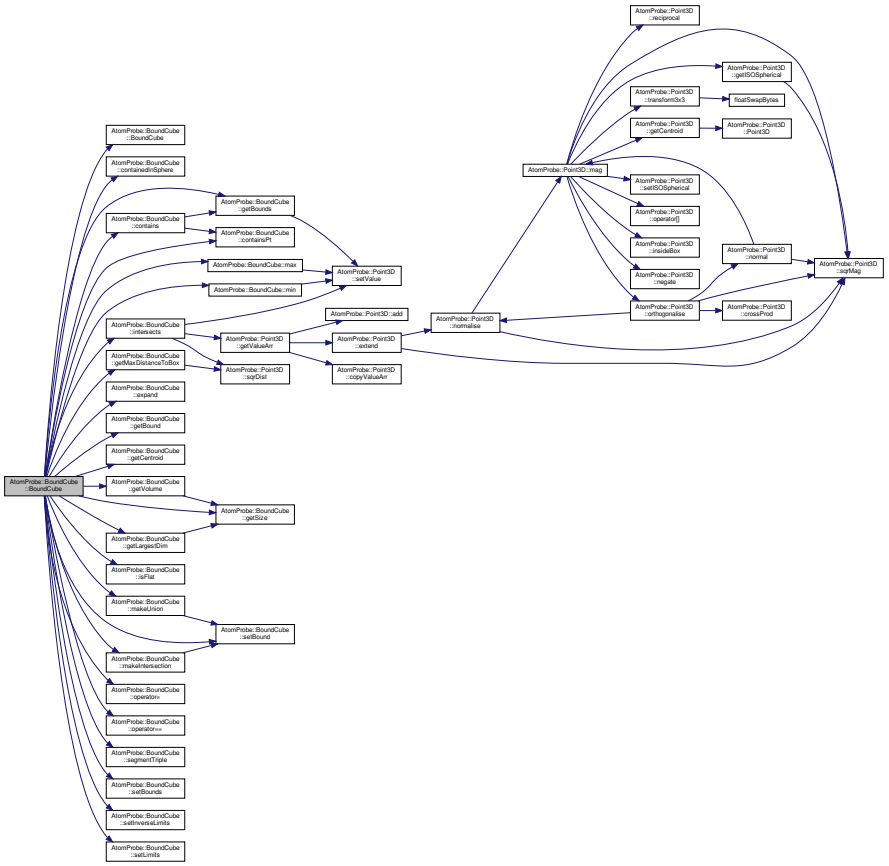
6.7.2.3 BoundCube() [3/4]

```
AtomProbe::BoundCube::BoundCube (
            const std::vector< IonHit > & pts )  [inline]
```

Definition at line 51 of file boundcube.h.

References BoundCube(), containedInSphere(), contains(), containsPt(), expand(), getBound(), getBounds(), getCentroid(), getLargestDim(), getMaxDistanceToBox(), getSize(), getVolume(), intersects(), isFlat(), makeIntersection(), makeUnion(), max(), min(), operator<<, operator=(), operator==(), segmentTriple(), setBound(), setBounds(), setInverseLimits(), and setLimits().

Here is the call graph for this function:



6.7.2.4 BoundCube() [4/4]

```
AtomProbe::BoundCube::BoundCube (
            const Point3D & p1,
            const Point3D & p2 )
```

Definition at line 26 of file boundcube.cpp.

6.7.3 Member Function Documentation

6.7.3.1 containedInSphere()

```
bool AtomProbe::BoundCube::containedInSphere (
            const Point3D & origin,
            float radius ) const
```

Returns true if this box is contained by the sphere, represented by the origin+radius.

Definition at line 379 of file boundcube.cpp.

Referenced by BoundCube(), and AtomProbe::K3DTreeExact::ptsInSphere().

6.7.3.2 contains()

```
bool AtomProbe::BoundCube::contains (
            const BoundCube & b ) const
```

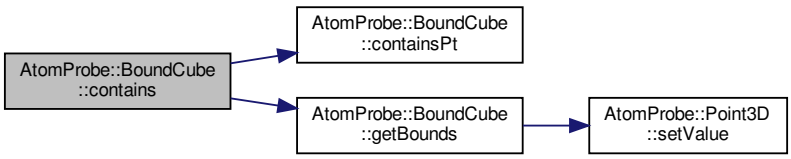
Does this bounding box entirely contain another.

Definition at line 360 of file boundcube.cpp.

References containsPt(), and getBounds().

Referenced by BoundCube().

Here is the call graph for this function:



6.7.3.3 containsPt()

```
bool AtomProbe::BoundCube::containsPt (
            const Point3D & pt ) const
```

Check to see if the point is contained in, or part of the walls of the cube.

Definition at line 367 of file boundcube.cpp.

References ASSERT.

Referenced by BoundCube(), contains(), AtomProbe::Mesh::getContainedNodes(), AtomProbe::Voxels< T >::getEdgeEnds(), AtomProbe::Voxels< T >::getInterpolatedData(), intersects(), AtomProbe::marchingCubes(), and AtomProbe::Mesh::pointsInside().

6.7.3.4 expand() [1/3]

```
void AtomProbe::BoundCube::expand (
            const BoundCube & b )
```

Expand (as needed) volume such that the argument bounding cube is enclosed by this one.

Definition at line 148 of file boundcube.cpp.

Referenced by BoundCube(), AtomProbe::Mesh::divideMeshSurface(), and AtomProbe::Voxels< T >::getEdgeEnds().

6.7.3.5 expand() [2/3]

```
void AtomProbe::BoundCube::expand (
            const Point3D & p )
```

Expand such that point is contained in this volume. Existing volume must be valid.

Definition at line 181 of file boundcube.cpp.

6.7.3.6 expand() [3/3]

```
void AtomProbe::BoundCube::expand (
            float f )
```

Expand the bounding cube by this value in each dimension (upper and lower)

Definition at line 197 of file boundcube.cpp.

6.7.3.7 getBound()

```
float AtomProbe::BoundCube::getBound (
            unsigned int bound,
            unsigned int minMax ) const
```

Return the bound on the given dimension.

bound - the dimension [x=0,y=1,z=2] minMax - 0 for lower bound, 1 for upper bound

Definition at line 86 of file boundcube.cpp.

References ASSERT.

Referenced by BoundCube().

6.7.3.8 getBounds()

```
void AtomProbe::BoundCube::getBounds (
            Point3D & low,
            Point3D & high ) const
```

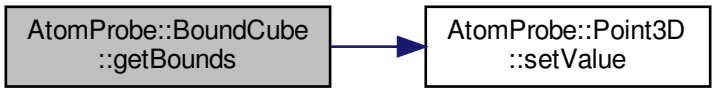
Get the bounds of the cube as two points, the lower left (minimum bound) and upper right corner (max bound)

Definition at line 302 of file boundcube.cpp.

References ASSERT, and AtomProbe::Point3D::setValue().

Referenced by BoundCube(), contains(), AtomProbe::Voxels< T >::init(), and intersects().

Here is the call graph for this function:



6.7.3.9 getCentroid()

```
Point3D AtomProbe::BoundCube::getCentroid ( ) const
```

Return the centroid.

Definition at line 486 of file boundcube.cpp.

References ASSERT.

Referenced by BoundCube().

6.7.3.10 getLargestDim()

```
float AtomProbe::BoundCube::getLargestDim ( ) const
```

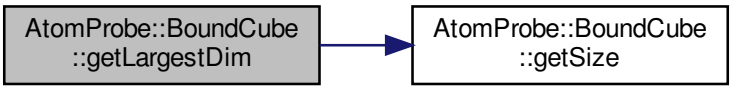
Get the largest dimension of the bound cube.

Definition at line 335 of file boundcube.cpp.

References getSize().

Referenced by BoundCube().

Here is the call graph for this function:



6.7.3.11 getMaxDistanceToBox()

```
float AtomProbe::BoundCube::getMaxDistanceToBox (
            const Point3D & pt ) const
```

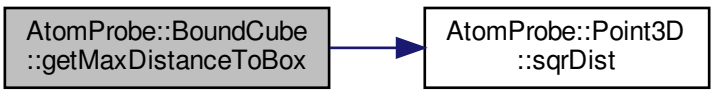
Returns maximum distance to box corners (which is an upper bound on max box distance).

Definition at line 499 of file boundcube.cpp.

References ASSERT, and AtomProbe::Point3D::sqrDist().

Referenced by BoundCube().

Here is the call graph for this function:



6.7.3.12 getSize()

```
float AtomProbe::BoundCube::getSize (
            unsigned int dim ) const
```

Return the size of the side parallel to the given dimension.

Definition at line 343 of file boundcube.cpp.

References ASSERT.

Referenced by BoundCube(), getLargestDim(), getVolume(), and AtomProbe::ReconstructionSphereOnCone↩ ::reconstruct().

6.7.3.13 getVolume()

```
float AtomProbe::BoundCube::getVolume ( ) const
```

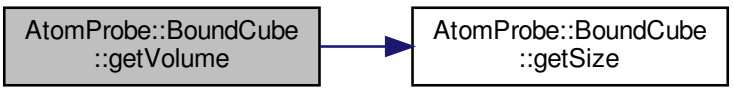
Obtain the volume of the cube.

Definition at line 355 of file boundcube.cpp.

References getSize().

Referenced by BoundCube(), and AtomProbe::ReconstructionSphereOnCone::reconstruct().

Here is the call graph for this function:



6.7.3.14 intersects() [1/2]

```
bool AtomProbe::BoundCube::intersects (
            const Point3D & pt,
            float sqrRad ) const
```

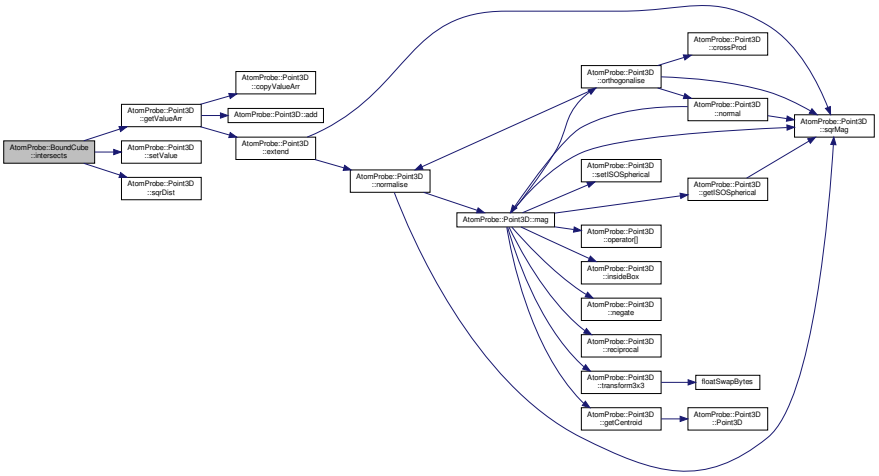
Checks if a point intersects a sphere of centre Pt, radius^2 sqrRad.

Definition at line 434 of file boundcube.cpp.

References AtomProbe::Point3D::getValueArr(), AtomProbe::Point3D::setValue(), and AtomProbe::Point3D::sqrDist().

Referenced by BoundCube(), AtomProbe::K3DTreeApprox::findNearest(), AtomProbe::K3DTreeExact::findNearestUntagged(), and AtomProbe::K3DTreeExact::ptsInSphere().

Here is the call graph for this function:



6.7.3.15 intersects() [2/2]

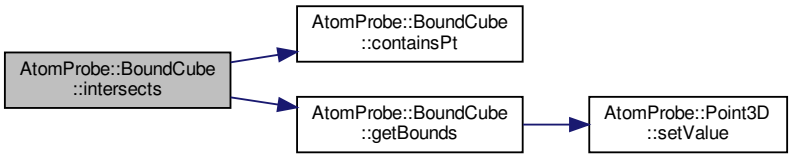
```
bool AtomProbe::BoundCube::intersects (
            const BoundCube & b ) const
```

Check to see if this box intersects another.

Definition at line 465 of file boundcube.cpp.

References containsPt(), and getBounds().

Here is the call graph for this function:



6.7.3.16 isFlat()

```
bool AtomProbe::BoundCube::isFlat ( ) const
```

Returns true if any bound is of null thickness.

Definition at line 136 of file boundcube.cpp.

Referenced by BoundCube(), and main().

6.7.3.17 makeIntersection()

```
BoundCube AtomProbe::BoundCube::makeIntersection (
            const BoundCube & b ) const
```

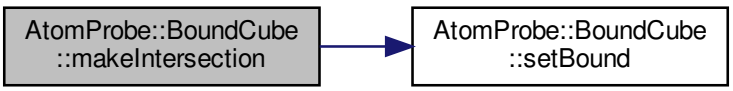
Create the box which is the intersection of two bounding cubes this is either null, or a box.

Definition at line 416 of file boundcube.cpp.

References setBound().

Referenced by BoundCube().

Here is the call graph for this function:



6.7.3.18 makeUnion()

```
BoundCube AtomProbe::BoundCube::makeUnion (
            const BoundCube & b ) const
```

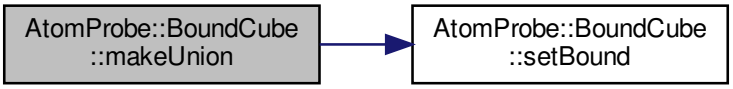
Create the box containing a union of two bounding cubes.

Definition at line 399 of file boundcube.cpp.

References setBound().

Referenced by BoundCube().

Here is the call graph for this function:



6.7.3.19 max()

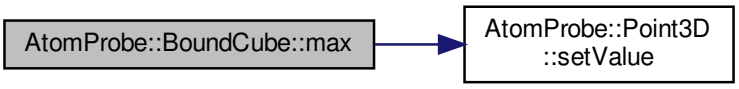
```
Point3D AtomProbe::BoundCube::max ( ) const
```

Definition at line 324 of file boundcube.cpp.

References ASSERT, and AtomProbe::Point3D::setValue().

Referenced by BoundCube(), and AtomProbe::Voxels< T >::setBounds().

Here is the call graph for this function:



6.7.3.20 min()

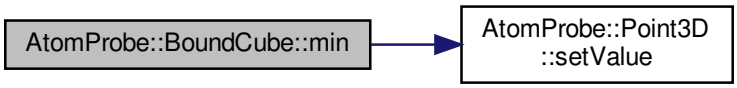
```
Point3D AtomProbe::BoundCube::min ( ) const
```

Definition at line 312 of file boundcube.cpp.

References ASSERT, and AtomProbe::Point3D::setValue().

Referenced by BoundCube(), and AtomProbe::Voxels< T >::setBounds().

Here is the call graph for this function:



6.7.3.21 operator=()

```
BoundCube AtomProbe::BoundCube::operator= (
            const BoundCube & b )
```

Definition at line 546 of file boundcube.cpp.

Referenced by BoundCube().

6.7.3.22 operator==()

```
bool AtomProbe::BoundCube::operator== (
            const BoundCube & other ) const
```

Definition at line 38 of file boundcube.cpp.

Referenced by BoundCube().

6.7.3.23 segmentTriple()

```
unsigned int AtomProbe::BoundCube::segmentTriple (
            unsigned int dim,
            float slice ) const
```

Return a triplet to indicate a spatial partition value lies in.

Returns which segment (lower:0, inside:1, higher:2) the given slice coordinate is at the specified dimension (eg, for a box [-1,1] in y, segmentTriple(1,-2) would return 0.

Definition at line 529 of file boundcube.cpp.

References ASSERT.

Referenced by BoundCube().

6.7.3.24 setBound()

```
void AtomProbe::BoundCube::setBound (
            unsigned int bound,
            unsigned int minMax,
            float value )
```

Set an individual bound.

bound : dimension of bound, 0=x,1=y,2=z minMax : 0 for lower bound, 1 for upper bound

Definition at line 76 of file boundcube.cpp.

References ASSERT.

Referenced by BoundCube(), makeIntersection(), and makeUnion().

6.7.3.25 setBounds() [1/7]

```
void AtomProbe::BoundCube::setBounds (
            float xMin,
            float yMin,
            float zMin,
            float xMax,
            float yMax,
            float zMax )
```

Set the bounds by passing in minima and maxima of each dimension.

Definition at line 49 of file boundcube.cpp.

Referenced by BoundCube(), AtomProbe::Mesh::divideMeshSurface(), AtomProbe::generate1DAxialDistHist(), AtomProbe::generate1DAxialDistHistSweep(), AtomProbe::BodyCentredCubicGen::generateLattice(), AtomProbe::IonHit::getBoundCube(), AtomProbe::K3DTreeExact::getBoundCube(), AtomProbe::Mesh::getBounds(), AtomProbe::Voxels< T >::getBounds(), AtomProbe::Voxels< T >::getEdgeEnds(), AtomProbe::marchingCubes(), AtomProbe::Mesh::pointsInside(), AtomProbe::Mesh::print(), AtomProbe::ReconstructionSphereOnCone::reconstruct(), AtomProbe::K3DTreeExact::resetPts(), and setBounds().

6.7.3.26 setBounds() [2/7]

```
void AtomProbe::BoundCube::setBounds (
            const BoundCube & b )
```

Set the bounding cube to be the same as a different cube.

Definition at line 60 of file boundcube.cpp.

6.7.3.27 setBounds() [3/7]

```
void AtomProbe::BoundCube::setBounds (
            const Point3D * ptArray,
            unsigned int nPoints )
```

Obtain bounds from an array of Point3Ds.

Definition at line 210 of file boundcube.cpp.

6.7.3.28 setBounds() [4/7]

```
void AtomProbe::BoundCube::setBounds (
            const Point3D & p,
            const Point3D & q )
```

Use two points to set bounds – does not need to be high,low. This is worked out.

Definition at line 244 of file boundcube.cpp.

6.7.3.29 setBounds() [5/7]

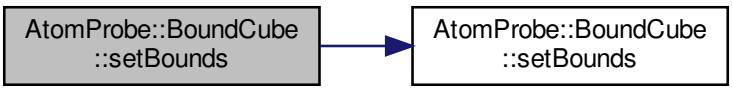
```
void AtomProbe::BoundCube::setBounds (
            const std::vector< Point3D > & ptArray )
```

Obtain bounds from an array of Point3Ds.

Definition at line 273 of file boundcube.cpp.

References setBounds().

Here is the call graph for this function:



6.7.3.30 setBounds() [6/7]

```
void AtomProbe::BoundCube::setBounds (
            const std::vector< IonHit > & ptArray )
```

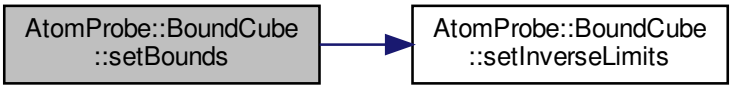
Obtain bounds from an array of IonHits.

Obtain bounds from an array of Point3Ds.

Definition at line 279 of file boundcube.cpp.

References setInverseLimits().

Here is the call graph for this function:



6.7.3.31 setBounds() [7/7]

```
void AtomProbe::BoundCube::setBounds (
            const Point3D & p,
            float radius )
```

Set the bounds using a single point and radius.

Bounds will be minimal sphere enclosing, where the sphere is defined by the (p,radius) pair

Definition at line 259 of file boundcube.cpp.

6.7.3.32 setInverseLimits()

```
void AtomProbe::BoundCube::setInverseLimits ( )
```

Set the cube to be "inside out" at the limits of numeric results;.

Definition at line 94 of file boundcube.cpp.

Referenced by BoundCube(), AtomProbe::Mesh::divideMeshSurface(), AtomProbe::IonHit::getIonDataLimits(), and setBounds().

6.7.3.33 setLimits()

```
void AtomProbe::BoundCube::setLimits ( )
```

Set min-max bounds to fp min/max.

Definition at line 115 of file boundcube.cpp.

Referenced by BoundCube().

6.7.4 Friends And Related Function Documentation

6.7.4.1 K3DTreeApprox

```
friend class K3DTreeApprox  [friend]
```

Definition at line 172 of file boundcube.h.

6.7.4.2 K3DTreeExact

```
friend class K3DTreeExact  [friend]
```

Definition at line 171 of file boundcube.h.

6.7.4.3 operator<<

```
std::ostream& operator<< (
            std::ostream & stream,
            const BoundCube & b )  [friend]
```

Definition at line 563 of file boundcube.cpp.

Referenced by BoundCube().

The documentation for this class was generated from the following files:

- include/atomprobe/primitives/boundcube.h
- src/primitives/boundcube.cpp

6.8 AtomProbe::ComparePairFirst Class Reference

```
#include <helpFuncs.h>
```

Public Member Functions

- template<class T1 , class T2 >
  bool operator() (const std::pair< T1, T2 > &p1, const std::pair< T1, T2 > &p2) const

6.8.1 Detailed Description

Definition at line 48 of file helpFuncs.h.

6.8.2 Member Function Documentation

6.8.2.1 operator()()

```
template<class T1 , class T2 >
bool AtomProbe::ComparePairFirst::operator() (
            const std::pair< T1, T2 > & p1,
            const std::pair< T1, T2 > & p2 ) const  [inline]
```

Definition at line 52 of file helpFuncs.h.

The documentation for this class was generated from the following file:

- src/helper/helpFuncs.h

6.9 AtomProbe::ComparePairFirstReverse Class Reference

```
#include <helpFuncs.h>
```

Public Member Functions

- template<class T1 , class T2 >
  bool operator() (const std::pair< T1, T2 > &p1, const std::pair< T1, T2 > &p2) const

6.9.1 Detailed Description

Definition at line 79 of file helpFuncs.h.

6.9.2 Member Function Documentation

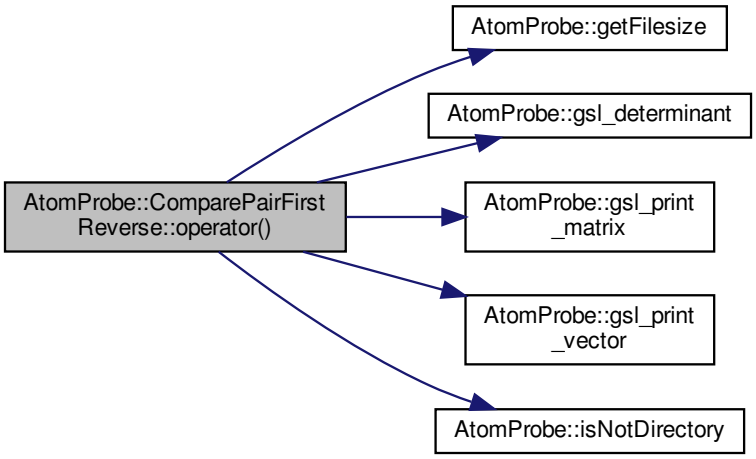
6.9.2.1 operator()()

```
template<class T1 , class T2 >
bool AtomProbe::ComparePairFirstReverse::operator() (
            const std::pair< T1, T2 > & p1,
            const std::pair< T1, T2 > & p2 ) const  [inline]
```

Definition at line 83 of file helpFuncs.h.

References AtomProbe::getFilesize(), AtomProbe::gsl_determinant(), AtomProbe::gsl_print_matrix(), AtomProbe::gsl_print_vector(), and AtomProbe::isNotDirectory().

Here is the call graph for this function:



The documentation for this class was generated from the following file:

- src/helper/helpFuncs.h

6.10 AtomProbe::ComparePairSecond Class Reference

```
#include <helpFuncs.h>
```

Public Member Functions

- template<class T1 , class T2 >
  bool operator() (const std::pair< T1, T2 > &p1, const std::pair< T1, T2 > &p2) const

6.10.1 Detailed Description

Definition at line 58 of file helpFuncs.h.

6.10.2 Member Function Documentation

6.10.2.1 operator()()

```
template<class T1 , class T2 >
bool AtomProbe::ComparePairSecond::operator() (
            const std::pair< T1, T2 > & p1,
            const std::pair< T1, T2 > & p2 ) const  [inline]
```

Definition at line 62 of file helpFuncs.h.

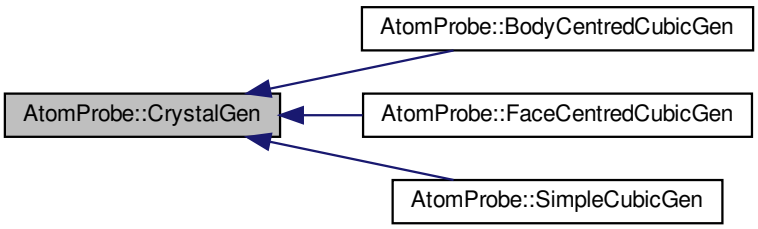
The documentation for this class was generated from the following file:

- src/helper/helpFuncs.h

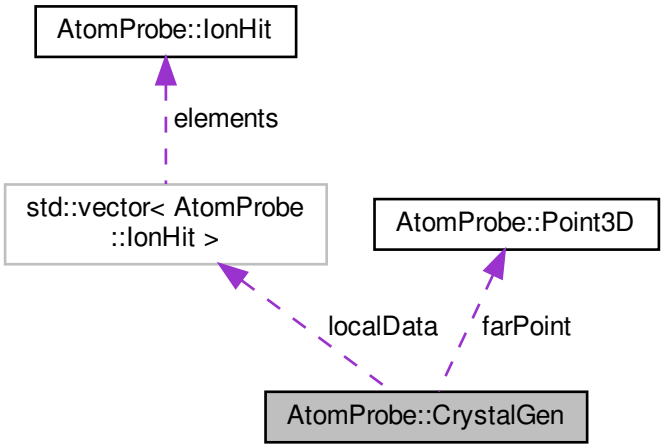
6.11 AtomProbe::CrystalGen Class Reference

```
#include <generate.h>
```

Inheritance diagram for AtomProbe::CrystalGen:



Collaboration diagram for AtomProbe::CrystalGen:



Public Member Functions

- CrystalGen ()
- virtual ~CrystalGen ()
- virtual unsigned int generateLattice ()=0
- virtual void swap (std::vector< IonHit > &data)
- virtual void extractPositions (std::vector< Point3D > &data)
- virtual void mirrorOut ()

Protected Attributes

- std::vector< IonHit > localData
- Point3D farPoint

6.11.1 Detailed Description

Definition at line 14 of file generate.h.

6.11.2 Constructor & Destructor Documentation

6.11.2.1 CrystalGen()

```
AtomProbe::CrystalGen::CrystalGen ( )  [inline]
```

Definition at line 25 of file generate.h.

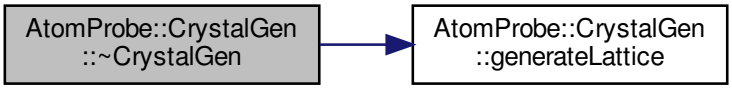
6.11.2.2 ~CrystalGen()

```
virtual AtomProbe::CrystalGen::~CrystalGen ( )  [inline], [virtual]
```

Definition at line 26 of file generate.h.

References generateLattice().

Here is the call graph for this function:



6.11.3 Member Function Documentation

6.11.3.1 extractPositions()

```
void AtomProbe::CrystalGen::extractPositions (
            std::vector< Point3D > & data )  [virtual]
```

Definition at line 7 of file generate.cpp.

References localData.

Referenced by AtomProbe::BodyCentredCubicGen::generateLattice(), main(), and swap().

6.11.3.2 generateLattice()

```
virtual unsigned int AtomProbe::CrystalGen::generateLattice ( )  [pure virtual]
```

Implemented in AtomProbe::BodyCentredCubicGen, AtomProbe::FaceCentredCubicGen, and AtomProbe::↩ SimpleCubicGen.

Referenced by main(), and ~CrystalGen().

6.11.3.3 mirrorOut()

```
void AtomProbe::CrystalGen::mirrorOut ( )  [virtual]
```

Definition at line 17 of file generate.cpp.

References localData.

Referenced by main(), and swap().

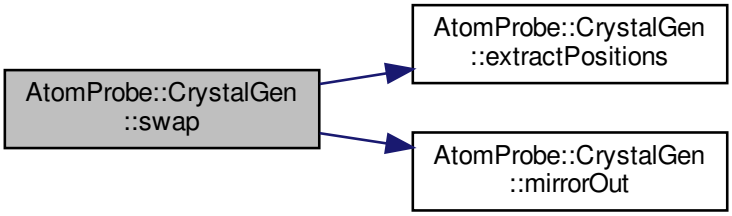
6.11.3.4 swap()

```
virtual void AtomProbe::CrystalGen::swap (
            std::vector< IonHit > & data )  [inline], [virtual]
```

Definition at line 32 of file generate.h.

References extractPositions(), and mirrorOut().

Here is the call graph for this function:



6.11.4 Member Data Documentation

6.11.4.1 farPoint

```
Point3D AtomProbe::CrystalGen::farPoint  [protected]
```

Definition at line 22 of file generate.h.

Referenced by AtomProbe::BodyCentredCubicGen::BodyCentredCubicGen(), AtomProbe::FaceCentredCubic↩Gen::FaceCentredCubicGen(), AtomProbe::SimpleCubicGen::generateLattice(), AtomProbe::FaceCentredCubic↩Gen::generateLattice(), AtomProbe::BodyCentredCubicGen::generateLattice(), and AtomProbe::SimpleCubic↩Gen::SimpleCubicGen().

6.11.4.2 localData

```
std::vector<IonHit> AtomProbe::CrystalGen::localData  [protected]
```

Definition at line 18 of file generate.h.

Referenced by extractPositions(), AtomProbe::SimpleCubicGen::generateLattice(), AtomProbe::FaceCentredCubicGen::generateLattice(), AtomProbe::BodyCentredCubicGen::generateLattice(), and mirrorOut().

The documentation for this class was generated from the following files:

- include/atomprobe/latticeplanes/generate.h
- src/lattice/generate.cpp

6.12 AtomProbe::EPOS_ENTRY Class Reference

```
#include <ionHit.h>
```

Public Member Functions

- IonHit getIonHit () const
- void getIonHit (IonHit &h) const
- bool operator== (const EPOS_ENTRY &obj) const

Public Attributes

- float x
- float y
- float z
- float massToCharge
- float timeOfFlight
- float voltDC
- float voltPulse
- float xDetector
- float yDetector
- int32_t deltaPulse
- int32_t hitMultiplicity

6.12.1 Detailed Description

Definition at line 113 of file ionHit.h.

6.12.2 Member Function Documentation

6.12.2.1 getIonHit() [1/2]

```
IonHit AtomProbe::EPOS_ENTRY::getIonHit ( ) const
```

Definition at line 231 of file dataFiles.cpp.

6.12.2.2 getIonHit() [2/2]

```
void AtomProbe::EPOS_ENTRY::getIonHit (
            IonHit & h ) const
```

Definition at line 223 of file dataFiles.cpp.

References AtomProbe::IONHIT::massToCharge.

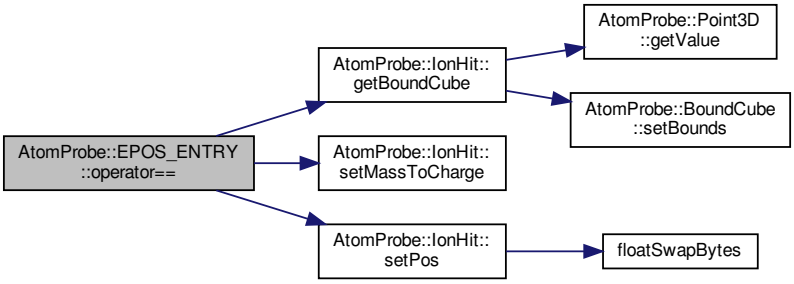
6.12.2.3 operator==()

```
bool AtomProbe::EPOS_ENTRY::operator== (
            const EPOS_ENTRY & obj ) const
```

Definition at line 271 of file ionhit.cpp.

References deltaPulse, AtomProbe::IonHit::getBoundCube(), hitMultiplicity, massToCharge, AtomProbe::IonHit↩ ::setMassToCharge(), AtomProbe::IonHit::setPos(), TEST, timeOfFlight, voltDC, voltPulse, x, xDetector, y, y↩ Detector, and z.

Here is the call graph for this function:



6.12.3 Member Data Documentation

6.12.3.1 deltaPulse

```
int32_t AtomProbe::EPOS_ENTRY::deltaPulse
```

Definition at line 130 of file ionHit.h.

Referenced by operator==(), and AtomProbe::readEposRecord().

6.12.3.2 hitMultiplicity

```
int32_t AtomProbe::EPOS_ENTRY::hitMultiplicity
```

Definition at line 130 of file ionHit.h.

Referenced by operator==(), and AtomProbe::readEposRecord().

6.12.3.3 massToCharge

```
float AtomProbe::EPOS_ENTRY::massToCharge
```

Definition at line 118 of file ionHit.h.

Referenced by operator==(), and AtomProbe::readEposRecord().

6.12.3.4 timeOfFlight

```
float AtomProbe::EPOS_ENTRY::timeOfFlight
```

Definition at line 122 of file ionHit.h.

Referenced by operator==(), and AtomProbe::readEposRecord().

6.12.3.5 voltDC

```
float AtomProbe::EPOS_ENTRY::voltDC
```

Definition at line 122 of file ionHit.h.

Referenced by operator==(), and AtomProbe::readEposRecord().

6.12.3.6 voltPulse

```
float AtomProbe::EPOS_ENTRY::voltPulse
```

Definition at line 122 of file ionHit.h.

Referenced by operator==(), and AtomProbe::readEposRecord().

6.12.3.7 x

```
float AtomProbe::EPOS_ENTRY::x
```

Definition at line 118 of file ionHit.h.

Referenced by operator==(), and AtomProbe::readEposRecord().

6.12.3.8 xDetector

```
float AtomProbe::EPOS_ENTRY::xDetector
```

Definition at line 124 of file ionHit.h.

Referenced by operator==(), and AtomProbe::readEposRecord().

6.12.3.9 y

```
float AtomProbe::EPOS_ENTRY::y
```

Definition at line 118 of file ionHit.h.

Referenced by operator==(), and AtomProbe::readEposRecord().

6.12.3.10 yDetector

```
float AtomProbe::EPOS_ENTRY::yDetector
```

Definition at line 124 of file ionHit.h.

Referenced by operator==(), and AtomProbe::readEposRecord().

6.12.3.11 z

```
float AtomProbe::EPOS_ENTRY::z
```

Definition at line 118 of file ionHit.h.

Referenced by operator==(), and AtomProbe::readEposRecord().

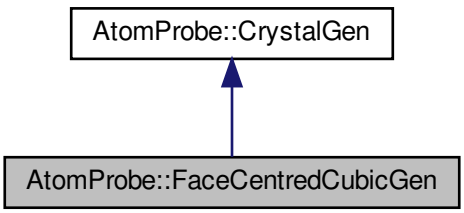
The documentation for this class was generated from the following files:

- include/atomprobe/primitives/ionHit.h
- src/io/dataFiles.cpp
- src/primitives/ionhit.cpp

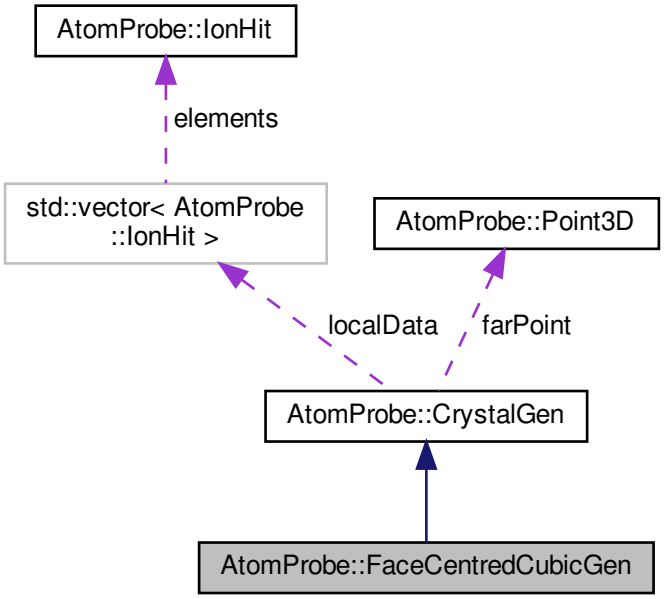
6.13 AtomProbe::FaceCentredCubicGen Class Reference

```
#include <generate.h>
```

Inheritance diagram for AtomProbe::FaceCentredCubicGen:



Collaboration diagram for AtomProbe::FaceCentredCubicGen:



Public Member Functions

- FaceCentredCubicGen (float latticeSpacing, float mToCCorner, const float ∗mToCFace, const Point3D &p)
- unsigned int generateLattice ()

Additional Inherited Members

6.13.1 Detailed Description

Definition at line 52 of file generate.h.

6.13.2 Constructor & Destructor Documentation

6.13.2.1 FaceCentredCubicGen()

```
AtomProbe::FaceCentredCubicGen::FaceCentredCubicGen (
            float latticeSpacing,
            float mToCCorner,
            const float * mToCFace,
            const Point3D & p )
```

Definition at line 104 of file generate.cpp.

References AtomProbe::CrystalGen::farPoint.

6.13.3 Member Function Documentation

6.13.3.1 generateLattice()

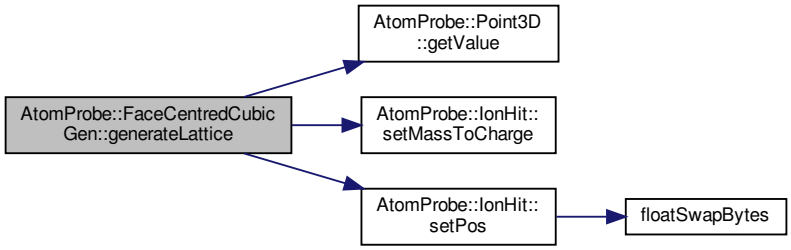
```
unsigned int AtomProbe::FaceCentredCubicGen::generateLattice ( )  [virtual]
```

Implements AtomProbe::CrystalGen.

Definition at line 114 of file generate.cpp.

References AtomProbe::CRYSTAL_BAD_UNIT_CELL, AtomProbe::CrystalGen::farPoint, AtomProbe::Point3D::getValue(), AtomProbe::CrystalGen::localData, AtomProbe::IonHit::setMassToCharge(), and AtomProbe::IonHit::setPos().

Here is the call graph for this function:



The documentation for this class was generated from the following files:

- include/atomprobe/latticeplanes/generate.h
- src/lattice/generate.cpp

6.14 FixedStack< T > Class Template Reference

Public Member Functions

- FixedStack (size_t size)
- FixedStack (const FixedStack &f)
- ~FixedStack ()
- T & top ()
- void pop ()
- void push (const T &t)
- bool empty () const

6.14.1 Detailed Description

template<class T>
class FixedStack< T >

Definition at line 51 of file massTool.cpp.

6.14.2 Constructor & Destructor Documentation

6.14.2.1 FixedStack() [1/2]

```
template<class T >
FixedStack< T >::FixedStack (
            size_t size )
```

Definition at line 68 of file massTool.cpp.

6.14.2.2 FixedStack() [2/2]

```
template<class T>
FixedStack< T >::FixedStack (
            const FixedStack< T > & f )
```

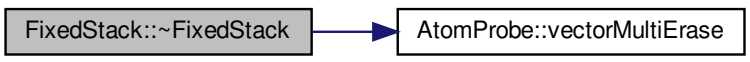
6.14.2.3 ~FixedStack()

```
template<class T >
FixedStack< T >::~FixedStack ( )
```

Definition at line 95 of file massTool.cpp.

References AtomProbe::vectorMultiErase().

Here is the call graph for this function:



6.14.3 Member Function Documentation

6.14.3.1 empty()

```
template<class T>
bool FixedStack< T >::empty ( ) const  [inline]
```

Definition at line 64 of file massTool.cpp.

Referenced by AtomProbe::MassTool::bruteKnapsack().

6.14.3.2 pop()

```
template<class T >
void FixedStack< T >::pop ( )
```

Definition at line 82 of file massTool.cpp.

References ASSERT.

Referenced by AtomProbe::MassTool::bruteKnapsack().

6.14.3.3 push()

```
template<class T >
void FixedStack< T >::push (
            const T & t )
```

Definition at line 75 of file massTool.cpp.

Referenced by AtomProbe::MassTool::bruteKnapsack().

6.14.3.4 top()

```
template<class T >
T & FixedStack< T >::top ( )
```

Definition at line 89 of file massTool.cpp.

Referenced by AtomProbe::MassTool::bruteKnapsack().

The documentation for this class was generated from the following file:

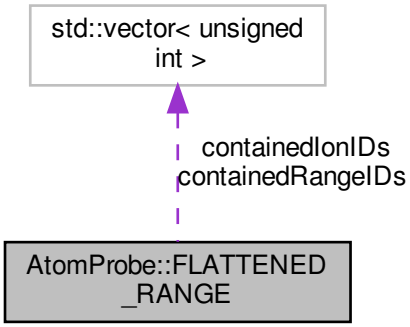
- src/algorithm/massTool.cpp

6.15 AtomProbe::FLATTENED_RANGE Struct Reference

Structure that allows for the multirange data to be mapped into.

`#include <multiRange.h>`

Collaboration diagram for AtomProbe::FLATTENED_RANGE:



Public Attributes

- float startMass
- float endMass
- std::vector< unsigned int > containedIonIDs
- std::vector< unsigned int > containedRangeIDs

6.15.1 Detailed Description

Structure that allows for the multirange data to be mapped into.

Definition at line 47 of file multiRange.h.

6.15.2 Member Data Documentation

6.15.2.1 containedIonIDs

`std::vector<unsigned int> AtomProbe::FLATTENED_RANGE::containedIonIDs`

Definition at line 52 of file multiRange.h.

6.15.2.2 containedRangeIDs

```
std::vector<unsigned int> AtomProbe::FLATTENED_RANGE::containedRangeIDs
```

Definition at line 52 of file multiRange.h.

6.15.2.3 endMass

```
float AtomProbe::FLATTENED_RANGE::endMass
```

Definition at line 50 of file multiRange.h.

6.15.2.4 startMass

```
float AtomProbe::FLATTENED_RANGE::startMass
```

Definition at line 50 of file multiRange.h.

Referenced by AtomProbe::MultiRange::flattenToMassAxis().

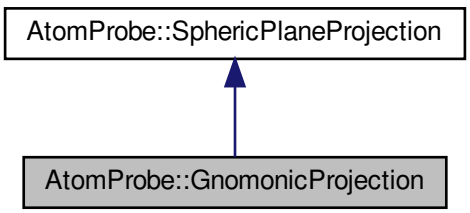
The documentation for this struct was generated from the following file:

- include/atomprobe/io/multiRange.h

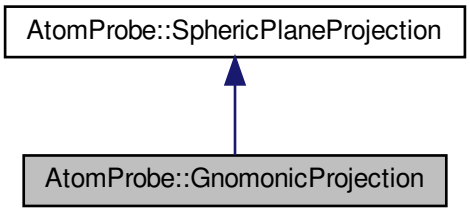
6.16 AtomProbe::GnomonicProjection Class Reference

```
#include <projection.h>
```

Inheritance diagram for AtomProbe::GnomonicProjection:



Collaboration diagram for AtomProbe::GnomonicProjection:



Public Member Functions

- virtual bool toAzimuthal (float fx, float fy, float &theta, float &phi) const
  Convert from plane coordinates to spherical coords.
- virtual bool toPlanar (float theta, float phi, float &fx, float &fy) const
  Convert from spherical coordinates to plane.
- virtual void scaleDown (float flightLength, float detX, float detY, float &scaledX, float &scaledY) const
  Convert from actual detector postion (eg. mm) and flight path to scaled-down transform.
- virtual void scaleUp (float flightLength, float scaledX, float scaledY, float &realX, float &realY) const
  Convert from scaled-down radius to actual radius.

6.16.1 Detailed Description

Definition at line 44 of file projection.h.

6.16.2 Member Function Documentation

6.16.2.1 scaleDown()

```
void AtomProbe::GnomonicProjection::scaleDown (
            float flightLength,
            float detX,
            float detY,
            float & scaledX,
            float & scaledY ) const  [virtual]
```

Convert from actual detector postion (eg. mm) and flight path to scaled-down transform.

Implements AtomProbe::SphericPlaneProjection.

Definition at line 84 of file projection.cpp.

References ASSERT.

6.16.2.2 scaleUp()

```
void AtomProbe::GnomonicProjection::scaleUp (
            float flightLength,
            float scaledX,
            float scaledY,
            float & realX,
            float & realY ) const  [virtual]
```

Convert from scaled-down radius to actual radius.

Implements AtomProbe::SphericPlaneProjection.

Definition at line 96 of file projection.cpp.

References ASSERT.

6.16.2.3 toAzimuthal()

```
bool AtomProbe::GnomonicProjection::toAzimuthal (
            float fx,
            float fy,
            float & theta,
            float & phi ) const  [virtual]
```

Convert from plane coordinates to spherical coords.

Implements AtomProbe::SphericPlaneProjection.

Definition at line 68 of file projection.cpp.

Referenced by AtomProbe::ModifiedFocusSphericProjection::scaleUp().

6.16.2.4 toPlanar()

```
bool AtomProbe::GnomonicProjection::toPlanar (
            float theta,
            float phi,
            float & fx,
            float & fy ) const  [virtual]
```

Convert from spherical coordinates to plane.

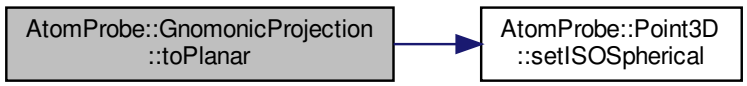
Implements AtomProbe::SphericPlaneProjection.

Definition at line 34 of file projection.cpp.

References ASSERT, M_PI, and AtomProbe::Point3D::setISOSpherical().

Referenced by AtomProbe::ModifiedFocusSphericProjection::scaleUp().

Here is the call graph for this function:



The documentation for this class was generated from the following files:

- include/atomprobe/projection/projection.h
- src/projection/projection.cpp

6.17 AtomProbe::IonHit Class Reference

This is a data holding class for POS file ions, from.

`#include <ionHit.h>`

Public Member Functions

- IonHit ()
- IonHit (float *)
- IonHit (const IonHit &)
- IonHit (const Point3D &p, float massToCharge)
- IonHit (float x, float y, float z, float mass)
- void setHit (float *arr)
- void setMassToCharge (float newMassToCharge)
- void setPos (const Point3D &pos)
- void setPos (unsigned int idx, float pos)
- void setPos (float fX, float fY, float fZ)
- Point3D getPos () const
- const Point3D & getPosRef () const
- bool hasNaN ()
- float getMassToCharge () const
- const IonHit & operator= (const IonHit &obj)
- bool operator== (const IonHit &obj) const
- float operator[ ] (unsigned int ui) const
- float & operator[ ] (unsigned int ui)
- IonHit operator+ (const Point3D &obj)

Static Public Member Functions

- static void getPoints (const std::vector< IonHit > &ions, std::vector< Point3D > &pts)
- static void getBoundCube (const std::vector< IonHit > &p, BoundCube &b)
- static void getCentroid (const std::vector< IonHit > &points, Point3D &centroid)
- static BoundCube getIonDataLimits (const std::vector< IonHit > &points)

Friends

- std::ostream & operator<< (std::ostream &stream, const IonHit &)

  Output streaming operator. Users (x,y,z,m) as format for output.

6.17.1 Detailed Description

This is a data holding class for POS file ions, from.

Definition at line 36 of file ionHit.h.

6.17.2 Constructor & Destructor Documentation

6.17.2.1 IonHit() [1/5]

```
AtomProbe::IonHit::IonHit ( )
```

Definition at line 38 of file ionhit.cpp.

6.17.2.2 IonHit() [2/5]

```
AtomProbe::IonHit::IonHit (
            float * buffer )
```

Definition at line 44 of file ionhit.cpp.

6.17.2.3 IonHit() [3/5]

```
AtomProbe::IonHit::IonHit (
            const IonHit & obj2 )
```

Definition at line 52 of file ionhit.cpp.

6.17.2.4 IonHit() [4/5]

```
AtomProbe::IonHit::IonHit (
            const Point3D & p,
            float massToCharge )
```

Definition at line 56 of file ionhit.cpp.

6.17.2.5 IonHit() [5/5]

```
AtomProbe::IonHit::IonHit (
            float x,
            float y,
            float z,
            float mass )
```

Definition at line 48 of file ionhit.cpp.

6.17.3 Member Function Documentation

6.17.3.1 getBoundCube()

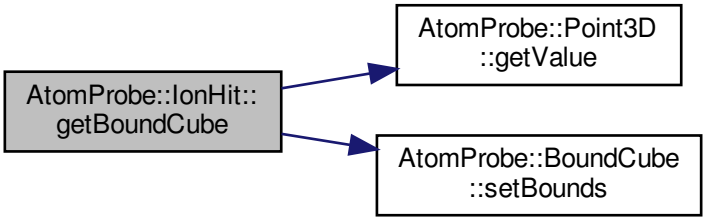
```
void AtomProbe::IonHit::getBoundCube (
            const std::vector< IonHit > & p,
            BoundCube & b )  [static]
```

Definition at line 153 of file ionhit.cpp.

References ASSERT, AtomProbe::Point3D::getValue(), and AtomProbe::BoundCube::setBounds().

Referenced by getPosRef(), and AtomProbe::EPOS_ENTRY::operator==().

Here is the call graph for this function:



6.17.3.2 getCentroid()

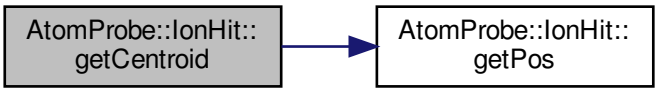
```
void AtomProbe::IonHit::getCentroid (
            const std::vector< IonHit > & points,
            Point3D & centroid )  [static]
```

Definition at line 128 of file ionhit.cpp.

References getPos().

Referenced by getPosRef().

Here is the call graph for this function:



6.17.3.3 getIonDataLimits()

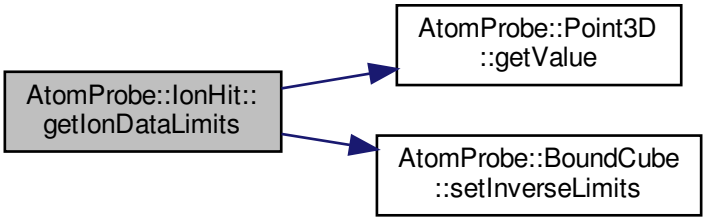
```
BoundCube AtomProbe::IonHit::getIonDataLimits (
            const std::vector< IonHit > & points )  [static]
```

Definition at line 188 of file ionhit.cpp.

References ASSERT, AtomProbe::Point3D::getValue(), and AtomProbe::BoundCube::setInverseLimits().

Referenced by getPosRef(), and AtomProbe::K3DTreeExact::resetPts().

Here is the call graph for this function:



6.17.3.4 getMassToCharge()

```
float AtomProbe::IonHit::getMassToCharge ( ) const
```

Definition at line 65 of file ionhit.cpp.

Referenced by AtomProbe::RangeFile::getIonID(), AtomProbe::RangeFile::getName(), getPosRef(), AtomProbe↩
::MultiRange::isRanged(), AtomProbe::RangeFile::isRanged(), main(), and AtomProbe::operator<<().

6.17.3.5 getPoints()

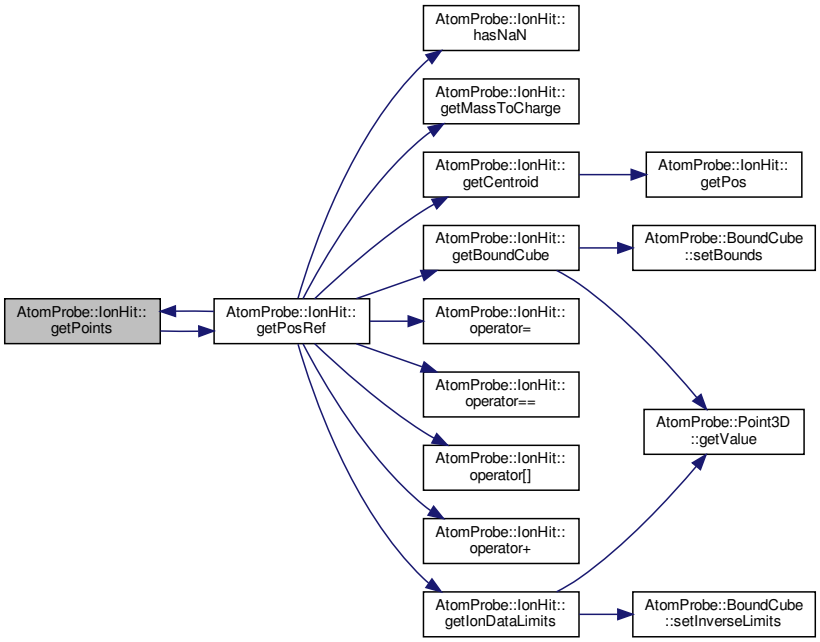
```
void AtomProbe::IonHit::getPoints (
            const std::vector< IonHit > & ions,
            std::vector< Point3D > & pts )  [static]
```

Definition at line 109 of file ionhit.cpp.

References getPosRef().

Referenced by getPosRef().

Here is the call graph for this function:



6.17.3.6 getPos()

```
Point3D AtomProbe::IonHit::getPos ( ) const
```

Definition at line 117 of file ionhit.cpp.

Referenced by getCentroid(), main(), AtomProbe::operator<<(), and setPos().

6.17.3.7 getPosRef()

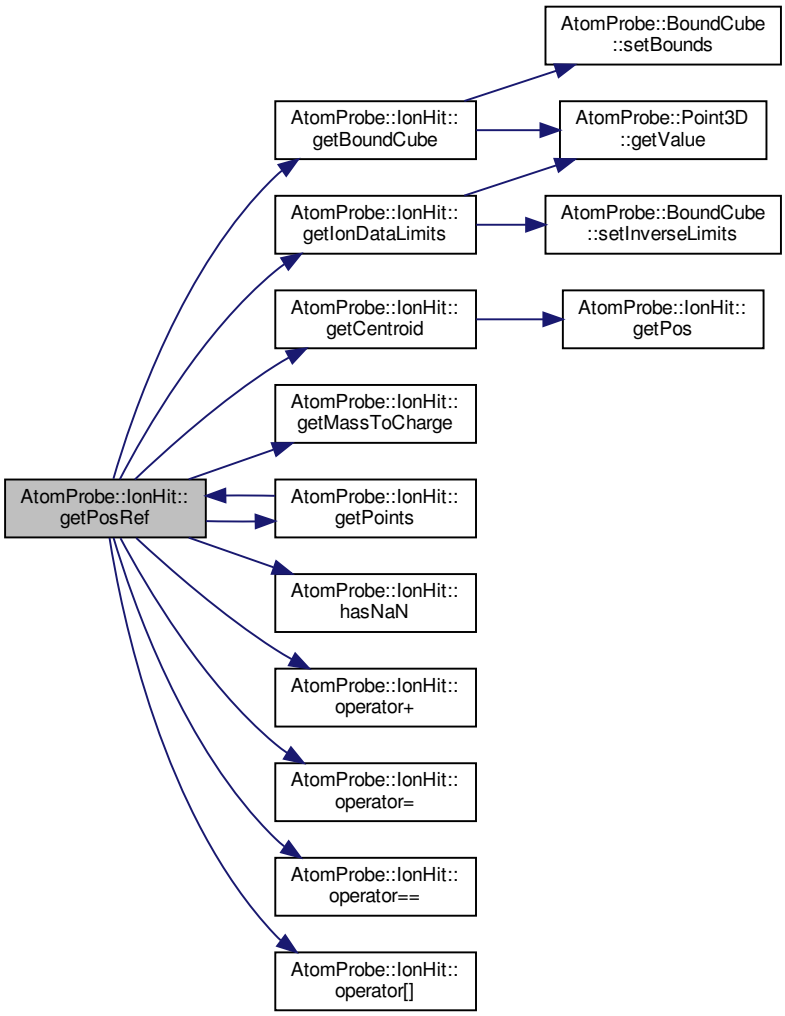
```
const Point3D& AtomProbe::IonHit::getPosRef ( ) const  [inline]
```

Definition at line 65 of file ionHit.h.

References getBoundCube(), getCentroid(), getIonDataLimits(), getMassToCharge(), getPoints(), hasNaN(), operator+(), operator<<, operator=(), operator==(), and operator[]().

Referenced by getPoints().

Here is the call graph for this function:



6.17.3.8 hasNaN()

```
bool AtomProbe::IonHit::hasNaN ( )
```

Definition at line 122 of file ionhit.cpp.

Referenced by getPosRef(), and AtomProbe::loadPosFile().

6.17.3.9 operator+()

```
IonHit AtomProbe::IonHit::operator+ (
            const Point3D & obj )
```

Definition at line 103 of file ionhit.cpp.

Referenced by getPosRef().

6.17.3.10 operator=()

```
const IonHit & AtomProbe::IonHit::operator= (
            const IonHit & obj )
```

Definition at line 90 of file ionhit.cpp.

Referenced by getPosRef().

6.17.3.11 operator==()

```
bool AtomProbe::IonHit::operator== (
            const IonHit & obj ) const
```

Definition at line 98 of file ionhit.cpp.

Referenced by getPosRef().

6.17.3.12 operator[]() [1/2]

```
float AtomProbe::IonHit::operator[] (
            unsigned int ui ) const
```

Definition at line 251 of file ionhit.cpp.

References ASSERT.

Referenced by getPosRef().

6.17.3.13 operator[]() [2/2]

```
float & AtomProbe::IonHit::operator[] (
            unsigned int ui )
```

Definition at line 260 of file ionhit.cpp.

References ASSERT.

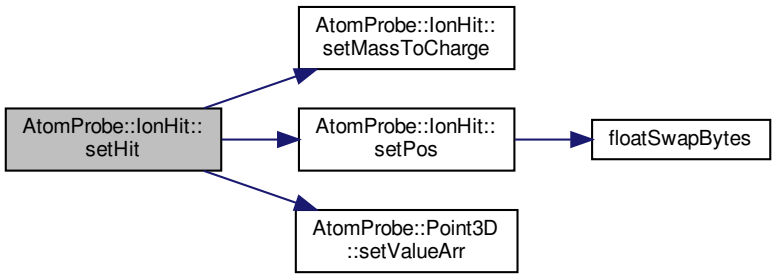
6.17.3.14 setHit()

```
void AtomProbe::IonHit::setHit (
            float * arr )  [inline]
```

Definition at line 50 of file ionHit.h.

References setMassToCharge(), setPos(), and AtomProbe::Point3D::setValueArr().

Here is the call graph for this function:



6.17.3.15 setMassToCharge()

```
void AtomProbe::IonHit::setMassToCharge (
            float newMassToCharge )
```

Definition at line 60 of file ionhit.cpp.

Referenced by AtomProbe::FaceCentredCubicGen::generateLattice(), AtomProbe::BodyCentredCubicGen↩
::generateLattice(), AtomProbe::loadPosFile(), AtomProbe::loadTapsimBinFile(), AtomProbe::EPOS_ENTRY↩
::operator==(), and setHit().

6.17.3.16 setPos() [1/3]

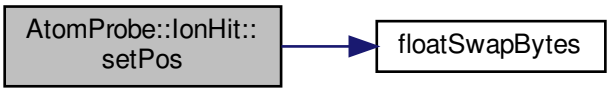
```
void AtomProbe::IonHit::setPos (
            const Point3D & pos )
```

Definition at line 76 of file ionhit.cpp.

References floatSwapBytes().

Referenced by AtomProbe::SimpleCubicGen::generateLattice(), AtomProbe::FaceCentredCubicGen::generate↩Lattice(), AtomProbe::BodyCentredCubicGen::generateLattice(), AtomProbe::loadPosFile(), AtomProbe::load↩TapsimBinFile(), AtomProbe::EPOS_ENTRY::operator==(), and setHit().

Here is the call graph for this function:



6.17.3.17 setPos() [2/3]

```
void AtomProbe::IonHit::setPos (
            unsigned int idx,
            float pos )
```

Definition at line 70 of file ionhit.cpp.

References ASSERT.

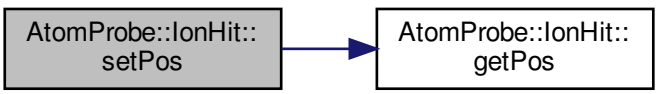
6.17.3.18 setPos() [3/3]

```
void AtomProbe::IonHit::setPos (
            float fX,
            float fY,
            float fZ )  [inline]
```

Definition at line 59 of file ionHit.h.

References getPos().

Here is the call graph for this function:



6.17.4 Friends And Related Function Documentation

6.17.4.1 operator<<

```
std::ostream& operator<< (
            std::ostream & stream,
            const IonHit & ion )  [friend]
```

Output streaming operator. Users (x,y,z,m) as format for output.

Definition at line 181 of file ionhit.cpp.

Referenced by getPosRef().

The documentation for this class was generated from the following files:

- include/atomprobe/primitives/ionHit.h
- src/primitives/ionhit.cpp

6.18 AtomProbe::IONHIT Struct Reference

Record as stored in a .POS file.

Public Attributes

- float pos [3]
- float massToCharge

6.18.1 Detailed Description

Record as stored in a .POS file.

Definition at line 45 of file dataFiles.cpp.

6.18.2 Member Data Documentation

6.18.2.1 massToCharge

```
float AtomProbe::IONHIT::massToCharge
```

Definition at line 48 of file dataFiles.cpp.

Referenced by AtomProbe::EPOS_ENTRY::getIonHit(), and AtomProbe::loadPosFile().

6.18.2.2 pos

```
float AtomProbe::IONHIT::pos[3]
```

Definition at line 47 of file dataFiles.cpp.

Referenced by AtomProbe::loadPosFile().

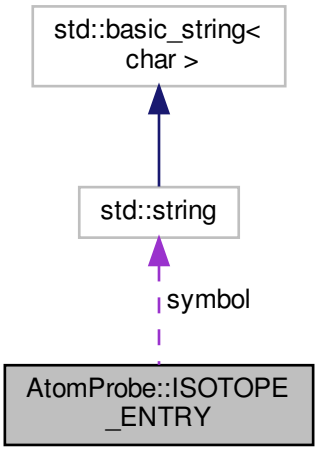
The documentation for this struct was generated from the following file:

- src/io/dataFiles.cpp

6.19 AtomProbe::ISOTOPE_ENTRY Struct Reference

```
#include <abundance.h>
```

Collaboration diagram for AtomProbe::ISOTOPE_ENTRY:



Public Attributes

- std::string symbol
- size_t massNumber
- size_t atomicNumber
- float mass
- float massError
- float abundance
- float abundanceError

6.19.1 Detailed Description

Definition at line 42 of file abundance.h.

6.19.2 Member Data Documentation

6.19.2.1 abundance

```
float AtomProbe::ISOTOPE_ENTRY::abundance
```

Definition at line 49 of file abundance.h.

Referenced by AtomProbe::filterBySolutionPPM(), and AtomProbe::AbundanceData::open().

6.19.2.2 abundanceError

```
float AtomProbe::ISOTOPE_ENTRY::abundanceError
```

Definition at line 50 of file abundance.h.

Referenced by AtomProbe::AbundanceData::open().

6.19.2.3 atomicNumber

```
size_t AtomProbe::ISOTOPE_ENTRY::atomicNumber
```

Definition at line 46 of file abundance.h.

Referenced by AtomProbe::MultiRange::copyDataFromRange(), AtomProbe::AbundanceData::elementName(), and AtomProbe::AbundanceData::open().

6.19.2.4 mass

```
float AtomProbe::ISOTOPE_ENTRY::mass
```

Definition at line 47 of file abundance.h.

Referenced by AtomProbe::AbundanceData::elementName(), AtomProbe::maxExplainedFraction(), and AtomProbe::AbundanceData::open().

6.19.2.5 massError

```
float AtomProbe::ISOTOPE_ENTRY::massError
```

Definition at line 48 of file abundance.h.

Referenced by AtomProbe::AbundanceData::open().

6.19.2.6 massNumber

```
size_t AtomProbe::ISOTOPE_ENTRY::massNumber
```

Definition at line 45 of file abundance.h.

Referenced by AtomProbe::AbundanceData::open().

6.19.2.7 symbol

```
std::string AtomProbe::ISOTOPE_ENTRY::symbol
```

Definition at line 44 of file abundance.h.

Referenced by AtomProbe::AbundanceData::open().

The documentation for this struct was generated from the following file:

- include/atomprobe/isotopes/abundance.h

6.20 AtomProbe::K3DNodeApprox Class Reference

Node Class for storing point.

```
#include <K3DTree-approx.h>
```

Public Member Functions

- Point3D getLoc () const
  Return the point data from the ndoe.
- const Point3D * getLocRef () const
  Return a pointer to the point from the node.
- void setLeft (K3DNodeApprox *node)
  Set the left child node.
- void setRight (K3DNodeApprox *node)
  Set the right child node.
- void setLoc (const Point3D &)
  Set the point data associated with this node.
- void setAxis (unsigned int newAxis)
  Set the axis that this node operates on.
- unsigned int getAxis () const
  Retrieve the axis that this node operates on.
- float getAxisVal () const
  retrieve the value associated with this axis
- float getLocVal (unsigned int pos) const
  Obtain the coordinates at dimension "pos".
- float sqrDist (const Point3D &pt) const
  Obtain the distance between this node and another point.
- K3DNodeApprox * left () const
  Obtain pointer to left child.
- K3DNodeApprox * right () const
  Obtain pointer to right child.
- void deleteChildren ()
  Recursively delete this node and all children.
- void dump (std::ostream &, unsigned int) const
  print the node data out to a given stream

6.20.1 Detailed Description

Node Class for storing point.

Definition at line 53 of file K3DTree-approx.h.

6.20.2 Member Function Documentation

6.20.2.1 deleteChildren()

```
void AtomProbe::K3DNodeApprox::deleteChildren ( )
```

Recursively delete this node and all children.

Definition at line 63 of file K3DTree-approx.cpp.

Referenced by AtomProbe::K3DTreeApprox::kill().

6.20.2.2 dump()

```
void AtomProbe::K3DNodeApprox::dump (
            std::ostream & strm,
            unsigned int depth ) const
```

print the node data out to a given stream

Definition at line 83 of file K3DTree-approx.cpp.

Referenced by AtomProbe::K3DTreeApprox::dump().

6.20.2.3 getAxis()

```
unsigned int AtomProbe::K3DNodeApprox::getAxis ( ) const  [inline]
```

Retrieve the axis that this node operates on.

Definition at line 79 of file K3DTree-approx.h.

6.20.2.4 getAxisVal()

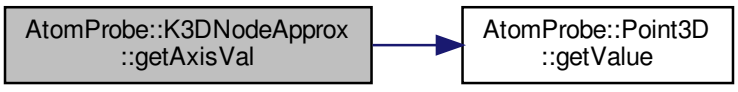
```
float AtomProbe::K3DNodeApprox::getAxisVal ( ) const  [inline]
```

retrieve the value associated with this axis

Definition at line 81 of file K3DTree-approx.h.

References AtomProbe::Point3D::getValue().

Here is the call graph for this function:



6.20.2.5 getLoc()

```
Point3D AtomProbe::K3DNodeApprox::getLoc ( ) const
```

Return the point data from the ndoe.

Definition at line 58 of file K3DTree-approx.cpp.

6.20.2.6 getLocRef()

```
const Point3D* AtomProbe::K3DNodeApprox::getLocRef ( ) const  [inline]
```

Return a pointer to the point from the node.

Definition at line 68 of file K3DTree-approx.h.

Referenced by AtomProbe::K3DTreeApprox::findNearest().

6.20.2.7 getLocVal()

```
float AtomProbe::K3DNodeApprox::getLocVal (
            unsigned int pos ) const  [inline]
```

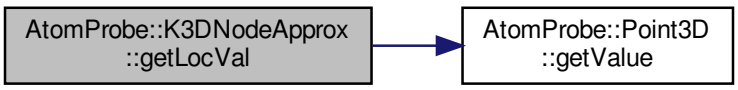
Obtain the coordinates at dimension "pos".

Definition at line 83 of file K3DTree-approx.h.

References AtomProbe::Point3D::getValue().

Referenced by AtomProbe::K3DTreeApprox::findNearest().

Here is the call graph for this function:



6.20.2.8 left()

```
K3DNodeApprox* AtomProbe::K3DNodeApprox::left ( ) const  [inline]
```

Obtain pointer to left child.

Definition at line 87 of file K3DTree-approx.h.

Referenced by AtomProbe::K3DTreeApprox::findNearest().

6.20.2.9 right()

```
K3DNodeApprox* AtomProbe::K3DNodeApprox::right ( ) const  [inline]
```

Obtain pointer to right child.

Definition at line 89 of file K3DTree-approx.h.

Referenced by AtomProbe::K3DTreeApprox::findNearest().

6.20.2.10 setAxis()

```
void AtomProbe::K3DNodeApprox::setAxis (
            unsigned int newAxis )  [inline]
```

Set the axis that this node operates on.

Definition at line 77 of file K3DTree-approx.h.

Referenced by AtomProbe::K3DTreeApprox::buildByRef().

6.20.2.11 setLeft()

```
void AtomProbe::K3DNodeApprox::setLeft (
            K3DNodeApprox * node )  [inline]
```

Set the left child node.

Definition at line 70 of file K3DTree-approx.h.

Referenced by AtomProbe::K3DTreeApprox::buildByRef().

6.20.2.12 setLoc()

```
void AtomProbe::K3DNodeApprox::setLoc (
            const Point3D & locNew )
```

Set the point data associated with this node.

Definition at line 53 of file K3DTree-approx.cpp.

Referenced by AtomProbe::K3DTreeApprox::buildByRef().

6.20.2.13 setRight()

```
void AtomProbe::K3DNodeApprox::setRight (
            K3DNodeApprox * node )  [inline]
```

Set the right child node.

Definition at line 72 of file K3DTree-approx.h.

Referenced by AtomProbe::K3DTreeApprox::buildByRef().

6.20.2.14 sqrDist()

```
float AtomProbe::K3DNodeApprox::sqrDist (
            const Point3D & pt ) const  [inline]
```

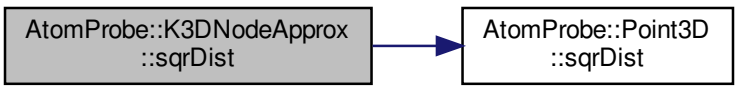
Obtain the distance between this node and another point.

Definition at line 85 of file K3DTree-approx.h.

References AtomProbe::Point3D::sqrDist().

Referenced by AtomProbe::K3DTreeApprox::findNearest().

Here is the call graph for this function:



The documentation for this class was generated from the following files:

- include/atomprobe/algorithm/K3DTree-approx.h
- src/algorithm/K3DTree-approx.cpp

6.21 AtomProbe::K3DNodeExact Class Reference

Node Class for storing point.

`#include <K3DTree-exact.h>`

Public Attributes

- size_t childLeft
- size_t childRight
- bool tagged

6.21.1 Detailed Description

Node Class for storing point.

Definition at line 41 of file K3DTree-exact.h.

6.21.2 Member Data Documentation

6.21.2.1 childLeft

`size_t AtomProbe::K3DNodeExact::childLeft`

Definition at line 45 of file K3DTree-exact.h.

6.21.2.2 childRight

`size_t AtomProbe::K3DNodeExact::childRight`

Definition at line 47 of file K3DTree-exact.h.

6.21.2.3 tagged

`bool AtomProbe::K3DNodeExact::tagged`

Definition at line 50 of file K3DTree-exact.h.

The documentation for this class was generated from the following file:

- include/atomprobe/algorithm/K3DTree-exact.h

6.22 AtomProbe::K3DTreeApprox Class Reference

3D specific KD tree

`#include <K3DTree-approx.h>`

Public Member Functions

- K3DTreeApprox ()
- ~K3DTreeApprox ()

  Cleans up tree, deallocates nodes.
- void build (const std::vector< Point3D > &pts)

  Builds a balanced KD tree from a list of points.
- void buildByRef (std::vector< Point3D > &pts)

  Builds a balanced KD tree from a list of points.
- void kill ()

  Destroy the tree contents.
- const Point3D * findNearest (const Point3D &, const BoundCube &, float deadDistSqr) const

  Find the nearest point to a given P that lies outsid some dead zone.
- void findKNearest (const Point3D &sourcePoint, const BoundCube &treeDomain, unsigned int numNNs, std::vector< const Point3D *> &results, float deadDistSqr=0.0f) const

  Find the nearest N points.
- void dump (std::ostream &) const

  Textual output of tree. tabs are used to separate different levels of the tree.
- unsigned int nodeCount () const

  Print the number of nodes stored in the tree.

6.22.1 Detailed Description

3D specific KD tree

Definition at line 98 of file K3DTree-approx.h.

6.22.2 Constructor & Destructor Documentation

6.22.2.1 K3DTreeApprox()

`AtomProbe::K3DTreeApprox::K3DTreeApprox ( )`

Definition at line 103 of file K3DTree-approx.cpp.

6.22.2.2 ~K3DTreeApprox()

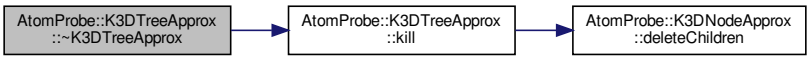
```
AtomProbe::K3DTreeApprox::~K3DTreeApprox ( )
```

Cleans up tree, deallocates nodes.

Definition at line 109 of file K3DTree-approx.cpp.

References kill().

Here is the call graph for this function:



6.22.3 Member Function Documentation

6.22.3.1 build()

```
void AtomProbe::K3DTreeApprox::build (
            const std::vector< Point3D > & pts )
```

Builds a balanced KD tree from a list of points.

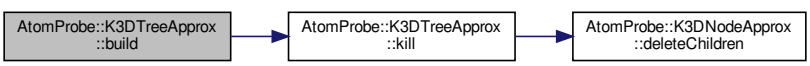
This call is const, and copies in order to prevent re-ordering of the points. If rordering points is unimportant, use buildByRef

Definition at line 127 of file K3DTree-approx.cpp.

References kill().

Referenced by findKNearest(), and testInexactKDTree().

Here is the call graph for this function:



6.22.3.2 buildByRef()

```
void AtomProbe::K3DTreeApprox::buildByRef (
            std::vector< Point3D > & pts )
```

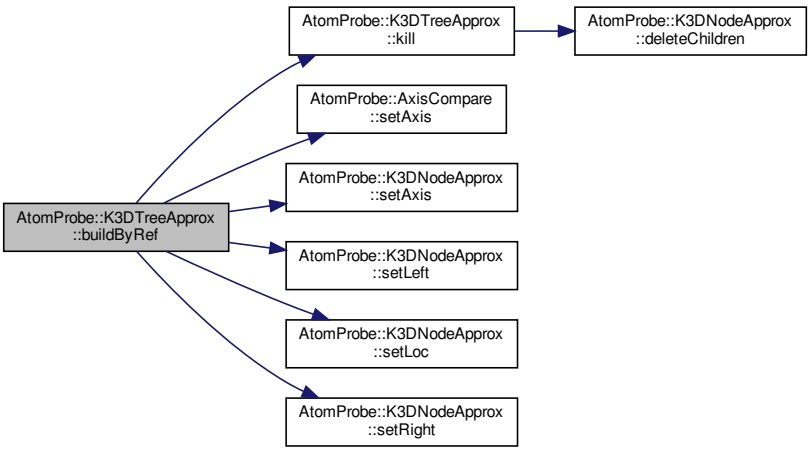
Builds a balanced KD tree from a list of points.

This uses a pass by ref where the points get scrambled (sorted). Resultant tree should be identical to that generated by build()

Definition at line 149 of file K3DTree-approx.cpp.

References kill(), AtomProbe::AxisCompare::setAxis(), AtomProbe::K3DNodeApprox::setAxis(), AtomProbe::K3↩DNodeApprox::setLeft(), AtomProbe::K3DNodeApprox::setLoc(), and AtomProbe::K3DNodeApprox::setRight().

Here is the call graph for this function:



6.22.3.3 dump()

```
void AtomProbe::K3DTreeApprox::dump (
            std::ostream & strm ) const
```

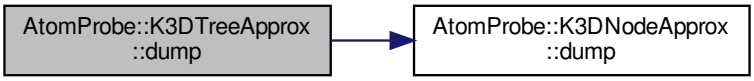
Textual output of tree. tabs are used to separate different levels of the tree.

The output from this function can be quite large for even modest trees. Recommended for debugging only

Definition at line 206 of file K3DTree-approx.cpp.

References AtomProbe::K3DNodeApprox::dump().

Here is the call graph for this function:



6.22.3.4 findKNearest()

```
void AtomProbe::K3DTreeApprox::findKNearest (
            const Point3D & sourcePoint,
            const BoundCube & treeDomain,
            unsigned int numNNs,
            std::vector< const Point3D *> & results,
            float deadDistSqr = 0.0f ) const
```

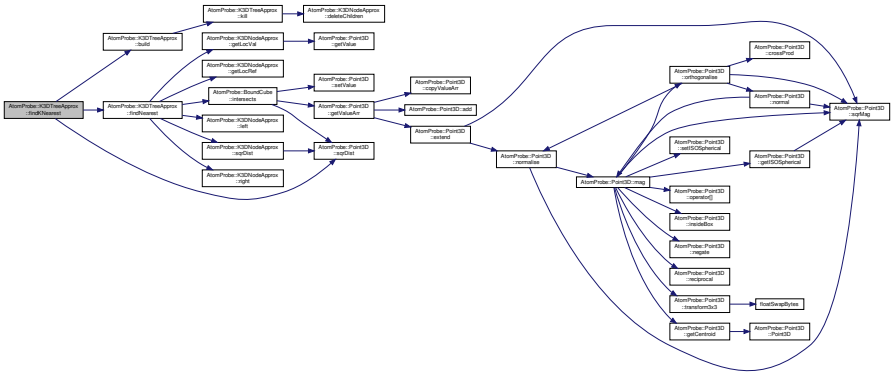
Find the nearest N points.

Finds the nearest N points, that lie outside a dead distance of deadDistSqr. k is the number to find

Definition at line 447 of file K3DTree-approx.cpp.

References build(), findNearest(), AtomProbe::Point3D::sqrDist(), and TEST.

Here is the call graph for this function:



6.22.3.5 findNearest()

```
const Point3D * AtomProbe::K3DTreeApprox::findNearest (
            const Point3D & searchPt,
            const BoundCube & domainCube,
            float deadDistSqr ) const
```

Find the nearest point to a given P that lies outsid some dead zone.

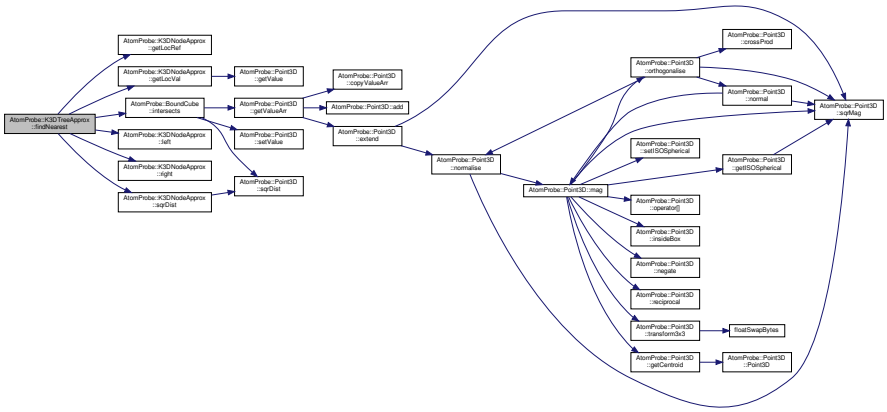
deadDistSqr can be used ot disallow exact matching on NN searching simply pass epsilon =std::numeric_↩ limits<float>::epsilon() (#include <limits>) Boundcube is the bounding box around the entire dataset

Definition at line 213 of file K3DTree-approx.cpp.

References ASSERT, AtomProbe::K3DNodeApprox::getLocRef(), AtomProbe::K3DNodeApprox::getLocVal(), AtomProbe::BoundCube::intersects(), AtomProbe::K3DNodeApprox::left(), AtomProbe::K3DNodeApprox::right(), and AtomProbe::K3DNodeApprox::sqrDist().

Referenced by findKNearest(), and testInexactKDTree().

Here is the call graph for this function:



6.22.3.6 kill()

```
void AtomProbe::K3DTreeApprox::kill ( )
```

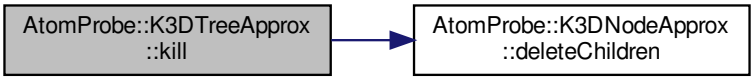
Destroy the tree contents.

Definition at line 115 of file K3DTree-approx.cpp.

References AtomProbe::K3DNodeApprox::deleteChildren().

Referenced by build(), buildByRef(), and ~K3DTreeApprox().

Here is the call graph for this function:



6.22.3.7 nodeCount()

```
unsigned int AtomProbe::K3DTreeApprox::nodeCount ( ) const  [inline]
```

Print the number of nodes stored in the tree.

Definition at line 159 of file K3DTree-approx.h.

The documentation for this class was generated from the following files:

- include/atomprobe/algorithm/K3DTree-approx.h
- src/algorithm/K3DTree-approx.cpp

6.23 AtomProbe::K3DTreeExact Class Reference

3D specific KD tree

```
#include <K3DTree-exact.h>
```

Public Member Functions

- K3DTreeExact ()
  KD Tree constructor. Tree is uninitialised at start.
- ~K3DTreeExact ()
  Cleans up tree, deallocates nodes.
- void resetPts (std::vector< Point3D > &pts, bool clear=true)
  Supply points to KD tree. Ouput vector will be erased if clear=true.
- void resetPts (std::vector< IonHit > &pts, bool clear=true)
  Supply points using IonHits to KD tree. Ouput vector will be erased if clear=true.
- bool build ()
  Build the KD tree using the previously supplied points.
- void getBoundCube (BoundCube &b)
  obtain the bounding rectangular prism volume for all elements in the KD tree
- void dump (std::ostream &, size_t depth=0, size_t offset=-1) const
  Textual output of tree. Tabs are used to separate different levels of the tree.

- size_t findNearestUntagged (const Point3D &queryPt, const BoundCube &b, bool tag=true)

  Find the nearest "untagged" point's internal index.
- void findUntaggedInRadius (const Point3D &queryPt, const BoundCube &b, float radius, std::vector< size_t > &result)

  Find untagged points within a given radius.
- void ptsInSphere (const Point3D &origin, float radius, std::vector< size_t > &pts) const
- const Point3D * getPt (size_t index) const
- const Point3D & getPtRef (size_t index) const
- void clearTags (std::vector< size_t > &tagsToClear)
- size_t getOrigIndex (size_t treeIndex) const
- void setCallback (bool(*cb)(void))
- void setProgressPointer (unsigned int *p)
- void clear ()
- void tag (size_t treeIndex, bool tagVal=true)
- void tag (const std::vector< size_t > &treeIndicies, bool tagVal=true)
- bool getTag (size_t treeIndex) const
- size_t size () const
- size_t rootIdx () const
- size_t tagCount () const
- void clearAllTags ()

6.23.1 Detailed Description

3D specific KD tree

Definition at line 54 of file K3DTree-exact.h.

6.23.2 Constructor & Destructor Documentation

6.23.2.1 K3DTreeExact()

```
K3DTreeExact::K3DTreeExact ( )
```

KD Tree constructor. Tree is uninitialised at start.

Note : must set progress pointer and callback

Definition at line 65 of file K3DTree-exact.cpp.

6.23.2.2 ~K3DTreeExact()

```
AtomProbe::K3DTreeExact::~K3DTreeExact ( )  [inline]
```

Cleans up tree, deallocates nodes.

Definition at line 85 of file K3DTree-exact.h.

6.23.3 Member Function Documentation

6.23.3.1 build()

```
bool K3DTreeExact::build ( )
```

Build the KD tree using the previously supplied points.

Builds a balanced KD tree from a list of points previously set by "resetPts". Callback and progress pointers must be set.

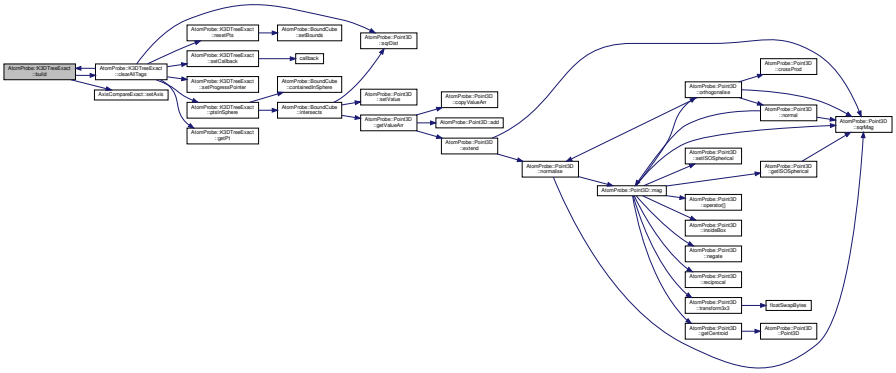
- Returns false if callback returns false;

Definition at line 162 of file K3DTree-exact.cpp.

References ASSERT, clearAllTags(), AtomProbe::PROGRESS_REDUCE, and AxisCompareExact::setAxis().

Referenced by clearAllTags(), kdExactFuzz(), and main().

Here is the call graph for this function:



6.23.3.2 clear()

```
void AtomProbe::K3DTreeExact::clear ( )  [inline]
```

Definition at line 149 of file K3DTree-exact.h.

6.23.3.3 clearAllTags()

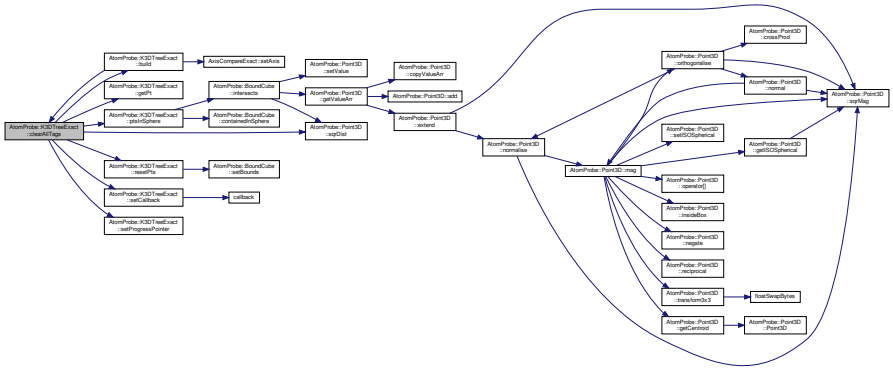
```
void K3DTreeExact::clearAllTags ( )
```

Definition at line 787 of file K3DTree-exact.cpp.

References ASSERT, build(), getPt(), ptsInSphere(), resetPts(), setCallback(), setProgressPointer(), AtomProbe↩
::Point3D::sqrDist(), and TEST.

Referenced by build().

Here is the call graph for this function:



6.23.3.4 clearTags()

```
void K3DTreeExact::clearTags (
            std::vector< size_t > & tagsToClear )
```

Definition at line 780 of file K3DTree-exact.cpp.

6.23.3.5 dump()

```
void K3DTreeExact::dump (
            std::ostream & strm,
            size_t depth = 0,
            size_t offset = -1 ) const
```

Textual output of tree. Tabs are used to separate different levels of the tree.

The output from this function can be quite large for even modest trees. Recommended for debugging only

Definition at line 333 of file K3DTree-exact.cpp.

6.23.3.6 findNearestUntagged()

```
size_t K3DTreeExact::findNearestUntagged (
            const Point3D & queryPt,
            const BoundCube & b,
            bool tag = true )
```

Find the nearest "untagged" point's internal index.

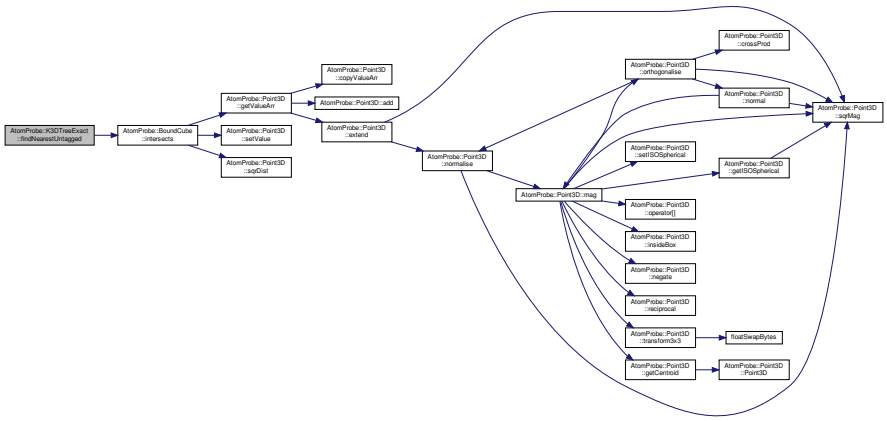
The point found is marked as "tagged" in the tree by default. -Returns -1 on failure (no untagged points), otherwise index of point

Definition at line 475 of file K3DTree-exact.cpp.

References ASSERT, and AtomProbe::BoundCube::intersects().

Referenced by findUntaggedInRadius(), and main().

Here is the call graph for this function:



6.23.3.7 findUntaggedInRadius()

```
void K3DTreeExact::findUntaggedInRadius (
            const Point3D & queryPt,
            const BoundCube & b,
            float radius,
            std::vector< size_t > & result )
```

Find untagged points within a given radius.

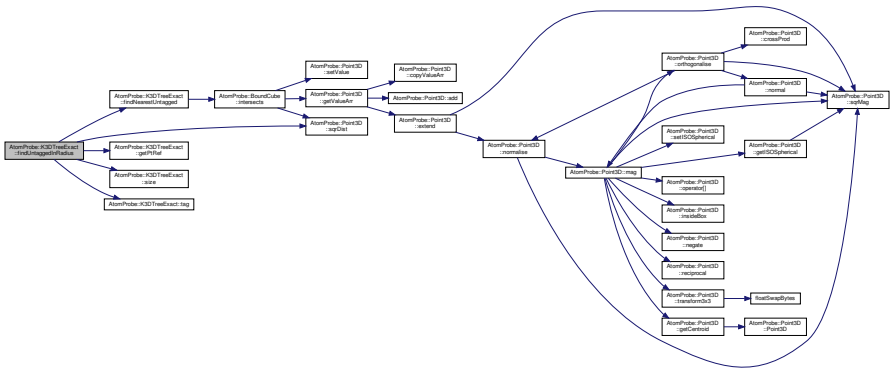
This is not thread safe - tags are read/written during operation

Definition at line 724 of file K3DTree-exact.cpp.

References ASSERT, findNearestUntagged(), getPtRef(), size(), AtomProbe::Point3D::sqrDist(), and tag().

Referenced by kdExactFuzz(), and main().

Here is the call graph for this function:



6.23.3.8 getBoundCube()

```
void K3DTreeExact::getBoundCube (
            BoundCube & b )
```

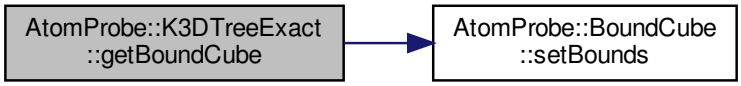
obtain the bounding rectangular prism volume for all elements in the KD tree

Definition at line 69 of file K3DTree-exact.cpp.

References ASSERT, and AtomProbe::BoundCube::setBounds().

Referenced by kdExactFuzz(), and main().

Here is the call graph for this function:



6.23.3.9 getOrigIndex()

```
size_t K3DTreeExact::getOrigIndex (
            size_t treeIndex ) const
```

Definition at line 87 of file K3DTree-exact.cpp.

References ASSERT.

Referenced by main().

6.23.3.10 getPt()

```
const Point3D * K3DTreeExact::getPt (
            size_t index ) const
```

Definition at line 75 of file K3DTree-exact.cpp.

References ASSERT.

Referenced by clearAllTags().

6.23.3.11 getPtRef()

```
const Point3D & K3DTreeExact::getPtRef (
            size_t index ) const
```

Definition at line 81 of file K3DTree-exact.cpp.

References ASSERT.

Referenced by findUntaggedInRadius(), AtomProbe::generate1DAxialDistHist(), AtomProbe::generate1DAxial↩DistHistSweep(), kdExactFuzz(), and main().

6.23.3.12 getTag()

```
bool K3DTreeExact::getTag (
            size_t treeIndex ) const
```

Definition at line 93 of file K3DTree-exact.cpp.

References ASSERT.

6.23.3.13 ptsInSphere()

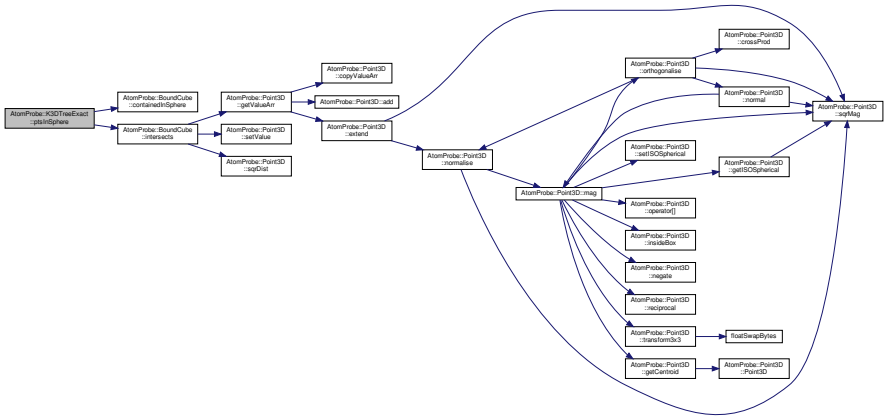
```
void K3DTreeExact::ptsInSphere (
            const Point3D & origin,
            float radius,
            std::vector< size_t > & pts ) const
```

Definition at line 379 of file K3DTree-exact.cpp.

References ASSERT, AtomProbe::BoundCube::containedInSphere(), and AtomProbe::BoundCube::intersects().

Referenced by clearAllTags(), AtomProbe::generate1DAxialDistHist(), AtomProbe::generate1DAxialDistHist↩Sweep(), kdExactFuzz(), and main().

Here is the call graph for this function:



6.23.3.14 resetPts() [1/2]

```
void K3DTreeExact::resetPts (
            std::vector< Point3D > & pts,
            bool clear = true )
```

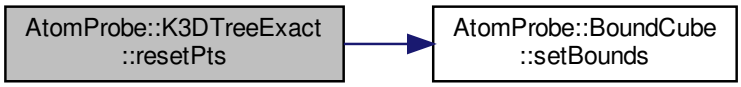
Supply points to KD tree. Ouput vector will be erased if clear=true.

Definition at line 119 of file K3DTree-exact.cpp.

References AtomProbe::BoundCube::setBounds().

Referenced by clearAllTags(), kdExactFuzz(), and main().

Here is the call graph for this function:



6.23.3.15 resetPts() [2/2]

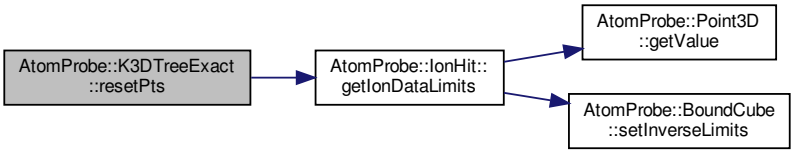
```
void K3DTreeExact::resetPts (
            std::vector< IonHit > & pts,
            bool clear = true )
```

Supply points using IonHits to KD tree. Ouput vector will be erased if clear=true.

Definition at line 138 of file K3DTree-exact.cpp.

References AtomProbe::IonHit::getIonDataLimits().

Here is the call graph for this function:



6.23.3.16 rootIdx()

```
size_t AtomProbe::K3DTreeExact::rootIdx ( ) const  [inline]
```

Definition at line 163 of file K3DTree-exact.h.

6.23.3.17 setCallback()

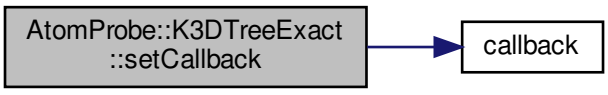
```
void AtomProbe::K3DTreeExact::setCallback (
            bool(*)(void) cb )  [inline]
```

Definition at line 143 of file K3DTree-exact.h.

References callback().

Referenced by clearAllTags(), kdExactFuzz(), and main().

Here is the call graph for this function:



6.23.3.18 setProgressPointer()

```
void AtomProbe::K3DTreeExact::setProgressPointer (
            unsigned int * p )  [inline]
```

Definition at line 146 of file K3DTree-exact.h.

Referenced by clearAllTags(), kdExactFuzz(), and main().

6.23.3.19 size()

```
size_t K3DTreeExact::size ( ) const
```

Definition at line 113 of file K3DTree-exact.cpp.

References ASSERT.

Referenced by findUntaggedInRadius(), AtomProbe::generate1DAxialDistHistSweep(), kdExactFuzz(), and main().

6.23.3.20 tag() [1/2]

```
void K3DTreeExact::tag (
            size_t treeIndex,
            bool tagVal = true )
```

Definition at line 99 of file K3DTree-exact.cpp.

References ASSERT.

Referenced by findUntaggedInRadius().

6.23.3.21 tag() [2/2]

```
void K3DTreeExact::tag (
            const std::vector< size_t > & treeIndicies,
            bool tagVal = true )
```

Definition at line 105 of file K3DTree-exact.cpp.

References ASSERT.

6.23.3.22 tagCount()

```
size_t K3DTreeExact::tagCount ( ) const
```

Definition at line 765 of file K3DTree-exact.cpp.

The documentation for this class was generated from the following files:

- include/atomprobe/algorithm/K3DTree-exact.h
- src/algorithm/K3DTree-exact.cpp

6.24 AtomProbe::LibVersion Class Reference

Class to hold the library version data.

```
#include <version.h>
```

Public Member Functions

- LibVersion ()
- void checkDebug ()

Static Public Member Functions

- static unsigned int getMajor ()
- static unsigned int getMinor ()
- static unsigned int getRevision ()
- static std::string getVersionStr ()

  Obtain the version of the program as a string.

6.24.1 Detailed Description

Class to hold the library version data.

Definition at line 19 of file version.h.

6.24.2 Constructor & Destructor Documentation

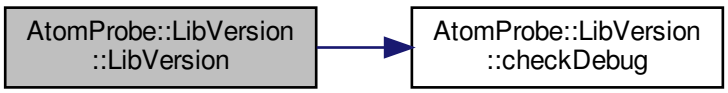
6.24.2.1 LibVersion()

```
AtomProbe::LibVersion::LibVersion ( )  [inline]
```

Definition at line 23 of file version.h.

References checkDebug(), LIBATOMPROBE_MAJOR, LIBATOMPROBE_MINOR, and LIBATOMPROBE_REV↩ ISION.

Here is the call graph for this function:



6.24.3 Member Function Documentation

6.24.3.1 checkDebug()

```
void AtomProbe::LibVersion::checkDebug ( )
```

Definition at line 39 of file atomprobe.cpp.

Referenced by LibVersion().

6.24.3.2 getMajor()

```
static unsigned int AtomProbe::LibVersion::getMajor ( )  [inline], [static]
```

Definition at line 37 of file version.h.

References LIBATOMPROBE_MAJOR.

Referenced by getVersionStr().

6.24.3.3 getMinor()

```
static unsigned int AtomProbe::LibVersion::getMinor ( )  [inline], [static]
```

Definition at line 38 of file version.h.

References LIBATOMPROBE_MINOR.

Referenced by getVersionStr().

6.24.3.4 getRevision()

```
static unsigned int AtomProbe::LibVersion::getRevision ( )  [inline], [static]
```

Definition at line 39 of file version.h.

References LIBATOMPROBE_REVISION.

Referenced by getVersionStr().

6.24.3.5 getVersionStr()

```
static std::string AtomProbe::LibVersion::getVersionStr ( )  [inline], [static]
```

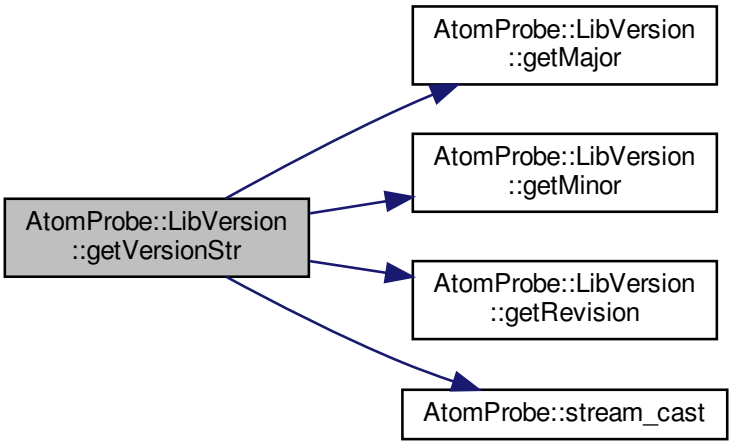
Obtain the version of the program as a string.

Definition at line 42 of file version.h.

References getMajor(), getMinor(), getRevision(), and AtomProbe::stream_cast().

Referenced by AtomProbe::MultiRange::write().

Here is the call graph for this function:



The documentation for this class was generated from the following files:

- include/atomprobe/helper/version.h
- src/atomprobe.cpp

6.25 AtomProbe::LINE Class Reference

`#include <mesh.h>`

Public Attributes

- unsigned int p [2]
- unsigned int physGroup

6.25.1 Detailed Description

Definition at line 66 of file mesh.h.

6.25.2 Member Data Documentation

6.25.2.1 p

`unsigned int AtomProbe::LINE::p[2]`

Definition at line 68 of file mesh.h.

Referenced by AtomProbe::Mesh::loadGmshMesh().

6.25.2.2 physGroup

`unsigned int AtomProbe::LINE::physGroup`

Definition at line 69 of file mesh.h.

Referenced by AtomProbe::Mesh::loadGmshMesh().

The documentation for this class was generated from the following file:

- include/atomprobe/primitives/mesh.h

6.26 AtomProbe::LinearFeedbackShiftReg Class Reference

This class implements a Linear Feedback Shift Register (in software)

`#include <lfsr.h>`

Public Member Functions

- size_t clock ()

  Get a value from the shift register, and advance.
- void setState (size_t newState)

  Set the internal lfsr state. Note 0 is the lock-up state.
- void setMaskPeriod (unsigned int newMask)

  Set the mask to use such that the period is 2^ n-1. 3 is minimum 60 is maximum.
- bool verifyTable (size_t maxLen=0)

  Check the validity of the table.

6.26.1 Detailed Description

This class implements a Linear Feedback Shift Register (in software)

This is a mathematical construct based upon polynomials over closed natural numbers (N mod p). This will generate a weakly random digit string, but with guaranteed no duplicates, using O(1) memory and O(n) calls. The no duplicate guarantee is weak-ish, only guaranteeing no repetition in the shift register for 2^n-1 iterations. n can be set by setMaskPeriod. After this the sequence will repeat

Definition at line 30 of file lfsr.h.

6.26.2 Member Function Documentation

6.26.2.1 clock()

```
size_t AtomProbe::LinearFeedbackShiftReg::clock ( )
```

Get a value from the shift register, and advance.

Definition at line 135 of file lfsr.cpp.

Referenced by AtomProbe::randomSelect(), and verifyTable().

6.26.2.2 setMaskPeriod()

```
void AtomProbe::LinearFeedbackShiftReg::setMaskPeriod (
            unsigned int newMask )
```

Set the mask to use such that the period is 2^n-1. 3 is minimum 60 is maximum.

Definition at line 81 of file lfsr.cpp.

References ASSERT.

Referenced by AtomProbe::randomSelect(), setState(), and verifyTable().

6.26.2.3 setState()

```
void AtomProbe::LinearFeedbackShiftReg::setState (
            size_t newState )  [inline]
```

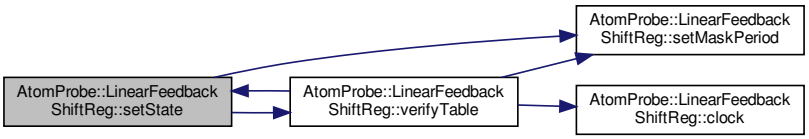
Set the internal lfsr state. Note 0 is the lock-up state.

Definition at line 39 of file lfsr.h.

References setMaskPeriod(), and verifyTable().

Referenced by AtomProbe::randomSelect(), and verifyTable().

Here is the call graph for this function:



6.26.2.4 verifyTable()

```
bool AtomProbe::LinearFeedbackShiftReg::verifyTable (
            size_t maxLen = 0 )
```

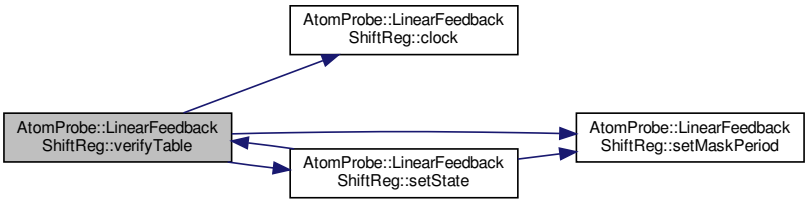
Check the validity of the table.

Definition at line 96 of file lfsr.cpp.

References ASSERT, clock(), AtomProbe::maximumLinearTable, setMaskPeriod(), and setState().

Referenced by setState().

Here is the call graph for this function:



The documentation for this class was generated from the following files:

- include/atomprobe/helper/maths/lfsr.h
- src/helper/maths/lfsr.cpp

6.27 AtomProbe::MassTool Class Reference

Class that brute-force solves the knapsack problem.

`#include <massTool.h>`

Static Public Member Functions

- static void bruteKnapsack (std::vector< Weight > &weights, float targetWeight, float tolerance, unsigned int maxObjects, std::vector< std::vector< Weight > > &solutions)

  Depth-First-Search based brute force solve the knapsack problem,.
- static void bruteKnapsack (std::vector< Weight > &weights, const std::vector< float > &targetWeight, float tolerance, unsigned int maxObjects, std::vector< std::vector< Weight > > &solutions)

  Multiple-target version of brute knapsack.

6.27.1 Detailed Description

Class that brute-force solves the knapsack problem.

Definition at line 43 of file massTool.h.

6.27.2 Member Function Documentation

6.27.2.1 bruteKnapsack() [1/2]

```
void MassTool::bruteKnapsack (
            std::vector< Weight > & weights,
            float targetWeight,
            float tolerance,
            unsigned int maxObjects,
            std::vector< std::vector< Weight > > & solutions )  [static]
```

Depth-First-Search based brute force solve the knapsack problem,.

Record all solutions within "tolerance" of the value "targetWeight". Solutions are reported as std::vectors of weights. All solutions are ensured unique.

"weights" vector should contain the masses of the input object. Note that the elemIdx and isotopeIdx values in the Weight structure are used for tracking purposes only. Elements may be removed from this input vector by MassTool.

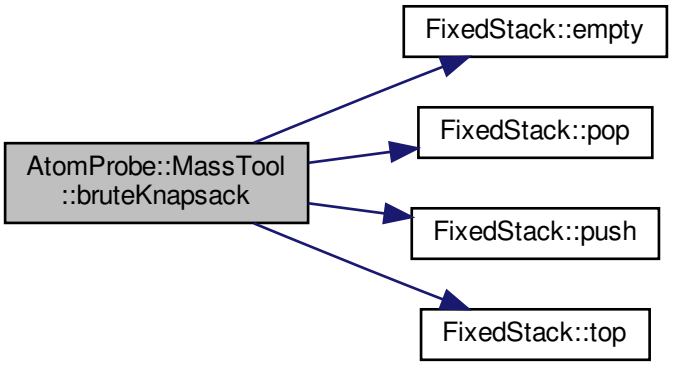
targetWeight is the total mass you want to find out what combination of weights matches. tolerance is the mass error from targetweight (+-tolerance) you are willing to accept maxObjects is the maximum nuber of weights you can combine to get the solution

Definition at line 117 of file massTool.cpp.

References WEIGHT_SEARCH_ENTRY::allowableWeights, WEIGHT_SEARCH_ENTRY::cumulativeWeight, WEIGHT_SEARCH_ENTRY::curWeights, FixedStack< T >::empty(), WEIGHT_SEARCH_ENTRY::offset, FixedStack< T >::pop(), FixedStack< T >::push(), and FixedStack< T >::top().

Referenced by main().

Here is the call graph for this function:



6.27.2.2 bruteKnapsack() [2/2]

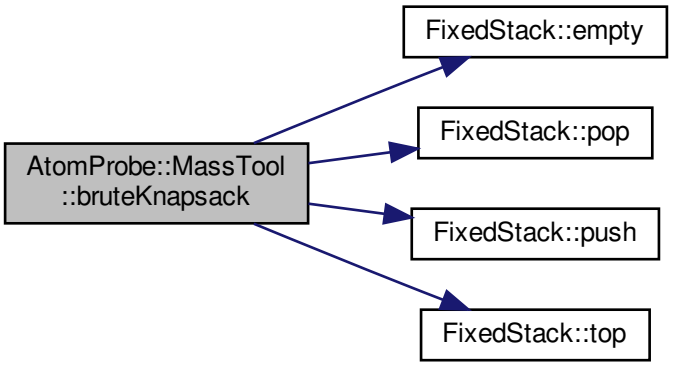
```
void MassTool::bruteKnapsack (
            std::vector< Weight > & weights,
            const std::vector< float > & targetWeight,
            float tolerance,
            unsigned int maxObjects,
            std::vector< std::vector< Weight > > & solutions )  [static]
```

Multiple-target version of brute knapsack.

Definition at line 220 of file massTool.cpp.

References WEIGHT_SEARCH_ENTRY::allowableWeights, WEIGHT_SEARCH_ENTRY::cumulativeWeight, WEIGHT_SEARCH_ENTRY::curWeights, FixedStack< T >::empty(), WEIGHT_SEARCH_ENTRY::offset, FixedStack< T >::pop(), FixedStack< T >::push(), TEST, and FixedStack< T >::top().

Here is the call graph for this function:



The documentation for this class was generated from the following files:

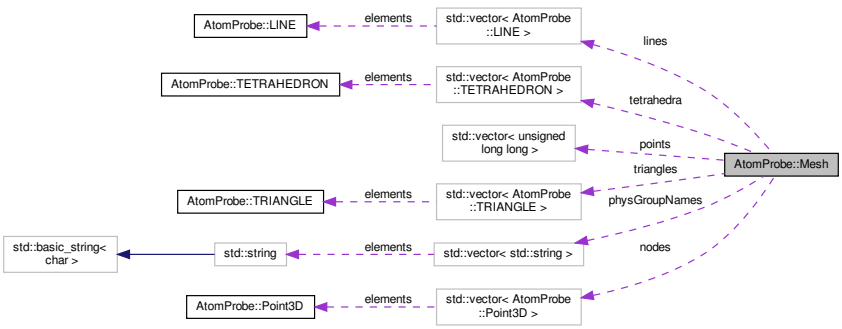
- include/atomprobe/algorithm/massTool.h
- src/algorithm/massTool.cpp

6.28 AtomProbe::Mesh Class Reference

Simple mesh class for storing and manipulating meshes consisting of 2 and 3D simplexes (triangles or tetrahedra)

```
#include <mesh.h>
```

Collaboration diagram for AtomProbe::Mesh:



Public Member Functions

- unsigned int loadGmshMesh (const char *meshfile, unsigned int &curLine, bool allowBadMeshes=true)
- unsigned int saveGmshMesh (const char *meshfile) const
- size_t elementCount () const
- void setTriangleMesh (const std::vector< float > &ptsA, const std::vector< float > &ptsB, const std::vector< float > &ptsC)
- void reassignGroups (unsigned int i)

  reassign the physical groups to a single number
- void removeDuplicateTris ()

  Remove exact duplicate triangles.
- void removeStrayTris ()
- void mergeDuplicateVertices (float tolerance)
- bool isSane (bool output=false, std::ostream &outStream=std::cerr) const

  Perform various sanity tests on mesh. Should return true if your mesh is sane.
- void getBounds (BoundCube &b) const

  Get the Axis aligned bounding box for this mesh.
- unsigned int countTriNodes () const

  Count the number of unique nodes shared by triangles.
- void translate ()

  Translate mesh around node centroid.
- void translate (const Point3D &origin)

  Translate mesh to specified position.
- void scale (const Point3D &origin, float scaleFactor)

  Scale the mesh around a specified origin.
- void scale (float scaleFactor)

  Scale the mesh around origin.
- void rotate (const Point3D &axis, const Point3D &origin, float angle)

  Rotate mesh.
- float getVolume () const

  Obtain the volume of the triangulated space.
- void resurface (unsigned int newPhys)

  place triangles over exposed tetrahedral faces
- void clear ()

  Clear the mesh.
- void getContainedNodes (const BoundCube &b, std::vector< size_t > &nodes) const

  Return all the nodes that are contained within specified bounding box.
- void getIntersectingPrimitives (std::vector< size_t > &searchNodes, std::vector< size_t > &lines, std::vector< size_t > &triangles, std::vector< size_t > &tetrahedra) const

  Return all primitives that are WHOLLY contained withing bounding box.
- unsigned int divideMeshSurface (float divisionAngle, unsigned int newPhysGroupStart, const std::vector< size_t > &physGroupsToSplit)
- void getCurPhysGroups (std::vector< std::pair< unsigned int, size_t > > &curPhys) const
- void erasePhysGroup (unsigned int group, unsigned int typeMask)
- unsigned int numDupVertices (float tolerance) const
- unsigned int numDupTris () const
- void print (std::ostream &o) const
- bool isOrientedCoherently () const
- void killOrphanNodes ()

  Kill specified orphan nodes within this dataset.
- void pointsInside (const std::vector< Point3D > &p, std::vector< bool > &meshResults, unsigned int &prog) const
- size_t getNearestTri (const Point3D &p, float &distance) const
- void getTriNormal (size_t tri, Point3D &normal) const

Public Attributes

- std::vector< Point3D > nodes

  Point storage for 3D Data (nodes/coords/vertices..)
- std::vector< std::string > physGroupNames

  Physical group storage.
- std::vector< TETRAHEDRON > tetrahedra

  Storage for node connectivity in tetrahedral form.
- std::vector< TRIANGLE > triangles

  Storage for node connectivity in triangle form (take in groups of 3)
- std::vector< LINE > lines

  Storage for line segments. .size()%2 should always==0.
- std::vector< unsigned long long > points

6.28.1 Detailed Description

Simple mesh class for storing and manipulating meshes consisting of 2 and 3D simplexes (triangles or tetrahedra)

Definition at line 73 of file mesh.h.

6.28.2 Member Function Documentation

6.28.2.1 clear()

```
void AtomProbe::Mesh::clear ( )
```

Clear the mesh.

Definition at line 922 of file mesh.cpp.

References lines, nodes, physGroupNames, points, tetrahedra, and triangles.

Referenced by setTriangleMesh().

6.28.2.2 countTriNodes()

```
unsigned int AtomProbe::Mesh::countTriNodes ( ) const
```

Count the number of unique nodes shared by triangles.

Definition at line 1336 of file mesh.cpp.

References triangles.

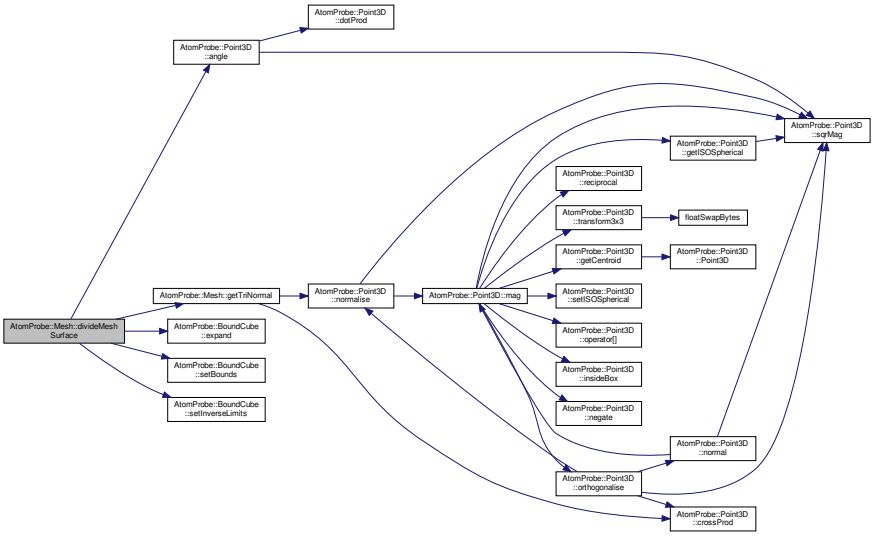
6.28.2.3 divideMeshSurface()

```
unsigned int AtomProbe::Mesh::divideMeshSurface (
            float divisionAngle,
            unsigned int newPhysGroupStart,
            const std::vector< size_t > & physGroupsToSplit )
```

Definition at line 1583 of file mesh.cpp.

References AtomProbe::Point3D::angle(), ASSERT, AtomProbe::BoundCube::expand(), getTriNormal(), nodes, AtomProbe::BoundCube::setBounds(), AtomProbe::BoundCube::setInverseLimits(), and triangles.

Here is the call graph for this function:



6.28.2.4 elementCount()

```
size_t AtomProbe::Mesh::elementCount ( ) const
```

Definition at line 1963 of file mesh.cpp.

References lines, points, tetrahedra, and triangles.

Referenced by loadGmshMesh().

6.28.2.5 erasePhysGroup()

```
void AtomProbe::Mesh::erasePhysGroup (
            unsigned int group,
            unsigned int typeMask )
```

Definition at line 1866 of file mesh.cpp.

References AtomProbe::ELEMENT_LINE, AtomProbe::ELEMENT_TETRAHEDRON, AtomProbe::ELEMENT_T↩ RIANGLE, tetrahedra, and triangles.

6.28.2.6 getBounds()

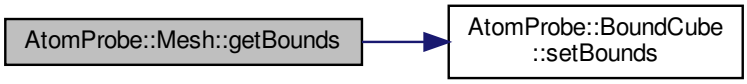
```
void AtomProbe::Mesh::getBounds (
            BoundCube & b ) const
```

Get the Axis aligned bounding box for this mesh.

Definition at line 1518 of file mesh.cpp.

References ASSERT, nodes, AtomProbe::BoundCube::setBounds(), and triangles.

Here is the call graph for this function:



6.28.2.7 getContainedNodes()

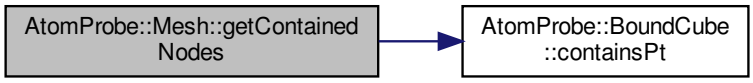
```
void AtomProbe::Mesh::getContainedNodes (
            const BoundCube & b,
            std::vector< size_t > & nodes ) const
```

Return all the nodes that are contained within specified bounding box.

Definition at line 1747 of file mesh.cpp.

References ASSERT, AtomProbe::BoundCube::containsPt(), and nodes.

Here is the call graph for this function:



6.28.2.8 getCurPhysGroups()

```
void AtomProbe::Mesh::getCurPhysGroups (
            std::vector< std::pair< unsigned int, size_t > > & curPhys ) const
```

Definition at line 1815 of file mesh.cpp.

References tetrahedra, and triangles.

6.28.2.9 getIntersectingPrimitives()

```
void AtomProbe::Mesh::getIntersectingPrimitives (
            std::vector< size_t > & searchNodes,
            std::vector< size_t > & lines,
            std::vector< size_t > & triangles,
            std::vector< size_t > & tetrahedra ) const
```

Return all primitives that are WHOLLY contained withing bounding box.

Definition at line 1758 of file mesh.cpp.

References ASSERT, lines, tetrahedra, and triangles.

6.28.2.10 getNearestTri()

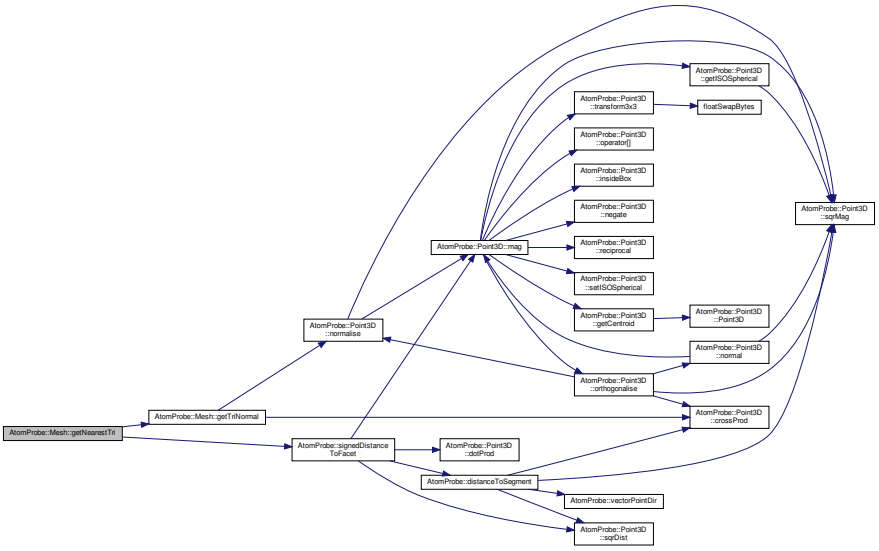
```
size_t AtomProbe::Mesh::getNearestTri (
            const Point3D & p,
            float & distance ) const
```

Definition at line 2105 of file mesh.cpp.

References getTriNormal(), nodes, AtomProbe::signedDistanceToFacet(), and triangles.

Referenced by AtomProbe::TRIANGLE::edgesMismatch(), and main().

Here is the call graph for this function:



6.28.2.11 getTriNormal()

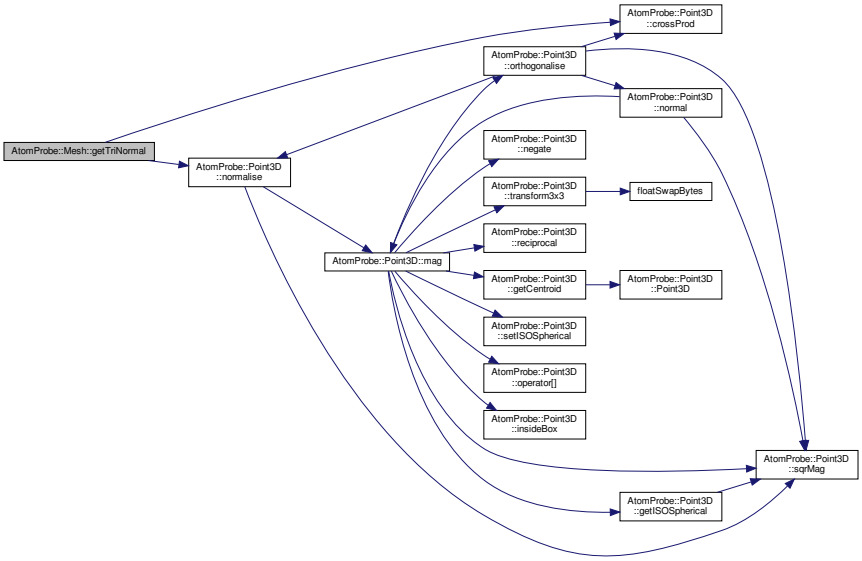
```
void AtomProbe::Mesh::getTriNormal (
            size_t tri,
            Point3D & normal ) const
```

Definition at line 1739 of file mesh.cpp.

References ASSERT, AtomProbe::Point3D::crossProd(), nodes, AtomProbe::Point3D::normalise(), and triangles.

Referenced by divideMeshSurface(), and getNearestTri().

Here is the call graph for this function:



6.28.2.12 getVolume()

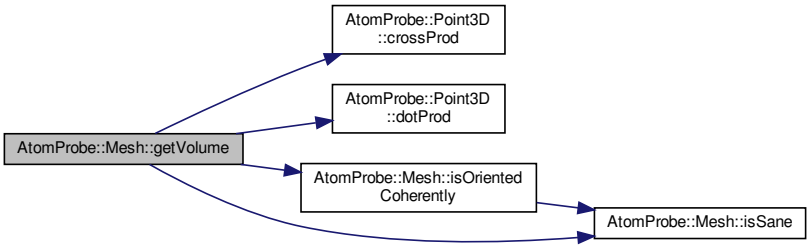
```
float AtomProbe::Mesh::getVolume ( ) const
```

Obtain the volume of the triangulated space.

Definition at line 1932 of file mesh.cpp.

References ASSERT, AtomProbe::Point3D::crossProd(), AtomProbe::Point3D::dotProd(), isOrientedCoherently(), isSane(), nodes, AtomProbe::TRIANGLE::p, and triangles.

Here is the call graph for this function:



6.28.2.13 isOrientedCoherently()

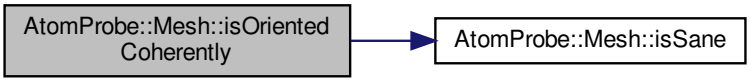
```
bool AtomProbe::Mesh::isOrientedCoherently ( ) const
```

Definition at line 2131 of file mesh.cpp.

References ASSERT, isSane(), and triangles.

Referenced by AtomProbe::TRIANGLE::edgesMismatch(), getVolume(), and pointsInside().

Here is the call graph for this function:



6.28.2.14 isSane()

```
bool AtomProbe::Mesh::isSane (
            bool output = false,
            std::ostream & outStream = std::cerr ) const
```

Perform various sanity tests on mesh. Should return true if your mesh is sane.

Definition at line 572 of file mesh.cpp.

References lines, nodes, tetrahedra, and triangles.

Referenced by AtomProbe::TRIANGLE::edgesMismatch(), getVolume(), isOrientedCoherently(), killOrphan↩ Nodes(), loadGmshMesh(), mergeDuplicateVertices(), numDupTris(), print(), removeDuplicateTris(), saveGmsh↩ Mesh(), and setTriangleMesh().

6.28.2.15 killOrphanNodes()

```
void AtomProbe::Mesh::killOrphanNodes ( )
```

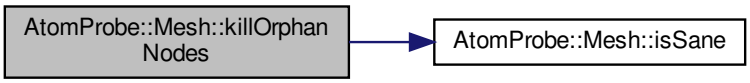
Kill specified orphan nodes within this dataset.

Definition at line 820 of file mesh.cpp.

References ASSERT, isSane(), lines, nodes, points, tetrahedra, and triangles.

Referenced by mergeDuplicateVertices(), and print().

Here is the call graph for this function:



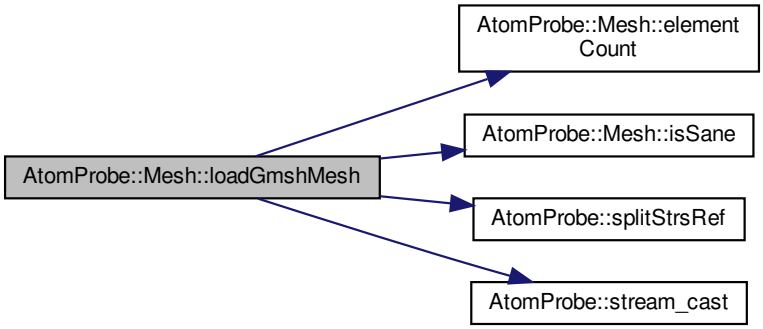
6.28.2.16 loadGmshMesh()

```
unsigned int AtomProbe::Mesh::loadGmshMesh (
            const char * meshfile,
            unsigned int & curLine,
            bool allowBadMeshes = true )
```

Definition at line 1025 of file mesh.cpp.

References ARRAYSIZE, AtomProbe::ELEM_FOUR_NODE_TETRAHEDRON, AtomProbe::ELEM_SINGLE_N↩ ODE_POINT, AtomProbe::ELEM_THREE_NODE_TRIANGLE, AtomProbe::ELEM_TWO_NODE_LINE, element↩ Count(), isSane(), lines, AtomProbe::MESH_LOAD_BAD_ELEMENTCOUNT, AtomProbe::MESH_LOAD_B↩ AD_NODECOUNT, AtomProbe::MESH_LOAD_ENUM_END, AtomProbe::MESH_LOAD_IS_INSANE, nodes, AtomProbe::TETRAHEDRON::p, AtomProbe::TRIANGLE::p, AtomProbe::LINE::p, AtomProbe::TETRAHEDR↩ ON::physGroup, AtomProbe::TRIANGLE::physGroup, AtomProbe::LINE::physGroup, points, AtomProbe::split↩ StrsRef(), AtomProbe::stream_cast(), tetrahedra, and triangles.

Here is the call graph for this function:



6.28.2.17 mergeDuplicateVertices()

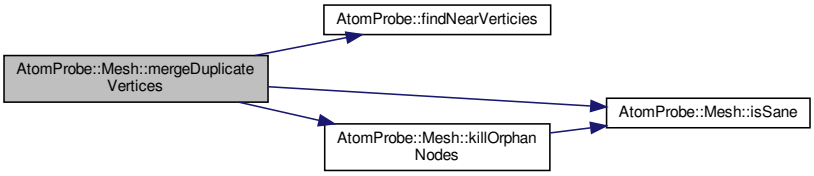
```
void AtomProbe::Mesh::mergeDuplicateVertices (
            float tolerance )
```

Definition at line 738 of file mesh.cpp.

References ASSERT, AtomProbe::findNearVerticies(), isSane(), killOrphanNodes(), lines, nodes, points, tetrahedra, and triangles.

Referenced by main().

Here is the call graph for this function:



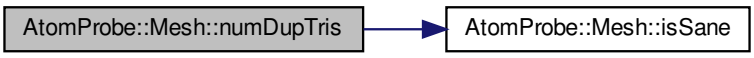
6.28.2.18 numDupTris()

```
unsigned int AtomProbe::Mesh::numDupTris ( ) const
```

Definition at line 854 of file mesh.cpp.

References ASSERT, isSane(), nodes, and triangles.

Here is the call graph for this function:



6.28.2.19 numDupVertices()

```
unsigned int AtomProbe::Mesh::numDupVertices (
            float tolerance ) const
```

Definition at line 897 of file mesh.cpp.

References nodes.

6.28.2.20 pointsInside()

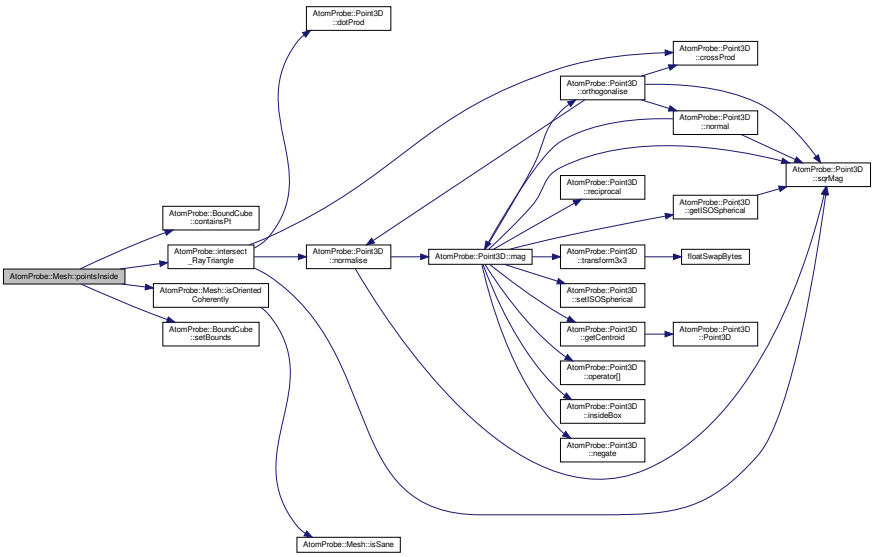
```
void AtomProbe::Mesh::pointsInside (
            const std::vector< Point3D > & p,
            std::vector< bool > & meshResults,
            unsigned int & prog ) const
```

Definition at line 1975 of file mesh.cpp.

References ASSERT, AtomProbe::BoundCube::containsPt(), AtomProbe::intersect_RayTriangle(), isOriented↩Coherently(), nodes, AtomProbe::PROGRESS_REDUCE, AtomProbe::BoundCube::setBounds(), tetrahedra, and triangles.

Referenced by main().

Here is the call graph for this function:



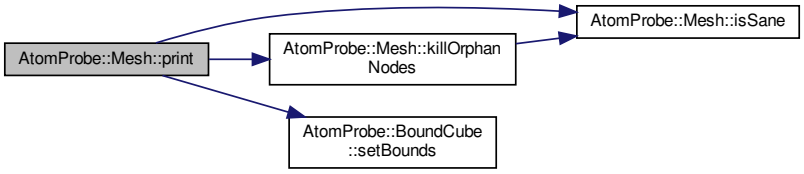
6.28.2.21 print()

```
void AtomProbe::Mesh::print (
            std::ostream & o ) const
```

Definition at line 445 of file mesh.cpp.

References ASSERT, isSane(), killOrphanNodes(), lines, nodes, AtomProbe::TRIANGLE::p, points, AtomProbe::↩ BoundCube::setBounds(), tetrahedra, and triangles.

Here is the call graph for this function:



6.28.2.22 reassignGroups()

```
void AtomProbe::Mesh::reassignGroups (
            unsigned int i )
```

reassign the physical groups to a single number

Definition at line 1361 of file mesh.cpp.

References lines, tetrahedra, and triangles.

6.28.2.23 removeDuplicateTris()

```
void AtomProbe::Mesh::removeDuplicateTris ( )
```

Remove exact duplicate triangles.

Definition at line 691 of file mesh.cpp.

References ASSERT, isSane(), nodes, and triangles.

Here is the call graph for this function:

6.28.2.24 removeStrayTris()

```
void AtomProbe::Mesh::removeStrayTris ( )
```

6.28.2.25 resurface()

```
void AtomProbe::Mesh::resurface (
            unsigned int newPhys )
```

place triangles over exposed tetrahedral faces

6.28.2.26 rotate()

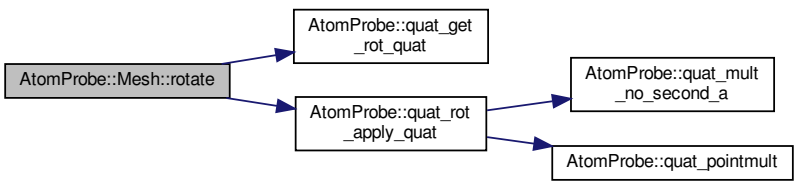
```
void AtomProbe::Mesh::rotate (
            const Point3D & axis,
            const Point3D & origin,
            float angle )
```

Rotate mesh.

Definition at line 1439 of file mesh.cpp.

References AtomProbe::Point3f::fx, AtomProbe::Point3f::fy, AtomProbe::Point3f::fz, nodes, AtomProbe::quat_get↩
_rot_quat(), and AtomProbe::quat_rot_apply_quat().

Here is the call graph for this function:



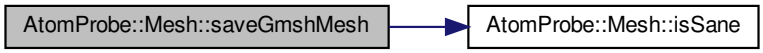
6.28.2.27 saveGmshMesh()

```
unsigned int AtomProbe::Mesh::saveGmshMesh (
            const char * meshfile ) const
```

Definition at line 1376 of file mesh.cpp.

References ASSERT, AtomProbe::ELEM_FOUR_NODE_TETRAHEDRON, AtomProbe::ELEM_SINGLE_NODE↩
_POINT, AtomProbe::ELEM_THREE_NODE_TRIANGLE, AtomProbe::ELEM_TWO_NODE_LINE, isSane(), lines, nodes, points, tetrahedra, and triangles.

Here is the call graph for this function:



6.28.2.28 scale() [1/2]

```
void AtomProbe::Mesh::scale (
            const Point3D & origin,
            float scaleFactor )
```

Scale the mesh around a specified origin.

Definition at line 1500 of file mesh.cpp.

References nodes.

6.28.2.29 scale() [2/2]

```
void AtomProbe::Mesh::scale (
            float scaleFactor )
```

Scale the mesh around origin.

Definition at line 1511 of file mesh.cpp.

References nodes.

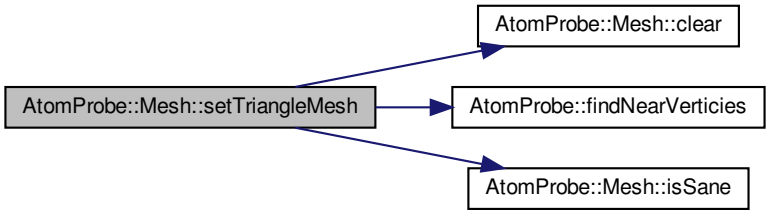
6.28.2.30 setTriangleMesh()

```
void AtomProbe::Mesh::setTriangleMesh (
            const std::vector< float > & ptsA,
            const std::vector< float > & ptsB,
            const std::vector< float > & ptsC )
```

Definition at line 932 of file mesh.cpp.

References ASSERT, clear(), AtomProbe::findNearVerticies(), isSane(), nodes, AtomProbe::TRIANGLE::p, and triangles.

Here is the call graph for this function:



6.28.2.31 translate() [1/2]

```
void AtomProbe::Mesh::translate ( )
```

Translate mesh around node centroid.

Definition at line 1482 of file mesh.cpp.

References nodes.

6.28.2.32 translate() [2/2]

```
void AtomProbe::Mesh::translate (
            const Point3D & origin )
```

Translate mesh to specified position.

Definition at line 1493 of file mesh.cpp.

References nodes.

6.28.3 Member Data Documentation

6.28.3.1 lines

```
std::vector<LINE> AtomProbe::Mesh::lines
```

Storage for line segments. .size()%2 should always==0.

Definition at line 118 of file mesh.h.

Referenced by clear(), elementCount(), getIntersectingPrimitives(), isSane(), killOrphanNodes(), loadGmshMesh(), mergeDuplicateVertices(), print(), reassignGroups(), and saveGmshMesh().

6.28.3.2 nodes

```
std::vector<Point3D> AtomProbe::Mesh::nodes
```

Point storage for 3D Data (nodes/coords/vertices..)

Definition at line 105 of file mesh.h.

Referenced by clear(), divideMeshSurface(), AtomProbe::TRIANGLE::edgesMismatch(), getBounds(), getContainedNodes(), getNearestTri(), getTriNormal(), getVolume(), isSane(), killOrphanNodes(), loadGmshMesh(), main(), mergeDuplicateVertices(), numDupTris(), numDupVertices(), pointsInside(), print(), removeDuplicateTris(), rotate(), saveGmshMesh(), scale(), setTriangleMesh(), and translate().

6.28.3.3 physGroupNames

```
std::vector<std::string> AtomProbe::Mesh::physGroupNames
```

Physical group storage.

Definition at line 108 of file mesh.h.

Referenced by clear().

6.28.3.4 points

```
std::vector<unsigned long long> AtomProbe::Mesh::points
```

Definition at line 120 of file mesh.h.

Referenced by clear(), elementCount(), killOrphanNodes(), loadGmshMesh(), mergeDuplicateVertices(), print(), and saveGmshMesh().

6.28.3.5 tetrahedra

```
std::vector<TETRAHEDRON> AtomProbe::Mesh::tetrahedra
```

Storage for node connectivity in tetrahedral form.

Definition at line 113 of file mesh.h.

Referenced by clear(), elementCount(), erasePhysGroup(), getCurPhysGroups(), getIntersectingPrimitives(), isSane(), killOrphanNodes(), loadGmshMesh(), mergeDuplicateVertices(), pointsInside(), print(), reassignGroups(), and saveGmshMesh().

6.28.3.6 triangles

```
std::vector<TRIANGLE> AtomProbe::Mesh::triangles
```

Storage for node connectivity in triangle form (take in groups of 3)

Definition at line 116 of file mesh.h.

Referenced by clear(), countTriNodes(), divideMeshSurface(), AtomProbe::TRIANGLE::edgesMismatch(), elementCount(), erasePhysGroup(), getBounds(), getCurPhysGroups(), getIntersectingPrimitives(), getNearestTri(), getTriNormal(), getVolume(), isOrientedCoherently(), isSane(), killOrphanNodes(), loadGmshMesh(), main(), mergeDuplicateVertices(), numDupTris(), pointsInside(), print(), reassignGroups(), removeDuplicateTris(), saveGmshMesh(), and setTriangleMesh().

The documentation for this class was generated from the following files:

- include/atomprobe/primitives/mesh.h
- src/primitives/mesh.cpp

6.29 AtomProbe::MILLER_TRIPLET Class Reference

```
#include <millerIndex.h>
```

Public Member Functions

- MILLER_TRIPLET (int a, int b, int c)
- int h () const
- int k () const
- int l () const
- bool operator== (const MILLER_TRIPLET &m) const
- void simplify ()
- Point3D tripletToNormal (unsigned int h, unsigned int k, unsigned int l)
- Point3D tripletToNormal (const MILLER_TRIPLET &m)

6.29.1 Detailed Description

Definition at line 20 of file millerIndex.h.

6.29.2 Constructor & Destructor Documentation

6.29.2.1 MILLER_TRIPLET()

```
AtomProbe::MILLER_TRIPLET::MILLER_TRIPLET (
            int a,
            int b,
            int c )
```

Definition at line 39 of file millerIndex.cpp.

Referenced by operator==().

6.29.3 Member Function Documentation

6.29.3.1 h()

```
int AtomProbe::MILLER_TRIPLET::h ( ) const
```

Definition at line 46 of file millerIndex.cpp.

6.29.3.2 k()

```
int AtomProbe::MILLER_TRIPLET::k ( ) const
```

Definition at line 51 of file millerIndex.cpp.

6.29.3.3 l()

```
int AtomProbe::MILLER_TRIPLET::l ( ) const
```

Definition at line 56 of file millerIndex.cpp.

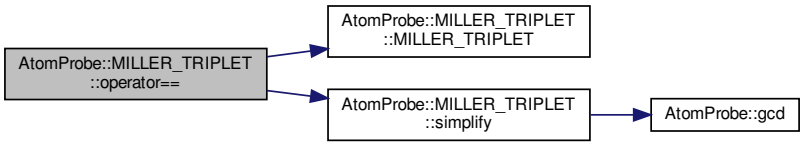
6.29.3.4 operator==()

```
bool AtomProbe::MILLER_TRIPLET::operator== (
            const MILLER_TRIPLET & m ) const
```

Definition at line 72 of file millerIndex.cpp.

References MILLER_TRIPLET(), simplify(), and TEST.

Here is the call graph for this function:



6.29.3.5 simplify()

```
void AtomProbe::MILLER_TRIPLET::simplify ( )
```

Definition at line 61 of file millerIndex.cpp.

References AtomProbe::gcd().

Referenced by operator==().

Here is the call graph for this function:

6.29.3.6 tripletToNormal() [1/2]

```
Point3D AtomProbe::MILLER_TRIPLET::tripletToNormal (
            unsigned int h,
            unsigned int k,
            unsigned int l )
```

6.29.3.7 tripletToNormal() [2/2]

```
Point3D AtomProbe::MILLER_TRIPLET::tripletToNormal (
            const MILLER_TRIPLET & m )
```

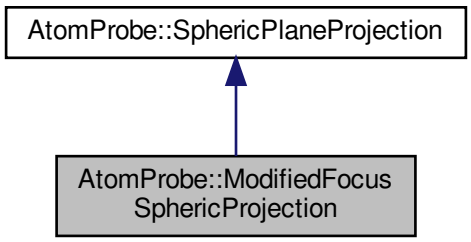
The documentation for this class was generated from the following files:

- include/atomprobe/latticeplanes/millerIndex.h
- src/lattice/millerIndex.cpp

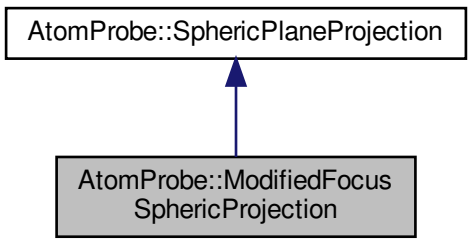
6.30 AtomProbe::ModifiedFocusSphericProjection Class Reference

```
#include <projection.h>
```

Inheritance diagram for AtomProbe::ModifiedFocusSphericProjection:



Collaboration diagram for AtomProbe::ModifiedFocusSphericProjection:



Public Member Functions

- ModifiedFocusSphericProjection (float focus)

  Create a Spheric projection, with a focal point that is moved behind the sphere.
- void setFocus (float focus)

  Set the focus position of the sphere. 0= sphere centre, 1=sphere end, >1 is outside sphere.
- float etaToTheta (float eta) const

  Convert the spherical angle to an azimuthal angle. See docs/figures for examples.
- float thetaToEta (float theta) const

  Convert azimuthal angle to spherical. See etaToTheta for description.
- virtual bool toAzimuthal (float fx, float fy, float &theta, float &phi) const

  Convert from plane coordinates to stereographic (NOT SPHERICAL) coords.
- virtual bool toPlanar (float theta, float phi, float &fx, float &fy) const

  Convert from stereographic (NOT SPHERICAL) coordinates to plane.
- virtual void scaleDown (float flightLength, float detX, float detY, float &scaledX, float &scaledY) const

  Convert from actual detector postion (eg. mm) and flight path to scaled-down transform.
- virtual void scaleUp (float flightLength, float scaledX, float scaledY, float &realX, float &realY) const

  Convert from scaled-down to actual dimension.
- float getMaxFOV () const

  Obtain angle spherical angle, eta, (i.e. angle from point of sphere, sphere centre and x axis) of the line that is tangent to the sphere.
- float getFOVRadius (float eta) const

  Obtain the radius in the XY plane of the sphere-angle (eta) that gives us a given FOV.

6.30.1 Detailed Description

Definition at line 95 of file projection.h.

6.30.2 Constructor & Destructor Documentation

6.30.2.1 ModifiedFocusSphericProjection()

```
AtomProbe::ModifiedFocusSphericProjection::ModifiedFocusSphericProjection (
            float focus )
```

Create a Spheric projection, with a focal point that is moved behind the sphere.

Definition at line 202 of file projection.cpp.

6.30.3 Member Function Documentation

6.30.3.1 etaToTheta()

```
float AtomProbe::ModifiedFocusSphericProjection::etaToTheta (
            float eta ) const
```

Convert the spherical angle to an azimuthal angle. See docs/figures for examples.

Definition at line 216 of file projection.cpp.

References ASSERT, and AtomProbe::SphericProjectionParams::focusDist.

Referenced by main(), and scaleUp().

6.30.3.2 getFOVRadius()

```
float AtomProbe::ModifiedFocusSphericProjection::getFOVRadius (
            float eta ) const
```

Obtain the radius in the XY plane of the sphere-angle (eta) that gives us a given FOV.

Definition at line 288 of file projection.cpp.

References AtomProbe::SphericProjectionParams::focusDist, and AtomProbe::SphericProjectionParams::theta.

6.30.3.3 getMaxFOV()

```
float AtomProbe::ModifiedFocusSphericProjection::getMaxFOV ( ) const
```

Obtain angle spherical angle, eta, (i.e. angle from point of sphere, sphere centre and x axis) of the line that is tangent to the sphere.

Beyond this there is no intersection, and no solution.

Definition at line 270 of file projection.cpp.

References AtomProbe::SphericProjectionParams::focusDist.

Referenced by main(), and scaleUp().

6.30.3.4 scaleDown()

```
void AtomProbe::ModifiedFocusSphericProjection::scaleDown (
            float flightLength,
            float detX,
            float detY,
            float & scaledX,
            float & scaledY ) const  [virtual]
```

Convert from actual detector postion (eg. mm) and flight path to scaled-down transform.

Implements AtomProbe::SphericPlaneProjection.

Definition at line 339 of file projection.cpp.

References ASSERT, and AtomProbe::SphericProjectionParams::focusDist.

6.30.3.5 scaleUp()

```
void AtomProbe::ModifiedFocusSphericProjection::scaleUp (
            float flightLength,
            float scaledX,
            float scaledY,
            float & realX,
            float & realY ) const  [virtual]
```

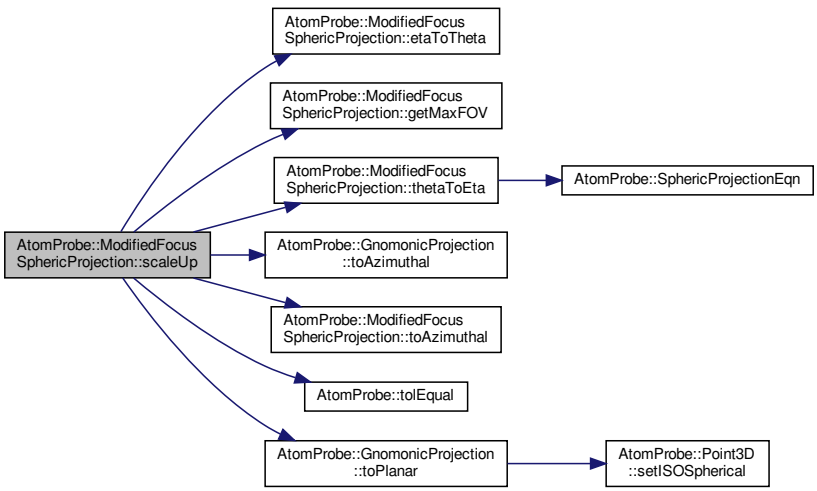
Convert from scaled-down to actual dimension.

Implements AtomProbe::SphericPlaneProjection.

Definition at line 350 of file projection.cpp.

References ASSERT, etaToTheta(), AtomProbe::SphericProjectionParams::focusDist, getMaxFOV(), M_PI, T↩EST, AtomProbe::SphericProjectionParams::theta, thetaToEta(), AtomProbe::GnomonicProjection::toAzimuthal(), toAzimuthal(), AtomProbe::tolEqual(), and AtomProbe::GnomonicProjection::toPlanar().

Here is the call graph for this function:



6.30.3.6 setFocus()

```
void AtomProbe::ModifiedFocusSphericProjection::setFocus (
            float focus )
```

Set the focus position of the sphere. 0= sphere centre, 1=sphere end, >1 is outside sphere.

Definition at line 207 of file projection.cpp.

References AtomProbe::SphericProjectionParams::focusDist.

6.30.3.7 thetaToEta()

```
float AtomProbe::ModifiedFocusSphericProjection::thetaToEta (
            float theta ) const
```

Convert azimuthal angle to spherical. See etaToTheta for description.

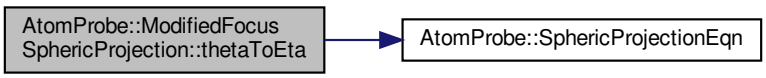
input range is limited to [0,getMaxFOV()]

Definition at line 225 of file projection.cpp.

References AtomProbe::SphericProjectionParams::focusDist, M_PI, AtomProbe::SphericProjectionEqn(), and AtomProbe::SphericProjectionParams::theta.

Referenced by scaleUp().

Here is the call graph for this function:



6.30.3.8 toAzimuthal()

```
bool AtomProbe::ModifiedFocusSphericProjection::toAzimuthal (
            float fx,
            float fy,
            float & theta,
            float & phi ) const  [virtual]
```

Convert from plane coordinates to stereographic (NOT SPHERICAL) coords.

Implements AtomProbe::SphericPlaneProjection.

Definition at line 324 of file projection.cpp.

References AtomProbe::SphericProjectionParams::focusDist.

Referenced by scaleUp().

6.30.3.9 toPlanar()

```
bool AtomProbe::ModifiedFocusSphericProjection::toPlanar (
            float theta,
            float phi,
            float & fx,
            float & fy ) const  [virtual]
```

Convert from stereographic (NOT SPHERICAL) coordinates to plane.

Implements AtomProbe::SphericPlaneProjection.

Definition at line 310 of file projection.cpp.

Referenced by main().

The documentation for this class was generated from the following files:

- include/atomprobe/projection/projection.h
- src/projection/projection.cpp

6.31 AtomProbe::MultiRange Class Reference

Data storage and retrieval class for "ranging" a spectra, where overlapping ranges are permitted.

```
#include <multiRange.h>
```

Public Member Functions

- MultiRange ()
- MultiRange (const RangeFile &rng, const AbundanceData &natData)

  Do our best to intialise from a rangefile.
- unsigned int addIon (const std::set< SIMPLE_SPECIES > &molecule, const std::string &name, const RGBf &ionCol)

  Add the ion to the database returns ion ID if successful, -1 otherwise.
- unsigned int addIon (const SIMPLE_SPECIES &molecule, const std::string &name, const RGBf &ionCol)

  Add a simple ion to the database - returns ion ID if successful, -1 otherwise.
- unsigned int addRange (float start, float end, unsigned int ionID)

  Add a range to the rangefile. Returns ID number of added range if adding successful, (unsigned int)-1 otherwise.
- unsigned int addRange (const std::pair< float, float > &rng, unsigned int ionID)

  Convenience wrapper for addRange(float,float, unsigned int)
- void setRangeGroups (const std::vector< unsigned int > &groups)

  Set the groupings for the ranges.
- bool write (const char *fileName, unsigned int format=MULTIRANGE_FORMAT_XML) const

  Save the structure to a file. format specifies output file format type.
- bool open (const char *fileName, unsigned int format=-1)

  read the contents of the file into class
- unsigned int getIonID (unsigned int rangeId) const

  Get the ion's ID from a specified mass.
- void setIonID (unsigned int range, unsigned int newIonId)

Set the ion ID for a given range.

- RGBf getColour (unsigned int ionID) const

  Obtain the colour for a given ion.
- void setColour (unsigned int, const RGBf &r)

  Set the colour using the ion ID.
- std::string getErrString () const

  Retrieve the human-readable error associated with the current range file state.
- std::string getIonName (unsigned int ionID) const

  Get the name of a specified ionID.
- unsigned int getNumRanges () const

  Get the number of unique ranges.
- unsigned int getNumRanges (unsigned int ionID) const

  Get the number of ranges for a given ion ID.
- unsigned int getNumIons () const

  Get the number of unique ions.
- std::set< SIMPLE_SPECIES > getMolecule (unsigned int ionID) const

  Return the molecule that is associated with this ion.
- std::pair< float, float > getRange (unsigned int rangeID) const

  Retrieve the start and end of a given range as a pair(start,end)
- std::vector< unsigned int > getRanges (float mass) const

  Retrieve all of the ranges that specify the given mass.
- std::vector< unsigned int > getRangeIdsFromIon (unsigned int ionId) const

  Retrieve all the ranges associated with a given ion.
- bool isRanged (float mass) const

  Returns true if a specified mass is ranged.
- bool isRanged (const IonHit &) const

  Returns true if an ion is ranged.
- void range (std::vector< IonHit > &ionHits) const

  Clips out ions that are not inside the rangefile's ranges.
- bool isSelfConsistent () const

  Check to see if data structure is internally consistent.
- void clear ()

  Erase the contents of the rangefile.
- void flattenToMassAxis (std::vector< FLATTENED_RANGE > &ionMapping) const

  Obtain a projection onto the mass axis of ranges that do not touch one another.
- void splitOverlapping (std::vector< MultiRange > &decomposedRanges) const
- void copyDataFromRange (const MultiRange &src, unsigned int srcRngId)

  Copy range from a different multirange into this one, including all dependant data.

6.31.1 Detailed Description

Data storage and retrieval class for "ranging" a spectra, where overlapping ranges are permitted.

Definition at line 63 of file multiRange.h.

6.31.2 Constructor & Destructor Documentation

6.31.2.1 MultiRange() [1/2]

```
AtomProbe::MultiRange::MultiRange ( )
```

Definition at line 136 of file multiRange.cpp.

6.31.2.2 MultiRange() [2/2]

```
AtomProbe::MultiRange::MultiRange (
            const RangeFile & rng,
            const AbundanceData & natData )
```

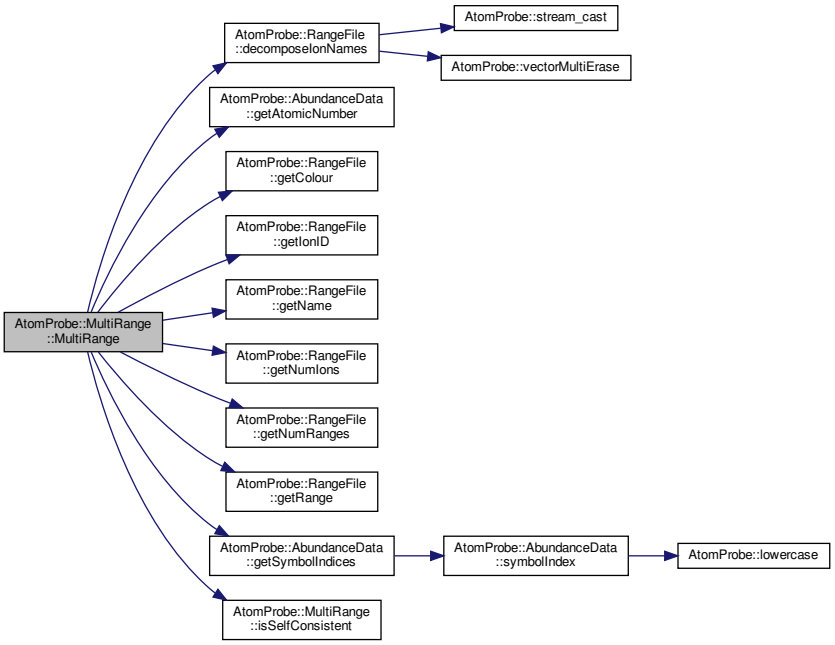
Do our best to intialise from a rangefile.

ions and their child ranges may be dropped if they cannot be identified

Definition at line 141 of file multiRange.cpp.

References ASSERT, AtomProbe::SIMPLE_SPECIES::atomicNumber, AtomProbe::SIMPLE_SPECIES::count, AtomProbe::RangeFile::decomposeIonNames(), AtomProbe::AbundanceData::getAtomicNumber(), AtomProbe::RangeFile::getColour(), AtomProbe::RangeFile::getIonID(), AtomProbe::RangeFile::getName(), AtomProbe::RangeFile::getNumIons(), AtomProbe::RangeFile::getNumRanges(), AtomProbe::RangeFile::getRange(), AtomProbe::AbundanceData::getSymbolIndices(), and isSelfConsistent().

Here is the call graph for this function:



6.31.3 Member Function Documentation

6.31.3.1 addIon() [1/2]

```
unsigned int AtomProbe::MultiRange::addIon (
            const std::set< SIMPLE_SPECIES > & molecule,
            const std::string & name,
            const RGBf & ionCol )
```

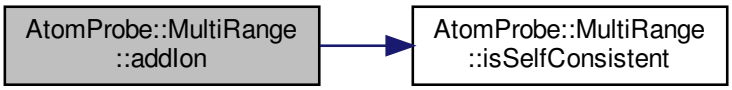
Add the ion to the database returns ion ID if successful, -1 otherwise.

Definition at line 250 of file multiRange.cpp.

References ASSERT, and isSelfConsistent().

Referenced by addIon(), AtomProbe::computeRangeAdjacency(), copyDataFromRange(), and AtomProbe::leastSquaresDeconvolve().

Here is the call graph for this function:



6.31.3.2 addIon() [2/2]

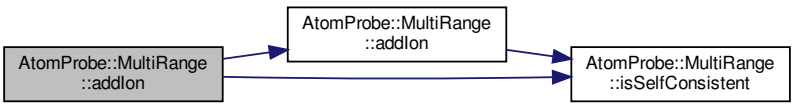
```
unsigned int AtomProbe::MultiRange::addIon (
            const SIMPLE_SPECIES & molecule,
            const std::string & name,
            const RGBf & ionCol )
```

Add a simple ion to the database - returns ion ID if successful, -1 otherwise.

Definition at line 272 of file multiRange.cpp.

References addIon(), ASSERT, and isSelfConsistent().

Here is the call graph for this function:



6.31.3.3 addRange() [1/2]

```
unsigned int AtomProbe::MultiRange::addRange (
            float start,
            float end,
            unsigned int ionID )
```

Add a range to the rangefile. Returns ID number of added range if adding successful, (unsigned int)-1 otherwise.

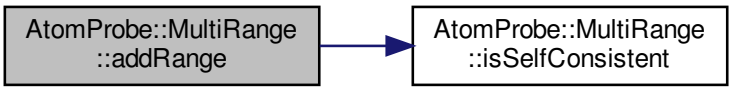
Note that ranges are, unlike RangeFile, allowed to overlap, and still be self consistent.

Definition at line 282 of file multiRange.cpp.

References ASSERT, and isSelfConsistent().

Referenced by AtomProbe::computeRangeAdjacency(), copyDataFromRange(), and AtomProbe::leastSquares↩Deconvolve().

Here is the call graph for this function:



6.31.3.4 addRange() [2/2]

```
unsigned int AtomProbe::MultiRange::addRange (
            const std::pair< float, float > & rng,
            unsigned int ionID )
```

Convenience wrapper for addRange(float,float, unsigned int)

6.31.3.5 clear()

```
void AtomProbe::MultiRange::clear ( )
```

Erase the contents of the rangefile.

Definition at line 806 of file multiRange.cpp.

Referenced by open().

6.31.3.6 copyDataFromRange()

```
void AtomProbe::MultiRange::copyDataFromRange (
            const MultiRange & src,
            unsigned int srcRngId )
```

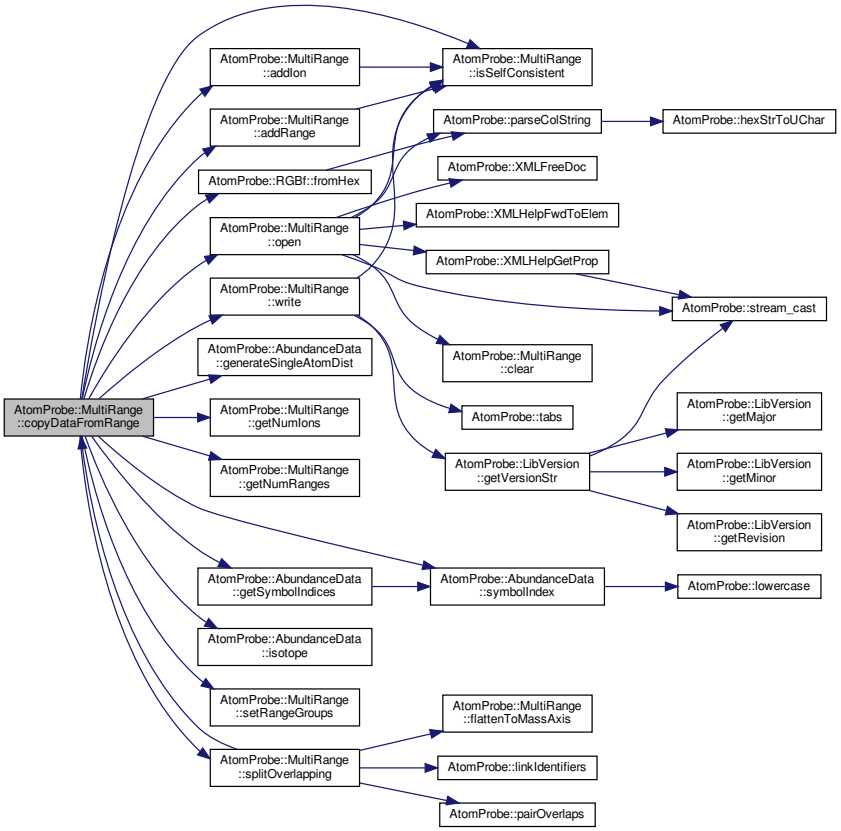
Copy range from a different multirange into this one, including all dependant data.

Definition at line 957 of file multiRange.cpp.

References addIon(), addRange(), ASSERT, AtomProbe::SIMPLE_SPECIES::atomicNumber, AtomProbe::ISOTOPE_ENTRY::atomicNumber, AtomProbe::RGBf::blue, AtomProbe::SIMPLE_SPECIES::count, AtomProbe::RGBf::fromHex(), AtomProbe::AbundanceData::generateSingleAtomDist(), getNumIons(), getNumRanges(), AtomProbe::AbundanceData::getSymbolIndices(), AtomProbe::RGBf::green, AtomProbe::AbundanceData::isotope(), isSelfConsistent(), MASS_TOL, open(), AtomProbe::RGBf::red, setRangeGroups(), splitOverlapping(), AtomProbe::AbundanceData::symbolIndex(), TEST, and write().

Referenced by splitOverlapping().

Here is the call graph for this function:



6.31.3.7 flattenToMassAxis()

```
void AtomProbe::MultiRange::flattenToMassAxis (
            std::vector< FLATTENED_RANGE > & ionMapping ) const
```

Obtain a projection onto the mass axis of ranges that do not touch one another.

Definition at line 889 of file multiRange.cpp.

References ASSERT, and AtomProbe::FLATTENED_RANGE::startMass.

Referenced by splitOverlapping().

6.31.3.8 getColour()

```
RGBf AtomProbe::MultiRange::getColour (
            unsigned int ionID ) const
```

Obtain the colour for a given ion.

Definition at line 765 of file multiRange.cpp.

References ASSERT.

6.31.3.9 getErrString()

```
std::string AtomProbe::MultiRange::getErrString ( ) const
```

Retrieve the human-readable error associated with the current range file state.

Definition at line 671 of file multiRange.cpp.

References ASSERT, and AtomProbe::MULTIRANGE_ERR_ENUM_END.

6.31.3.10 getIonID()

```
unsigned int AtomProbe::MultiRange::getIonID (
            unsigned int rangeId ) const
```

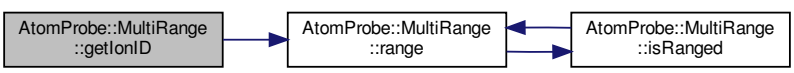
Get the ion's ID from a specified mass.

Returns the ions ID if there exists a range that contains this mass. Otherwise (unsigned int)-1 is returned

Definition at line 732 of file multiRange.cpp.

References ASSERT, and range().

Here is the call graph for this function:



6.31.3.11 getIonName()

```
std::string AtomProbe::MultiRange::getIonName (
            unsigned int ionID ) const
```

Get the name of a specified ionID.

Definition at line 713 of file multiRange.cpp.

References ASSERT.

Referenced by AtomProbe::leastSquaresDeconvolve().

6.31.3.12 getMolecule()

```
set< SIMPLE_SPECIES > AtomProbe::MultiRange::getMolecule (
            unsigned int ionID ) const
```

Return the molecule that is associated with this ion.

Definition at line 707 of file multiRange.cpp.

References ASSERT.

Referenced by AtomProbe::computeIonDistAdjacency().

6.31.3.13 getNumIons()

```
unsigned int AtomProbe::MultiRange::getNumIons ( ) const
```

Get the number of unique ions.

Definition at line 727 of file multiRange.cpp.

Referenced by AtomProbe::computeIonDistAdjacency(), copyDataFromRange(), and AtomProbe::leastSquares↩Deconvolve().

6.31.3.14 getNumRanges() [1/2]

```
unsigned int AtomProbe::MultiRange::getNumRanges ( ) const
```

Get the number of unique ranges.

Definition at line 700 of file multiRange.cpp.

Referenced by AtomProbe::computeRangeAdjacency(), copyDataFromRange(), and AtomProbe::leastSquares↩Deconvolve().

6.31.3.15 getNumRanges() [2/2]

```
unsigned int AtomProbe::MultiRange::getNumRanges (
            unsigned int ionID ) const
```

Get the number of ranges for a given ion ID.

Definition at line 719 of file multiRange.cpp.

References ASSERT.

6.31.3.16 getRange()

```
std::pair< float, float > AtomProbe::MultiRange::getRange (
            unsigned int rangeID ) const
```

Retrieve the start and end of a given range as a pair(start,end)

Definition at line 739 of file multiRange.cpp.

References ASSERT.

Referenced by AtomProbe::computeRangeAdjacency().

6.31.3.17 getRangeIdsFromIon()

```
std::vector<unsigned int> AtomProbe::MultiRange::getRangeIdsFromIon (
            unsigned int ionId ) const
```

Retrieve all the ranges associated with a given ion.

6.31.3.18 getRanges()

```
std::vector< unsigned int > AtomProbe::MultiRange::getRanges (
            float mass ) const
```

Retrieve all of the ranges that specify the given mass.

Definition at line 745 of file multiRange.cpp.

6.31.3.19 isRanged() [1/2]

```
bool AtomProbe::MultiRange::isRanged (
            float mass ) const
```

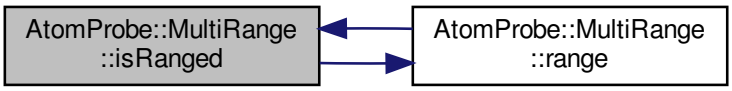
Returns true if a specified mass is ranged.

Definition at line 772 of file multiRange.cpp.

References range().

Referenced by isRanged(), and range().

Here is the call graph for this function:



6.31.3.20 isRanged() [2/2]

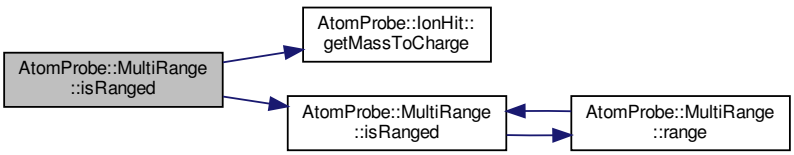
```
bool AtomProbe::MultiRange::isRanged (
            const IonHit & ion ) const
```

Returns true if an ion is ranged.

Definition at line 784 of file multiRange.cpp.

References AtomProbe::IonHit::getMassToCharge(), and isRanged().

Here is the call graph for this function:



6.31.3.21 isSelfConsistent()

```
bool AtomProbe::MultiRange::isSelfConsistent ( ) const
```

Check to see if data structure is internally consistent.

Definition at line 209 of file multiRange.cpp.

Referenced by addIon(), addRange(), copyDataFromRange(), MultiRange(), open(), and write().

6.31.3.22 open()

```
bool AtomProbe::MultiRange::open (
            const char * fileName,
            unsigned int format = -1 )
```

read the contents of the file into class

returns true if successful, otherwise false

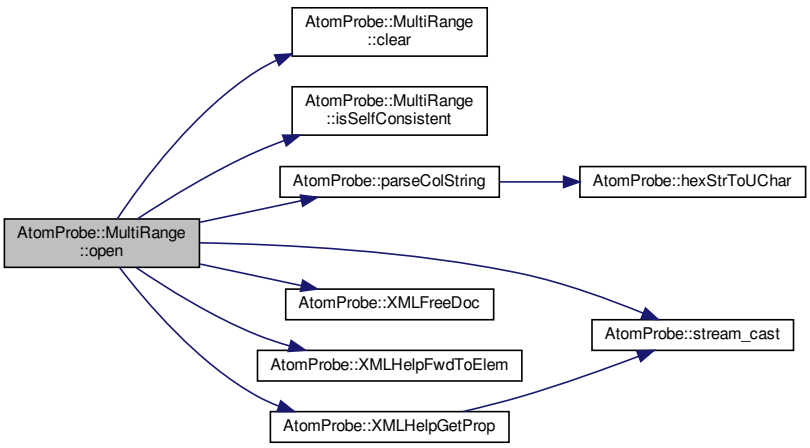
- if not successful then the errState will contain the error information, and the calling object (rangefile) will be in an invalid state

Definition at line 376 of file multiRange.cpp.

References AtomProbe::SIMPLE_SPECIES::atomicNumber, AtomProbe::RGBf::blue, clear(), AtomProbe::SIMPLE_SPECIES::count, AtomProbe::RGBf::green, isSelfConsistent(), AtomProbe::MULTIRANGE_ERR_BAD_GROUP, AtomProbe::MULTIRANGE_ERR_BAD_RANGE, AtomProbe::MULTIRANGE_ERR_BAD_RANGES, AtomProbe::MULTIRANGE_ERR_MOL_BAD_COLOUR, AtomProbe::MULTIRANGE_ERR_MOL_MISSING_COLOUR, AtomProbe::MULTIRANGE_ERR_MOL_MISSING_COMPONENTS, AtomProbe::MULTIRANGE_ERR_MOL_MISSING_ENTRY, AtomProbe::MULTIRANGE_ERR_MOL_MISSING_NAME, AtomProbe::MULTIRANGE_ERR_NO_CONTENT, AtomProbe::MULTIRANGE_ERR_NO_MOLECULE_ENTRIES, AtomProbe::MULTIRANGE_ERR_NO_MOLECULES, AtomProbe::MULTIRANGE_ERR_NO_NODEPTR, AtomProbe::MULTIRANGE_ERR_NO_PARSER, AtomProbe::MULTIRANGE_ERR_NO_RANGES, AtomProbe::MULTIRANGE_ERR_NO_TIMESTAMP, AtomProbe::MULTIRANGE_ERR_NO_XML_CONTEXT, AtomProbe::MULTIRANGE_ERR_NO_XML_DOC, AtomProbe::MULTIRANGE_ERR_RANGE_NOPARENT, AtomProbe::MULTIRANGE_ERR_SELF_INCONSISTENT, AtomProbe::MULTIRANGE_NOT_VALID_ROOTNODE, AtomProbe::parseColString(), AtomProbe::RGBf::red, AtomProbe::stream_cast(), AtomProbe::XMLFreeDoc(), AtomProbe::XMLHelpFwdToElem(), and AtomProbe::XMLHelpGetProp().

Referenced by copyDataFromRange().

Here is the call graph for this function:



6.31.3.23 range()

```
void AtomProbe::MultiRange::range (
            std::vector< IonHit > & ionHits ) const
```

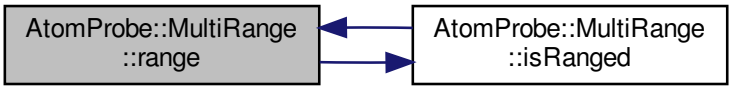
Clips out ions that are not inside the rangefile's ranges.

Definition at line 789 of file multiRange.cpp.

References isRanged().

Referenced by getIonID(), isRanged(), and setIonID().

Here is the call graph for this function:



6.31.3.24 setColour()

```
void AtomProbe::MultiRange::setColour (
            unsigned int,
            const RGBf & r )
```

Set the colour using the ion ID.

6.31.3.25 setIonID()

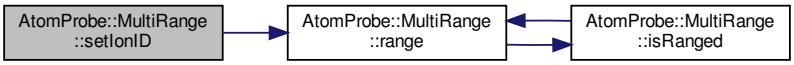
```
void AtomProbe::MultiRange::setIonID (
            unsigned int range,
            unsigned int newIonId )
```

Set the ion ID for a given range.

Definition at line 758 of file multiRange.cpp.

References ASSERT, and range().

Here is the call graph for this function:



6.31.3.26 setRangeGroups()

```
void AtomProbe::MultiRange::setRangeGroups (
            const std::vector< unsigned int > & groups )
```

Set the groupings for the ranges.

Definition at line 300 of file multiRange.cpp.

Referenced by copyDataFromRange().

6.31.3.27 splitOverlapping()

```
void AtomProbe::MultiRange::splitOverlapping (
            std::vector< MultiRange > & decomposedRanges ) const
```

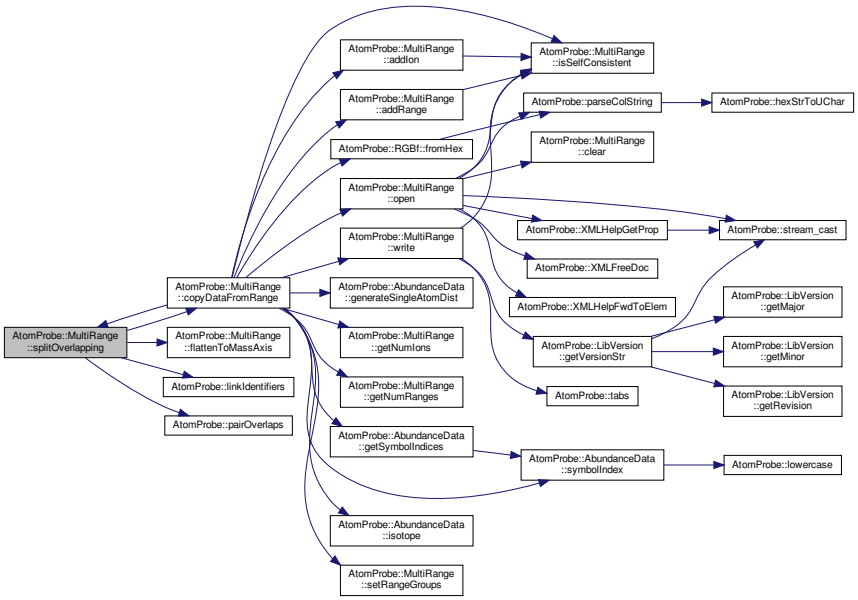
Separate out the non-interacting parts of the multi-ranges into their own multiRange entries The vector of maps converts the ioniDs of the child MultiRange to the parent

Definition at line 819 of file multiRange.cpp.

References ASSERT, copyDataFromRange(), flattenToMassAxis(), AtomProbe::linkIdentifiers(), and AtomProbe::pairOverlaps().

Referenced by copyDataFromRange().

Here is the call graph for this function:



6.31.3.28 write()

```
bool AtomProbe::MultiRange::write (
            const char * fileName,
            unsigned int format = MULTIRANGE_FORMAT_XML ) const
```

Save the structure to a file. format specifies output file format type.

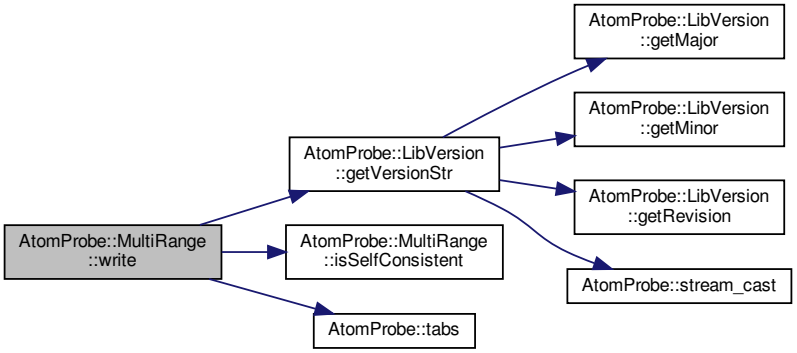
Returns true if successful, otherwise false

Definition at line 305 of file multiRange.cpp.

References ASSERT, AtomProbe::LibVersion::getVersionStr(), isSelfConsistent(), AtomProbe::MULTIRANGE_F↩ ORMAT_XML, and AtomProbe::tabs().

Referenced by copyDataFromRange().

Here is the call graph for this function:

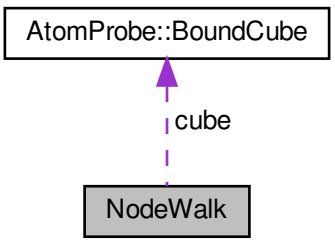


The documentation for this class was generated from the following files:

- include/atomprobe/io/multiRange.h
- src/io/multiRange.cpp

6.32 NodeWalk Class Reference

Collaboration diagram for NodeWalk:



Public Member Functions

- NodeWalk (unsigned int idx, const BoundCube &bc, unsigned int dpth)

Public Attributes

- size_t index
- BoundCube cube
- unsigned int depth

6.32.1 Detailed Description

Definition at line 55 of file K3DTree-exact.cpp.

6.32.2 Constructor & Destructor Documentation

6.32.2.1 NodeWalk()

```
NodeWalk::NodeWalk (
            unsigned int idx,
            const BoundCube & bc,
            unsigned int dpth )  [inline]
```

Definition at line 61 of file K3DTree-exact.cpp.

6.32.3 Member Data Documentation

6.32.3.1 cube

```
BoundCube NodeWalk::cube
```

Definition at line 59 of file K3DTree-exact.cpp.

6.32.3.2 depth

```
unsigned int NodeWalk::depth
```

Definition at line 60 of file K3DTree-exact.cpp.

6.32.3.3 index

```
size_t NodeWalk::index
```

Definition at line 58 of file K3DTree-exact.cpp.

The documentation for this class was generated from the following file:

- src/algorithm/K3DTree-exact.cpp

6.33 AtomProbe::OVERLAP_PROBLEM_SETTINGS Struct Reference

```
#include <componentAnalysis.h>
```

Public Attributes

- float massTolerance

  Tolerance in Da, above which we consider problems to be.
- float intensityTolerance

  The minimal natural abundance for which we consider the ions.
- unsigned int maxDefaultCharge

  Maximum charge state to consider.

6.33.1 Detailed Description

Definition at line 24 of file componentAnalysis.h.

6.33.2 Member Data Documentation

6.33.2.1 intensityTolerance

```
float AtomProbe::OVERLAP_PROBLEM_SETTINGS::intensityTolerance
```

The minimal natural abundance for which we consider the ions.

Definition at line 31 of file componentAnalysis.h.

Referenced by AtomProbe::computeIonDistAdjacency().

6.33.2.2 massTolerance

```
float AtomProbe::OVERLAP_PROBLEM_SETTINGS::massTolerance
```

Tolerance in Da, above which we consider problems to be.

Definition at line 27 of file componentAnalysis.h.

Referenced by AtomProbe::computeIonDistAdjacency(), and AtomProbe::computeRangeAdjacency().

6.33.2.3 maxDefaultCharge

```
unsigned int AtomProbe::OVERLAP_PROBLEM_SETTINGS::maxDefaultCharge
```

Maximum charge state to consider.

Definition at line 34 of file componentAnalysis.h.

Referenced by AtomProbe::computeIonDistAdjacency(), and AtomProbe::computeRangeAdjacency().

The documentation for this struct was generated from the following file:

- include/atomprobe/algorithm/componentAnalysis.h

6.34 AtomProbe::Point3D Class Reference

A 3D point data class storage.

```
#include <point3D.h>
```

Public Member Functions

- Point3D ()
  Constructor with no initialisation.
- Point3D (const float *f)
  Constructor initialising values from an array of length 4(sizeof(float))*
- Point3D (float x, float y, float z)
  Constructor with initialising values, X, Y and Z.
- void setValue (unsigned int ui, float val)
  Set value val of the ui-th dimension, ui in (0,1,2)
- void setValue (float fX, float fY, float fZ)
  Set the XYZ value fo the point.
- bool parse (const std::string &s)
  Set from string representation.
- void setValueArr (const float *val)
  Set value by pointer (X, Y, Z from array of len 3)
- float getValue (unsigned int ui) const

Get value of ith dimension (0, 1, 2)

- const float * getValueArr () const

  Obtain a pointer to internal array (3 floats)
- void copyValueArr (float *value) const

  Copy data from internal into target array of length 3 : Pointer MUST be allocated.
- void add (const Point3D &obj)

  Add a point to this, without generating a return value.
- void extend (float distance)

  Extend the vector by the specified distance.
- bool hasNaN () const

  Returns true if any of the 3 data pts are NaN.
- bool operator== (const Point3D &pt) const

  Equality operator.
- const Point3D & operator= (const Point3D &pt)

  Assignment operator.
- const Point3D & operator+= (const Point3D &pt)

  += operator
- const Point3D & operator-= (const Point3D &pt)

  -= operator
- Point3D operator*= (const float scale)

  **= operator, multiplies the whole Point3D by a scalar*
- const Point3D operator+ (const Point3D &pt) const

  Addition of Point3D objects (X1+X2, Y1+Y2, Z1+Z2)
- const Point3D operator+ (float f) const

  Addition of a scalar to a Point3D object (X+f, Y+f, Z+f)
- const Point3D operator* (float scale) const

  *Scalar multiplication (X*f, Y*f, Z*f)*
- const Point3D operator* (const Point3D &pt) const

  *Elemental multiplication of two Point3D objects (X1*X2, Y1*Y2, Z1*Z2)*
- const Point3D operator/ (float scale) const

  Scalar division of Point3D by scale (X/scale, Y/scale, Z/scale)
- const Point3D operator/ (const Point3D &pt) const

  Elemental division of two Point3D objects (X1/X2, Y1/Y2, Z1/Z2)
- const Point3D operator- (const Point3D &pt) const

  Subtraction of two Point3D objects (X1-X2, Y1-Y2, Z1-Z2)
- const Point3D operator- () const

  Negation, Returns a Point3D object with the negative of the previous value.
- void normalise ()

  Make point unit magnitude, maintaining direction.
- Point3D normal () const

  Return point unit magnitude, maintianing direction.
- float sqrDist (const Point3D &pt) const

  Returns the square of distance to another Point3D.
- float dotProd (const Point3D &pt) const

  Calculate the dot product of this and another point.
- Point3D crossProd (const Point3D &pt) const

  Calculate the cross product of this and another point.
- float angle (const Point3D &pt) const

  Calculate the angle between two position vectors in radians.
- float sqrMag () const

  Returns magnitude^2, taking this as a position vector.

- float mag () const

  Magnitude of position vector.
- float operator[ ] (unsigned int ui) const

  Array indexing operator, Point3D[1] returns the value of the ui-th dim.
- float & operator[ ] (unsigned int ui)

  Array reference operator, Point3D[1].
- bool insideBox (const Point3D &farPoint) const

  Is this point inside a box bounded by orign and farPoint?
- bool insideBox (const Point3D &lowPt, const Point3D &hiPt) const

  Is this point inside a box bounded by lowPt and hiPt?
- void negate ()

  Makes each value negative of old value (-X, -Y, -Z)
- void reciprocal ()

  Makes each value its reciprocal (1/X, 1/Y, 1/Z)
- void transform3x3 (const gsl_matrix *matrix)

  Perform a 3x3 matrix transformation using a GSL matrix.
- bool orthogonalise (const Point3D &p)

  Perform a cross-product based orthogonalisation with the specified vector.
- void setISOSpherical (float radius, float theta, float phi)

  Assign the vector using spherical coordinates.
- void getISOSpherical (float &radius, float &theta, float &phi) const

  Get the Point3D value as spherical coordinates (ISO 30-11)

Static Public Member Functions

- static void getCentroid (const std::vector< Point3D > &pts, Point3D &p)

  find the centroid of a set of points

Friends

- std::ostream & operator<< (std::ostream &stream, const Point3D &)

  Output streaming operator. Streams values in the text format (x,y,z)

6.34.1 Detailed Description

A 3D point data class storage.

Definition at line 43 of file point3D.h.

6.34.2 Constructor & Destructor Documentation

6.34.2.1 Point3D() [1/3]

```
AtomProbe::Point3D::Point3D ( )  [inline]
```

Constructor with no initialisation.

Definition at line 50 of file point3D.h.

Referenced by getCentroid().

6.34.2.2 Point3D() [2/3]

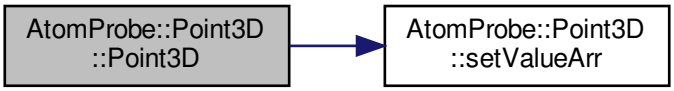
```
AtomProbe::Point3D::Point3D (
            const float * f )  [inline]
```

Constructor initialising values from an array of length 4∗(sizeof(float))

Definition at line 53 of file point3D.h.

References setValueArr().

Here is the call graph for this function:



6.34.2.3 Point3D() [3/3]

```
AtomProbe::Point3D::Point3D (
            float x,
            float y,
            float z )  [inline]
```

Constructor with initialising values, X, Y and Z.

Definition at line 56 of file point3D.h.

6.34.3 Member Function Documentation

6.34.3.1 add()

```
void AtomProbe::Point3D::add (
            const Point3D & obj )
```

Add a point to this, without generating a return value.

Add a *Point3D* set of values to this Point3D.

This is different to +=, because it generates no return value.

Definition at line 333 of file point3D.cpp.

Referenced by getValueArr().

6.34.3.2 angle()

```
float AtomProbe::Point3D::angle (
            const Point3D & pt ) const
```

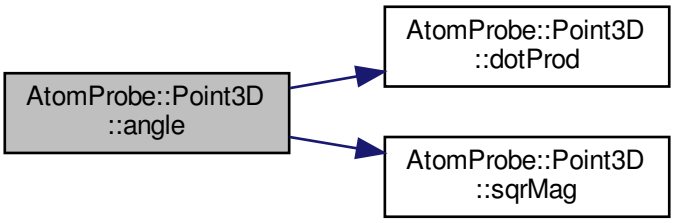
Calculate the angle between two position vectors in radians.

Definition at line 396 of file point3D.cpp.

References dotProd(), and sqrMag().

Referenced by AtomProbe::Mesh::divideMeshSurface(), and hasNaN().

Here is the call graph for this function:



6.34.3.3 copyValueArr()

```
void AtomProbe::Point3D::copyValueArr (
            float * value ) const
```

Copy data from internal into target array of length 3 : Pointer MUST be allocated.

As a quick example, you can copy into a buffer you own Point3D p(1,2,3); float x[3]; p.copyValueArr(x[0]);

Definition at line 147 of file point3D.cpp.

References ASSERT.

Referenced by getValueArr().

6.34.3.4 crossProd()

```
Point3D AtomProbe::Point3D::crossProd (
            const Point3D & pt ) const
```

Calculate the cross product of this and another point.

Definition at line 293 of file point3D.cpp.

Referenced by AtomProbe::TriangleWithVertexNorm::computeACWNormal(), AtomProbe::TriangleWithVertex↩Norm::computeArea(), AtomProbe::computeRotationMatrix(), AtomProbe::distanceToSegment(), AtomProbe::↩Mesh::getTriNormal(), AtomProbe::Mesh::getVolume(), hasNaN(), AtomProbe::intersect_RayTriangle(), main(), orthogonalise(), and AtomProbe::TriangleWithVertexNorm::safeComputeACWNormal().

6.34.3.5 dotProd()

```
float AtomProbe::Point3D::dotProd (
            const Point3D & pt ) const
```

Calculate the dot product of this and another point.

(X1∗X2 + Y1∗Y2 ...)

Definition at line 287 of file point3D.cpp.

Referenced by angle(), AtomProbe::generate1DAxialDistHistSweep(), AtomProbe::Mesh::getVolume(), hasNaN(), AtomProbe::intersect_RayTriangle(), main(), and AtomProbe::signedDistanceToFacet().

6.34.3.6 extend()

```
void AtomProbe::Point3D::extend (
            float distance )
```

Extend the vector by the specified distance.

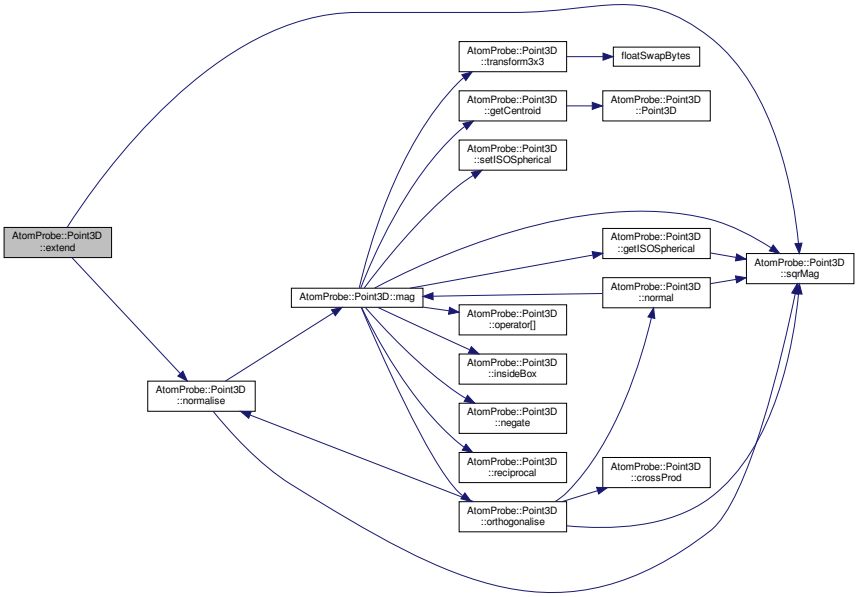
Assumes Point3D is a vector from the origin, and adds on a vector parallel to Point3D of length *distance*.

Definition at line 306 of file point3D.cpp.

References ASSERT, normalise(), and sqrMag().

Referenced by getValueArr().

Here is the call graph for this function:



6.34.3.7 getCentroid()

```
void AtomProbe::Point3D::getCentroid (
            const std::vector< Point3D > & pts,
            Point3D & p )  [static]
```

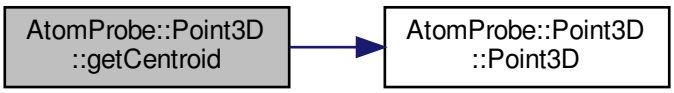
find the centroid of a set of points

Definition at line 401 of file point3D.cpp.

References Point3D().

Referenced by mag().

Here is the call graph for this function:



6.34.3.8 getISOSpherical()

```
void AtomProbe::Point3D::getISOSpherical (
            float & radius,
            float & theta,
            float & phi ) const
```

Get the Point3D value as spherical coordinates (ISO 30-11)

Internal cartesian representation converted to ISO 30-11 and returned in the pointers provided as input.

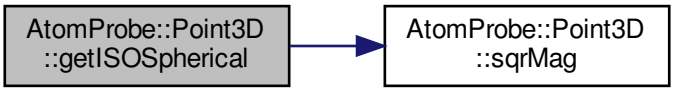
theta - inclination (angle from +z). phi - azimuth (angle from +x), r - radius

Definition at line 441 of file point3D.cpp.

References sqrMag().

Referenced by mag().

Here is the call graph for this function:



6.34.3.9 getValue()

```
float AtomProbe::Point3D::getValue (
            unsigned int ui ) const  [inline]
```

Get value of ith dimension (0, 1, 2)

Definition at line 102 of file point3D.h.

Referenced by AtomProbe::SimpleCubicGen::generateLattice(), AtomProbe::FaceCentredCubicGen::generate↩Lattice(), AtomProbe::BodyCentredCubicGen::generateLattice(), AtomProbe::K3DNodeApprox::getAxisVal(), AtomProbe::IonHit::getBoundCube(), AtomProbe::IonHit::getIonDataLimits(), and AtomProbe::K3DNodeApprox↩::getLocVal().

6.34.3.10 getValueArr()

```
const float* AtomProbe::Point3D::getValueArr ( ) const  [inline]
```

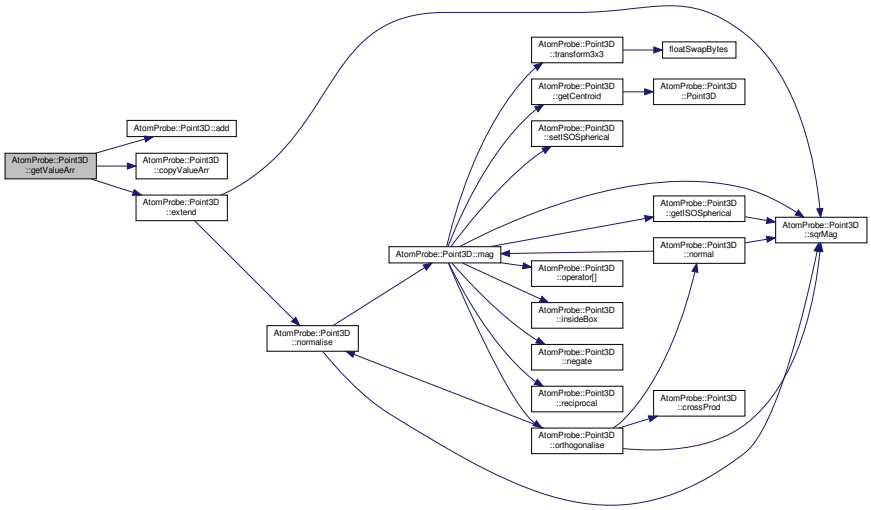
Obtain a pointer to internal array (3 floats)

Definition at line 105 of file point3D.h.

References add(), copyValueArr(), and extend().

Referenced by AtomProbe::BoundCube::intersects().

Here is the call graph for this function:



6.34.3.11 hasNaN()

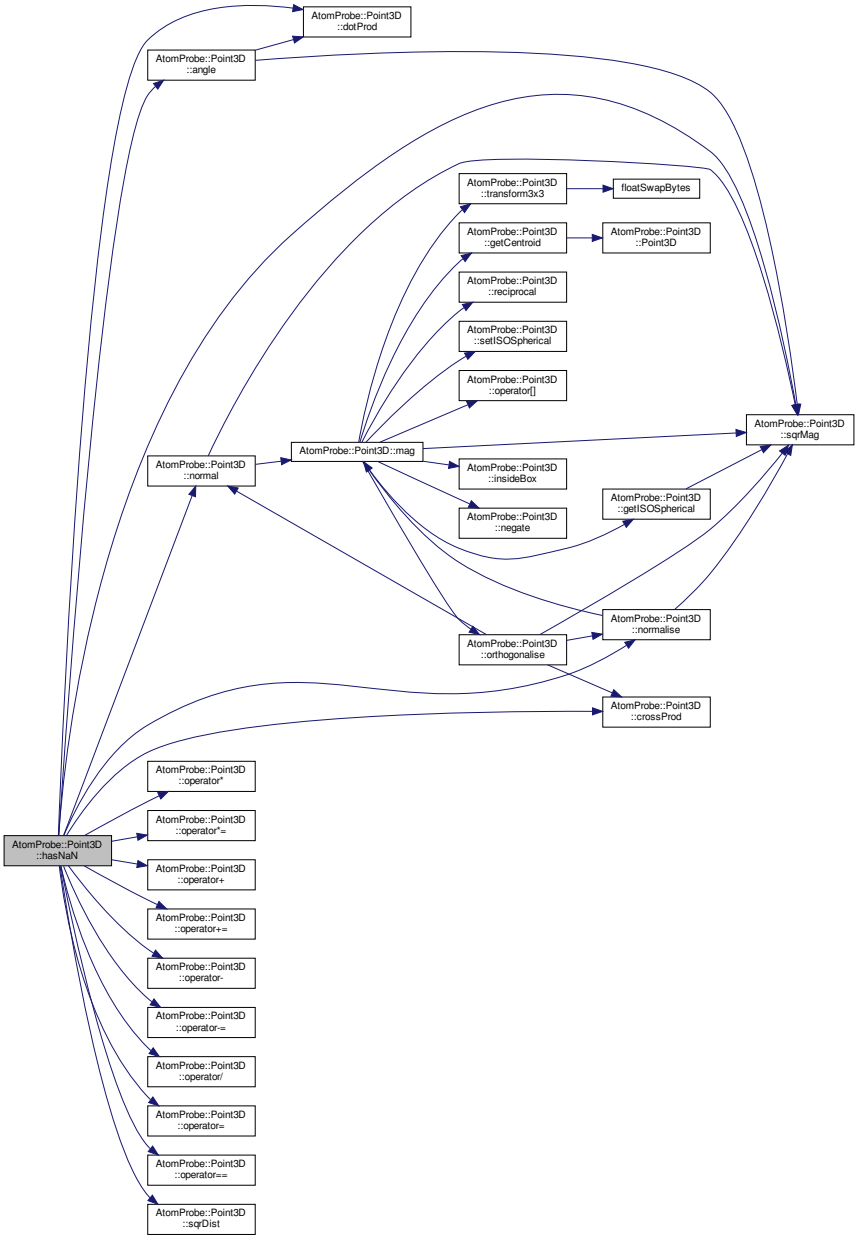
```
bool AtomProbe::Point3D::hasNaN ( ) const  [inline]
```

Returns true if any of the 3 data pts are NaN.

Definition at line 132 of file point3D.h.

References angle(), crossProd(), dotProd(), normal(), normalise(), operator∗(), operator∗=(), operator+(), operator+=(), operator-(), operator-=(), operator/(), operator<<, operator=(), operator==(), sqrDist(), and sqrMag().

Here is the call graph for this function:



6.34.3.12 insideBox() [1/2]

```
bool AtomProbe::Point3D::insideBox (
            const Point3D & farPoint ) const
```

Is this point inside a box bounded by orign and *farPoint*?

Returns true if this point is located inside (0,0,0) -> *farPoint*

Assuming box shape (non zero edges return false)

farPoint must be positive in all dim

Definition at line 316 of file point3D.cpp.

Referenced by mag().

6.34.3.13 insideBox() [2/2]

```
bool AtomProbe::Point3D::insideBox (
            const Point3D & lowPt,
            const Point3D & hiPt ) const
```

Is this point inside a box bounded by *lowPt* and *hiPt*?

Returns true if this point is located inside *lowPt* -> *hiPt*

Assuming box shape.

Definition at line 324 of file point3D.cpp.

6.34.3.14 mag()

```
float AtomProbe::Point3D::mag ( ) const  [inline]
```

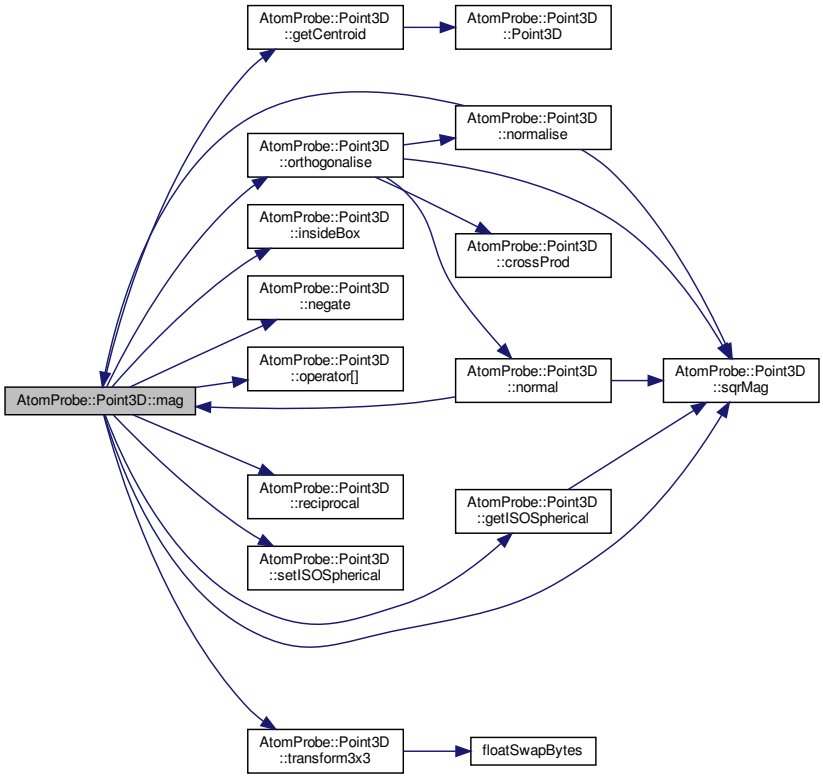
Magnitude of position vector.

Definition at line 201 of file point3D.h.

References getCentroid(), getISOSpherical(), insideBox(), negate(), operator[ ](), orthogonalise(), reciprocal(), set↩ ISOSpherical(), sqrMag(), and transform3x3().

Referenced by normal(), normalise(), AtomProbe::signedDistanceToFacet(), and AtomProbe::triIsDegenerate().

Here is the call graph for this function:



6.34.3.15 negate()

```
void AtomProbe::Point3D::negate ( )
```

Makes each value negative of old value (-X, -Y, -Z)

Definition at line 366 of file point3D.cpp.

Referenced by mag().

6.34.3.16 normal()

```
Point3D AtomProbe::Point3D::normal ( ) const
```

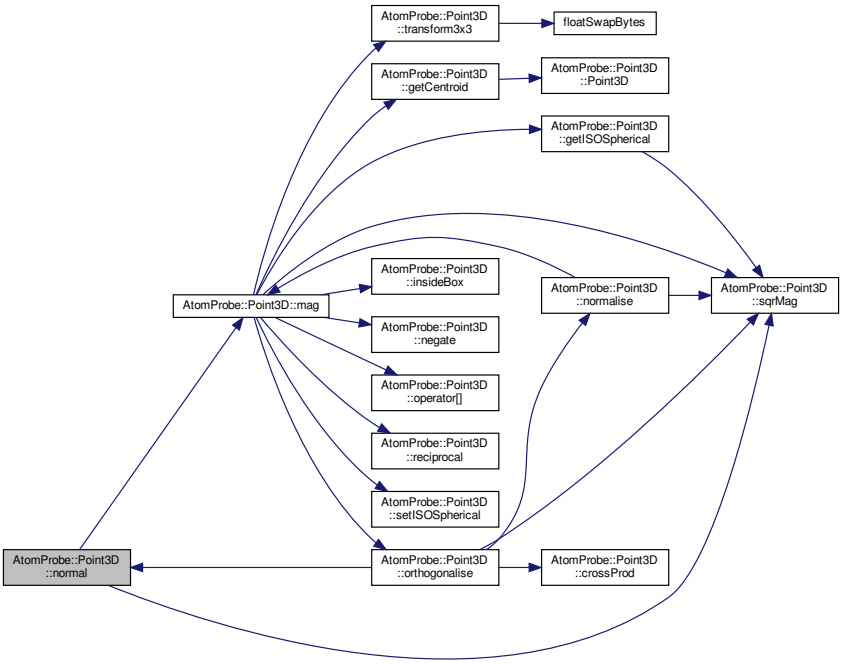
Return point unit magnitude, maintianing direction.

Definition at line 355 of file point3D.cpp.

References mag(), and sqrMag().

Referenced by hasNaN(), and orthogonalise().

Here is the call graph for this function:



6.34.3.17 normalise()

```
void AtomProbe::Point3D::normalise ( )
```

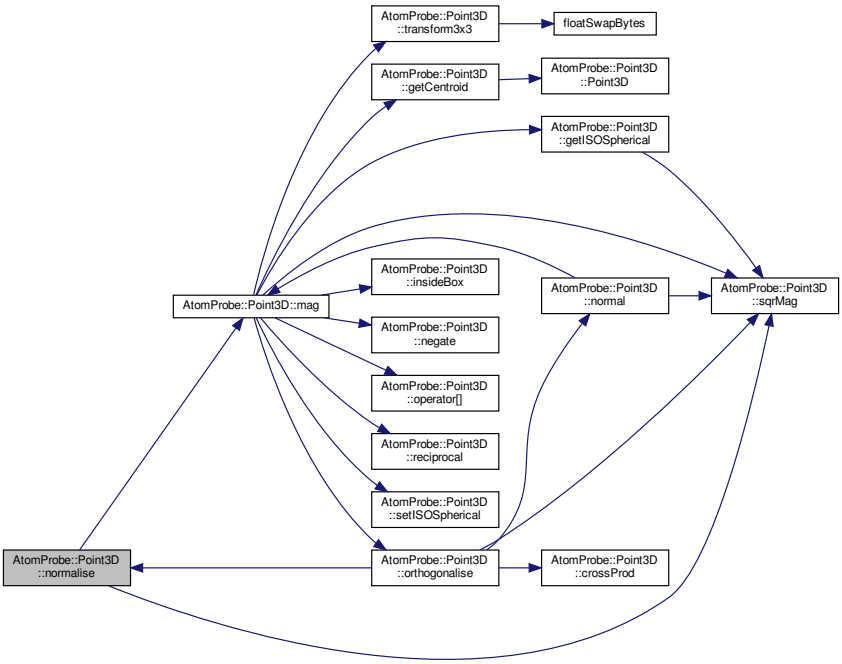
Make point unit magnitude, maintaining direction.

Definition at line 345 of file point3D.cpp.

References mag(), and sqrMag().

Referenced by AtomProbe::TriangleWithVertexNorm::computeACWNormal(), AtomProbe::computeRotation↩ Matrix(), extend(), AtomProbe::Mesh::getTriNormal(), hasNaN(), AtomProbe::intersect_RayTriangle(), main(), orthogonalise(), and AtomProbe::TriangleWithVertexNorm::safeComputeACWNormal().

Here is the call graph for this function:



6.34.3.18 operator∗() [1/2]

```
const Point3D AtomProbe::Point3D::operator* (
            float scale ) const
```

Scalar multiplication (X∗f, Y∗f, Z∗f)

Definition at line 234 of file point3D.cpp.

Referenced by hasNaN().

6.34.3.19 operator∗() [2/2]

```
const Point3D AtomProbe::Point3D::operator* (
            const Point3D & pt ) const
```

Elemental multiplication of two Point3D objects (X1∗X2, Y1∗Y2, Z1∗Z2)

Definition at line 245 of file point3D.cpp.

6.34.3.20 operator*=()

```
Point3D AtomProbe::Point3D::operator*= (
            const float scale )
```

*= operator, multiplies the whole Point3D by a scalar

Definition at line 225 of file point3D.cpp.

Referenced by hasNaN().

6.34.3.21 operator+() [1/2]

```
const Point3D AtomProbe::Point3D::operator+ (
            const Point3D & pt ) const
```

Addition of Point3D objects (X1+X2, Y1+Y2, Z1+Z2)

Definition at line 186 of file point3D.cpp.

Referenced by hasNaN().

6.34.3.22 operator+() [2/2]

```
const Point3D AtomProbe::Point3D::operator+ (
            float f ) const
```

Addition of a scalar to a Point3D object (X+f, Y+f, Z+f)

Definition at line 196 of file point3D.cpp.

6.34.3.23 operator+=()

```
const Point3D & AtomProbe::Point3D::operator+= (
            const Point3D & pt )
```

+= operator

Definition at line 178 of file point3D.cpp.

Referenced by hasNaN().

6.34.3.24 operator-() [1/2]

```
const Point3D AtomProbe::Point3D::operator- (
            const Point3D & pt ) const
```

Subtraction of two Point3D objects (X1-X2, Y1-Y2, Z1-Z2)

Definition at line 205 of file point3D.cpp.

6.34.3.25 operator-() [2/2]

```
const Point3D AtomProbe::Point3D::operator- ( ) const
```

Negation, Returns a Point3D object with the negative of the previous value.

Definition at line 215 of file point3D.cpp.

Referenced by hasNaN().

6.34.3.26 operator-=()

```
const Point3D & AtomProbe::Point3D::operator-= (
            const Point3D & pt )
```

-= operator

Definition at line 157 of file point3D.cpp.

Referenced by hasNaN().

6.34.3.27 operator/() [1/2]

```
const Point3D AtomProbe::Point3D::operator/ (
            float scale ) const
```

Scalar division of Point3D by *scale* (X/scale, Y/scale, Z/scale)

Definition at line 256 of file point3D.cpp.

Referenced by hasNaN().

6.34.3.28 operator/() [2/2]

```
const Point3D AtomProbe::Point3D::operator/ (
            const Point3D & pt ) const
```

Elemental division of two Point3D objects (X1/X2, Y1/Y2, Z1/Z2)

Definition at line 268 of file point3D.cpp.

6.34.3.29 operator=()

```
const Point3D & AtomProbe::Point3D::operator= (
            const Point3D & pt )
```

Assignment operator.

Definition at line 170 of file point3D.cpp.

Referenced by hasNaN().

6.34.3.30 operator==()

```
bool AtomProbe::Point3D::operator== (
            const Point3D & pt ) const
```

Equality operator.

Definition at line 165 of file point3D.cpp.

Referenced by hasNaN().

6.34.3.31 operator[]() [1/2]

```
float AtomProbe::Point3D::operator[] (
            unsigned int ui ) const
```

Array indexing operator, Point3D[1] returns the value of the ui-th dim.

Definition at line 135 of file point3D.cpp.

References ASSERT.

Referenced by mag().

6.34.3.32 operator[]() [2/2]

```
float & AtomProbe::Point3D::operator[] (
            unsigned int ui )
```

Array reference operator, Point3D[1].

returns reference to data in ui-th dim

Definition at line 141 of file point3D.cpp.

References ASSERT.

6.34.3.33 orthogonalise()

```
bool AtomProbe::Point3D::orthogonalise (
            const Point3D & p )
```

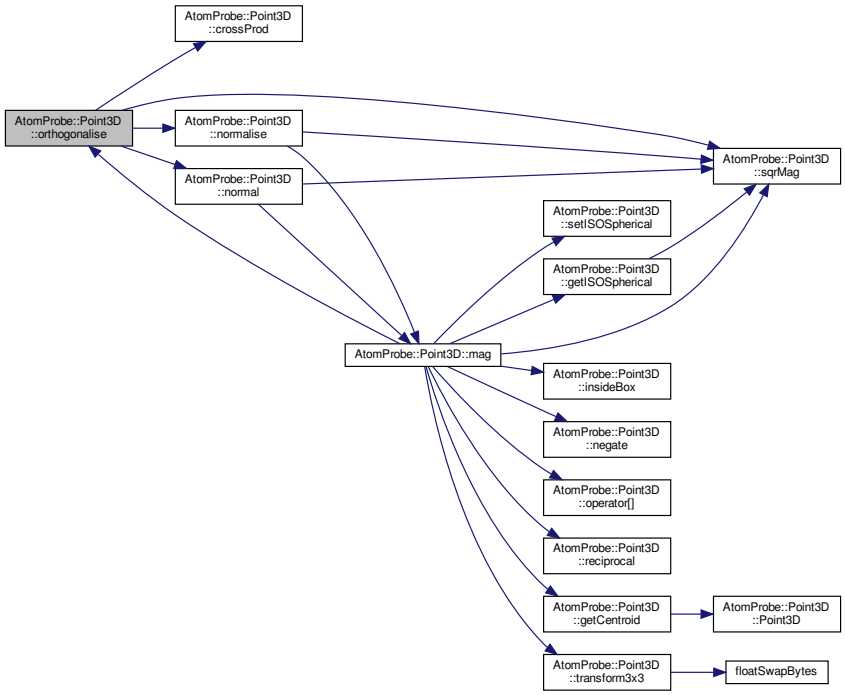
Perform a cross-product based orthogonalisation with the specified vector.

Definition at line 380 of file point3D.cpp.

References crossProd(), normal(), normalise(), and sqrMag().

Referenced by mag().

Here is the call graph for this function:



6.34.3.34 parse()

```
bool AtomProbe::Point3D::parse (
            const std::string & s )
```

Set from string representation.

From a string representation of a 3D point, parse and store the data in a Point3D.

Must contain 3 entries.

Values can be separated by whitespace or any of ,;|_

Polar notation is indicated by < ... >

Polar notation assumes <radius,theta,phi> in degrees (they will be converted to radians internally) and then converted into cartesian coordinates (X,Y,Z)

```
Point3D mypoint;
mypoint.parse("<1,45,90>");
cout << mypoint << endl;
```

Returns:

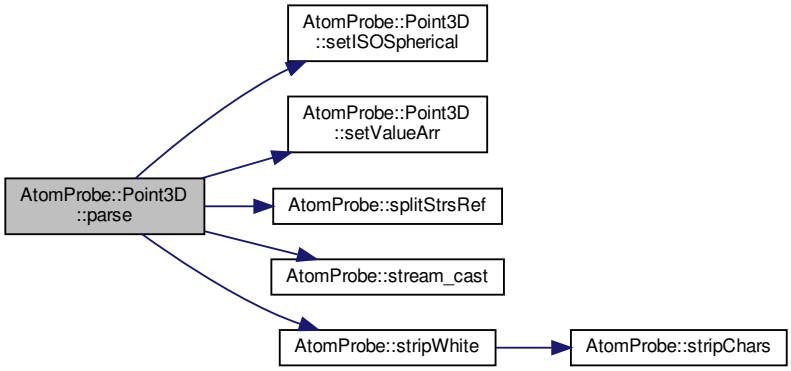
```
(-3.09086e-08,0.707107,0.707107)
```

Definition at line 47 of file point3D.cpp.

References M_PI, setISOSpherical(), setValueArr(), AtomProbe::splitStrsRef(), AtomProbe::stream_cast(), and AtomProbe::stripWhite().

Referenced by main(), and setValue().

Here is the call graph for this function:



6.34.3.35 reciprocal()

```
void AtomProbe::Point3D::reciprocal ( )
```

Makes each value its reciprocal (1/X, 1/Y, 1/Z)

Definition at line 373 of file point3D.cpp.

Referenced by mag().

6.34.3.36 setISOSpherical()

```
void AtomProbe::Point3D::setISOSpherical (
            float radius,
            float theta,
            float phi )
```

Assign the vector using spherical coordinates.

theta - inclination (angle from +z). phi - azimuth (angle from +x), r - radius

The value of the point is stored in cartesian coords.

Definition at line 433 of file point3D.cpp.

Referenced by AtomProbe::generate1DAxialDistHistSweep(), mag(), parse(), and AtomProbe::Gnomonic↩ Projection::toPlanar().

6.34.3.37 setValue() [1/2]

```
void AtomProbe::Point3D::setValue (
            unsigned int ui,
            float val )  [inline]
```

Set value *val* of the *ui-th* dimension, *ui* in (0,1,2)

Definition at line 61 of file point3D.h.

Referenced by AtomProbe::BoundCube::getBounds(), AtomProbe::BoundCube::intersects(), AtomProbe::Bound↩ Cube::max(), and AtomProbe::BoundCube::min().

6.34.3.38 setValue() [2/2]

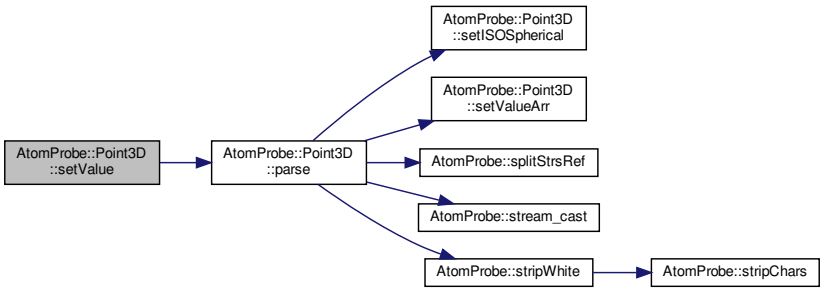
```
void AtomProbe::Point3D::setValue (
            float fX,
            float fY,
            float fZ )  [inline]
```

Set the XYZ value fo the point.

Definition at line 64 of file point3D.h.

References parse().

Here is the call graph for this function:



6.34.3.39 setValueArr()

```
void AtomProbe::Point3D::setValueArr (
            const float * val )  [inline]
```

Set value by pointer (X, Y, Z from array of len 3)

Definition at line 94 of file point3D.h.

Referenced by parse(), Point3D(), and AtomProbe::IonHit::setHit().

6.34.3.40 sqrDist()

```
float AtomProbe::Point3D::sqrDist (
            const Point3D & pt ) const
```

Returns the square of distance to another Point3D.

(X1-X2)^2 + (Y1-Y2)^2 ...

Definition at line 280 of file point3D.cpp.

Referenced by AtomProbe::K3DTreeExact::clearAllTags(), AtomProbe::computeConvexHull(), AtomProbe::computeRotationMatrix(), AtomProbe::distanceToSegment(), AtomProbe::K3DTreeApprox::findKNearest(), AtomProbe::K3DTreeExact::findUntaggedInRadius(), AtomProbe::generate1DAxialDistHist(), AtomProbe::generate1DAxialDistHistSweep(), AtomProbe::BoundCube::getMaxDistanceToBox(), hasNaN(), AtomProbe::incrementDataDistanceWeight(), AtomProbe::BoundCube::intersects(), main(), AtomProbe::signedDistanceToFacet(), AtomProbe::K3DNodeApprox::sqrDist(), and testInexactKDTree().

6.34.3.41 sqrMag()

```
float AtomProbe::Point3D::sqrMag ( ) const
```

Returns magnitude^2, taking this as a position vector.

Definition at line 340 of file point3D.cpp.

Referenced by angle(), AtomProbe::TriangleWithVertexNorm::computeArea(), AtomProbe::computeRotationMatrix(), AtomProbe::distanceToSegment(), extend(), AtomProbe::generate1DAxialDistHist(), getISOSpherical(), hasNaN(), AtomProbe::intersect_RayTriangle(), mag(), main(), normal(), normalise(), orthogonalise(), and AtomProbe::TriangleWithVertexNorm::safeComputeACWNormal().

6.34.3.42 transform3x3()

```
void AtomProbe::Point3D::transform3x3 (
            const gsl_matrix * matrix )
```

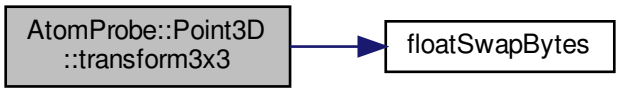
Perform a 3x3 matrix transformation using a GSL matrix.

Definition at line 453 of file point3D.cpp.

References floatSwapBytes().

Referenced by AtomProbe::computeRotationMatrix(), and mag().

Here is the call graph for this function:



6.34.4 Friends And Related Function Documentation

6.34.4.1 operator<<

```
std::ostream& operator<< (
            std::ostream & stream,
            const Point3D & pt )  [friend]
```

Output streaming operator. Streams values in the text format (x,y,z)

Definition at line 425 of file point3D.cpp.

Referenced by hasNaN().

The documentation for this class was generated from the following files:

- include/atomprobe/primitives/point3D.h
- src/primitives/point3D.cpp

6.35 AtomProbe::Point3f Struct Reference

Data storage structure for points.

`#include <quat.h>`

Public Attributes

- float fx
- float fy
- float fz

6.35.1 Detailed Description

Data storage structure for points.

Definition at line 45 of file quat.h.

6.35.2 Member Data Documentation

6.35.2.1 fx

`float AtomProbe::Point3f::fx`

Definition at line 47 of file quat.h.

Referenced by AtomProbe::quat_get_rot_quat(), AtomProbe::quat_pointmult(), AtomProbe::quat_rot(), AtomProbe::quat_rot_apply_quat(), AtomProbe::quat_rot_array(), and AtomProbe::Mesh::rotate().

6.35.2.2 fy

`float AtomProbe::Point3f::fy`

Definition at line 48 of file quat.h.

Referenced by AtomProbe::quat_get_rot_quat(), AtomProbe::quat_pointmult(), AtomProbe::quat_rot(), AtomProbe::quat_rot_apply_quat(), AtomProbe::quat_rot_array(), and AtomProbe::Mesh::rotate().

6.35.2.3 fz

```
float AtomProbe::Point3f::fz
```

Definition at line 49 of file quat.h.

Referenced by AtomProbe::quat_get_rot_quat(), AtomProbe::quat_pointmult(), AtomProbe::quat_rot(), AtomProbe::quat_rot_apply_quat(), AtomProbe::quat_rot_array(), and AtomProbe::Mesh::rotate().

The documentation for this struct was generated from the following file:

- include/atomprobe/helper/maths/quat.h

6.36 AtomProbe::ProgressBar Class Reference

```
#include <progress.h>
```

Public Member Functions

- ProgressBar ()
- ~ProgressBar ()
- void setLength (unsigned int l)

  Set the number of markers in the progress bar.
- void init ()

  Draw the initial progress bar.
- void reset ()

  reset the progress bar internals, in case we want to re-use it
- void update (unsigned int newProgress)

  Draw the progress bar as needed, using the given progress value [0,100].
- void finish ()

  Finalise the progress bar. It is not necessary for the progress to be set to 100%, this is done for you.
- void abort ()

  Abort drawing the progress.

6.36.1 Detailed Description

Definition at line 25 of file progress.h.

6.36.2 Constructor & Destructor Documentation

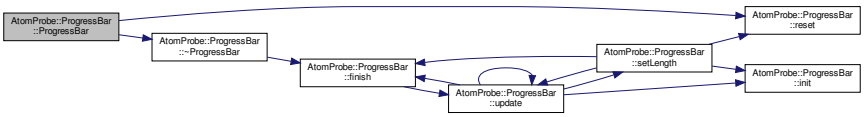
6.36.2.1 ProgressBar()

```
AtomProbe::ProgressBar::ProgressBar ( )  [inline]
```

Definition at line 37 of file progress.h.

References reset(), and ~ProgressBar().

Here is the call graph for this function:



6.36.2.2 ~ProgressBar()

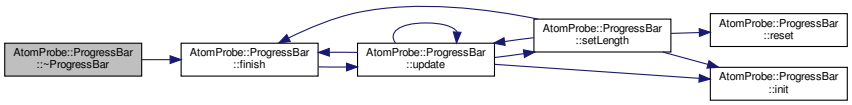
```
AtomProbe::ProgressBar::~ProgressBar ( )
```

Definition at line 29 of file progress.cpp.

References finish().

Referenced by ProgressBar().

Here is the call graph for this function:



6.36.3 Member Function Documentation

6.36.3.1 abort()

```
void AtomProbe::ProgressBar::abort ( )  [inline]
```

Abort drawing the progress.

Definition at line 55 of file progress.h.

6.36.3.2 finish()

```
void AtomProbe::ProgressBar::finish ( )
```

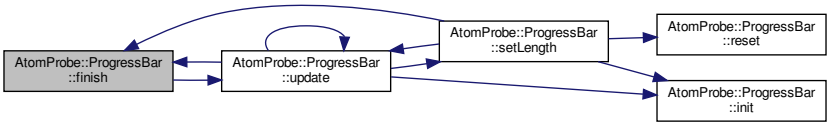
Finalise the progress bar. It is not necessary for the progress to be set to 100%, this is done for you.

Definition at line 52 of file progress.cpp.

References update().

Referenced by main(), setLength(), update(), and ~ProgressBar().

Here is the call graph for this function:



6.36.3.3 init()

```
void AtomProbe::ProgressBar::init ( )
```

Draw the initial progress bar.

Definition at line 35 of file progress.cpp.

Referenced by main(), setLength(), and update().

6.36.3.4 reset()

```
void AtomProbe::ProgressBar::reset ( )
```

reset the progress bar internals, in case we want to re-use it

Definition at line 43 of file progress.cpp.

Referenced by ProgressBar(), and setLength().

6.36.3.5 setLength()

```
void AtomProbe::ProgressBar::setLength (
            unsigned int l )  [inline]
```

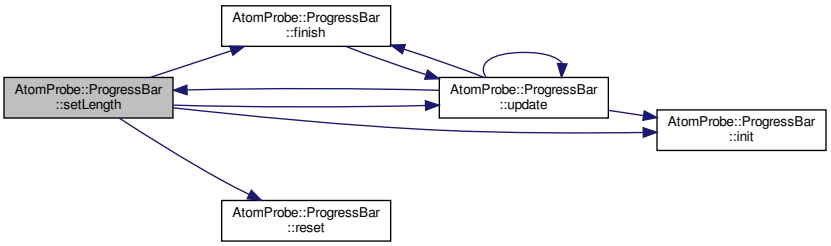
Set the number of markers in the progress bar.

Definition at line 40 of file progress.h.

References finish(), init(), reset(), and update().

Referenced by main(), and update().

Here is the call graph for this function:



6.36.3.6 update()

```
void AtomProbe::ProgressBar::update (
            unsigned int newProgress )
```

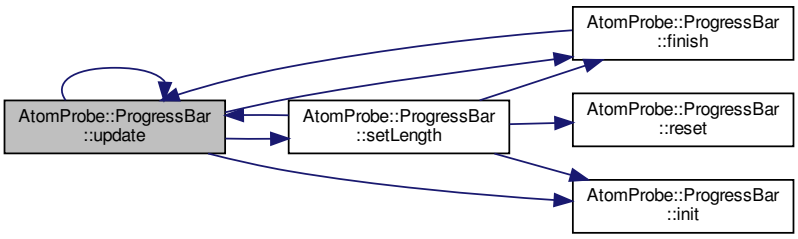
Draw the progress bar as needed, using the given progress value [0,100].

Definition at line 58 of file progress.cpp.

References finish(), init(), progress, setLength(), and update().

Referenced by callback(), finish(), AtomProbe::generate1DAxialDistHistSweep(), main(), setLength(), and update().

Here is the call graph for this function:



The documentation for this class was generated from the following files:

- include/atomprobe/helper/progress.h
- src/helper/progress.cpp

6.37 AtomProbe::Quaternion Struct Reference

Data storage structure for quaternions.

`#include <quat.h>`

Public Attributes

- float a
- float b
- float c
- float d

6.37.1 Detailed Description

Data storage structure for quaternions.

Definition at line 35 of file quat.h.

6.37.2 Member Data Documentation

6.37.2.1 a

`float AtomProbe::Quaternion::a`

Definition at line 37 of file quat.h.

Referenced by AtomProbe::quat_get_rot_quat(), AtomProbe::quat_mult_no_second_a(), AtomProbe::quat_pointmult(), AtomProbe::quat_rot(), and AtomProbe::quat_rot_array().

6.37.2.2 b

`float AtomProbe::Quaternion::b`

Definition at line 38 of file quat.h.

Referenced by AtomProbe::quat_get_rot_quat(), AtomProbe::quat_invert(), AtomProbe::quat_mult_no_second_a(), AtomProbe::quat_pointmult(), AtomProbe::quat_rot(), AtomProbe::quat_rot_apply_quat(), and AtomProbe::quat_rot_array().

6.37.2.3 c

```
float AtomProbe::Quaternion::c
```

Definition at line 39 of file quat.h.

Referenced by AtomProbe::quat_get_rot_quat(), AtomProbe::quat_invert(), AtomProbe::quat_mult_no_second_a(), AtomProbe::quat_pointmult(), AtomProbe::quat_rot(), AtomProbe::quat_rot_apply_quat(), and AtomProbe::quat_↩ rot_array().

6.37.2.4 d

```
float AtomProbe::Quaternion::d
```

Definition at line 40 of file quat.h.

Referenced by AtomProbe::quat_get_rot_quat(), AtomProbe::quat_invert(), AtomProbe::quat_mult_no_second_a(), AtomProbe::quat_pointmult(), AtomProbe::quat_rot(), AtomProbe::quat_rot_apply_quat(), and AtomProbe::quat_↩ rot_array().

The documentation for this struct was generated from the following file:

- include/atomprobe/helper/maths/quat.h

6.38 AtomProbe::RandNumGen Class Reference

```
#include <atomprobe.h>
```

Public Member Functions

- RandNumGen ()
- ∼RandNumGen ()
- gsl_rng ∗ getRng () const

  Obtain a GSL random number generator.

6.38.1 Detailed Description

Library-wide singleton random number source. Uses GSL as backend Defaults to marsenne twister

Definition at line 86 of file atomprobe.h.

6.38.2 Constructor & Destructor Documentation

6.38.2.1 RandNumGen()

```
AtomProbe::RandNumGen::RandNumGen ( )
```

Definition at line 52 of file atomprobe.cpp.

6.38.2.2 ~RandNumGen()

```
AtomProbe::RandNumGen::~RandNumGen ( )
```

Definition at line 63 of file atomprobe.cpp.

6.38.3 Member Function Documentation

6.38.3.1 getRng()

```
gsl_rng* AtomProbe::RandNumGen::getRng ( ) const  [inline]
```

Obtain a GSL random number generator.

Definition at line 95 of file atomprobe.h.

References AtomProbe::libVersion, and AtomProbe::randGen.

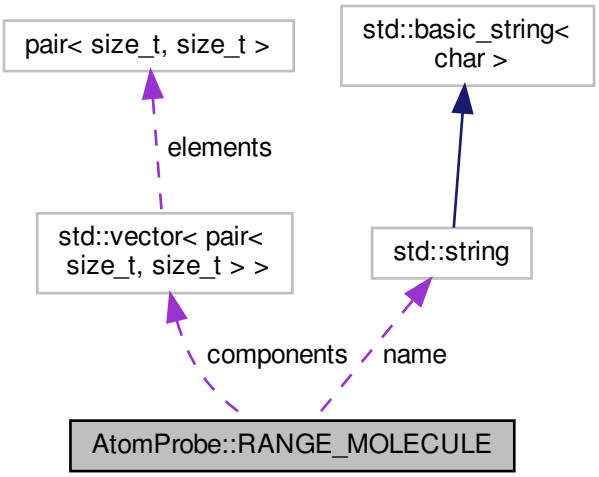
Referenced by AtomProbe::leastSquaresDeconvolve(), AtomProbe::loadATOFile(), AtomProbe::loadPosFile(), main(), AtomProbe::poissonConfidenceObservation(), and AtomProbe::sampleIons().

The documentation for this class was generated from the following files:

- include/atomprobe/atomprobe.h
- src/atomprobe.cpp

6.39 AtomProbe::RANGE_MOLECULE Struct Reference

Collaboration diagram for AtomProbe::RANGE_MOLECULE:



Public Attributes

- bool isOK
- string name
- vector< pair< size_t, size_t > > components

6.39.1 Detailed Description

Definition at line 34 of file rangeCheck.cpp.

6.39.2 Member Data Documentation

6.39.2.1 components

```
vector<pair<size_t,size_t> > AtomProbe::RANGE_MOLECULE::components
```

Definition at line 41 of file rangeCheck.cpp.

Referenced by AtomProbe::checkMassRangingCorrectness(), and AtomProbe::getRangeMolecule().

6.39.2.2 isOK

```
bool AtomProbe::RANGE_MOLECULE::isOK
```

Definition at line 36 of file rangeCheck.cpp.

Referenced by AtomProbe::checkMassRangingCorrectness(), and AtomProbe::getRangeMolecule().

6.39.2.3 name

```
string AtomProbe::RANGE_MOLECULE::name
```

Definition at line 38 of file rangeCheck.cpp.

Referenced by AtomProbe::getRangeMolecule().

The documentation for this struct was generated from the following file:

- src/algorithm/rangeCheck.cpp

6.40 AtomProbe::RangeFile Class Reference

Data storage and retrieval class for various range files.

```
#include <ranges.h>
```

Public Member Functions

- RangeFile ()
- const RangeFile & operator= (const RangeFile &other)
- bool open (const char *rangeFile)

  Open a specified range file - returns true on success.
- unsigned int openFormat (const char *rangeFile, unsigned int format)

  Open a specified range file using a given file format. Returns nonzero on failure.
- bool isSelfConsistent () const

  Performs checks for self consistency.
- bool isSelfConsistent (std::vector< std::string > &consistencyMessages) const

  Performs checks for self consistency, whilst providing information on the inconsistent components.
- bool makeSelfConsistent ()

  Modify range file to ensure self-consistency, by arbitrary heuristics.
- std::string getErrString () const

  Retrieve the translated error associated with the current range file state.
- unsigned int getErrState () const

  Obtain the error state last set for this rangefile.
- unsigned int getNumRanges () const

  Get the number of unique ranges.
- unsigned int getNumRanges (unsigned int ionID) const

Get the number of ranges for a given ion ID.

- unsigned int getNumIons () const

  Get the number of unique ions.
- std::pair< float, float > getRange (unsigned int) const

  Retrieve the start and end of a given range as a pair(start,end)
- std::pair< float, float > & getRangeByRef (unsigned int)

  Retrieve the start and end of a given range as a pair(start,end)
- bool haveRangeVolumes () const

  Return true if we have range volume data, false otherwise.
- float getRangeVolume (unsigned int rangeId) const

  Obtain an ions volume, if we have it. Zero may indicate no ion volume specfied for that range.
- void setRangeVolume (unsigned int rangeId, float newVolume)

  Set the ion volume for a given range. If ion volumes are not tracked, these will be created.
- RGBf getColour (unsigned int) const

  Retrieve a given colour from the ion ID.
- void setColour (unsigned int, const RGBf &r)

  Set the colour using the ion ID.
- unsigned int getIonID (float mass) const

  Retrieve the colour from a given ion ID.
- unsigned int getIonID (const IonHit &hit) const

  Get the ion's ID from a specified mass, using an IonHit.
- unsigned int getIonID (unsigned int range) const

  Get the ion ID from a given range ID.
- unsigned int getIonID (const char *name, bool useShortName=true) const

  Get the ion ID from its short or long name, returns -1 if name does not exist. Case must match.
- unsigned int getIonID (const std::string &name) const
- void setIonID (unsigned int range, unsigned int newIonId)

  Set the ion ID for a given range.
- bool isRanged (float mass) const

  Returns true if a specified mass is ranged.
- bool isRanged (const IonHit &) const

  Returns true if an ion is ranged.
- void range (std::vector< IonHit > &ionHits) const

  Clips out ions that are not inside the rangefile's ranges.
- void rangeInvertable (std::vector< IonHit > &ionHits, bool invert)

  Clips out ions that are inside the rangefile's ranges, if invert is false. If true, then reverse the set.
- bool range (std::vector< IonHit > &ionHits, const std::string &shortIonName)

  Clips out ions that don't match the specified ion name.
- bool rangeByID (std::vector< IonHit > &ionHits, unsigned int range)

  Clips out ions that don't lie in the specified range number.
- void rangeByRangeID (std::vector< IonHit > &ionHits, unsigned int rangeID)

  Range the given ions, allowing only ions in the specified range. Input data will be modified to return result.
- void extractIons (const std::vector< IonHit > &ionHits, const std::vector< unsigned int > &ionIDs, std::vector< IonHit > &hits) const

  Extract ion hit events in the specified ion ID values, from the input ion ionhit sequence.
- std::string getName (unsigned int ionID, bool shortName=true) const

  Get the short name or long name of a specified ionID.
- std::string getName (const IonHit &ion, bool shortName=true) const

  Obtain the short name for a given IonHit. If not ranged, an empty string will be returned.
- void setIonShortName (unsigned int ionID, const std::string &newName)

  set the short name for a given ion

- void setIonLongName (unsigned int ionID, const std::string &newName)

  Set the long name for a given ion.
- bool isRanged (std::string shortName, bool caseSensitive=true)

  Check to see if an atom is ranged.
- unsigned int write (std::ostream &o, size_t format=RANGE_FORMAT_ORNL) const

  Write the rangefile to the specified output stream (default ORNL format)
- unsigned int write (const char *datafile, size_t format=RANGE_FORMAT_ORNL) const

  Write the rangefile to a file (ORNL format)
- unsigned int getRangeID (float mass) const

  Get a range ID from mass to charge.
- void swap (RangeFile &rng)

  Swap a range file with this one.
- bool moveRange (unsigned int range, bool limit, float newMass)

  Move a range's mass to a new location.
- bool moveBothRanges (unsigned int range, float newLow, float newHigh)

  Move both of a range's masses to a new location.
- unsigned int addRange (float start, float end, unsigned int ionID)

  Add a range to the rangefile. Returns ID number of added range.
- unsigned int addIon (const std::string &shortName, const std::string &longName, const RGBf &ionCol)

  Add the ion to the database returns ion ID if successful, -1 otherwise.
- bool setRangeStart (unsigned int rangeID, float v)

  Set the lower bound of the given range.
- bool setRangeEnd (unsigned int rangeID, float v)

  Set the upper bound of the given range.
- void eraseRange (unsigned int rangeId)

  Erase given range - this will reorder rangeIDs, so any ids you had previously will not longer be valid.
- void eraseIon (unsigned int ionId)

  erase given ions and associated ranges)
- bool decomposeIonById (unsigned int ionId, std::vector< std::pair< std::string, size_t > > &fragments) const

  Perform decomposeIonNames(...) for a given ionID.
- bool guessChargeState (unsigned int rangeId, const AtomProbe::AbundanceData &massTable, unsigned int &charge, float tolerance=0.5f) const

  Guess the charge state for the ion that corresponds to the given range's midpoint.

Static Public Member Functions

- static bool extensionIsRange (const char *ext)

  is the extension string the same as that for a range file? I don't advocate this method, but it is convenient in a pinch.
- static void getAllExts (std::vector< std::string > &exts)

  Grab a vector that contains all the extensions that are valid for range files.
- static unsigned int detectFileType (const char *file)

  Attempt to detect the file format of an unknown rangefile.
- static std::string rangeTypeString (unsigned int rangeType)

  Return the human readable name for the given RANGE_FORMAT value.
- static void setEnforceConsistent (bool shouldEnforce=true)

  Set whether the class will attempt to enfore consistency when running.
- static bool decomposeIonNames (const std::string &name, std::vector< std::pair< std::string, size_t > > &fragments)

6.40.1 Detailed Description

Data storage and retrieval class for various range files.

Definition at line 92 of file ranges.h.

6.40.2 Constructor & Destructor Documentation

6.40.2.1 RangeFile()

```
AtomProbe::RangeFile::RangeFile ( )
```

Definition at line 370 of file ranges.cpp.

References ARRAYSIZE, and AtomProbe::RANGE_FORMAT_END_OF_ENUM.

6.40.3 Member Function Documentation

6.40.3.1 addIon()

```
unsigned int AtomProbe::RangeFile::addIon (
            const std::string & shortName,
            const std::string & longName,
            const RGBf & ionCol )
```

Add the ion to the database returns ion ID if successful, -1 otherwise.

Definition at line 3143 of file ranges.cpp.

References ASSERT, and isSelfConsistent().

Referenced by AtomProbe::checkMassRangingCorrectness(), AtomProbe::findOverlaps(), getIonID(), guessChargeState(), and main().

Here is the call graph for this function:

6.40.3.2 addRange()

```
unsigned int AtomProbe::RangeFile::addRange (
            float start,
            float end,
            unsigned int ionID )
```

Add a range to the rangefile. Returns ID number of added range.

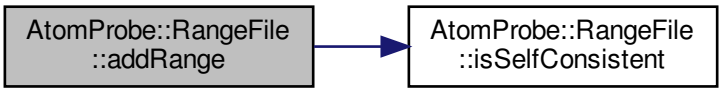
if adding successful, (unsigned int)-1 otherwise. If enforceConsistency is true, this will disallow addition of ranges that collide with existing ranges

Definition at line 3104 of file ranges.cpp.

References ASSERT, and isSelfConsistent().

Referenced by AtomProbe::checkMassRangingCorrectness(), AtomProbe::findOverlaps(), getIonID(), guessChargeState(), and main().

Here is the call graph for this function:



6.40.3.3 decomposeIonById()

```
bool AtomProbe::RangeFile::decomposeIonById (
            unsigned int ionId,
            std::vector< std::pair< std::string, size_t > > & fragments ) const
```

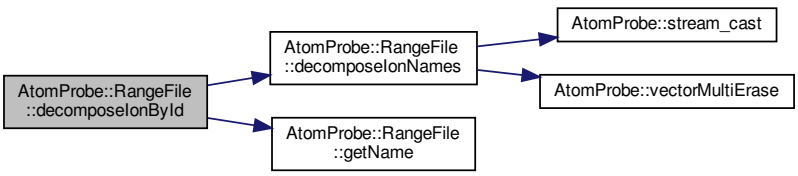
Perform decomposeIonNames(...) for a given ionID.

Definition at line 226 of file ranges.cpp.

References decomposeIonNames(), and getName().

Referenced by AtomProbe::findOverlaps(), and getIonID().

Here is the call graph for this function:



6.40.3.4 decomposeIonNames()

```
bool AtomProbe::RangeFile::decomposeIonNames (
            const std::string & name,
            std::vector< std::pair< std::string, size_t > > & fragments )  [static]
```

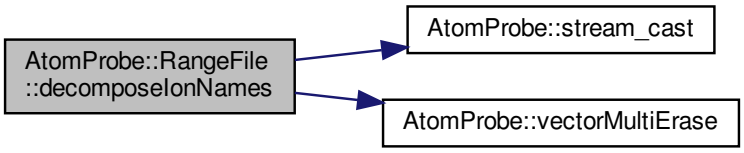
Break a given string down into a series of substring-count pairs depicting basic ionic components returns false if the name cannot be broken down. E.g. H2O will be converted to [{H,2}, {O,1}]

Definition at line 95 of file ranges.cpp.

References AtomProbe::stream_cast(), and AtomProbe::vectorMultiErase().

Referenced by decomposeIonById(), getIonID(), AtomProbe::getRangeMolecule(), guessChargeState(), AtomProbe::matchComposedName(), and AtomProbe::MultiRange::MultiRange().

Here is the call graph for this function:



6.40.3.5 detectFileType()

```
unsigned int AtomProbe::RangeFile::detectFileType (
            const char * file )  [static]
```

Attempt to detect the file format of an unknown rangefile.

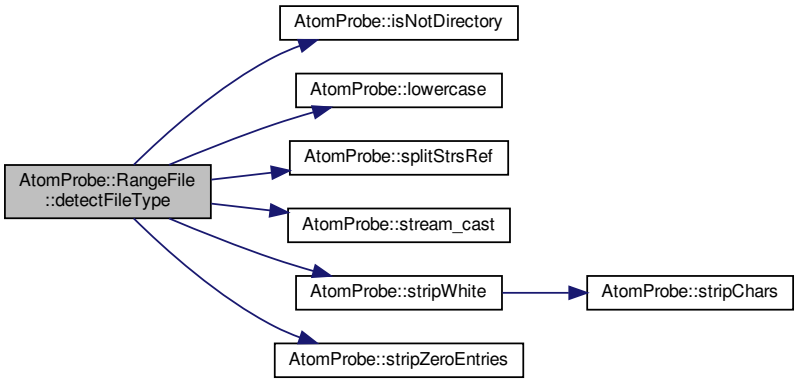
Returns one of RANGE_FORMAT_ enum value on success, or RANGE_FORMAT_END_OF_ENUM on failure

Definition at line 1074 of file ranges.cpp.

References AtomProbe::isNotDirectory(), AtomProbe::lowercase(), AtomProbe::RANGE_FORMAT_DBL_ORNL, AtomProbe::RANGE_FORMAT_END_OF_ENUM, AtomProbe::RANGE_FORMAT_ENV, AtomProbe::RANGE_FORMAT_ORNL, AtomProbe::RANGE_FORMAT_RRNG, AtomProbe::splitStrsRef(), AtomProbe::stream_cast(), AtomProbe::stripWhite(), and AtomProbe::stripZeroEntries().

Referenced by open().

Here is the call graph for this function:



6.40.3.6 eraseIon()

```
void AtomProbe::RangeFile::eraseIon (
            unsigned int ionId )
```

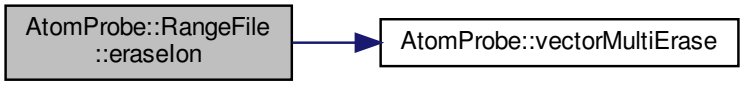
erase given ions and associated ranges)

Definition at line 3183 of file ranges.cpp.

References ASSERT, and AtomProbe::vectorMultiErase().

Referenced by getIonID().

Here is the call graph for this function:



6.40.3.7 eraseRange()

```
void AtomProbe::RangeFile::eraseRange (
            unsigned int rangeId )
```

Erase given range - this will reorder rangeIDs, so any ids you had previously will not longer be valid.

Definition at line 3167 of file ranges.cpp.

References ASSERT.

Referenced by getIonID().

6.40.3.8 extensionIsRange()

```
bool AtomProbe::RangeFile::extensionIsRange (
            const char * ext )  [static]
```

is the extension string the same as that for a range file? I don't advocate this method, but it is convenient in a pinch.

Definition at line 2329 of file ranges.cpp.

6.40.3.9 extractIons()

```
void AtomProbe::RangeFile::extractIons (
            const std::vector< IonHit > & ionHits,
            const std::vector< unsigned int > & ionIDs,
            std::vector< IonHit > & hits ) const
```

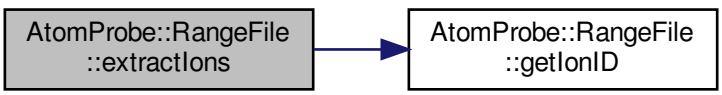
Extract ion hit events in the specified ion ID values, from the input ion ionhit sequence.

Definition at line 2871 of file ranges.cpp.

References getIonID().

Referenced by getIonID().

Here is the call graph for this function:



6.40.3.10 getAllExts()

```
void AtomProbe::RangeFile::getAllExts (
            std::vector< std::string > & exts )  [static]
```

Grab a vector that contains all the extensions that are valid for range files.

Definition at line 2347 of file ranges.cpp.

References ARRAYSIZE, and ASSERT.

6.40.3.11 getColour()

```
RGBf AtomProbe::RangeFile::getColour (
            unsigned int ui ) const
```

Retrieve a given colour from the ion ID.

Definition at line 2774 of file ranges.cpp.

References ASSERT.

Referenced by getErrState(), and AtomProbe::MultiRange::MultiRange().

6.40.3.12 getErrState()

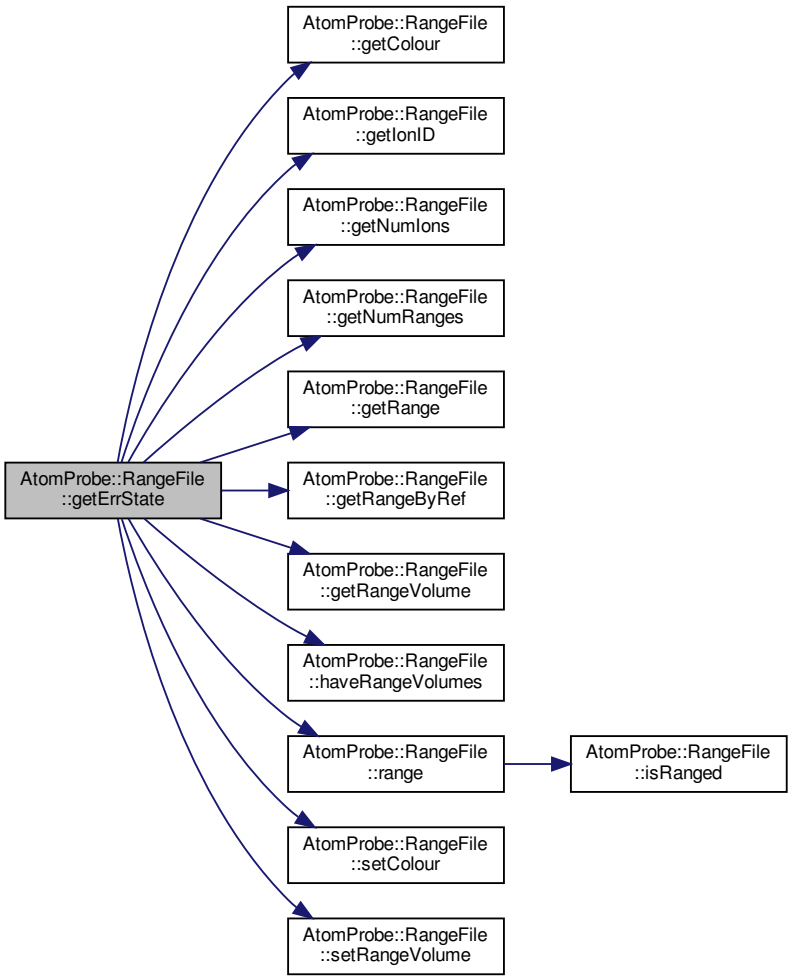
```
unsigned int AtomProbe::RangeFile::getErrState ( ) const  [inline]
```

Obtain the error state last set for this rangefile.

Definition at line 198 of file ranges.h.

References getColour(), getIonID(), getNumIons(), getNumRanges(), getRange(), getRangeByRef(), getRange↩Volume(), haveRangeVolumes(), range(), setColour(), and setRangeVolume().

Here is the call graph for this function:



6.40.3.13 getErrString()

```
std::string AtomProbe::RangeFile::getErrString ( ) const
```

Retrieve the translated error associated with the current range file state.

Definition at line 3219 of file ranges.cpp.

References ARRAYSIZE, and AtomProbe::RANGE_ERR_ENUM_END.

Referenced by main(), and setEnforceConsistent().

6.40.3.14 getIonID() [1/5]

```
unsigned int AtomProbe::RangeFile::getIonID (
            float mass ) const
```

Retrieve the colour from a given ion ID.

Get the ion's ID from a specified mass

Returns the ions ID if there exists a range that contains this mass. Otherwise (unsigned int)-1 is returned

Definition at line 2780 of file ranges.cpp.

Referenced by extractIons(), getErrState(), getIonID(), getName(), getNumRanges(), AtomProbe::getRangeMolecule(), guessChargeState(), main(), AtomProbe::MultiRange::MultiRange(), and open().

6.40.3.15 getIonID() [2/5]

```
unsigned int AtomProbe::RangeFile::getIonID (
            const IonHit & hit ) const
```

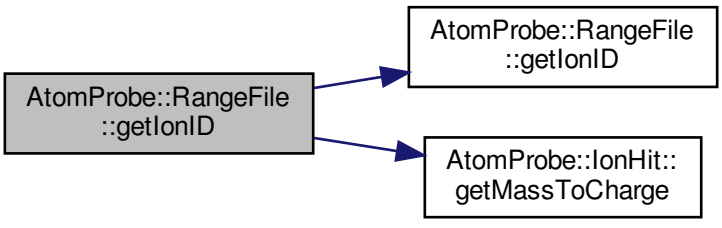
Get the ion's ID from a specified mass, using an IonHit.

Returns the ions ID if there exists a range that contains this mass. Otherwise (unsigned int)-1 is returned

Definition at line 2794 of file ranges.cpp.

References getIonID(), and AtomProbe::IonHit::getMassToCharge().

Here is the call graph for this function:



6.40.3.16 getIonID() [3/5]

```
unsigned int AtomProbe::RangeFile::getIonID (
            unsigned int range ) const
```

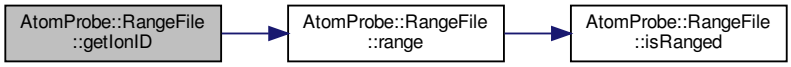
Get the ion ID from a given range ID.

No validation checks are performed outside debug mode. Ion range *must* exist

Definition at line 2814 of file ranges.cpp.

References ASSERT, and range().

Here is the call graph for this function:



6.40.3.17 getIonID() [4/5]

```
unsigned int AtomProbe::RangeFile::getIonID (
            const char * name,
            bool useShortName = true ) const
```

Get the ion ID from its short or long name, returns -1 if name does not exist. Case must match.

Definition at line 2821 of file ranges.cpp.

6.40.3.18 getIonID() [5/5]

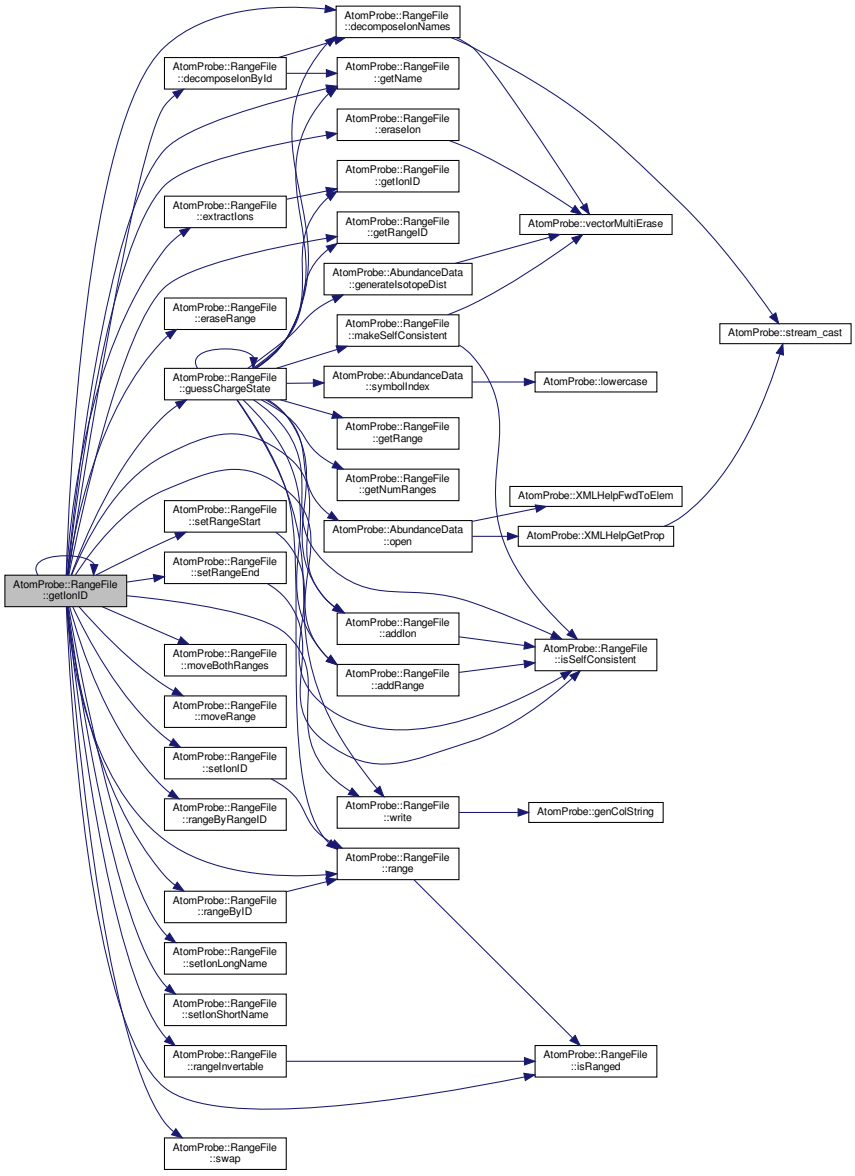
```
unsigned int AtomProbe::RangeFile::getIonID (
            const std::string & name ) const  [inline]
```

Definition at line 248 of file ranges.h.

References addIon(), addRange(), decomposeIonById(), decomposeIonNames(), eraseIon(), eraseRange(), extractIons(), getIonID(), getName(), getRangeID(), guessChargeState(), isRanged(), moveBothRanges(), moveRange(), range(), AtomProbe::RANGE_FORMAT_ORNL, rangeByID(), rangeByRangeID(), rangeInvertable(), setIonID(), setIonLongName(), setIonShortName(), setRangeEnd(), setRangeStart(), swap(), and write().

Referenced by getIonID().

Here is the call graph for this function:



6.40.3.19 getName() [1/2]

```
std::string AtomProbe::RangeFile::getName (
            unsigned int ionID,
            bool shortName = true ) const
```

Get the short name or long name of a specified ionID.

Pass shortname=false to retrieve the long name ionID passed in must exist. No checking outside debug mode

Definition at line 2845 of file ranges.cpp.

References ASSERT.

Referenced by decomposeIonById(), dumpAutocorrelation(), getIonID(), AtomProbe::getRangeMolecule(), guessChargeState(), main(), and AtomProbe::MultiRange::MultiRange().

6.40.3.20 getName() [2/2]

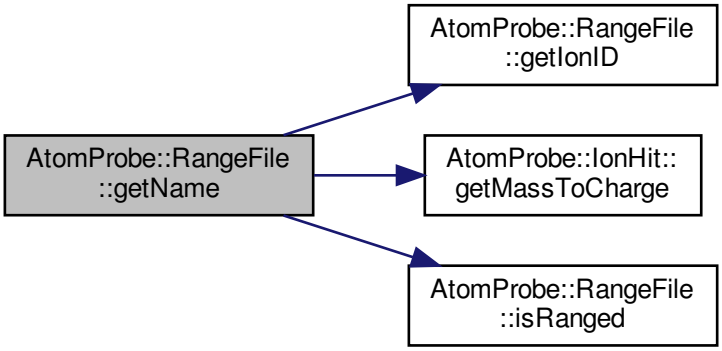
```
std::string AtomProbe::RangeFile::getName (
            const IonHit & ion,
            bool shortName = true ) const
```

Obtain the short name for a given IonHit. If not ranged, an empty string will be returned.

Definition at line 2854 of file ranges.cpp.

References getIonID(), AtomProbe::IonHit::getMassToCharge(), and isRanged().

Here is the call graph for this function:



6.40.3.21 getNumIons()

```
unsigned int AtomProbe::RangeFile::getNumIons ( ) const
```

Get the number of unique ions.

Definition at line 2759 of file ranges.cpp.

Referenced by dumpAutocorrelation(), AtomProbe::findOverlaps(), getErrState(), main(), and AtomProbe::MultiRange::MultiRange().

6.40.3.22 getNumRanges() [1/2]

```
unsigned int AtomProbe::RangeFile::getNumRanges ( ) const
```

Get the number of unique ranges.

Definition at line 2742 of file ranges.cpp.

Referenced by AtomProbe::checkMassRangingCorrectness(), getErrState(), guessChargeState(), AtomProbe::↩ MultiRange::MultiRange(), and open().

6.40.3.23 getNumRanges() [2/2]

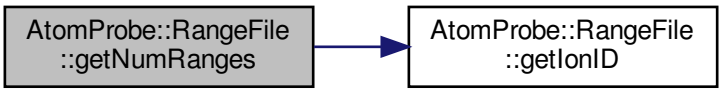
```
unsigned int AtomProbe::RangeFile::getNumRanges (
            unsigned int ionID ) const
```

Get the number of ranges for a given ion ID.

Definition at line 2747 of file ranges.cpp.

References getIonID().

Here is the call graph for this function:



6.40.3.24 getRange()

```
pair< float, float > AtomProbe::RangeFile::getRange (
            unsigned int ui ) const
```

Retrieve the start and end of a given range as a pair(start,end)

Definition at line 2764 of file ranges.cpp.

Referenced by AtomProbe::checkMassRangingCorrectness(), getErrState(), guessChargeState(), AtomProbe::↩ MultiRange::MultiRange(), and open().

6.40.3.25 getRangeByRef()

```
pair< float, float > & AtomProbe::RangeFile::getRangeByRef (
            unsigned int ui )
```

Retrieve the start and end of a given range as a pair(start,end)

Definition at line 2769 of file ranges.cpp.

Referenced by getErrState().

6.40.3.26 getRangeID()

```
unsigned int AtomProbe::RangeFile::getRangeID (
            float mass ) const
```

Get a range ID from mass to charge.

Definition at line 2800 of file ranges.cpp.

Referenced by getIonID(), and guessChargeState().

6.40.3.27 getRangeVolume()

```
float AtomProbe::RangeFile::getRangeVolume (
            unsigned int rangeId ) const
```

Obtain an ions volume, if we have it. Zero may indicate no ion volume specfied for that range.

Definition at line 3285 of file ranges.cpp.

References ASSERT.

Referenced by getErrState().

6.40.3.28 guessChargeState()

```
bool AtomProbe::RangeFile::guessChargeState (
            unsigned int rangeId,
            const AtomProbe::AbundanceData & massTable,
            unsigned int & charge,
            float tolerance = 0.5f ) const
```

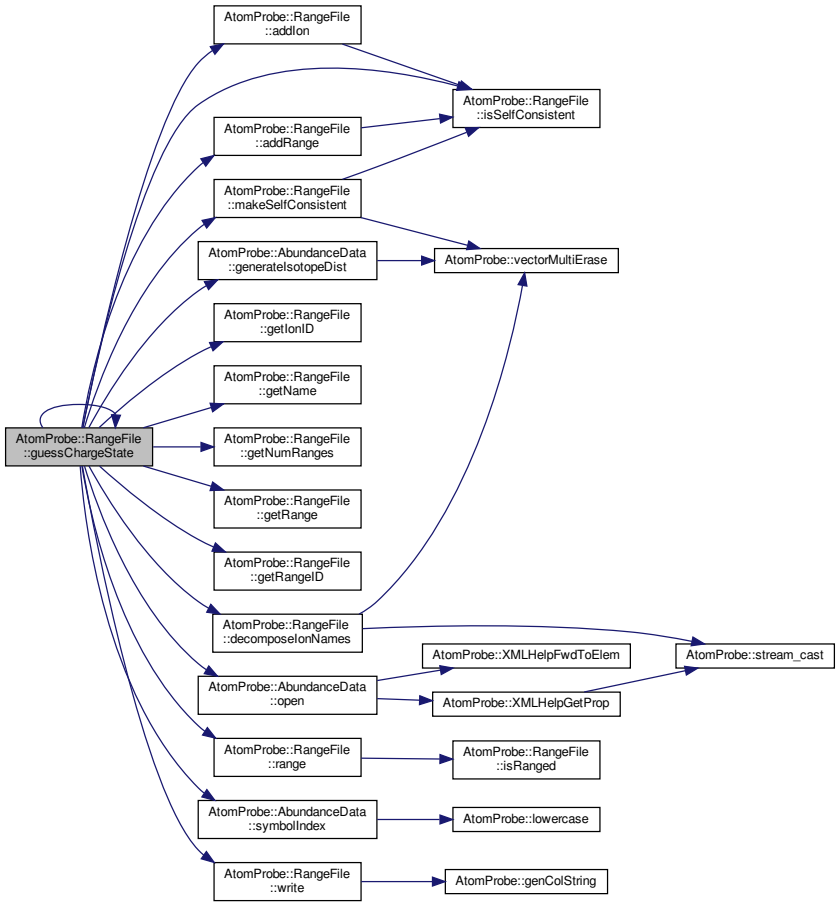
Guess the charge state for the ion that corresponds to the given range's midpoint.

Definition at line 3300 of file ranges.cpp.

References addIon(), addRange(), AtomProbe::RGBf::blue, decomposeIonNames(), AtomProbe::AbundanceData::generateIsotopeDist(), getIonID(), getName(), getNumRanges(), getRange(), getRangeID(), AtomProbe::RGBf::green, guessChargeState(), isSelfConsistent(), makeSelfConsistent(), AtomProbe::AbundanceData::open(), range(), AtomProbe::RANGE_FORMAT_DBL_ORNL, AtomProbe::RANGE_FORMAT_END_OF_ENUM, AtomProbe::RGBf::red, AtomProbe::AbundanceData::symbolIndex(), TEST, and write().

Referenced by getIonID(), guessChargeState(), and main().

Here is the call graph for this function:



6.40.3.29 haveRangeVolumes()

```
bool AtomProbe::RangeFile::haveRangeVolumes ( ) const
```

Return true if we have range volume data, false otherwise.

Definition at line 3295 of file ranges.cpp.

Referenced by getErrState().

6.40.3.30 isRanged() [1/3]

```
bool AtomProbe::RangeFile::isRanged (
            float mass ) const
```

Returns true if a specified mass is ranged.

Definition at line 2609 of file ranges.cpp.

Referenced by getIonID(), getName(), isRanged(), range(), and rangeInvertable().

6.40.3.31 isRanged() [2/3]

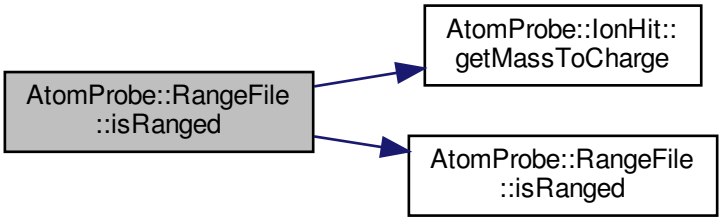
```
bool AtomProbe::RangeFile::isRanged (
            const IonHit & ion ) const
```

Returns true if an ion is ranged.

Definition at line 2623 of file ranges.cpp.

References AtomProbe::IonHit::getMassToCharge(), and isRanged().

Here is the call graph for this function:



6.40.3.32 isRanged() [3/3]

```
bool AtomProbe::RangeFile::isRanged (
            std::string shortName,
            bool caseSensitive = true )
```

Check to see if an atom is ranged.

Returns true if rangefile holds at least one range with shortname corresponding input value. Case sensitivity search is default

Definition at line 2894 of file ranges.cpp.

6.40.3.33 isSelfConsistent() [1/2]

```
bool AtomProbe::RangeFile::isSelfConsistent ( ) const
```

Performs checks for self consistency.

Definition at line 2360 of file ranges.cpp.

References ASSERT.

Referenced by addIon(), addRange(), guessChargeState(), main(), makeSelfConsistent(), open(), openFormat(), runTests(), setEnforceConsistent(), setRangeEnd(), and setRangeStart().

6.40.3.34 isSelfConsistent() [2/2]

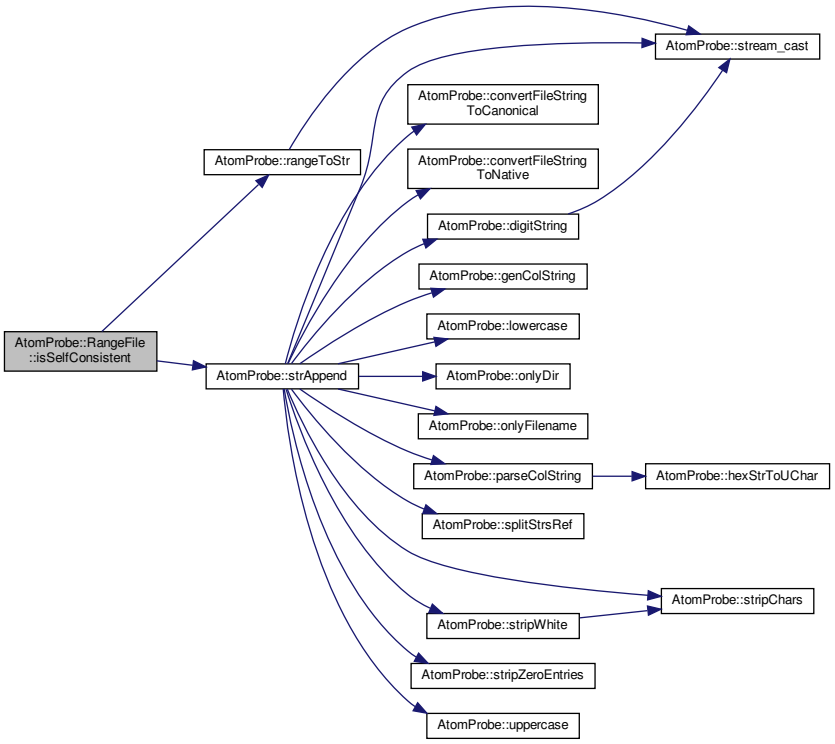
```
bool AtomProbe::RangeFile::isSelfConsistent (
            std::vector< std::string > & consistencyMessages ) const
```

Performs checks for self consistency, whilst providing information on the inconsistent components.

Definition at line 2487 of file ranges.cpp.

References AtomProbe::rangeToStr(), and AtomProbe::strAppend().

Here is the call graph for this function:



6.40.3.35 makeSelfConsistent()

```
bool AtomProbe::RangeFile::makeSelfConsistent ( )
```

Modify range file to ensure self-consistency, by arbitrary heuristics.

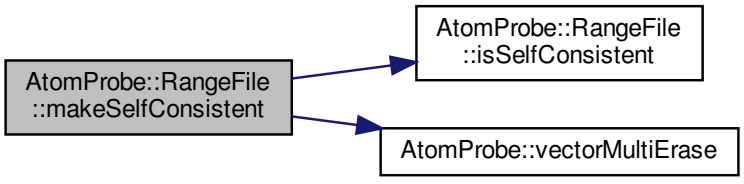
Returns true if self consistant after corrections. false otherwise

Definition at line 2432 of file ranges.cpp.

References isSelfConsistent(), and AtomProbe::vectorMultiErase().

Referenced by guessChargeState(), and setEnforceConsistent().

Here is the call graph for this function:



6.40.3.36 moveBothRanges()

```
bool AtomProbe::RangeFile::moveBothRanges (
            unsigned int range,
            float newLow,
            float newHigh )
```

Move both of a range's masses to a new location.

Definition at line 3066 of file ranges.cpp.

Referenced by AtomProbe::checkMassRangingCorrectness(), and getIonID().

6.40.3.37 moveRange()

```
bool AtomProbe::RangeFile::moveRange (
            unsigned int range,
            bool limit,
            float newMass )
```

Move a range's mass to a new location.

Definition at line 3005 of file ranges.cpp.

Referenced by getIonID().

6.40.3.38 open()

```
bool AtomProbe::RangeFile::open (
            const char * rangeFile )
```

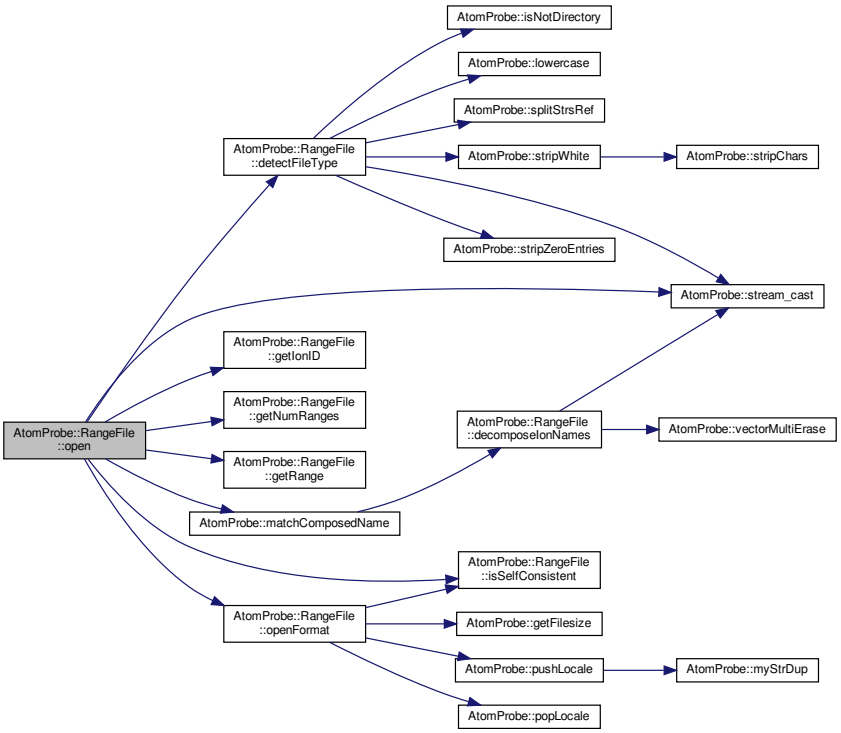
Open a specified range file - returns true on success.

Definition at line 637 of file ranges.cpp.

References ASSERT, AtomProbe::RGBf::blue, detectFileType(), getIonID(), getNumRanges(), getRange(), AtomProbe::RGBf::green, isSelfConsistent(), AtomProbe::matchComposedName(), AtomProbe::MAX_LINE_SIZE, openFormat(), AtomProbe::RANGE_ERR_DASHHEADER, AtomProbe::RANGE_ERR_DATA_NOMAPPED_IONNAME, AtomProbe::RANGE_ERR_FORMAT, AtomProbe::RANGE_ERR_FORMAT_EMPTY_RANGEROW, AtomProbe::RANGE_ERR_FORMAT_TABLESEPARATOR, AtomProbe::RANGE_ERR_NONUNIQUE_POLYATOMIC, AtomProbe::RANGE_FORMAT_END_OF_ENUM, AtomProbe::RGBf::red, and AtomProbe::stream_cast().

Referenced by main(), and runTests().

Here is the call graph for this function:



6.40.3.39 openFormat()

```
unsigned int AtomProbe::RangeFile::openFormat (
            const char * rangeFile,
            unsigned int format )
```

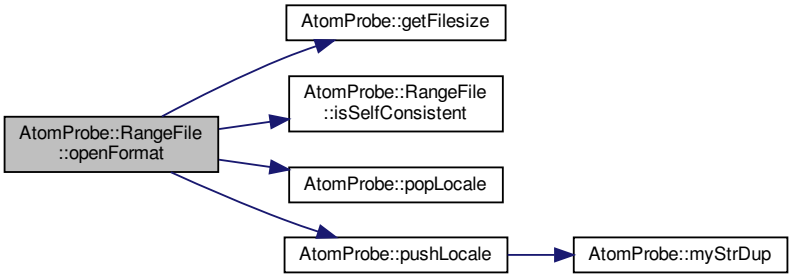
Open a specified range file using a given file format. Returns nonzero on failure.

Definition at line 568 of file ranges.cpp.

References ASSERT, AtomProbe::getFilesize(), isSelfConsistent(), AtomProbe::popLocale(), AtomProbe::pushLocale(), AtomProbe::RANGE_ERR_DATA_INCONSISTENT, AtomProbe::RANGE_ERR_FILESIZE, AtomProbe::RANGE_ERR_FORMAT, AtomProbe::RANGE_ERR_OPEN, AtomProbe::RANGE_FORMAT_DBL_ORNL, AtomProbe::RANGE_FORMAT_ENV, AtomProbe::RANGE_FORMAT_ORNL, and AtomProbe::RANGE_FORMAT_RRNG.

Referenced by open().

Here is the call graph for this function:



6.40.3.40 operator=()

```
const RangeFile & AtomProbe::RangeFile::operator= (
            const RangeFile & other )
```

Definition at line 375 of file ranges.cpp.

6.40.3.41 range() [1/2]

```
void AtomProbe::RangeFile::range (
            std::vector< IonHit > & ionHits ) const
```

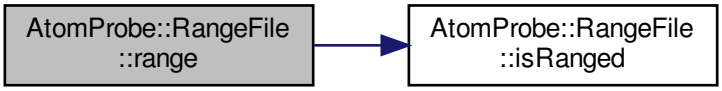
Clips out ions that are not inside the rangefile's ranges.

Definition at line 2679 of file ranges.cpp.

References isRanged().

Referenced by getErrState(), getIonID(), guessChargeState(), main(), rangeByID(), and setIonID().

Here is the call graph for this function:



6.40.3.42 range() [2/2]

```
bool AtomProbe::RangeFile::range (
            std::vector< IonHit > & ionHits,
            const std::string & shortIonName )
```

Clips out ions that don't match the specified ion name.

Returns false if the ion name given doesn't match any in the rangefile (case sensitive)

Definition at line 2628 of file ranges.cpp.

6.40.3.43 rangeByID()

```
bool AtomProbe::RangeFile::rangeByID (
            std::vector< IonHit > & ionHits,
            unsigned int range )
```

Clips out ions that don't lie in the specified range number.

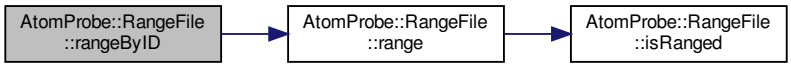
Returns false if the range does not exist any in the rangefile (case sensitive)

Definition at line 2865 of file ranges.cpp.

References range().

Referenced by getIonID().

Here is the call graph for this function:



6.40.3.44 rangeByRangeID()

```
void AtomProbe::RangeFile::rangeByRangeID (
            std::vector< IonHit > & ionHits,
            unsigned int rangeID )
```

Range the given ions, allowing only ions in the specified range. Input data will be modified to return result.

Definition at line 2718 of file ranges.cpp.

Referenced by getIonID().

6.40.3.45 rangeInvertable()

```
void AtomProbe::RangeFile::rangeInvertable (
            std::vector< IonHit > & ionHits,
            bool invert )
```

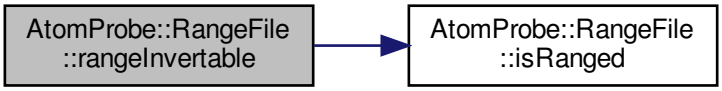
Clips out ions that are inside the rangefile's ranges, if invert is false. If true, then reverse the set.

Definition at line 2699 of file ranges.cpp.

References isRanged(), and XOR.

Referenced by getIonID().

Here is the call graph for this function:



6.40.3.46 rangeTypeString()

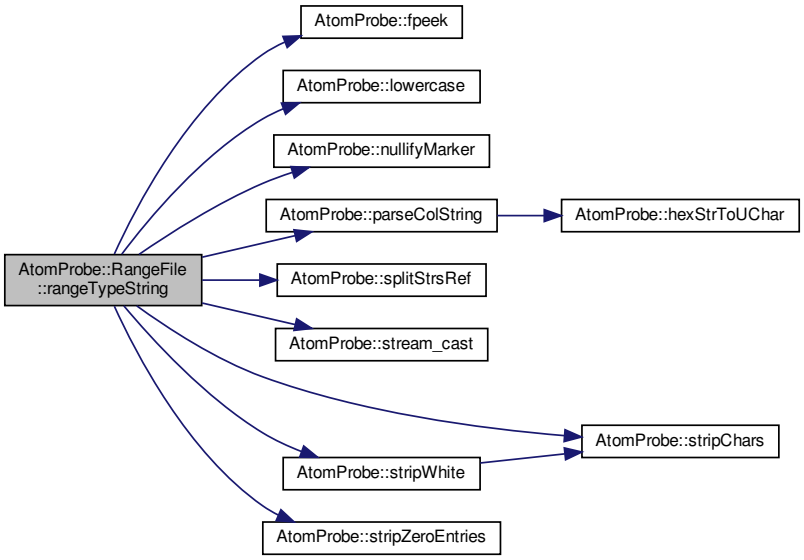
```
string AtomProbe::RangeFile::rangeTypeString (
            unsigned int rangeType )  [static]
```

Return the human readable name for the given RANGE_FORMAT value.

Definition at line 1298 of file ranges.cpp.

References ARRAYSIZE, ASSERT, AtomProbe::RGBf::blue, AtomProbe::fpeek(), AtomProbe::RGBf::green, AtomProbe::lowercase(), AtomProbe::MAX_LINE_SIZE, AtomProbe::nullifyMarker(), AtomProbe::parseColString(), AtomProbe::RANGE_ERR_BAD_MULTIPLICITY, AtomProbe::RANGE_ERR_BADSTART, AtomProbe::RANGE↩_ERR_DATA_FLIPPED, AtomProbe::RANGE_ERR_DATA_TOO_MANY_USELESS_RANGES, AtomProbe::R↩ANGE_ERR_DUPLICATE_NUMRANGES, AtomProbe::RANGE_ERR_EMPTY, AtomProbe::RANGE_ERR_FO↩RMAT, AtomProbe::RANGE_ERR_FORMAT_COLOUR, AtomProbe::RANGE_ERR_FORMAT_HEADER, Atom↩Probe::RANGE_ERR_FORMAT_LONGNAME, AtomProbe::RANGE_ERR_FORMAT_MASS_PAIR, AtomProbe↩::RANGE_ERR_FORMAT_RANGETABLE, AtomProbe::RANGE_ERR_FORMAT_SHORTNAME, AtomProbe↩::RANGE_ERR_FORMAT_TABLE_ENTRY, AtomProbe::RANGE_ERR_FORMAT_TABLEHEADER_NUMIONS, AtomProbe::RANGE_ERR_FORMAT_TABLESEPARATOR, AtomProbe::RANGE_ERR_ION_BLOCK_NOT_P↩RESENT, AtomProbe::RANGE_ERR_ION_NOT_MAPPED, AtomProbe::RANGE_ERR_IONBLOCK_CONTENT, AtomProbe::RANGE_ERR_NUMIONS, AtomProbe::RANGE_ERR_NUMIONS_DUPLICATED, AtomProbe::R↩ANGE_ERR_NUMRANGE_PARSE, AtomProbe::RANGE_ERR_RANGEBLOCK_FORMAT, AtomProbe::RAN↩GE_ERR_RRNG_COLON_SEPARATOR, AtomProbe::RANGE_ERR_RRNG_IONS_TOOSHORT, AtomProbe↩::RANGE_ERR_TOO_MANYIONS, AtomProbe::RANGE_FORMAT_END_OF_ENUM, AtomProbe::RGBf::red, AtomProbe::splitStrsRef(), AtomProbe::stream_cast(), AtomProbe::stripChars(), AtomProbe::stripWhite(), and AtomProbe::stripZeroEntries().

Here is the call graph for this function:



6.40.3.47 setColour()

```
void AtomProbe::RangeFile::setColour (
            unsigned int id,
            const RGBf & r )
```

Set the colour using the ion ID.

Definition at line 2936 of file ranges.cpp.

References ASSERT.

Referenced by getErrState().

6.40.3.48 setEnforceConsistent()

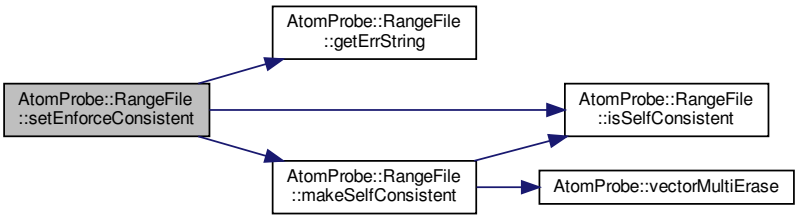
```
static void AtomProbe::RangeFile::setEnforceConsistent (
            bool shouldEnforce = true )  [inline], [static]
```

Set whether the class will attempt to enfore consistency when running.

Definition at line 181 of file ranges.h.

References getErrString(), isSelfConsistent(), and makeSelfConsistent().

Here is the call graph for this function:



6.40.3.49 setIonID()

```
void AtomProbe::RangeFile::setIonID (
            unsigned int range,
            unsigned int newIonId )
```

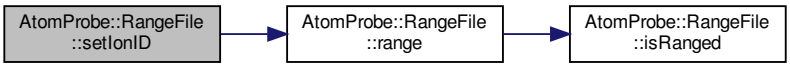
Set the ion ID for a given range.

Definition at line 3161 of file ranges.cpp.

References ASSERT, and range().

Referenced by getIonID().

Here is the call graph for this function:



6.40.3.50 setIonLongName()

```
void AtomProbe::RangeFile::setIonLongName (
            unsigned int ionID,
            const std::string & newName )
```

Set the long name for a given ion.

Definition at line 2948 of file ranges.cpp.

Referenced by getIonID().

6.40.3.51 setIonShortName()

```
void AtomProbe::RangeFile::setIonShortName (
            unsigned int ionID,
            const std::string & newName )
```

set the short name for a given ion

Definition at line 2943 of file ranges.cpp.

Referenced by getIonID().

6.40.3.52 setRangeEnd()

```
bool AtomProbe::RangeFile::setRangeEnd (
            unsigned int rangeID,
            float v )
```

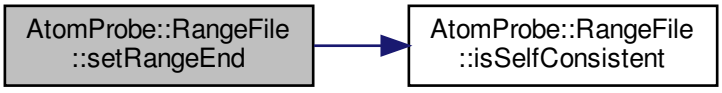
Set the upper bound of the given range.

Definition at line 2973 of file ranges.cpp.

References ASSERT, and isSelfConsistent().

Referenced by getIonID().

Here is the call graph for this function:



6.40.3.53 setRangeStart()

```
bool AtomProbe::RangeFile::setRangeStart (
            unsigned int rangeID,
            float v )
```

Set the lower bound of the given range.

Definition at line 2953 of file ranges.cpp.

References ASSERT, and isSelfConsistent().

Referenced by getIonID().

Here is the call graph for this function:

6.40.3.54 setRangeVolume()

```
void AtomProbe::RangeFile::setRangeVolume (
            unsigned int rangeId,
            float newVolume )
```

Set the ion volume for a given range. If ion volumes are not tracked, these will be created.

Definition at line 3274 of file ranges.cpp.

References ASSERT.

Referenced by getErrState().

6.40.3.55 swap()

```
void AtomProbe::RangeFile::swap (
            RangeFile & rng )
```

Swap a range file with this one.

Definition at line 2993 of file ranges.cpp.

Referenced by getIonID().

6.40.3.56 write() [1/2]

```
unsigned int AtomProbe::RangeFile::write (
            std::ostream & o,
            size_t format = RANGE_FORMAT_ORNL ) const
```

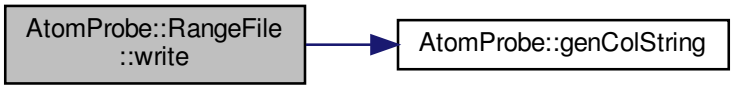
Write the rangefile to the specified output stream (default ORNL format)

Definition at line 396 of file ranges.cpp.

References ASSERT, AtomProbe::genColString(), AtomProbe::RANGE_FORMAT_ENV, AtomProbe::RANGE_F↩ ORMAT_ORNL, and AtomProbe::RANGE_FORMAT_RRNG.

Referenced by getIonID(), guessChargeState(), and write().

Here is the call graph for this function:



6.40.3.57 write() [2/2]

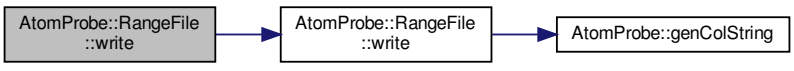
```
unsigned int AtomProbe::RangeFile::write (
            const char * datafile,
            size_t format = RANGE_FORMAT_ORNL ) const
```

Write the rangefile to a file (ORNL format)

Definition at line 547 of file ranges.cpp.

References write().

Here is the call graph for this function:



The documentation for this class was generated from the following files:

- include/atomprobe/io/ranges.h
- src/io/ranges.cpp

6.41 AtomProbe::ReconstructionSphereOnCone Class Reference

`#include <reconstruction-simple.h>`

Public Member Functions

- ReconstructionSphereOnCone ()

  Default constructor.
- void setProjModel (SphericPlaneProjection *model)

  Set a given projection model.
- void setRadiusEvolutionMode (unsigned int evolutionMode)

  Set the method of evolution for the shank, as per EVOLUTION_MODE_ enum.
- void setInitialRadius (float rInit)

  Set the initial tip radius.
- void setShankAngle (float angle)

  Set initial angle, in radiians.
- void setDetectorEfficiency (float detEff)

  Set detector efficiency in range (0,1].
- void setFlightPath (float detEff)

  Set flight path. Units must match detector units (eg mm)
- void setReconFOV (float angle)

  Set the angle (between 0 and pi radiaans). This is.
- bool reconstruct (const std::vector< float > &detectorX, const std::vector< float > &detectorY, const std::vector< float > &timeOfFlight, const std::vector< float > &ionVolume, std::vector< IonHit > &outputPts) const

  Using the current reconstruction model, reconstruct a detector sequence.

6.41.1 Detailed Description

Definition at line 35 of file reconstruction-simple.h.

6.41.2 Constructor & Destructor Documentation

6.41.2.1 ReconstructionSphereOnCone()

`AtomProbe::ReconstructionSphereOnCone::ReconstructionSphereOnCone ( )`

Default constructor.

Definition at line 14 of file reconstruction-simple.cpp.

References AtomProbe::EVOLUTION_MODE_SHANKANGLE.

6.41.3 Member Function Documentation

6.41.3.1 reconstruct()

```
bool AtomProbe::ReconstructionSphereOnCone::reconstruct (
            const std::vector< float > & detectorX,
            const std::vector< float > & detectorY,
            const std::vector< float > & timeOfFlight,
            const std::vector< float > & ionVolume,
            std::vector< IonHit > & outputPts ) const
```

Using the current reconstruction model, reconstruct a detector sequence.

Uses the projection model given in ::setProjModel, to perform the reconstruction

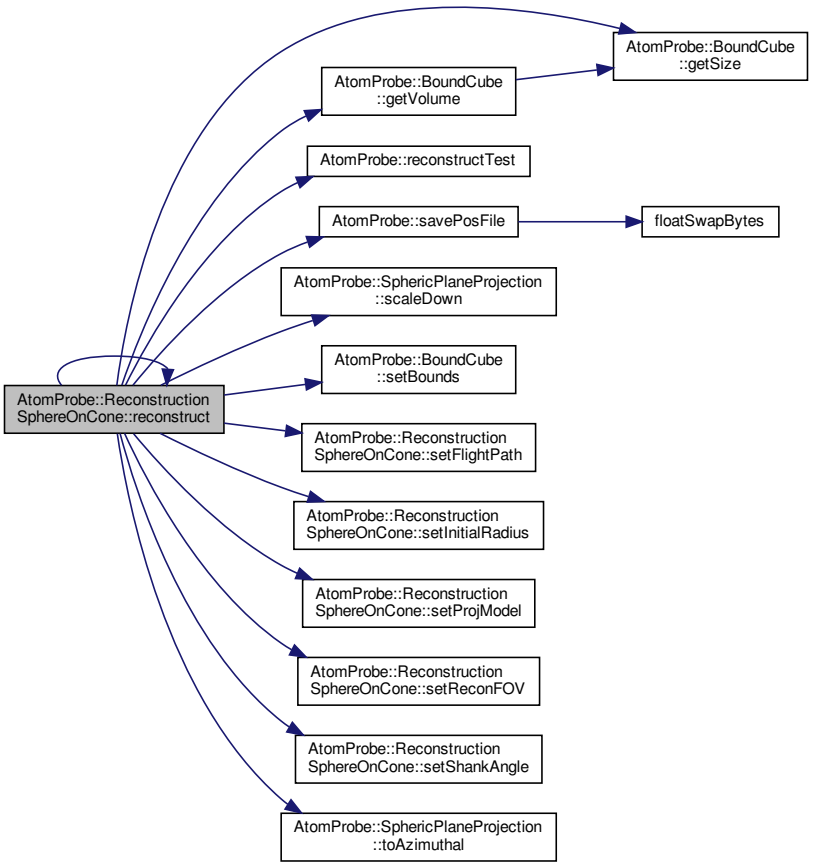
- This is a "shank" reconstruction
- Detector sequence input should typically be centered around 0,0 - automatic recentring may not be desired, so this will not be performed
- Sequence scale should match flight path (e.g. mm)
- Ions may not be reconstructed if outside FOV, so $|\text{outputPts}| < |\text{detector events}|$

Definition at line 62 of file reconstruction-simple.cpp.

References ASSERT, AtomProbe::EVOLUTION_MODE_SHANKANGLE, AtomProbe::BoundCube::getSize(), AtomProbe::BoundCube::getVolume(), M_PI, reconstruct(), AtomProbe::reconstructTest(), AtomProbe::savePos↩File(), AtomProbe::SphericPlaneProjection::scaleDown(), AtomProbe::BoundCube::setBounds(), setFlightPath(), setInitialRadius(), setProjModel(), setReconFOV(), setShankAngle(), TEST, and AtomProbe::SphericPlane↩Projection::toAzimuthal().

Referenced by reconstruct().

Here is the call graph for this function:



6.41.3.2 setDetectorEfficiency()

```
void AtomProbe::ReconstructionSphereOnCone::setDetectorEfficiency (
            float detEff )
```

Set detector efficiency in range (0,1].

Definition at line 31 of file reconstruction-simple.cpp.

References ASSERT.

6.41.3.3 setFlightPath()

```
void AtomProbe::ReconstructionSphereOnCone::setFlightPath (
            float detEff )
```

Set flight path. Units must match detector units (eg mm)

Definition at line 37 of file reconstruction-simple.cpp.

References ASSERT.

Referenced by reconstruct().

6.41.3.4 setInitialRadius()

```
void AtomProbe::ReconstructionSphereOnCone::setInitialRadius (
            float rInit )
```

Set the initial tip radius.

Definition at line 56 of file reconstruction-simple.cpp.

References ASSERT.

Referenced by reconstruct().

6.41.3.5 setProjModel()

```
void AtomProbe::ReconstructionSphereOnCone::setProjModel (
            SphericPlaneProjection * model )
```

Set a given projection model.

Definition at line 21 of file reconstruction-simple.cpp.

Referenced by reconstruct().

6.41.3.6 setRadiusEvolutionMode()

```
void AtomProbe::ReconstructionSphereOnCone::setRadiusEvolutionMode (
            unsigned int evolutionMode )
```

Set the method of evolution for the shank, as per EVOLUTION_MODE_ enum.

Definition at line 26 of file reconstruction-simple.cpp.

6.41.3.7 setReconFOV()

```
void AtomProbe::ReconstructionSphereOnCone::setReconFOV (
            float angle )
```

Set the angle (between 0 and pi radiaans). This is.

Definition at line 43 of file reconstruction-simple.cpp.

References ASSERT, and M_PI.

Referenced by reconstruct().

6.41.3.8 setShankAngle()

```
void AtomProbe::ReconstructionSphereOnCone::setShankAngle (
            float angle )
```

Set initial angle, in radiians.

Definition at line 49 of file reconstruction-simple.cpp.

References ASSERT, and M_PI.

Referenced by reconstruct().

The documentation for this class was generated from the following files:

- include/atomprobe/reconstruction/reconstruction-simple.h
- src/reconstruction/reconstruction-simple.cpp

6.42 AtomProbe::RGBf Class Reference

Data holder for colour as float.

```
#include <misc.h>
```

Public Member Functions

- std::string toHex () const

  Convert to hex-256 representation #rrggbb.
- void fromHex (const std::string &s)

Public Attributes

- float red
- float green
- float blue

6.42.1 Detailed Description

Data holder for colour as float.

Definition at line 26 of file misc.h.

6.42.2 Member Function Documentation

6.42.2.1 fromHex()

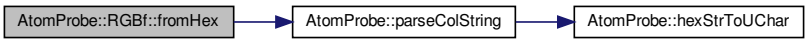
```
void AtomProbe::RGBf::fromHex (
            const std::string & s )  [inline]
```

Definition at line 40 of file misc.h.

References AtomProbe::parseColString().

Referenced by AtomProbe::MultiRange::copyDataFromRange().

Here is the call graph for this function:



6.42.2.2 toHex()

```
std::string AtomProbe::RGBf::toHex ( ) const  [inline]
```

Convert to hex-256 representation #rrggbb.

Definition at line 34 of file misc.h.

References AtomProbe::genColString().

Here is the call graph for this function:

6.42.3 Member Data Documentation

6.42.3.1 blue

```
float AtomProbe::RGBf::blue
```

Definition at line 31 of file misc.h.

Referenced by AtomProbe::checkMassRangingCorrectness(), AtomProbe::computeRangeAdjacency(), AtomProbe::MultiRange::copyDataFromRange(), AtomProbe::findOverlaps(), AtomProbe::RangeFile::guessChargeState(), AtomProbe::leastSquaresDeconvolve(), main(), AtomProbe::MultiRange::open(), AtomProbe::RangeFile::open(), and AtomProbe::RangeFile::rangeTypeString().

6.42.3.2 green

```
float AtomProbe::RGBf::green
```

Definition at line 30 of file misc.h.

Referenced by AtomProbe::checkMassRangingCorrectness(), AtomProbe::computeRangeAdjacency(), AtomProbe::MultiRange::copyDataFromRange(), AtomProbe::findOverlaps(), AtomProbe::RangeFile::guessChargeState(), AtomProbe::leastSquaresDeconvolve(), main(), AtomProbe::MultiRange::open(), AtomProbe::RangeFile::open(), and AtomProbe::RangeFile::rangeTypeString().

6.42.3.3 red

```
float AtomProbe::RGBf::red
```

Definition at line 29 of file misc.h.

Referenced by AtomProbe::checkMassRangingCorrectness(), AtomProbe::computeRangeAdjacency(), AtomProbe::MultiRange::copyDataFromRange(), AtomProbe::findOverlaps(), AtomProbe::RangeFile::guessChargeState(), AtomProbe::leastSquaresDeconvolve(), main(), AtomProbe::MultiRange::open(), AtomProbe::RangeFile::open(), and AtomProbe::RangeFile::rangeTypeString().

The documentation for this class was generated from the following file:

- include/atomprobe/helper/misc.h

6.43 AtomProbe::SIMPLE_SPECIES Struct Reference

```
#include <multiRange.h>
```

Public Member Functions

- bool operator== (const SIMPLE_SPECIES &oth) const

Public Attributes

- unsigned int atomicNumber

  Number of protons (element number)
- unsigned int count

  Number of copies of this isotope.

6.43.1 Detailed Description

Definition at line 34 of file multiRange.h.

6.43.2 Member Function Documentation

6.43.2.1 operator==()

```
bool AtomProbe::SIMPLE_SPECIES::operator== (
            const SIMPLE_SPECIES & oth ) const
```

Definition at line 112 of file multiRange.cpp.

References atomicNumber, and count.

6.43.3 Member Data Documentation

6.43.3.1 atomicNumber

```
unsigned int AtomProbe::SIMPLE_SPECIES::atomicNumber
```

Number of protons (element number)

Definition at line 37 of file multiRange.h.

Referenced by AtomProbe::computeRangeAdjacency(), AtomProbe::MultiRange::copyDataFromRange(), AtomProbe::leastSquaresDeconvolve(), AtomProbe::MultiRange::MultiRange(), AtomProbe::MultiRange::open(), AtomProbe::operator<(), and operator==().

6.43.3.2 count

```
unsigned int AtomProbe::SIMPLE_SPECIES::count
```

Number of copies of this isotope.

Definition at line 40 of file multiRange.h.

Referenced by AtomProbe::computeRangeAdjacency(), AtomProbe::MultiRange::copyDataFromRange(), AtomProbe::leastSquaresDeconvolve(), AtomProbe::MultiRange::MultiRange(), AtomProbe::MultiRange::open(), AtomProbe::operator<(), and operator==().

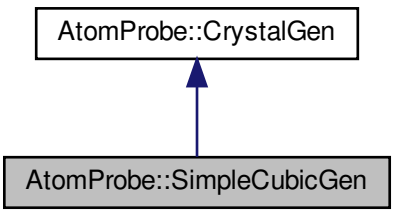
The documentation for this struct was generated from the following files:

- include/atomprobe/io/multiRange.h
- src/io/multiRange.cpp

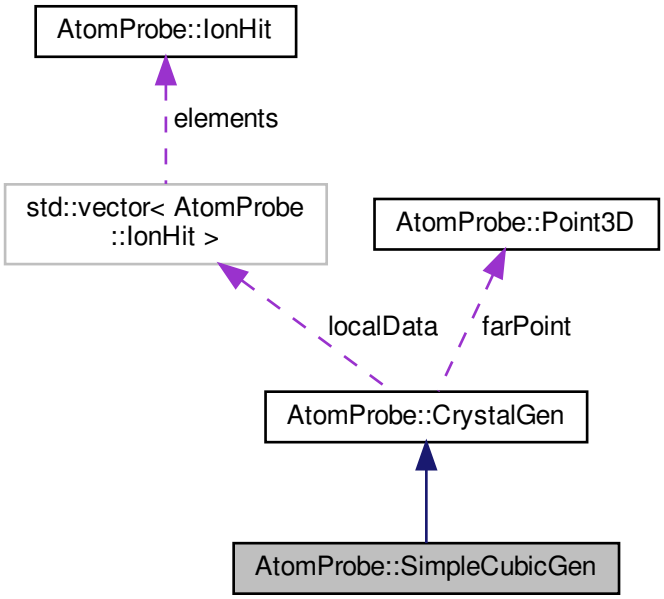
6.44 AtomProbe::SimpleCubicGen Class Reference

```
#include <generate.h>
```

Inheritance diagram for AtomProbe::SimpleCubicGen:



Collaboration diagram for AtomProbe::SimpleCubicGen:



Public Member Functions

- SimpleCubicGen (float latticeSpacing, float massToC, const Point3D &p)
- unsigned int generateLattice ()

Additional Inherited Members

6.44.1 Detailed Description

Definition at line 40 of file generate.h.

6.44.2 Constructor & Destructor Documentation

6.44.2.1 SimpleCubicGen()

```
AtomProbe::SimpleCubicGen::SimpleCubicGen (
            float latticeSpacing,
            float massToC,
            const Point3D & p )
```

Definition at line 46 of file generate.cpp.

References AtomProbe::CrystalGen::farPoint.

6.44.3 Member Function Documentation

6.44.3.1 generateLattice()

```
unsigned int AtomProbe::SimpleCubicGen::generateLattice ( )  [virtual]
```

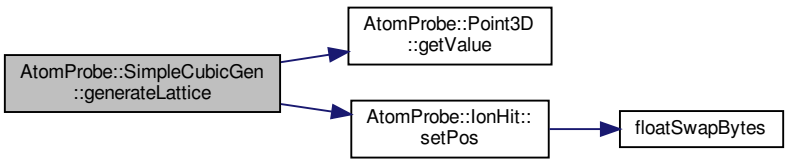
Implements AtomProbe::CrystalGen.

Definition at line 53 of file generate.cpp.

References AtomProbe::CRYSTAL_BAD_UNIT_CELL, AtomProbe::CrystalGen::farPoint, AtomProbe::Point3D::getValue(), AtomProbe::CrystalGen::localData, and AtomProbe::IonHit::setPos().

Referenced by AtomProbe::BodyCentredCubicGen::generateLattice().

Here is the call graph for this function:



The documentation for this class was generated from the following files:

- include/atomprobe/latticeplanes/generate.h
- src/lattice/generate.cpp

6.45 AtomProbe::SINGLE_HIT Struct Reference

Single 3DAP hit event.

```
#include <dataFiles.h>
```

Public Attributes

- float x

  Position on the detector.
- float y
- float tof

  Reported time of flight.

6.45.1 Detailed Description

Single 3DAP hit event.

Definition at line 197 of file dataFiles.h.

6.45.2 Member Data Documentation

6.45.2.1 tof

```
float AtomProbe::SINGLE_HIT::tof
```

Reported time of flight.

Definition at line 202 of file dataFiles.h.

Referenced by AtomProbe::readPosapOps().

6.45.2.2 x

```
float AtomProbe::SINGLE_HIT::x
```

Position on the detector.

Definition at line 200 of file dataFiles.h.

6.45.2.3 y

```
float AtomProbe::SINGLE_HIT::y
```

Definition at line 200 of file dataFiles.h.

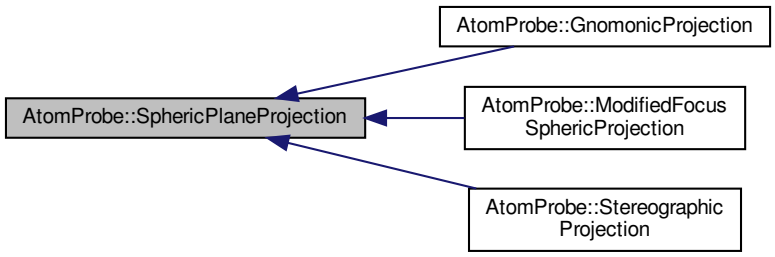
The documentation for this struct was generated from the following file:

- include/atomprobe/io/dataFiles.h

6.46 AtomProbe::SphericPlaneProjection Class Reference

`#include <projection.h>`

Inheritance diagram for AtomProbe::SphericPlaneProjection:



Public Member Functions

- virtual bool toAzimuthal (float fx, float fy, float &theta, float &phi) const =0
  Convert from plane coordinates to projection coords.
- virtual bool toPlanar (float theta, float phi, float &fx, float &fy) const =0
  Convert from spherical planar coordinates to projection coords.
- virtual void scaleDown (float flightLength, float detX, float detY, float &scaledX, float &scaledY) const =0
  Convert from actual detector postion (eg. mm) and flight path to scaled-down transform.
- virtual void scaleUp (float flightLength, float scaledX, float scaledY, float &realX, float &realY) const =0
  Convert from scaled-down coordinates to actual size.

6.46.1 Detailed Description

Definition at line 20 of file projection.h.

6.46.2 Member Function Documentation

6.46.2.1 scaleDown()

```
virtual void AtomProbe::SphericPlaneProjection::scaleDown (
            float flightLength,
            float detX,
            float detY,
            float & scaledX,
            float & scaledY ) const  [pure virtual]
```

Convert from actual detector postion (eg. mm) and flight path to scaled-down transform.

Implemented in AtomProbe::ModifiedFocusSphericProjection, AtomProbe::StereographicProjection, and AtomProbe::GnomonicProjection.

Referenced by AtomProbe::ReconstructionSphereOnCone::reconstruct().

6.46.2.2 scaleUp()

```
virtual void AtomProbe::SphericPlaneProjection::scaleUp (
            float flightLength,
            float scaledX,
            float scaledY,
            float & realX,
            float & realY ) const  [pure virtual]
```

Convert from scaled-down coordinates to actual size.

Implemented in AtomProbe::ModifiedFocusSphericProjection, AtomProbe::StereographicProjection, and AtomProbe::GnomonicProjection.

6.46.2.3 toAzimuthal()

```
virtual bool AtomProbe::SphericPlaneProjection::toAzimuthal (
            float fx,
            float fy,
            float & theta,
            float & phi ) const  [pure virtual]
```

Convert from plane coordinates to projection coords.

- Returns false if transform is not possible

Implemented in AtomProbe::ModifiedFocusSphericProjection, AtomProbe::StereographicProjection, and AtomProbe::GnomonicProjection.

Referenced by AtomProbe::ReconstructionSphereOnCone::reconstruct().

6.46.2.4 toPlanar()

```
virtual bool AtomProbe::SphericPlaneProjection::toPlanar (
            float theta,
            float phi,
            float & fx,
            float & fy ) const  [pure virtual]
```

Convert from spherical planar coordinates to projection coords.

Implemented in AtomProbe::ModifiedFocusSphericProjection, AtomProbe::StereographicProjection, and AtomProbe::GnomonicProjection.

The documentation for this class was generated from the following file:

- include/atomprobe/projection/projection.h

6.47 AtomProbe::SphericProjectionParams Struct Reference

Public Attributes

- double theta
- double focusDist

6.47.1 Detailed Description

Definition at line 19 of file projection.cpp.

6.47.2 Member Data Documentation

6.47.2.1 focusDist

```
double AtomProbe::SphericProjectionParams::focusDist
```

Definition at line 22 of file projection.cpp.

Referenced by AtomProbe::ModifiedFocusSphericProjection::etaToTheta(), AtomProbe::ModifiedFocusSpheric↩ Projection::getFOVRadius(), AtomProbe::ModifiedFocusSphericProjection::getMaxFOV(), AtomProbe::Modified↩ FocusSphericProjection::scaleDown(), AtomProbe::ModifiedFocusSphericProjection::scaleUp(), AtomProbe::↩ ModifiedFocusSphericProjection::setFocus(), AtomProbe::SphericProjectionEqn(), AtomProbe::Stereographic↩ Projection::thetaToEta(), AtomProbe::ModifiedFocusSphericProjection::thetaToEta(), and AtomProbe::Modified↩ FocusSphericProjection::toAzimuthal().

6.47.2.2 theta

```
double AtomProbe::SphericProjectionParams::theta
```

Definition at line 21 of file projection.cpp.

Referenced by AtomProbe::ModifiedFocusSphericProjection::getFOVRadius(), AtomProbe::ModifiedFocus↩ SphericProjection::scaleUp(), AtomProbe::SphericProjectionEqn(), AtomProbe::StereographicProjection::theta↩ ToEta(), and AtomProbe::ModifiedFocusSphericProjection::thetaToEta().

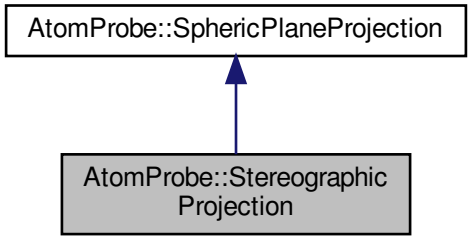
The documentation for this struct was generated from the following file:

- src/projection/projection.cpp

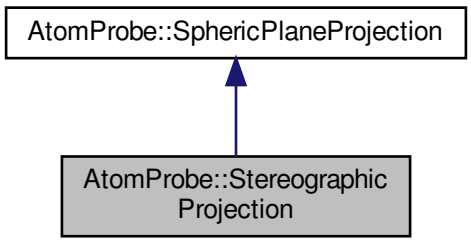
6.48 AtomProbe::StereographicProjection Class Reference

`#include <projection.h>`

Inheritance diagram for AtomProbe::StereographicProjection:



Collaboration diagram for AtomProbe::StereographicProjection:



Public Member Functions

- virtual bool toAzimuthal (float fx, float fy, float &theta, float &phi) const

  Convert from plane coordinates to stereographic (NOT SPHERICAL) coords.
- virtual bool toPlanar (float theta, float phi, float &fx, float &fy) const

  Convert from stereographic (NOT SPHERICAL) coordinates to plane.
- virtual void scaleDown (float flightLength, float detX, float detY, float &scaledX, float &scaledY) const

  Convert from actual detector postion (eg. mm) and flight path to scaled-down transform.
- virtual void scaleUp (float flightLength, float scaledX, float scaledY, float &realX, float &realY) const

  Convert from scaled-down radius to actual radius.

Static Public Member Functions

- static float thetaToEta (float theta)

  Convert azimuthal angle to spherical. See etaToTheta for description.

6.48.1 Detailed Description

Definition at line 68 of file projection.h.

6.48.2 Member Function Documentation

6.48.2.1 scaleDown()

```
void AtomProbe::StereographicProjection::scaleDown (
            float flightLength,
            float detX,
            float detY,
            float & scaledX,
            float & scaledY ) const  [virtual]
```

Convert from actual detector postion (eg. mm) and flight path to scaled-down transform.

Implements AtomProbe::SphericPlaneProjection.

Definition at line 119 of file projection.cpp.

References ASSERT.

6.48.2.2 scaleUp()

```
void AtomProbe::StereographicProjection::scaleUp (
            float flightLength,
            float scaledX,
            float scaledY,
            float & realX,
            float & realY ) const  [virtual]
```

Convert from scaled-down radius to actual radius.

Implements AtomProbe::SphericPlaneProjection.

Definition at line 130 of file projection.cpp.

References ASSERT.

6.48.2.3 thetaToEta()

```
float AtomProbe::StereographicProjection::thetaToEta (
            float theta )  [static]
```

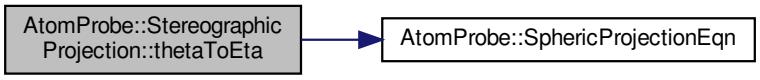
Convert azimuthal angle to spherical. See etaToTheta for description.

-input range is limited to [0,90)

Definition at line 158 of file projection.cpp.

References AtomProbe::SphericProjectionParams::focusDist, M_PI, AtomProbe::SphericProjectionEqn(), and AtomProbe::SphericProjectionParams::theta.

Here is the call graph for this function:



6.48.2.4 toAzimuthal()

```
bool AtomProbe::StereographicProjection::toAzimuthal (
            float fx,
            float fy,
            float & theta,
            float & phi ) const  [virtual]
```

Convert from plane coordinates to stereographic (NOT SPHERICAL) coords.

Implements AtomProbe::SphericPlaneProjection.

Definition at line 141 of file projection.cpp.

6.48.2.5 toPlanar()

```
bool AtomProbe::StereographicProjection::toPlanar (
            float theta,
            float phi,
            float & fx,
            float & fy ) const  [virtual]
```

Convert from stereographic (NOT SPHERICAL) coordinates to plane.

Implements AtomProbe::SphericPlaneProjection.

Definition at line 107 of file projection.cpp.

The documentation for this class was generated from the following files:

- include/atomprobe/projection/projection.h
- src/projection/projection.cpp

6.49 AtomProbe::TETRAHEDRON Class Reference

`#include <mesh.h>`

Public Attributes

- unsigned int p [4]
- unsigned int physGroup

6.49.1 Detailed Description

Definition at line 51 of file mesh.h.

6.49.2 Member Data Documentation

6.49.2.1 p

`unsigned int AtomProbe::TETRAHEDRON::p[4]`

Definition at line 53 of file mesh.h.

Referenced by AtomProbe::Mesh::loadGmshMesh().

6.49.2.2 physGroup

`unsigned int AtomProbe::TETRAHEDRON::physGroup`

Definition at line 54 of file mesh.h.

Referenced by AtomProbe::Mesh::loadGmshMesh().

The documentation for this class was generated from the following file:

- include/atomprobe/primitives/mesh.h

6.50 AtomProbe::THREEDAP_DATA Struct Reference

experimental setup data

`#include <dataFiles.h>`

Public Attributes

- float flightPath

  The flight path to the virtual (or real) projected tip image.
- float alpha

  Pulse coupling coefficient (1 of 2)
- float beta

  Pulse coupling coefficient (2 of 2)
- float tZero

  Time offset for pulse, in nanoseconds.
- float detectorRadius

  The size of the detector, in mm.
- unsigned int detectorChannels

  The number of channels on the detector.

6.50.1 Detailed Description

experimental setup data

Definition at line 222 of file dataFiles.h.

6.50.2 Member Data Documentation

6.50.2.1 alpha

```
float AtomProbe::THREEDAP_DATA::alpha
```

Pulse coupling coefficient (1 of 2)

Definition at line 227 of file dataFiles.h.

Referenced by AtomProbe::readPosapOps().

6.50.2.2 beta

```
float AtomProbe::THREEDAP_DATA::beta
```

Pulse coupling coefficient (2 of 2)

Definition at line 229 of file dataFiles.h.

Referenced by AtomProbe::readPosapOps().

6.50.2.3 detectorChannels

```
unsigned int AtomProbe::THREEDAP_DATA::detectorChannels
```

The number of channels on the detector.

Definition at line 235 of file dataFiles.h.

Referenced by AtomProbe::readPosapOps().

6.50.2.4 detectorRadius

```
float AtomProbe::THREEDAP_DATA::detectorRadius
```

The size of the detector, in mm.

Definition at line 233 of file dataFiles.h.

Referenced by AtomProbe::readPosapOps().

6.50.2.5 flightPath

```
float AtomProbe::THREEDAP_DATA::flightPath
```

The flight path to the virtual (or real) projected tip image.

Definition at line 225 of file dataFiles.h.

Referenced by AtomProbe::readPosapOps().

6.50.2.6 tZero

```
float AtomProbe::THREEDAP_DATA::tZero
```

Time offset for pulse, in nanoseconds.

Definition at line 231 of file dataFiles.h.

Referenced by AtomProbe::readPosapOps().

The documentation for this struct was generated from the following file:

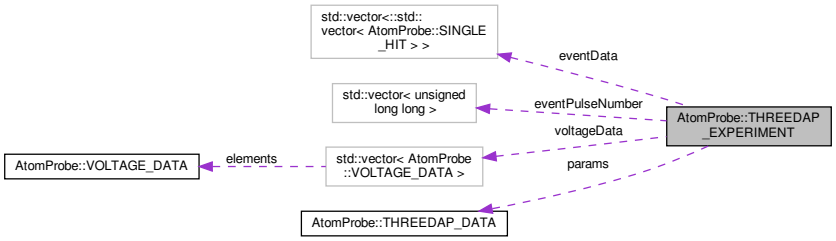
- include/atomprobe/io/dataFiles.h

6.51 AtomProbe::THREEDAP_EXPERIMENT Struct Reference

Data structure that contains the experiment information present in a 3Dap file.

`#include <dataFiles.h>`

Collaboration diagram for AtomProbe::THREEDAP_EXPERIMENT:



Public Attributes

- THREEDAP_DATA params
  Experiment parameters.
- std::vector<::std::vector< SINGLE_HIT > > eventData
  vector of event vectors. Each interior event vector describes a group of hits on one pulse
- std::vector< VOLTAGE_DATA > voltageData
  Voltage information.
- std::vector< unsigned long long > eventPulseNumber
  The pulse number associated with an event group.

6.51.1 Detailed Description

Data structure that contains the experiment information present in a 3Dap file.

Definition at line 239 of file dataFiles.h.

6.51.2 Member Data Documentation

6.51.2.1 eventData

`std::vector<::std::vector<SINGLE_HIT> > AtomProbe::THREEDAP_EXPERIMENT::eventData`

vector of event vectors. Each interior event vector describes a group of hits on one pulse

Definition at line 244 of file dataFiles.h.

Referenced by AtomProbe::readPosapOps().

6.51.2.2 eventPulseNumber

```
std::vector<unsigned long long> AtomProbe::THREEDAP_EXPERIMENT::eventPulseNumber
```

The pulse number associated with an event group.

Definition at line 248 of file dataFiles.h.

Referenced by AtomProbe::readPosapOps().

6.51.2.3 params

```
THREEDAP_DATA AtomProbe::THREEDAP_EXPERIMENT::params
```

Experiment parameters.

Definition at line 242 of file dataFiles.h.

Referenced by AtomProbe::readPosapOps().

6.51.2.4 voltageData

```
std::vector<VOLTAGE_DATA> AtomProbe::THREEDAP_EXPERIMENT::voltageData
```

Voltage information.

Definition at line 246 of file dataFiles.h.

Referenced by AtomProbe::readPosapOps().

The documentation for this struct was generated from the following file:

- include/atomprobe/io/dataFiles.h

6.52 AtomProbe::TRIANGLE Class Reference

```
#include <mesh.h>
```

Public Member Functions

- bool isSane (size_t pLimit=(size_t) -1) const
- bool edgesMismatch (const TRIANGLE &tOther) const

Public Attributes

- unsigned int p [3]
- unsigned int physGroup

6.52.1 Detailed Description

Definition at line 57 of file mesh.h.

6.52.2 Member Function Documentation

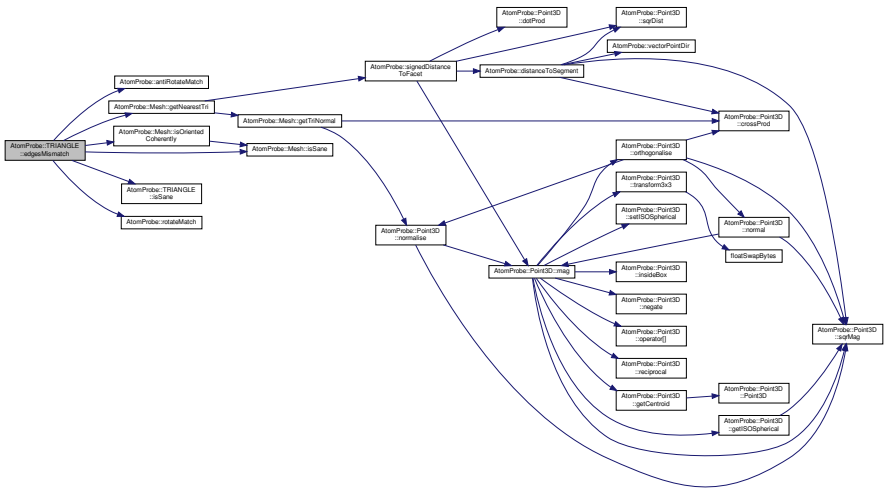
6.52.2.1 edgesMismatch()

```
bool AtomProbe::TRIANGLE::edgesMismatch (
            const TRIANGLE & tOther ) const
```

Definition at line 2201 of file mesh.cpp.

References AtomProbe::antiRotateMatch(), ASSERT, AtomProbe::Mesh::getNearestTri(), AtomProbe::Mesh::isOrientedCoherently(), isSane(), AtomProbe::Mesh::isSane(), AtomProbe::Mesh::nodes, p, AtomProbe::rotateMatch(), TEST, and AtomProbe::Mesh::triangles.

Here is the call graph for this function:



6.52.2.2 isSane()

```
bool AtomProbe::TRIANGLE::isSane (
            size_t pLimit = (size_t)-1 ) const
```

Definition at line 2185 of file mesh.cpp.

Referenced by edgesMismatch().

6.52.3 Member Data Documentation

6.52.3.1 p

```
unsigned int AtomProbe::TRIANGLE::p[3]
```

Definition at line 59 of file mesh.h.

Referenced by edgesMismatch(), AtomProbe::Mesh::getVolume(), AtomProbe::Mesh::loadGmshMesh(), AtomProbe::marchingCubes(), AtomProbe::Mesh::print(), and AtomProbe::Mesh::setTriangleMesh().

6.52.3.2 physGroup

```
unsigned int AtomProbe::TRIANGLE::physGroup
```

Definition at line 60 of file mesh.h.

Referenced by AtomProbe::Mesh::loadGmshMesh(), and AtomProbe::marchingCubes().

The documentation for this class was generated from the following files:

- include/atomprobe/primitives/mesh.h
- src/primitives/mesh.cpp

6.53 AtomProbe::TriangleWithIndexedVertices Struct Reference

```
#include <isoSurface.h>
```

Public Attributes

- size_t p [3]

6.53.1 Detailed Description

Definition at line 40 of file isoSurface.h.

6.53.2 Member Data Documentation

6.53.2.1 p

```
size_t AtomProbe::TriangleWithIndexedVertices::p[3]
```

Definition at line 42 of file isoSurface.h.

Referenced by AtomProbe::marchingCubes().

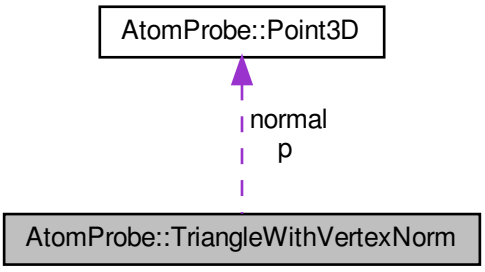
The documentation for this struct was generated from the following file:

- include/atomprobe/algorithm/isoSurface.h

6.54 AtomProbe::TriangleWithVertexNorm Class Reference

```
#include <isoSurface.h>
```

Collaboration diagram for AtomProbe::TriangleWithVertexNorm:



Public Member Functions

- void getCentroid (Point3D &p) const
- void computeACWNormal (Point3D &p) const
- void safeComputeACWNormal (Point3D &p) const
- float computeArea () const
- bool isDegenerate () const

Public Attributes

- Point3D p [3]
- Point3D normal [3]

6.54.1 Detailed Description

Definition at line 27 of file isoSurface.h.

6.54.2 Member Function Documentation

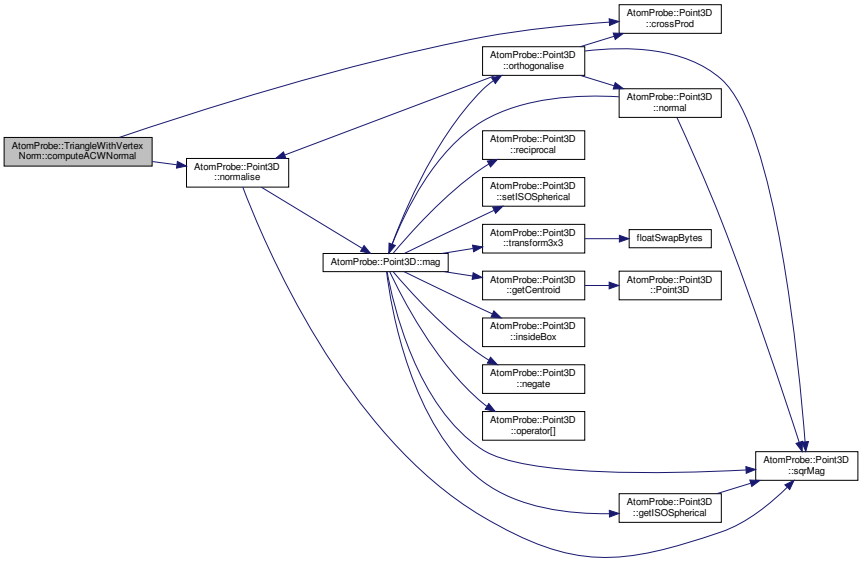
6.54.2.1 computeACWNormal()

```
void AtomProbe::TriangleWithVertexNorm::computeACWNormal (
            Point3D & p ) const
```

Definition at line 89 of file isoSurface.cpp.

References AtomProbe::Point3D::crossProd(), AtomProbe::Point3D::normalise(), and p.

Here is the call graph for this function:



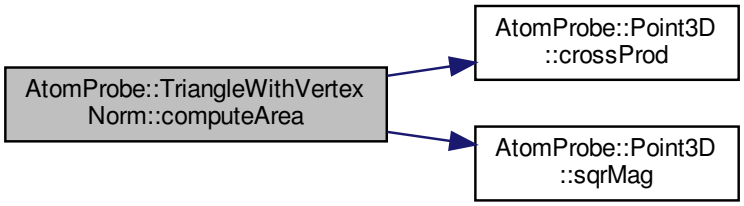
6.54.2.2 computeArea()

```
float AtomProbe::TriangleWithVertexNorm::computeArea ( ) const
```

Definition at line 117 of file isoSurface.cpp.

References AtomProbe::Point3D::crossProd(), p, and AtomProbe::Point3D::sqrMag().

Here is the call graph for this function:



6.54.2.3 getCentroid()

```
void AtomProbe::TriangleWithVertexNorm::getCentroid (
             Point3D & p ) const
```

Definition at line 135 of file isoSurface.cpp.

References p.

6.54.2.4 isDegenerate()

```
bool AtomProbe::TriangleWithVertexNorm::isDegenerate ( ) const
```

Definition at line 128 of file isoSurface.cpp.

References p.

Referenced by AtomProbe::marchingCubes().

6.54.2.5 safeComputeACWNormal()

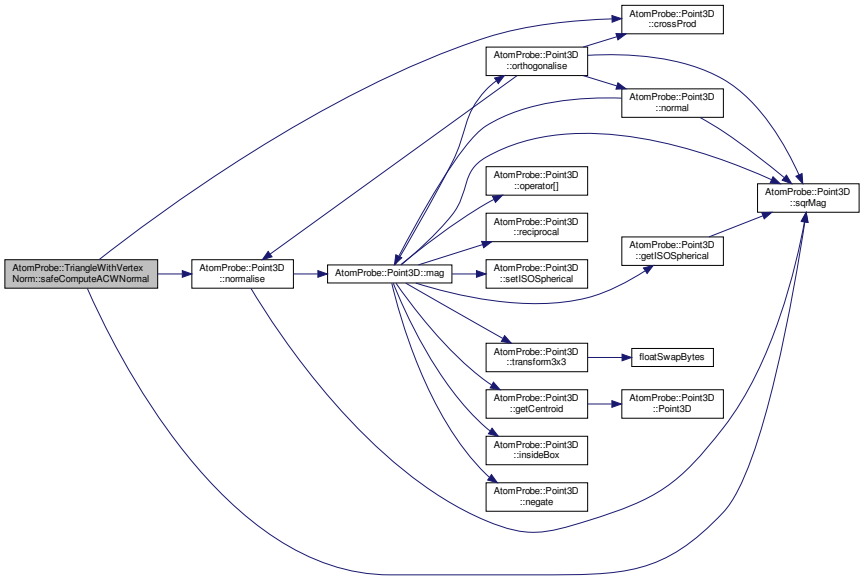
```
void AtomProbe::TriangleWithVertexNorm::safeComputeACWNormal (
            Point3D & p ) const
```

Definition at line 100 of file isoSurface.cpp.

References AtomProbe::Point3D::crossProd(), AtomProbe::Point3D::normalise(), p, and AtomProbe::Point3D::sqrMag().

Referenced by AtomProbe::marchingCubes().

Here is the call graph for this function:



6.54.3 Member Data Documentation

6.54.3.1 normal

```
Point3D AtomProbe::TriangleWithVertexNorm::normal[3]
```

Definition at line 31 of file isoSurface.h.

Referenced by AtomProbe::marchingCubes().

6.54.3.2 p

```
Point3D AtomProbe::TriangleWithVertexNorm::p[3]
```

Definition at line 30 of file isoSurface.h.

Referenced by computeACWNormal(), computeArea(), getCentroid(), isDegenerate(), AtomProbe::marching↩ Cubes(), and safeComputeACWNormal().

The documentation for this class was generated from the following files:

- include/atomprobe/algorithm/isoSurface.h
- src/algorithm/isoSurface.cpp

6.55 AtomProbe::VOLTAGE_DATA Struct Reference

Voltage data structure – these updates occur periodically during the experiment.

```
#include <dataFiles.h>
```

Public Attributes

- size_t nextHitGroupOffset
  FIXME: Document me.
- float voltage
  Standing Voltage applied to specimen (V)
- float pulseVolt
  Pulse voltage applied to specimen (V)
- float beta
  Coupling coefficient to specimen.

6.55.1 Detailed Description

Voltage data structure – these updates occur periodically during the experiment.

Definition at line 206 of file dataFiles.h.

6.55.2 Member Data Documentation

6.55.2.1 beta

```
float AtomProbe::VOLTAGE_DATA::beta
```

Coupling coefficient to specimen.

Definition at line 216 of file dataFiles.h.

Referenced by AtomProbe::readPosapOps().

6.55.2.2 nextHitGroupOffset

```
size_t AtomProbe::VOLTAGE_DATA::nextHitGroupOffset
```

FIXME: Document me.

Definition at line 209 of file dataFiles.h.

Referenced by AtomProbe::readPosapOps().

6.55.2.3 pulseVolt

```
float AtomProbe::VOLTAGE_DATA::pulseVolt
```

Pulse voltage applied to specimen (V)

Definition at line 213 of file dataFiles.h.

Referenced by AtomProbe::readPosapOps().

6.55.2.4 voltage

```
float AtomProbe::VOLTAGE_DATA::voltage
```

Standing Voltage applied to specimen (V)

Definition at line 211 of file dataFiles.h.

Referenced by AtomProbe::readPosapOps().

The documentation for this struct was generated from the following file:

- include/atomprobe/io/dataFiles.h

6.56 AtomProbe::Voxels< T > Class Template Reference

Template class that stores 3D voxel data.

```
#include <voxels.h>
```

Public Member Functions

- Voxels ()

  Constructor.
- ~Voxels ()

  Destructor.
- void swap (Voxels< T > &v)

  Swap object contents with other voxel object.
- void copy (Voxels< T > &newCopy) const

  Clone data into another object.
- void setPoint (const AtomProbe::Point3D &pt, const T &val)

  Set the value of a point in the dataset.
- T getPointData (const AtomProbe::Point3D &pt) const

  Retrieve the value of a datapoint, this is rounded to the nearest voxel.
- void getIndex (size_t &x, size_t &y, size_t &z, const AtomProbe::Point3D &p) const

  Retrieve the XYZ voxel location associated with a given position.
- void getIndexWithUpper (size_t &x, size_t &y, size_t &z, const AtomProbe::Point3D &p) const

  Retrieve the XYZ voxel location associated with a given position,.
- AtomProbe::Point3D getPoint (size_t x, size_t y, size_t z) const

  Get the position associated with an XYZ voxel.
- T getData (size_t x, size_t y, size_t z) const

  Retrieve the value of a specific voxel.
- T getData (size_t i) const

  Retrieve value of the nth voxel.
- size_t getOffset (size_t x, size_t y, size_t z) const

  Convert xyz to offset.
- void setEntry (size_t n, const T &val)
- void setData (size_t x, size_t y, size_t z, const T &val)

  Retrieve a reference to the data ata given position.
- void setData (size_t n, const T &val)

  Set the value of nth point in the dataset.
- void getInterpolatedData (const AtomProbe::Point3D &pt, T &v) const
- void getInterpSlice (size_t normal, float offset, T *p, size_t interpMode=VOX_INTERP_NONE) const
- void getSlice (size_t normal, size_t offset, T *p) const
- void getSize (size_t &x, size_t &y, size_t &z) const

  Get the size of the data field.
- size_t resize (size_t newX, size_t newY, size_t newZ, const AtomProbe::Point3D &newMinBound=AtomProbe::Point3D(0.0f, 0.0f, 0.0f), const AtomProbe::Point3D &newMaxBound=AtomProbe::Point3D(1.0f, 1.0f, 1.0f))

  Resize the data field.
- size_t resize (const Voxels< T > &v)
- size_t resizeKeepData (size_t newX, size_t newY, size_t newZ, unsigned int direction=CLIP_LOWER_SOUTH_WEST, const AtomProbe::Point3D &newMinBound=AtomProbe::Point3D(0.0f, 0.0f, 0.0f), const AtomProbe::Point3D &newMaxBound=AtomProbe::Point3D(1.0f, 1.0f, 1.0f), const T &fill=T(0), bool doFill=false)

  Resize the data field, maintaining data as best as possible.
- size_t deprecatedGetEdgeUniqueIndex (size_t x, size_t y, size_t z, unsigned int edge) const

  DEPRECATED FUNCTION : Get a unique integer that corresponds to the edge index for the voxel; where edges are shared between voxels.
- size_t getCellUniqueEdgeIndex (size_t x, size_t y, size_t z, unsigned int edge) const

  Get a unique integer that corresponds to an edge index for the voxel; where edges are shared between voxels.
- void getEdgeEnds (size_t edgeIndex, AtomProbe::Point3D &a, AtomProbe::Point3D &b) const

  Convert the edge index (as generated by getEdgeUniqueIndex) into a cenre position.

- void getEdgeCell (size_t edgeUniqId, size_t &x, size_t &y, size_t &z, size_t &axis) const

  Convert edge index (only as generted by getCellUniqueEdgeIndex) into a cell & axis value.
- void getEdgeEndApproxVals (size_t edgeUniqId, T &a, T &b) const

  Return the values that are associated with the edge ends, as returned by getEdgeEnds.
- void rebin (Voxels< T > &dest, size_t rate, size_t clipMode=CLIP_NONE) const

  Rebin the data by a given rate.
- T getSum (const T &initialVal=T(0.0)) const

  Get the total value of the data field.
- size_t count (const T &minIntensity) const

  count the number of cells with at least this intensity
- void fill (const T &val)

  Fill all voxels with a given value.
- AtomProbe::Point3D getMinBounds () const

  Get the bounding box vertex (min/max)
- AtomProbe::Point3D getMaxBounds () const
- void getAxisBounds (size_t axis, float &minV, float &maxV) const
- AtomProbe::Point3D getPitch () const

  ! Get the spacing for a unit cell
- void setBounds (const AtomProbe::Point3D &pMin, const AtomProbe::Point3D &pMax)

  Set the bounding size.
- void setBounds (const BoundCube &b)
- void getBounds (AtomProbe::Point3D &pMin, AtomProbe::Point3D &pMax) const

  Get the bounding size.
- void getBounds (BoundCube &bc) const
- size_t init (size_t nX, size_t nY, size_t nZ, const BoundCube &bound)

  Initialise the voxel storage.
- size_t init (size_t nX, size_t nY, size_t nZ)

  Initialise the voxel storage.
- size_t loadFile (const char *cpFilename, size_t nX, size_t nY, size_t nZ, bool silent=false)

  Load the voxels from file.
- size_t writeFile (const char *cpFilename) const

  Write the voxel objects in column major written out to file.
- size_t convolve (const Voxels< T > &templateVec, Voxels< T > &result, size_t boundMode=BOUND_CLIP) const

  Run convolution over this data, placing the correlation data into "result".
- size_t separableConvolve (const Voxels< T > &templateVec, Voxels< T > &result, size_t boundMode=BOUND_CLIP)

  Similar to convolve, but faster – only works with separable kernels.
- void threshold (const T &thresh, bool keepUpper, const T &newVal)

  Threshold the voxels, keeping either the lower or upper values above this threshold.
- void thresholdToBoolMask (const T &thresh, bool keepUpper, Voxels< bool > &result) const

  Generate a boolean voxel field stating whether the data is above or below the threshold specified.
- void applyMask (const Voxels< bool > &mask, const T &newVal, bool invert=false)

  Apply a mask to this dataset, where the mask is true (if not inverting), replace with specified val (newVal)
- void thresholdForPosition (std::vector< AtomProbe::Point3D > &p, const T &thresh, bool lowerEq=false) const

  Find the positions of the voxels that are above or below a given value.
- void binarise (Voxels< T > &result, const T &thresh, const T &onThresh, const T &offThresh) const

  Binarise the data into a result vector.
- void clear ()

  Empty the data.

- T min () const
  Find minimum in dataset.
- T max () const
  Find maximum in dataset.
- void minMax (T &min, T &max) const
  Find both min and max in dataset in the same loop.
- int countPoints (const std::vector< AtomProbe::Point3D > &points, bool noWrap=true, bool doErase=false)
  Generate a dataset that consists of the counts of points in a given voxel.
- T trapezIntegral () const
  Integrate the datataset via the trapezoidal method.
- void calculateDensity ()
  Convert voxel intensity into voxel density.
- float getBinVolume () const
- void operator/= (const Voxels< T > &v)
  Element wise division.
- void operator/= (const T &v)
- bool operator== (const Voxels< T > &v) const
- size_t size () const

Static Public Member Functions

- static size_t sizeofType ()
  Return the sizeof value for the T type.

6.56.1 Detailed Description

template<class T>
class AtomProbe::Voxels< T >

Template class that stores 3D voxel data.

To instantiate this class, objects must have basic mathematical operators, such as * + - and =

Definition at line 104 of file voxels.h.

6.56.2 Constructor & Destructor Documentation

6.56.2.1 Voxels()

```
template<class T >
AtomProbe::Voxels< T >::Voxels ( )
```

Constructor.

Definition at line 407 of file voxels.h.

6.56.2.2 ~Voxels()

```
template<class T >
AtomProbe::Voxels< T >::~Voxels ( )
```

Destructor.

Definition at line 412 of file voxels.h.

6.56.3 Member Function Documentation

6.56.3.1 applyMask()

```
template<class T >
void AtomProbe::Voxels< T >::applyMask (
            const Voxels< bool > & mask,
            const T & newVal,
            bool invert = false )
```

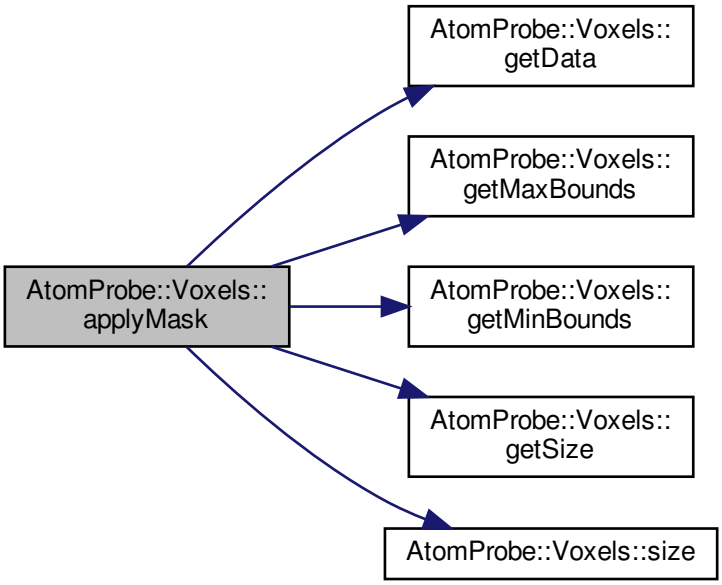
Apply a mask to this dataset, where the mask is true (if not inverting), replace with specified val (newVal)

Definition at line 1335 of file voxels.h.

References ASSERT, AtomProbe::Voxels< T >::getData(), AtomProbe::Voxels< T >::getMaxBounds(), AtomProbe::Voxels< T >::getMinBounds(), AtomProbe::Voxels< T >::getSize(), and AtomProbe::Voxels< T >::size().

Referenced by AtomProbe::Voxels< T >::getBounds().

Here is the call graph for this function:



6.56.3.2 binarise()

```
template<class T >
void AtomProbe::Voxels< T >::binarise (
            Voxels< T > & result,
            const T & thresh,
            const T & onThresh,
            const T & offThresh ) const
```

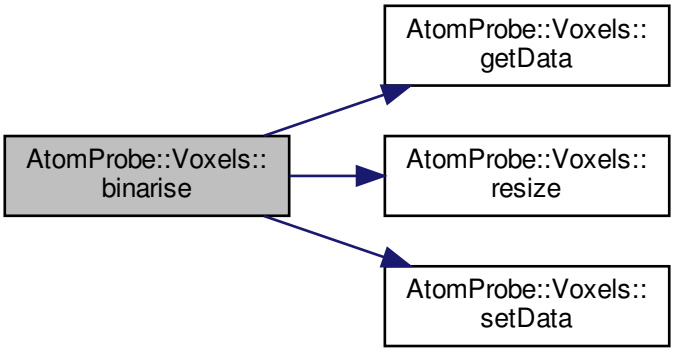
Binarise the data into a result vector.

Definition at line 1368 of file voxels.h.

References AtomProbe::Voxels< T >::getData(), AtomProbe::Voxels< T >::resize(), and AtomProbe::Voxels< T >::setData().

Referenced by AtomProbe::Voxels< T >::sizeofType().

Here is the call graph for this function:



6.56.3.3 calculateDensity()

```
template<class T >
void AtomProbe::Voxels< T >::calculateDensity ( )
```

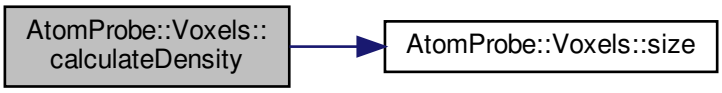
Convert voxel intensity into voxel density.

Definition at line 1458 of file voxels.h.

References AtomProbe::Voxels< T >::size().

Referenced by AtomProbe::Voxels< T >::clear().

Here is the call graph for this function:



6.56.3.4 clear()

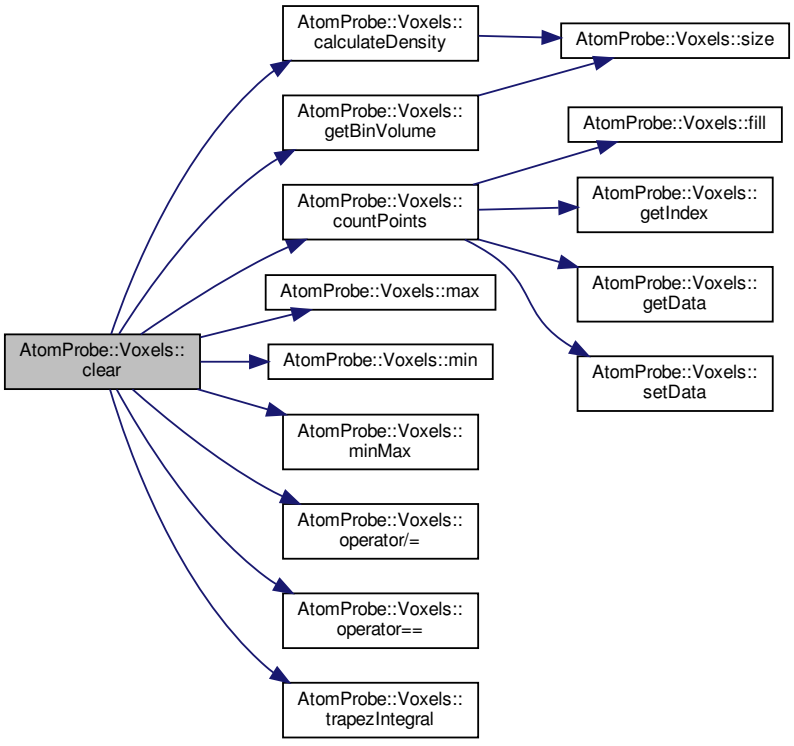
```
template<class T>
void AtomProbe::Voxels< T >::clear ( )  [inline]
```

Empty the data.

Definition at line 341 of file voxels.h.

References AtomProbe::Voxels< T >::calculateDensity(), AtomProbe::Voxels< T >::countPoints(), AtomProbe::Voxels< T >::getBinVolume(), AtomProbe::Voxels< T >::max(), AtomProbe::Voxels< T >::min(), AtomProbe::Voxels< T >::minMax(), AtomProbe::Voxels< T >::operator/=(), AtomProbe::Voxels< T >::operator==(), and AtomProbe::Voxels< T >::trapezIntegral().

Here is the call graph for this function:



6.56.3.5 convolve()

```
template<class T>
size_t AtomProbe::Voxels< T >::convolve (
            const Voxels< T > & templateVec,
            Voxels< T > & result,
            size_t boundMode = BOUND_CLIP ) const
```

Run convolution over this data, placing the correlation data into "result".

Datasets MUST have the same pitch (spacing) for the result to be defined template type must have a T(0.0) constructor that intialises it to some "zero"

Referenced by AtomProbe::Voxels< T >::getBounds().

6.56.3.6 copy()

```
template<class T >
void AtomProbe::Voxels< T >::copy (
            Voxels< T > & newCopy ) const
```

Clone data into another object.

Definition at line 424 of file voxels.h.

6.56.3.7 count()

```
template<class T >
size_t AtomProbe::Voxels< T >::count (
            const T & minIntensity ) const
```

count the number of cells with at least this intensity

Definition at line 1194 of file voxels.h.

Referenced by AtomProbe::countDataDistanceWeight(), and AtomProbe::Voxels< T >::setEntry().

6.56.3.8 countPoints()

```
template<class T >
int AtomProbe::Voxels< T >::countPoints (
            const std::vector< AtomProbe::Point3D > & points,
            bool noWrap = true,
            bool doErase = false )
```

Generate a dataset that consists of the counts of points in a given voxel.

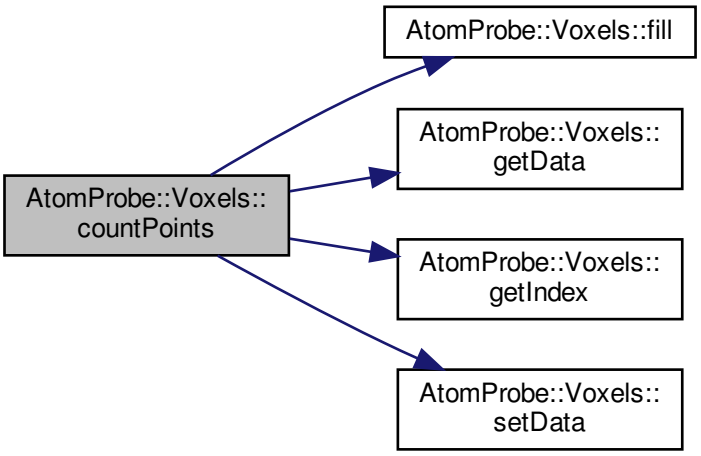
Ensure that the voxel scaling factors are set by calling ::setBounds() with the appropriate parameters for your data. Disabling nowrap allows you to "saturate" your data field in the case of dense regions, rather than let wrap-around errors occur

Definition at line 1420 of file voxels.h.

References AtomProbe::Voxels< T >::fill(), AtomProbe::Voxels< T >::getData(), AtomProbe::Voxels< T >::getIndex(), AtomProbe::Voxels< T >::setData(), and AtomProbe::VOXEL_ABORT_ERR.

Referenced by AtomProbe::Voxels< T >::clear().

Here is the call graph for this function:



6.56.3.9 deprecatedGetEdgeUniqueIndex()

```
template<class T >
size_t AtomProbe::Voxels< T >::deprecatedGetEdgeUniqueIndex (
            size_t x,
            size_t y,
            size_t z,
            unsigned int edge ) const
```

DEPRECATED FUNCTION : Get a unique integer that corresponds to the edge index for the voxel; where edges are shared between voxels.

Each voxel has 12 edges. These are shared (except voxels that on zero or positive boundary). Return a unique index that corresponds to a specified edge (0->11). Index *CANNOT* be inverted to yield cell

Definition at line 512 of file voxels.h.

Referenced by AtomProbe::marchingCubes(), and AtomProbe::Voxels< T >::setEntry().

6.56.3.10 fill()

```
template<class T >
void AtomProbe::Voxels< T >::fill (
            const T & val )
```

Fill all voxels with a given value.

Definition at line 1525 of file voxels.h.

Referenced by AtomProbe::countDataDistanceWeight(), AtomProbe::Voxels< T >::countPoints(), main(), AtomProbe::marchingCubes(), and AtomProbe::Voxels< T >::setEntry().

6.56.3.11 getAxisBounds()

```
template<class T >
void AtomProbe::Voxels< T >::getAxisBounds (
            size_t axis,
            float & minV,
            float & maxV ) const
```

Definition at line 843 of file voxels.h.

Referenced by AtomProbe::Voxels< T >::setEntry().

6.56.3.12 getBinVolume()

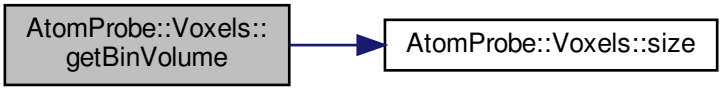
```
template<class T >
float AtomProbe::Voxels< T >::getBinVolume ( ) const
```

Definition at line 1474 of file voxels.h.

References AtomProbe::Voxels< T >::size().

Referenced by AtomProbe::Voxels< T >::clear().

Here is the call graph for this function:



6.56.3.13 getBounds() [1/2]

```
template<class T>
void AtomProbe::Voxels< T >::getBounds (
            AtomProbe::Point3D & pMin,
            AtomProbe::Point3D & pMax ) const  [inline]
```

Get the bounding size.

Definition at line 260 of file voxels.h.

Referenced by main(), and AtomProbe::marchingCubes().

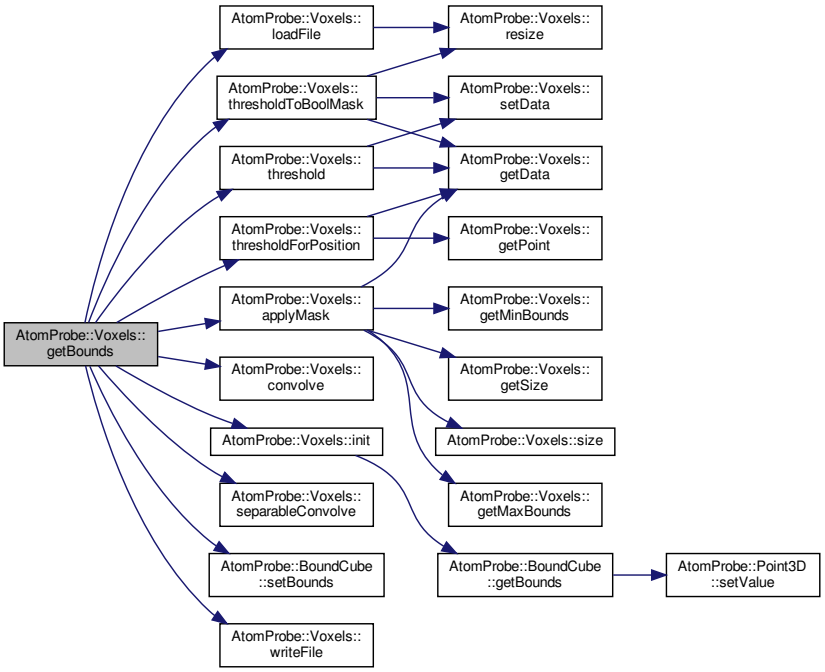
6.56.3.14 getBounds() [2/2]

```
template<class T>
void AtomProbe::Voxels< T >::getBounds (
            BoundCube & bc ) const  [inline]
```

Definition at line 261 of file voxels.h.

References AtomProbe::Voxels< T >::applyMask(), AtomProbe::BOUND_CLIP, AtomProbe::Voxels< T >::convolve(), AtomProbe::Voxels< T >::init(), AtomProbe::Voxels< T >::loadFile(), AtomProbe::Voxels< T >::separableConvolve(), AtomProbe::BoundCube::setBounds(), AtomProbe::Voxels< T >::threshold(), AtomProbe::Voxels< T >::thresholdForPosition(), AtomProbe::Voxels< T >::thresholdToBoolMask(), and AtomProbe::Voxels< T >::writeFile().

Here is the call graph for this function:



6.56.3.15 getCellUniqueEdgeIndex()

```
template<class T >
size_t AtomProbe::Voxels< T >::getCellUniqueEdgeIndex (
            size_t x,
            size_t y,
            size_t z,
            unsigned int edge ) const
```

Get a unique integer that corresponds to an edge index for the voxel; where edges are shared between voxels.

Each voxel has 12 edges. These are shared (except voxels that on zero or positive boundary). Return a NON-unique index that corresponds to a specified edge (0->11) Index can be inverted to yield cell

Definition at line 716 of file voxels.h.

Referenced by AtomProbe::Voxels< T >::setEntry().

6.56.3.16 getData() [1/2]

```
template<class T >
T AtomProbe::Voxels< T >::getData (
            size_t x,
            size_t y,
            size_t z ) const  [inline]
```

Retrieve the value of a specific voxel.

Definition at line 1224 of file voxels.h.

References ASSERT.

Referenced by AtomProbe::Voxels< T >::applyMask(), AtomProbe::Voxels< T >::binarise(), AtomProbe::Voxels< T >::countPoints(), AtomProbe::Voxels< T >::getInterpolatedData(), AtomProbe::Voxels< T >::getSlice(), AtomProbe::incrementDataDistanceWeight(), AtomProbe::marchingCubes(), AtomProbe::Voxels< T >::resizeKeepData(), AtomProbe::sumVoxels(), AtomProbe::Voxels< T >::threshold(), AtomProbe::Voxels< T >::thresholdForPosition(), and AtomProbe::Voxels< T >::thresholdToBoolMask().

6.56.3.17 getData() [2/2]

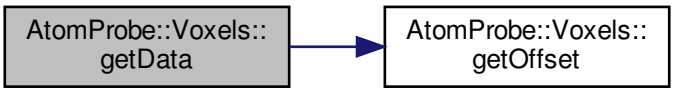
```
template<class T>
T AtomProbe::Voxels< T >::getData (
            size_t i ) const  [inline]
```

Retrieve value of the nth voxel.

Definition at line 154 of file voxels.h.

References AtomProbe::Voxels< T >::getOffset().

Here is the call graph for this function:



6.56.3.18 getEdgeCell()

```
template<class T >
void AtomProbe::Voxels< T >::getEdgeCell (
            size_t edgeUniqId,
            size_t & x,
            size_t & y,
            size_t & z,
            size_t & axis ) const
```

Convert edge index (only as generted by getCellUniqueEdgeIndex) into a cell & axis value.

Definition at line 766 of file voxels.h.

References ASSERT.

Referenced by AtomProbe::Voxels< T >::getEdgeEnds(), and AtomProbe::Voxels< T >::setEntry().

6.56.3.19 getEdgeEndApproxVals()

```
template<class T >
void AtomProbe::Voxels< T >::getEdgeEndApproxVals (
            size_t edgeUniqId,
            T & a,
            T & b ) const
```

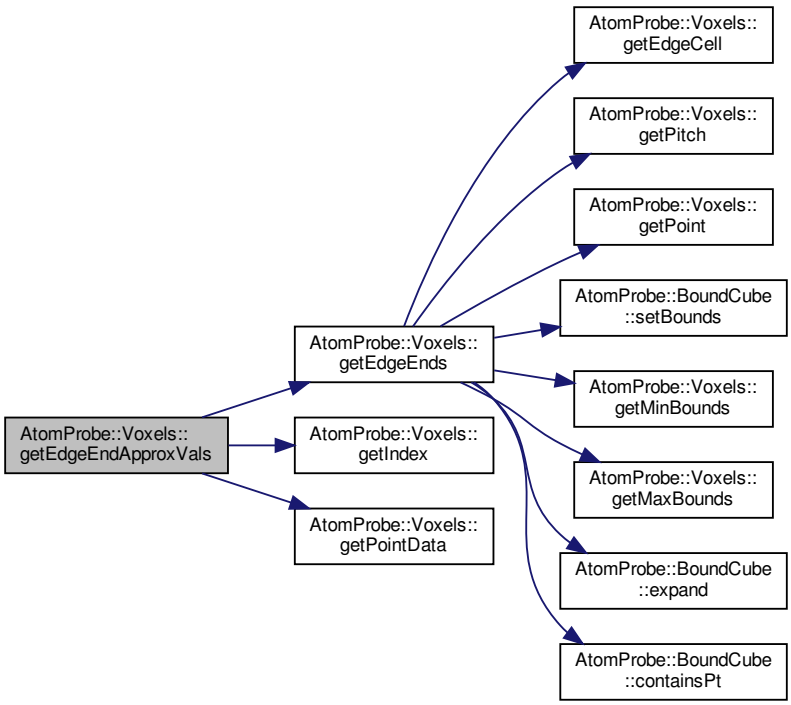
Return the values that are associated with the edge ends, as returned by getEdgeEnds.

Definition at line 828 of file voxels.h.

References AtomProbe::Voxels< T >::getEdgeEnds(), AtomProbe::Voxels< T >::getIndex(), and AtomProbe::↩ Voxels< T >::getPointData().

Referenced by AtomProbe::marchingCubes(), and AtomProbe::Voxels< T >::setEntry().

Here is the call graph for this function:



6.56.3.20 getEdgeEnds()

```
template<class T >
void AtomProbe::Voxels< T >::getEdgeEnds (
            size_t edgeIndex,
            AtomProbe::Point3D & a,
            AtomProbe::Point3D & b ) const
```

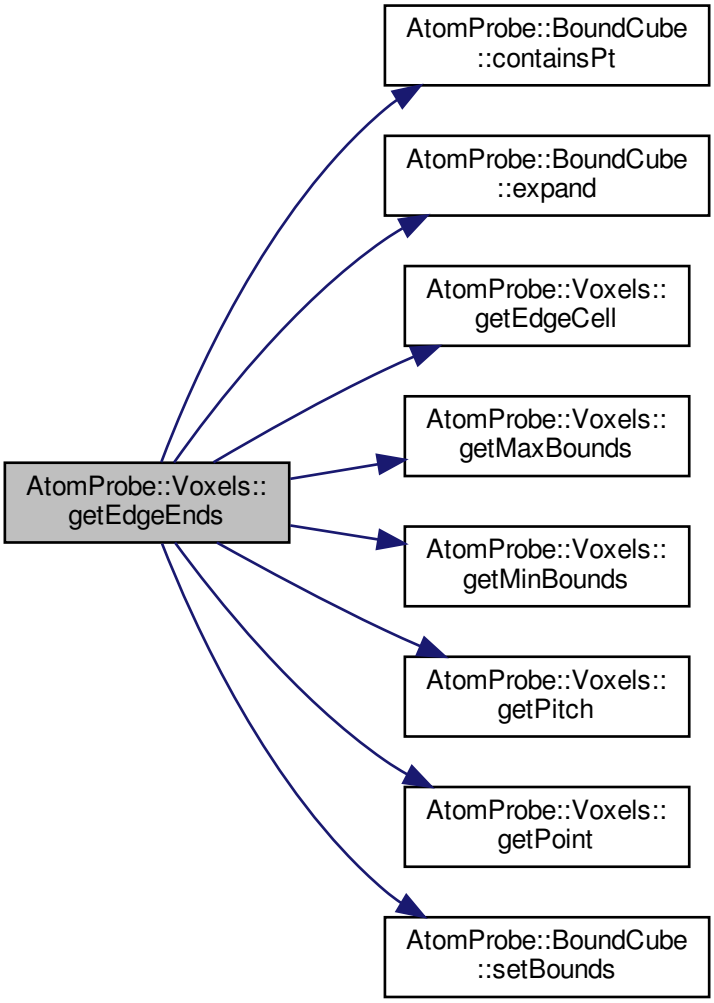
Convert the edge index (as generated by getEdgeUniqueIndex) into a cenre position.

Definition at line 786 of file voxels.h.

References ASSERT, AtomProbe::BoundCube::containsPt(), AtomProbe::BoundCube::expand(), AtomProbe::↩ Voxels< T >::getEdgeCell(), AtomProbe::Voxels< T >::getMaxBounds(), AtomProbe::Voxels< T >::getMin↩ Bounds(), AtomProbe::Voxels< T >::getPitch(), AtomProbe::Voxels< T >::getPoint(), and AtomProbe::Bound↩ Cube::setBounds().

Referenced by AtomProbe::Voxels< T >::getEdgeEndApproxVals(), AtomProbe::marchingCubes(), and Atom↩ Probe::Voxels< T >::setEntry().

Here is the call graph for this function:



6.56.3.21 getIndex()

```
template<class T >
void AtomProbe::Voxels< T >::getIndex (
            size_t & x,
            size_t & y,
            size_t & z,
            const AtomProbe::Point3D & p ) const
```

Retrieve the XYZ voxel location associated with a given position.

Definition at line 1485 of file voxels.h.

References ASSERT.

Referenced by AtomProbe::Voxels< T >::countPoints(), AtomProbe::Voxels< T >::getEdgeEndApproxVals(), AtomProbe::Voxels< T >::getIndexWithUpper(), AtomProbe::Voxels< T >::getInterpolatedData(), and AtomProbe::incrementDataDistanceWeight().

6.56.3.22 getIndexWithUpper()

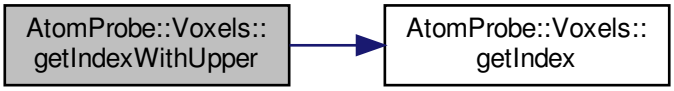
```
template<class T >
void AtomProbe::Voxels< T >::getIndexWithUpper (
            size_t & x,
            size_t & y,
            size_t & z,
            const AtomProbe::Point3D & p ) const
```

Retrieve the XYZ voxel location associated with a given position,.

Definition at line 1504 of file voxels.h.

References AtomProbe::Voxels< T >::getIndex().

Here is the call graph for this function:



6.56.3.23 getInterpolatedData()

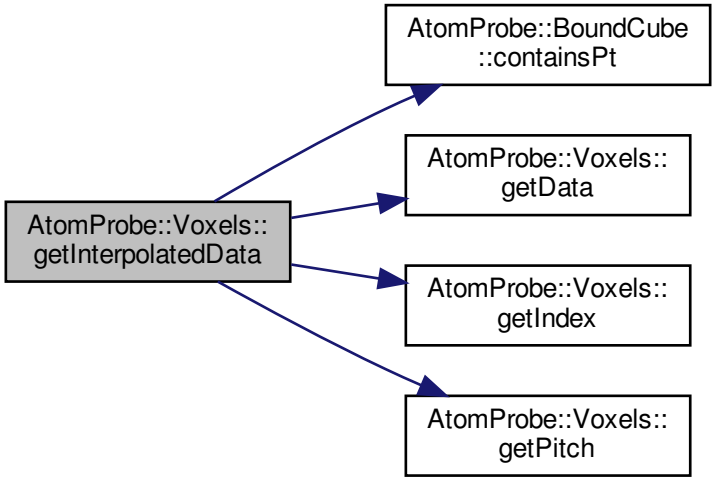
```
template<class T >
void AtomProbe::Voxels< T >::getInterpolatedData (
            const AtomProbe::Point3D & pt,
            T & v ) const
```

Definition at line 1667 of file voxels.h.

References ASSERT, AtomProbe::BoundCube::containsPt(), AtomProbe::Voxels< T >::getData(), AtomProbe::Voxels< T >::getIndex(), and AtomProbe::Voxels< T >::getPitch().

Referenced by AtomProbe::countDataDistanceWeight(), and AtomProbe::Voxels< T >::setEntry().

Here is the call graph for this function:



6.56.3.24 getInterpSlice()

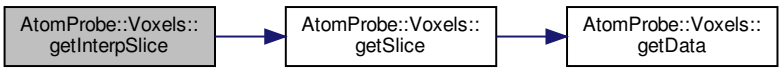
```
template<class T >
void AtomProbe::Voxels< T >::getInterpSlice (
            size_t normal,
            float offset,
            T * p,
            size_t interpMode = VOX_INTERP_NONE ) const
```

Definition at line 1603 of file voxels.h.

References ASSERT, AtomProbe::Voxels< T >::getSlice(), AtomProbe::VOX_INTERP_LINEAR, and AtomProbe↩
::VOX_INTERP_NONE.

Referenced by AtomProbe::Voxels< T >::setEntry().

Here is the call graph for this function:



6.56.3.25 getMaxBounds()

```
template<class T >
AtomProbe::Point3D AtomProbe::Voxels< T >::getMaxBounds ( ) const
```

Definition at line 990 of file voxels.h.

References ASSERT.

Referenced by AtomProbe::Voxels< T >::applyMask(), AtomProbe::Voxels< T >::getEdgeEnds(), AtomProbe::marchingCubes(), and AtomProbe::Voxels< T >::setEntry().

6.56.3.26 getMinBounds()

```
template<class T >
AtomProbe::Point3D AtomProbe::Voxels< T >::getMinBounds ( ) const
```

Get the bounding box vertex (min/max)

Definition at line 983 of file voxels.h.

References ASSERT.

Referenced by AtomProbe::Voxels< T >::applyMask(), AtomProbe::Voxels< T >::getEdgeEnds(), AtomProbe::marchingCubes(), and AtomProbe::Voxels< T >::setEntry().

6.56.3.27 getOffset()

```
template<class T>
size_t AtomProbe::Voxels< T >::getOffset (
            size_t x,
            size_t y,
            size_t z ) const
```

Convert xyz to offset.

Referenced by AtomProbe::Voxels< T >::getData().

6.56.3.28 getPitch()

```
template<class T >
AtomProbe::Point3D AtomProbe::Voxels< T >::getPitch ( ) const
```

! Get the spacing for a unit cell

Definition at line 495 of file voxels.h.

Referenced by AtomProbe::Voxels< T >::getEdgeEnds(), AtomProbe::Voxels< T >::getInterpolatedData(), AtomProbe::marchingCubes(), and AtomProbe::Voxels< T >::setEntry().

6.56.3.29 getPoint()

```
template<class T >
AtomProbe::Point3D AtomProbe::Voxels< T >::getPoint (
            size_t x,
            size_t y,
            size_t z ) const
```

Get the position associated with an XYZ voxel.

Definition at line 485 of file voxels.h.

Referenced by AtomProbe::Voxels< T >::getEdgeEnds(), AtomProbe::incrementDataDistanceWeight(), main(), and AtomProbe::Voxels< T >::thresholdForPosition().

6.56.3.30 getPointData()

```
template<class T >
T AtomProbe::Voxels< T >::getPointData (
            const AtomProbe::Point3D & pt ) const
```

Retrieve the value of a datapoint, this is rounded to the nearest voxel.

Definition at line 469 of file voxels.h.

References ASSERT.

Referenced by AtomProbe::Voxels< T >::getEdgeEndApproxVals().

6.56.3.31 getSize()

```
template<class T >
void AtomProbe::Voxels< T >::getSize (
            size_t & x,
            size_t & y,
            size_t & z ) const
```

Get the size of the data field.

Definition at line 503 of file voxels.h.

References ASSERT.

Referenced by AtomProbe::Voxels< T >::applyMask(), AtomProbe::countDataDistanceWeight(), AtomProbe::incrementDataDistanceWeight(), AtomProbe::marchingCubes(), AtomProbe::Voxels< T >::setEntry(), and AtomProbe::sumVoxels().

6.56.3.32 getSlice()

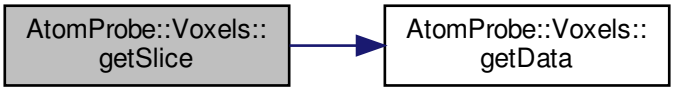
```
template<class T >
void AtomProbe::Voxels< T >::getSlice (
            size_t normal,
            size_t offset,
            T * p ) const
```

Definition at line 1534 of file voxels.h.

References ASSERT, and AtomProbe::Voxels< T >::getData().

Referenced by AtomProbe::Voxels< T >::getInterpSlice(), and AtomProbe::Voxels< T >::setEntry().

Here is the call graph for this function:



6.56.3.33 getSum()

```
template<class T >
T AtomProbe::Voxels< T >::getSum (
            const T & initialVal = T(0.0) ) const
```

Get the total value of the data field.

An "initial value" is provided to provide the definition of a zero value

Definition at line 1155 of file voxels.h.

References ASSERT.

Referenced by AtomProbe::countDataDistanceWeight(), and AtomProbe::Voxels< T >::setEntry().

6.56.3.34 init() [1/2]

```
template<class T >
size_t AtomProbe::Voxels< T >::init (
            size_t nX,
            size_t nY,
            size_t nZ,
            const BoundCube & bound )
```

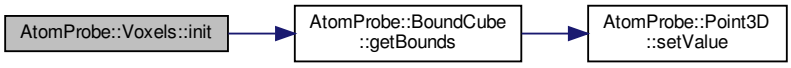
Initialise the voxel storage.

Definition at line 1018 of file voxels.h.

References AtomProbe::BoundCube::getBounds().

Referenced by AtomProbe::Voxels< T >::getBounds(), and AtomProbe::Voxels< T >::init().

Here is the call graph for this function:



6.56.3.35 init() [2/2]

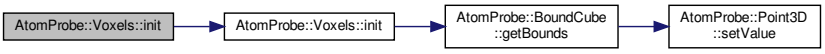
```
template<class T >
size_t AtomProbe::Voxels< T >::init (
            size_t nX,
            size_t nY,
            size_t nZ )
```

Initialise the voxel storage.

Definition at line 1035 of file voxels.h.

References AtomProbe::Voxels< T >::init().

Here is the call graph for this function:



6.56.3.36 loadFile()

```
template<class T >
size_t AtomProbe::Voxels< T >::loadFile (
            const char * cpFilename,
            size_t nX,
            size_t nY,
            size_t nZ,
            bool silent = false )
```

Load the voxels from file.

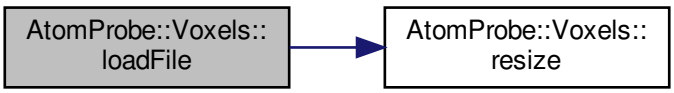
Format is flat size_ts in column major return codes: 1: File open error 2: Data size error

Definition at line 1044 of file voxels.h.

References AtomProbe::Voxels< T >::resize(), AtomProbe::VOXELS_BAD_FILE_OPEN, AtomProbe::VOXELS↩
_BAD_FILE_READ, and AtomProbe::VOXELS_BAD_FILE_SIZE.

Referenced by AtomProbe::Voxels< T >::getBounds().

Here is the call graph for this function:



6.56.3.37 max()

```
template<class T >
T AtomProbe::Voxels< T >::max ( ) const
```

Find maximum in dataset.

Definition at line 1402 of file voxels.h.

References ASSERT.

Referenced by AtomProbe::Voxels< T >::clear(), and AtomProbe::countDataDistanceWeight().

6.56.3.38 min()

```
template<class T >
T AtomProbe::Voxels< T >::min ( ) const
```

Find minimum in dataset.

Definition at line 1395 of file voxels.h.

References ASSERT.

Referenced by AtomProbe::Voxels< T >::clear().

6.56.3.39 minMax()

```
template<class T >
void AtomProbe::Voxels< T >::minMax (
            T & min,
            T & max ) const
```

Find both min and max in dataset in the same loop.

Definition at line 1410 of file voxels.h.

References ASSERT.

Referenced by AtomProbe::Voxels< T >::clear().

6.56.3.40 operator/=() [1/2]

```
template<class T >
void AtomProbe::Voxels< T >::operator/= (
            const Voxels< T > & v )
```

Element wise division.

Definition at line 1725 of file voxels.h.

References ASSERT.

Referenced by AtomProbe::Voxels< T >::clear().

6.56.3.41 operator/=() [2/2]

```
template<class T >
void AtomProbe::Voxels< T >::operator/= (
            const T & v )
```

Definition at line 1745 of file voxels.h.

References ASSERT.

6.56.3.42 operator==()

```
template<class T >
bool AtomProbe::Voxels< T >::operator== (
            const Voxels< T > & v ) const
```

Definition at line 1764 of file voxels.h.

Referenced by AtomProbe::Voxels< T >::clear().

6.56.3.43 rebin()

```
template<class T>
void AtomProbe::Voxels< T >::rebin (
            Voxels< T > & dest,
            size_t rate,
            size_t clipMode = CLIP_NONE ) const
```

Rebin the data by a given rate.

This will perform a quick and dirty rebin operation, where groups of datablocks are binned into a single cell. Number of blocks binned is rate^3. Field must be larger than rate in all directions. Currently only CLIP_NONE is supported.

Referenced by AtomProbe::Voxels< T >::setEntry().

6.56.3.44 resize() [1/2]

```
template<class T >
size_t AtomProbe::Voxels< T >::resize (
            size_t newX,
            size_t newY,
            size_t newZ,
            const AtomProbe::Point3D & newMinBound = AtomProbe::Point3D(0.0f,0.0f,0.0f),
            const AtomProbe::Point3D & newMaxBound = AtomProbe::Point3D(1.0f,1.0f,1.0f) )
```

Resize the data field.

This will destroy any data that was already in place If the data needs to be preserved use "resizeKeepData" Data will *not* be initialised

Definition at line 850 of file voxels.h.

Referenced by AtomProbe::Voxels< T >::binarise(), AtomProbe::countDataDistanceWeight(), AtomProbe::Voxels< T >::loadFile(), main(), AtomProbe::marchingCubes(), AtomProbe::Voxels< T >::resize(), AtomProbe::Voxels< T >::resizeKeepData(), AtomProbe::Voxels< T >::setEntry(), and AtomProbe::Voxels< T >::thresholdToBoolMask().

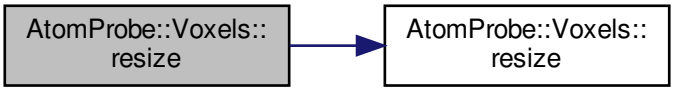
6.56.3.45 resize() [2/2]

```
template<class T >
size_t AtomProbe::Voxels< T >::resize (
            const Voxels< T > & v )
```

Definition at line 873 of file voxels.h.

References AtomProbe::Voxels< T >::resize().

Here is the call graph for this function:



6.56.3.46 resizeKeepData()

```
template<class T >
size_t AtomProbe::Voxels< T >::resizeKeepData (
            size_t newX,
            size_t newY,
            size_t newZ,
            unsigned int direction = CLIP_LOWER_SOUTH_WEST,
            const AtomProbe::Point3D & newMinBound = AtomProbe::Point3D(0.0f,0.0f,0.0f),
            const AtomProbe::Point3D & newMaxBound = AtomProbe::Point3D(1.0f,1.0f,1.0f),
            const T & fill = T(0),
            bool doFill = false )
```

Resize the data field, maintaining data as best as possible.

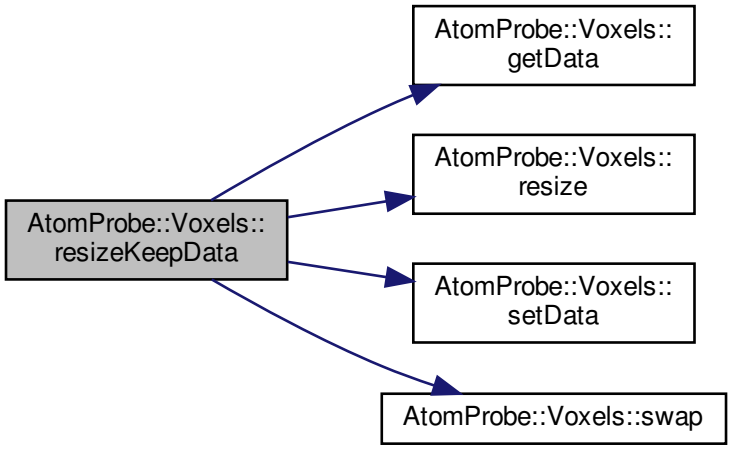
This will preserve data by resizing as much as possible about the origin. If the bounds are extended, the "fill" value is used by default iff doFill is set to true.

Definition at line 879 of file voxels.h.

References ASSERT, AtomProbe::CLIP_LOWER_SOUTH_WEST, AtomProbe::Voxels< T >::getData(), AtomProbe::Voxels< T >::resize(), AtomProbe::Voxels< T >::setData(), AtomProbe::Voxels< T >::swap(), and AtomProbe::VOXEL_ABORT_ERR.

Referenced by AtomProbe::countDataDistanceWeight(), and AtomProbe::Voxels< T >::setEntry().

Here is the call graph for this function:



6.56.3.47 separableConvolve()

```
template<class T>
size_t AtomProbe::Voxels< T >::separableConvolve (
            const Voxels< T > & templateVec,
            Voxels< T > & result,
            size_t boundMode = BOUND_CLIP )
```

Similar to convolve, but faster – only works with separable kernels.

Datasets MUST have the same pitch (spacing) for the result to be defined template type must have a T(0.0) constructor that intialises it to some "zero"

Referenced by AtomProbe::Voxels< T >::getBounds().

6.56.3.48 setBounds() [1/2]

```
template<class T >
void AtomProbe::Voxels< T >::setBounds (
            const AtomProbe::Point3D & pMin,
            const AtomProbe::Point3D & pMax )
```

Set the bounding size.

Definition at line 997 of file voxels.h.

References ASSERT.

Referenced by AtomProbe::countDataDistanceWeight(), main(), AtomProbe::Voxels< T >::setBounds(), and AtomProbe::Voxels< T >::setEntry().

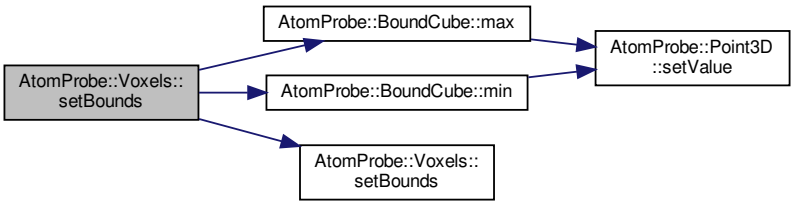
6.56.3.49 setBounds() [2/2]

```
template<class T >
void AtomProbe::Voxels< T >::setBounds (
            const BoundCube & b )
```

Definition at line 1012 of file voxels.h.

References AtomProbe::BoundCube::max(), AtomProbe::BoundCube::min(), and AtomProbe::Voxels< T >::setBounds().

Here is the call graph for this function:



6.56.3.50 setData() [1/2]

```
template<class T >
void AtomProbe::Voxels< T >::setData (
            size_t x,
            size_t y,
            size_t z,
            const T & val )
```

Retrieve a reference to the data ata given position.

Set the value of a point in the dataset

Definition at line 450 of file voxels.h.

References ASSERT.

Referenced by AtomProbe::Voxels< T >::binarise(), AtomProbe::countDataDistanceWeight(), AtomProbe::Voxels< T >::countPoints(), AtomProbe::incrementDataDistanceWeight(), main(), AtomProbe::marchingCubes(), AtomProbe::Voxels< T >::resizeKeepData(), AtomProbe::Voxels< T >::setEntry(), AtomProbe::Voxels< T >::threshold(), and AtomProbe::Voxels< T >::thresholdToBoolMask().

6.56.3.51 setData() [2/2]

```
template<class T >
void AtomProbe::Voxels< T >::setData (
            size_t n,
            const T & val )  [inline]
```

Set the value of nth point in the dataset.

Definition at line 460 of file voxels.h.

References ASSERT.

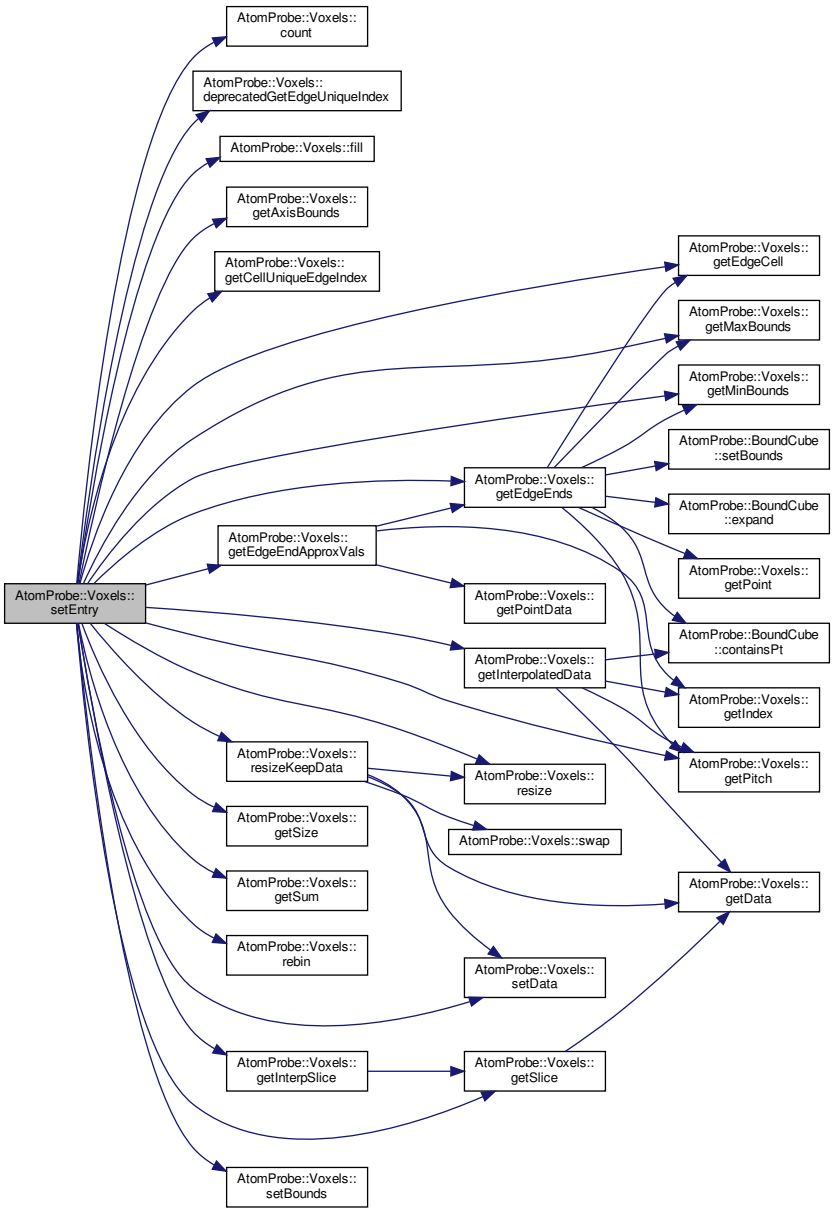
6.56.3.52 setEntry()

```
template<class T>
void AtomProbe::Voxels< T >::setEntry (
            size_t n,
            const T & val )  [inline]
```

Definition at line 159 of file voxels.h.

References AtomProbe::CLIP_LOWER_SOUTH_WEST, AtomProbe::CLIP_NONE, AtomProbe::Voxels< T >::count(), AtomProbe::Voxels< T >::deprecatedGetEdgeUniqueIndex(), AtomProbe::Voxels< T >::fill(), AtomProbe::Voxels< T >::getAxisBounds(), AtomProbe::Voxels< T >::getCellUniqueEdgeIndex(), AtomProbe::Voxels< T >::getEdgeCell(), AtomProbe::Voxels< T >::getEdgeEndApproxVals(), AtomProbe::Voxels< T >::getEdgeEnds(), AtomProbe::Voxels< T >::getInterpolatedData(), AtomProbe::Voxels< T >::getInterpSlice(), AtomProbe::Voxels< T >::getMaxBounds(), AtomProbe::Voxels< T >::getMinBounds(), AtomProbe::Voxels< T >::getPitch(), AtomProbe::Voxels< T >::getSize(), AtomProbe::Voxels< T >::getSlice(), AtomProbe::Voxels< T >::getSum(), AtomProbe::Voxels< T >::rebin(), AtomProbe::Voxels< T >::resize(), AtomProbe::Voxels< T >::resizeKeepData(), AtomProbe::Voxels< T >::setBounds(), AtomProbe::Voxels< T >::setData(), and AtomProbe::VOX_INTERP_NONE.

Here is the call graph for this function:



6.56.3.53 setPoint()

```
template<class T >
void AtomProbe::Voxels< T >::setPoint (
            const AtomProbe::Point3D & pt,
            const T & val )
```

Set the value of a point in the dataset.

Definition at line 438 of file voxels.h.

References ASSERT.

6.56.3.54 size()

```
template<class T>
size_t AtomProbe::Voxels< T >::size ( ) const  [inline]
```

Definition at line 378 of file voxels.h.

Referenced by AtomProbe::Voxels< T >::applyMask(), AtomProbe::Voxels< T >::calculateDensity(), AtomProbe::Voxels< T >::getBinVolume(), and AtomProbe::sumVoxels().

6.56.3.55 sizeofType()

```
template<class T>
static size_t AtomProbe::Voxels< T >::sizeofType ( )  [inline], [static]
```

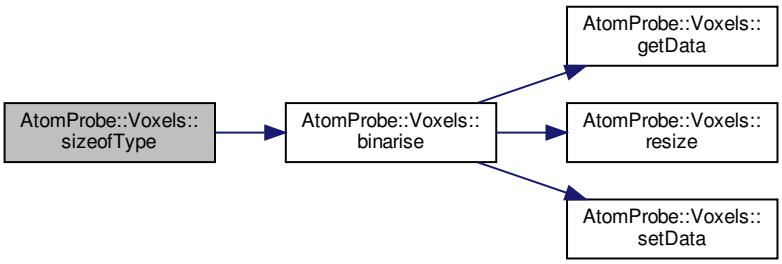
Return the sizeof value for the T type.

Maybe there is a better way to do this, I don't know

Definition at line 327 of file voxels.h.

References AtomProbe::Voxels< T >::binarise().

Here is the call graph for this function:



6.56.3.56 swap()

```
template<class T >
void AtomProbe::Voxels< T >::swap (
            Voxels< T > & v )
```

Swap object contents with other voxel object.

Definition at line 1211 of file voxels.h.

Referenced by AtomProbe::Voxels< T >::resizeKeepData().

6.56.3.57 threshold()

```
template<class T >
void AtomProbe::Voxels< T >::threshold (
            const T & thresh,
            bool keepUpper,
            const T & newVal )
```

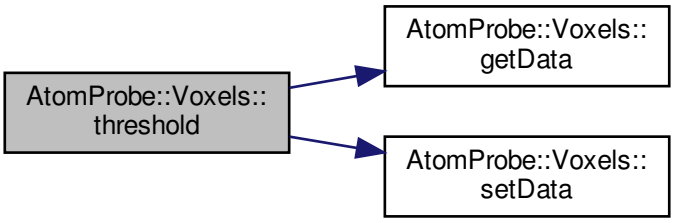
Threshold the voxels, keeping either the lower or upper values above this threshold.

Definition at line 1276 of file voxels.h.

References AtomProbe::Voxels< T >::getData(), and AtomProbe::Voxels< T >::setData().

Referenced by AtomProbe::Voxels< T >::getBounds().

Here is the call graph for this function:



6.56.3.58 thresholdForPosition()

```
template<class T >
void AtomProbe::Voxels< T >::thresholdForPosition (
            std::vector< AtomProbe::Point3D > & p,
            const T & thresh,
            bool lowerEq = false ) const
```

Find the positions of the voxels that are above or below a given value.

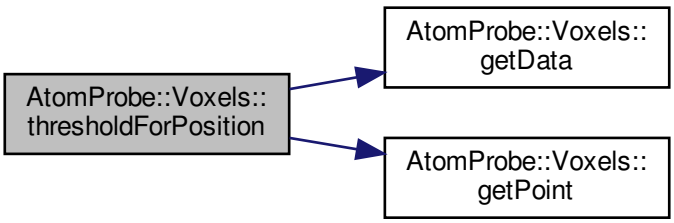
Returns the positions of the voxels' centroids for voxels that have, by default, a value greater than that of thresh. This behaviour can by reversed to "lesser than" by setting lowerEq to false

Definition at line 1231 of file voxels.h.

References AtomProbe::Voxels< T >::getData(), and AtomProbe::Voxels< T >::getPoint().

Referenced by AtomProbe::Voxels< T >::getBounds().

Here is the call graph for this function:



6.56.3.59 thresholdToBoolMask()

```
template<class T >
void AtomProbe::Voxels< T >::thresholdToBoolMask (
            const T & thresh,
            bool keepUpper,
            Voxels< bool > & result ) const
```

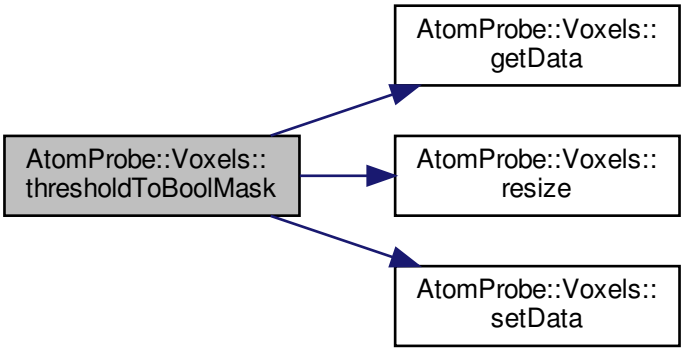
Generate a boolean voxel field stating whether the data is above or below the threshold specified.

Definition at line 1312 of file voxels.h.

References AtomProbe::Voxels< T >::getData(), AtomProbe::Voxels< T >::resize(), AtomProbe::Voxels< T >::setData(), and XOR.

Referenced by AtomProbe::Voxels< T >::getBounds().

Here is the call graph for this function:



6.56.3.60 trapezIntegral()

```
template<class T >
T AtomProbe::Voxels< T >::trapezIntegral ( ) const
```

Integrate the datataset via the trapezoidal method.

Definition at line 1168 of file voxels.h.

Referenced by AtomProbe::Voxels< T >::clear().

6.56.3.61 writeFile()

```
template<class T >
size_t AtomProbe::Voxels< T >::writeFile (
            const char * cpFilename ) const
```

Write the voxel objects in column major written out to file.

Format is flat objects ("T"s) in column major format. Returns nonzero on failure

Definition at line 1131 of file voxels.h.

References ASSERT.

Referenced by AtomProbe::Voxels< T >::getBounds().

The documentation for this class was generated from the following file:

- include/atomprobe/helper/voxels.h

6.57 AtomProbe::Weight Class Reference

Placeholder class for containing input weights for MassTool.

`#include <massTool.h>`

Public Member Functions

- Weight ()
- Weight (float m, size_t uniqId=0)
- bool operator== (const Weight &b) const
- bool operator< (const Weight &b) const

Public Attributes

- float mass
- size_t uniqueId

6.57.1 Detailed Description

Placeholder class for containing input weights for MassTool.

Definition at line 29 of file massTool.h.

6.57.2 Constructor & Destructor Documentation

6.57.2.1 Weight() [1/2]

```
AtomProbe::Weight::Weight ( )  [inline]
```

Definition at line 32 of file massTool.h.

6.57.2.2 Weight() [2/2]

```
AtomProbe::Weight::Weight (
            float m,
            size_t uniqId = 0 )  [inline]
```

Definition at line 33 of file massTool.h.

References mass, and uniqueId.

6.57.3 Member Function Documentation

6.57.3.1 operator<()

```
bool AtomProbe::Weight::operator< (
            const Weight & b ) const  [inline]
```

Definition at line 39 of file massTool.h.

References mass.

6.57.3.2 operator==()

```
bool AtomProbe::Weight::operator== (
            const Weight & b ) const  [inline]
```

Definition at line 38 of file massTool.h.

References mass, and uniqueId.

6.57.4 Member Data Documentation

6.57.4.1 mass

```
float AtomProbe::Weight::mass
```

Definition at line 35 of file massTool.h.

Referenced by operator<(), operator==(), printSolution(), and Weight().

6.57.4.2 uniqueId

```
size_t AtomProbe::Weight::uniqueId
```

Definition at line 36 of file massTool.h.

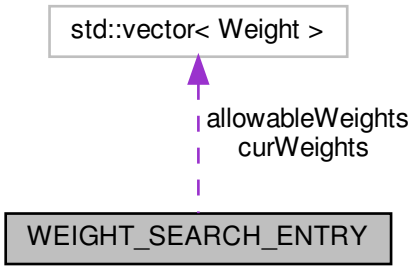
Referenced by operator==(), printSolution(), and Weight().

The documentation for this class was generated from the following file:

- include/atomprobe/algorithm/massTool.h

6.58 WEIGHT_SEARCH_ENTRY Class Reference

Collaboration diagram for WEIGHT_SEARCH_ENTRY:



Public Attributes

- vector< Weight > curWeights
- vector< Weight > allowableWeights
- size_t offset
- float cumulativeWeight

6.58.1 Detailed Description

Definition at line 40 of file massTool.cpp.

6.58.2 Member Data Documentation

6.58.2.1 allowableWeights

```
vector<Weight> WEIGHT_SEARCH_ENTRY::allowableWeights
```

Definition at line 43 of file massTool.cpp.

Referenced by AtomProbe::MassTool::bruteKnapsack().

6.58.2.2 cumulativeWeight

```
float WEIGHT_SEARCH_ENTRY::cumulativeWeight
```

Definition at line 45 of file massTool.cpp.

Referenced by AtomProbe::MassTool::bruteKnapsack().

6.58.2.3 curWeights

```
vector<Weight> WEIGHT_SEARCH_ENTRY::curWeights
```

Definition at line 43 of file massTool.cpp.

Referenced by AtomProbe::MassTool::bruteKnapsack().

6.58.2.4 offset

```
size_t WEIGHT_SEARCH_ENTRY::offset
```

Definition at line 44 of file massTool.cpp.

Referenced by AtomProbe::MassTool::bruteKnapsack().

The documentation for this class was generated from the following file:

- src/algorithm/massTool.cpp

6.59 AtomProbe::ZECH_ROOT Struct Reference

Public Attributes

- float alpha
- float lambdaBack
- float observation

6.59.1 Detailed Description

Definition at line 362 of file confidence.cpp.

6.59.2 Member Data Documentation

6.59.2.1 alpha

```
float AtomProbe::ZECH_ROOT::alpha
```

Definition at line 364 of file confidence.cpp.

Referenced by AtomProbe::zechConfidenceLimits(), and AtomProbe::zechRoot().

6.59.2.2 lambdaBack

```
float AtomProbe::ZECH_ROOT::lambdaBack
```

Definition at line 365 of file confidence.cpp.

Referenced by AtomProbe::zechConfidenceLimits(), and AtomProbe::zechRoot().

6.59.2.3 observation

```
float AtomProbe::ZECH_ROOT::observation
```

Definition at line 366 of file confidence.cpp.

Referenced by AtomProbe::zechConfidenceLimits(), and AtomProbe::zechRoot().

The documentation for this struct was generated from the following file:

- src/statistics/confidence.cpp

Chapter 7

File Documentation

7.1 CMakeFiles/3.10.2/CompilerIdCXX/CMakeCXXCompilerId.cpp File Reference

Macros

- #define COMPILER_ID ""
- #define STRINGIFY_HELPER(X) #X
- #define STRINGIFY(X) STRINGIFY_HELPER(X)
- #define PLATFORM_ID
- #define ARCHITECTURE_ID
- #define DEC(n)
- #define HEX(n)
- #define CXX_STD __cplusplus

Functions

- int main (int argc, char *argv[ ])

Variables

- char const * info_compiler = "INFO" ":" "compiler[" COMPILER_ID "]"
- char const * info_platform = "INFO" ":" "platform[" PLATFORM_ID "]"
- char const * info_arch = "INFO" ":" "arch[" ARCHITECTURE_ID "]"
- const char * info_language_dialect_default

7.1.1 Macro Definition Documentation

7.1.1.1 ARCHITECTURE_ID

```
#define ARCHITECTURE_ID
```

Definition at line 453 of file CMakeCXXCompilerId.cpp.

7.1.1.2 COMPILER_ID

```
#define COMPILER_ID ""
```

Definition at line 273 of file CMakeCXXCompilerId.cpp.

7.1.1.3 CXX_STD

```
#define CXX_STD __cplusplus
```

Definition at line 536 of file CMakeCXXCompilerId.cpp.

7.1.1.4 DEC

```
#define DEC(
              n )
```

Value:

```
('0' + (((n) / 10000000)%10)), \
  ('0' + (((n) / 1000000)%10)),  \
  ('0' + (((n) / 100000)%10)),   \
  ('0' + (((n) / 10000)%10)),    \
  ('0' + (((n) / 1000)%10)),     \
  ('0' + (((n) / 100)%10)),      \
  ('0' + (((n) / 10)%10)),       \
  ('0' +  ((n) % 10))
```

Definition at line 457 of file CMakeCXXCompilerId.cpp.

7.1.1.5 HEX

```
#define HEX(
              n )
```

Value:

```
('0' + ((n)>>28 & 0xF)), \
  ('0' + ((n)>>24 & 0xF)), \
  ('0' + ((n)>>20 & 0xF)), \
  ('0' + ((n)>>16 & 0xF)), \
  ('0' + ((n)>>12 & 0xF)), \
  ('0' + ((n)>>8  & 0xF)), \
  ('0' + ((n)>>4  & 0xF)), \
  ('0' + ((n)     & 0xF))
```

Definition at line 468 of file CMakeCXXCompilerId.cpp.

7.1.1.6 PLATFORM_ID

```
#define PLATFORM_ID
```

Definition at line 390 of file CMakeCXXCompilerId.cpp.

7.1.1.7 STRINGIFY

```
#define STRINGIFY(
              X ) STRINGIFY_HELPER(X)
```

Definition at line 294 of file CMakeCXXCompilerId.cpp.

7.1.1.8 STRINGIFY_HELPER

```
#define STRINGIFY_HELPER(
              X ) #X
```

Definition at line 293 of file CMakeCXXCompilerId.cpp.

7.1.2 Function Documentation

7.1.2.1 main()

```
int main (
             int argc,
             char * argv[] )
```

Definition at line 553 of file CMakeCXXCompilerId.cpp.

References info_compiler, info_language_dialect_default, and info_platform.

7.1.3 Variable Documentation

7.1.3.1 info_arch

```
char const* info_arch = "INFO" ":" "arch[" ARCHITECTURE_ID "]"
```

Definition at line 528 of file CMakeCXXCompilerId.cpp.

7.1.3.2 info_compiler

```
char const* info_compiler = "INFO" ":" "compiler[" COMPILER_ID "]"
```

Definition at line 280 of file CMakeCXXCompilerId.cpp.

Referenced by main().

7.1.3.3 info_language_dialect_default

```
const char* info_language_dialect_default
```

Initial value:

```
= "INFO" ":" "dialect_default["



  "98"

"]"
```

Definition at line 539 of file CMakeCXXCompilerId.cpp.

Referenced by main().

7.1.3.4 info_platform

```
char const* info_platform = "INFO" ":" "platform[" PLATFORM_ID "]"
```

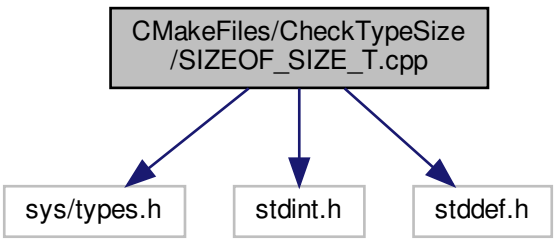
Definition at line 527 of file CMakeCXXCompilerId.cpp.

Referenced by main().

7.2 CMakeFiles/CheckTypeSize/SIZEOF_SIZE_T.cpp File Reference

```
#include <sys/types.h>
#include <stdint.h>
#include <stddef.h>
```

Include dependency graph for SIZEOF_SIZE_T.cpp:



Macros

- #define SIZE (sizeof(size_t))

Functions

- int main (int argc, char ∗argv[ ])

Variables

- char info_size [ ]

7.2.1 Macro Definition Documentation

7.2.1.1 SIZE

```
#define SIZE (sizeof(size_t))
```

Definition at line 23 of file SIZEOF_SIZE_T.cpp.

7.2.2 Function Documentation

7.2.2.1 main()

```
int main (
            int argc,
            char * argv[] )
```

Definition at line 39 of file SIZEOF_SIZE_T.cpp.

References info_size.

7.2.3 Variable Documentation

7.2.3.1 info_size

```
char info_size[]
```

Initial value:

```
= {'I', 'N', 'F', 'O', ':', 's','i','z','e','[',
  ('0' + ((SIZE / 10000)%10)),
  ('0' + ((SIZE / 1000)%10)),
  ('0' + ((SIZE / 100)%10)),
  ('0' + ((SIZE / 10)%10)),
  ('0' +  (SIZE    % 10)),
  ']',


  '\0'}
```

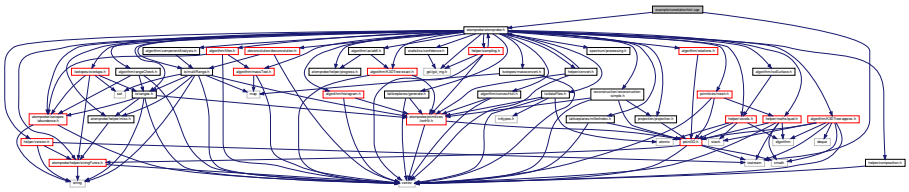
Definition at line 24 of file SIZEOF_SIZE_T.cpp.

Referenced by main().

7.3 example/correlationhist.cpp File Reference

```
#include <iostream>
#include "atomprobe/atomprobe.h"
```

Include dependency graph for correlationhist.cpp:



Functions

- void dumpHistogram (std::vector< std::vector< unsigned int > > &hist, float step)
- int main (int argc, char *argv[])

7.3.1 Function Documentation

7.3.1.1 dumpHistogram()

```
void dumpHistogram (
            std::vector< std::vector< unsigned int > > & hist,
            float step )
```

Definition at line 31 of file correlationhist.cpp.

Referenced by main().

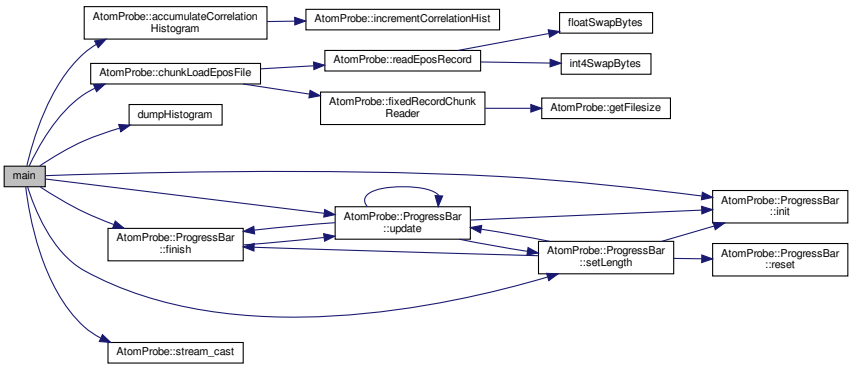
7.3.1.2 main()

```
int main (
            int argc,
            char * argv[] )
```

Definition at line 48 of file correlationhist.cpp.

References AtomProbe::accumulateCorrelationHistogram(), AtomProbe::chunkLoadEposFile(), dumpHistogram(), AtomProbe::ProgressBar::finish(), AtomProbe::ProgressBar::init(), AtomProbe::ProgressBar::setLength(), AtomProbe::stream_cast(), and AtomProbe::ProgressBar::update().

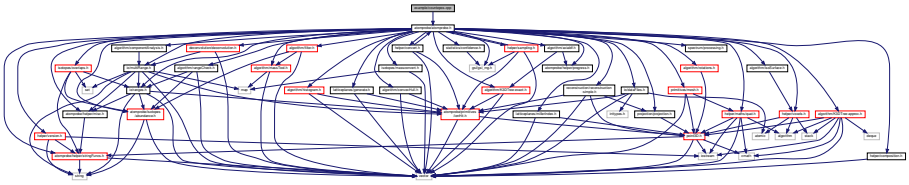
Here is the call graph for this function:



7.4 example/countepos.cpp File Reference

```
#include "atomprobe/atomprobe.h"
```

Include dependency graph for countepos.cpp:



Functions

- int main (int argc, char ∗argv[ ])

7.4.1 Function Documentation

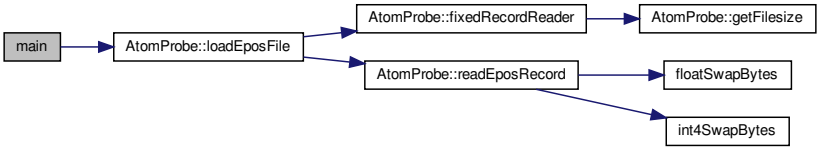
7.4.1.1 main()

```
int main (
            int argc,
            char * argv[] )
```

Definition at line 6 of file countepos.cpp.

References AtomProbe::loadEposFile().

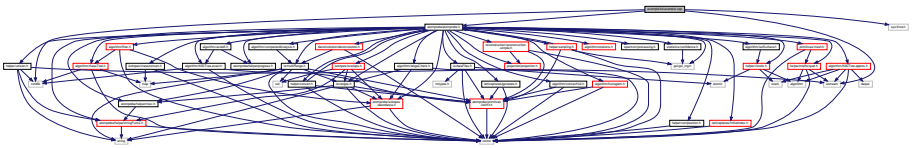
Here is the call graph for this function:



7.5 example/kd-example.cpp File Reference

```
#include <iostream>
#include <cstdlib>
#include <sys/time.h>
#include "atomprobe/atomprobe.h"
```

Include dependency graph for kd-example.cpp:



Macros

- #define TIME_START() timeval TIME_DEBUG_t; gettimeofday(&TIME_DEBUG_t,NULL);
- #define TIME_END()
- #define M_PI 3.141596254

Functions

- bool callback ()
- int main ()

Variables

- unsigned int progress =0

7.5.1 Macro Definition Documentation

7.5.1.1 M_PI

```
#define M_PI 3.141596254
```

Definition at line 34 of file kd-example.cpp.

Referenced by AtomProbe::gauss_ratio_pdf(), AtomProbe::generate1DAxialDistHistSweep(), main(), AtomProbe::Point3D::parse(), AtomProbe::ReconstructionSphereOnCone::reconstruct(), AtomProbe::ModifiedFocusSphericProjection::scaleUp(), AtomProbe::ReconstructionSphereOnCone::setReconFOV(), AtomProbe::ReconstructionSphereOnCone::setShankAngle(), AtomProbe::StereographicProjection::thetaToEta(), AtomProbe::ModifiedFocusSphericProjection::thetaToEta(), and AtomProbe::GnomonicProjection::toPlanar().

7.5.1.2 TIME_END

```
#define TIME_END( )
```

Value:

```
float TIME_DELTA; {timeval TIME_DEBUG_tend; gettimeofday(&TIME_DEBUG_tend,NULL); \
TIME_DELTA=(TIME_DEBUG_tend.tv_sec - TIME_DEBUG_t.tv_sec) + ((float)TIME_DEBUG_tend.tv_usec-(float)
      TIME_DEBUG_t.tv_usec)/1.0e6;}
```

Definition at line 29 of file kd-example.cpp.

Referenced by main().

7.5.1.3 TIME_START

```
#define TIME_START( ) timeval TIME_DEBUG_t; gettimeofday(&TIME_DEBUG_t,NULL);
```

Definition at line 28 of file kd-example.cpp.

Referenced by main().

7.5.2 Function Documentation

7.5.2.1 callback()

```
bool callback ( )
```

Definition at line 37 of file kd-example.cpp.

References progress.

Referenced by AtomProbe::computeConvexHull(), AtomProbe::GetReducedHullPts(), main(), and AtomProbe::↩ K3DTreeExact::setCallback().

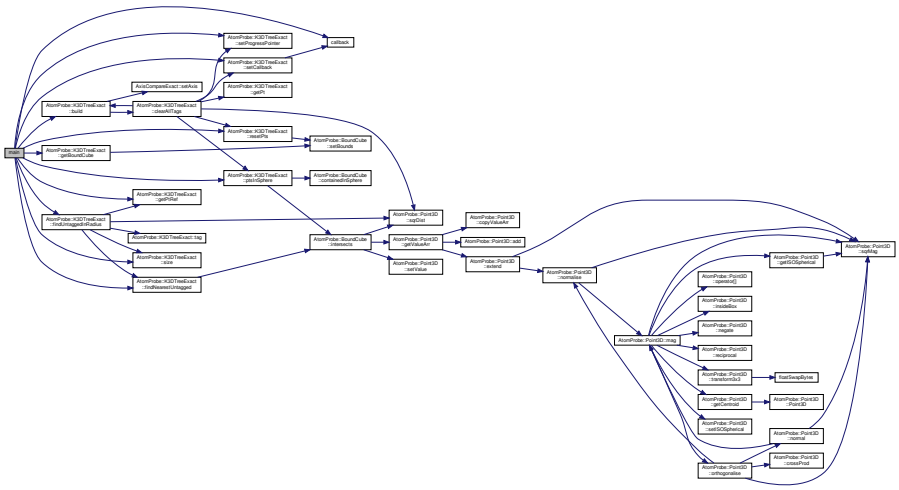
7.5.2.2 main()

```
int main ( )
```

Definition at line 49 of file kd-example.cpp.

References AtomProbe::K3DTreeExact::build(), callback(), AtomProbe::K3DTreeExact::findNearestUntagged(), AtomProbe::K3DTreeExact::findUntaggedInRadius(), AtomProbe::K3DTreeExact::getBoundCube(), AtomProbe::↩ K3DTreeExact::getPtRef(), M_PI, NUM_IONS, progress, AtomProbe::K3DTreeExact::ptsInSphere(), AtomProbe↩ ::K3DTreeExact::resetPts(), SCALE, SEARCH_RAD, AtomProbe::K3DTreeExact::setCallback(), AtomProbe::K3↩ DTreeExact::setProgressPointer(), AtomProbe::K3DTreeExact::size(), TIME_END, and TIME_START.

Here is the call graph for this function:



7.5.3 Variable Documentation

7.5.3.1 progress

```
unsigned int progress =0
```

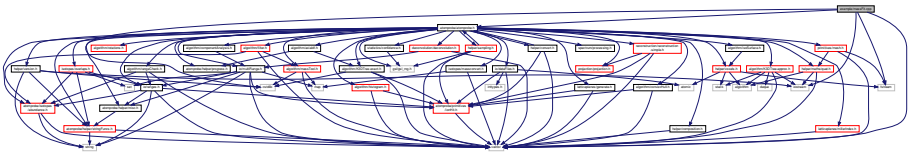
Definition at line 26 of file kd-example.cpp.

Referenced by callback(), main(), and AtomProbe::ProgressBar::update().

7.6 example/massFit.cpp File Reference

```
#include <atomprobe/atomprobe.h>
#include <iostream>
#include <cstdlib>
#include <vector>
#include <fstream>
```

Include dependency graph for massFit.cpp:



Functions

- void printSolution (const vector< Weight > &solnComponents, const vector< string > &labels)
- int main (int argc, const char *argv[])

7.6.1 Function Documentation

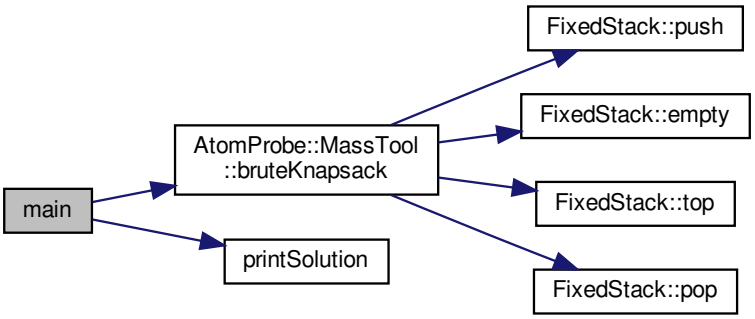
7.6.1.1 main()

```
int main (
            int argc,
            const char * argv[] )
```

Definition at line 52 of file massFit.cpp.

References AtomProbe::MassTool::bruteKnapsack(), and printSolution().

Here is the call graph for this function:



7.6.1.2 printSolution()

```
void printSolution (
            const vector< Weight > & solnComponents,
            const vector< string > & labels )
```

Definition at line 34 of file massFit.cpp.

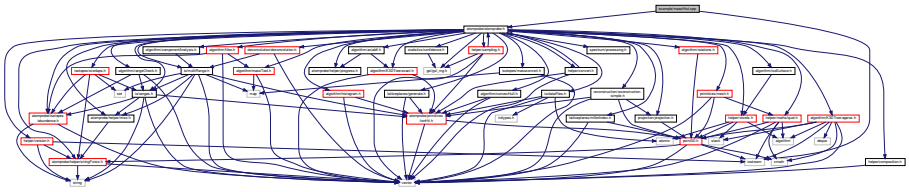
References AtomProbe::Weight::mass, and AtomProbe::Weight::uniqueId.

Referenced by main().

7.7 example/massHist.cpp File Reference

```
#include <iostream>
#include "atomprobe/atomprobe.h"
```

Include dependency graph for massHist.cpp:



Functions

- int main (int argc, char ∗argv[ ])

7.7.1 Function Documentation

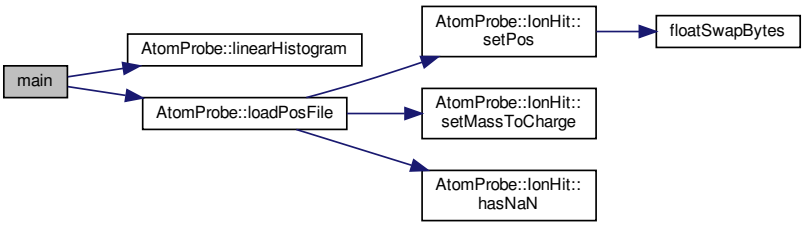
7.7.1.1 main()

```
int main (
            int argc,
            char * argv[] )
```

Definition at line 11 of file massHist.cpp.

References AtomProbe::linearHistogram(), and AtomProbe::loadPosFile().

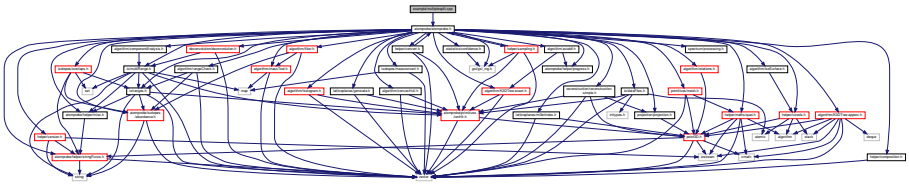
Here is the call graph for this function:



7.8 example/multiplesplit.cpp File Reference

```
#include "atomprobe/atomprobe.h"
```

Include dependency graph for multiplesplit.cpp:



Functions

- int main (int argc, char ∗argv[ ])

7.8.1 Function Documentation

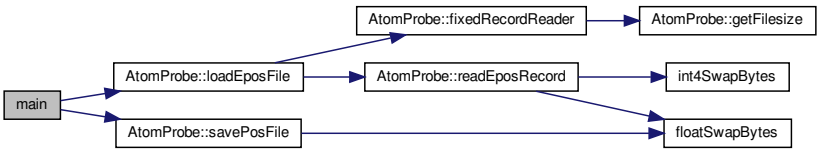
7.8.1.1 main()

```
int main (
            int argc,
            char * argv[] )
```

Definition at line 6 of file multiplesplit.cpp.

References AtomProbe::loadEposFile(), and AtomProbe::savePosFile().

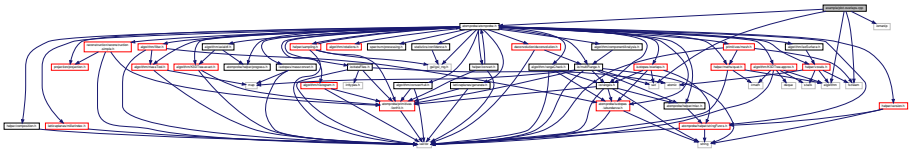
Here is the call graph for this function:



7.9 example/plot-overlaps.cpp File Reference

```
#include "atomprobe/atomprobe.h"
#include <fstream>
#include <set>
#include <iomanip>
#include <algorithm>
```

Include dependency graph for plot-overlaps.cpp:



Functions

- int main (int argc, char ∗argv[ ])

7.9.1 Function Documentation

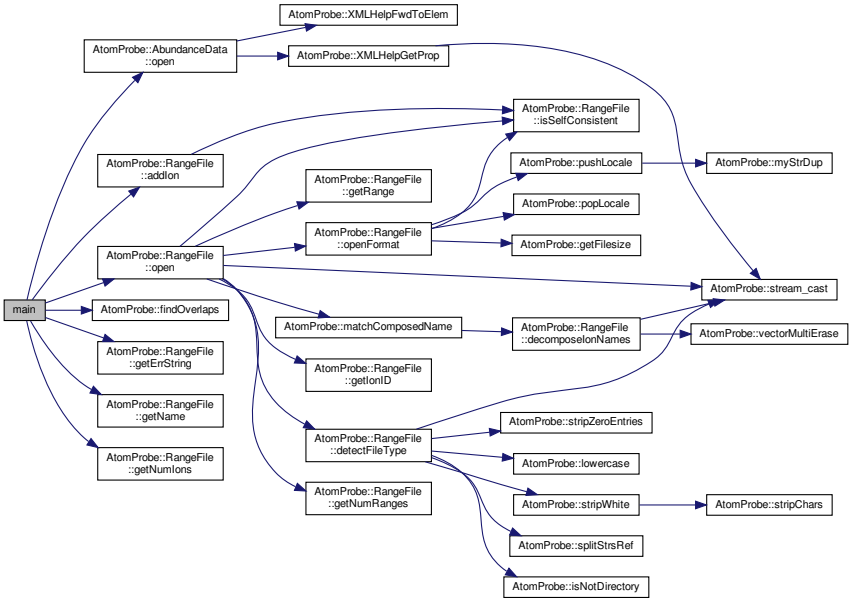
7.9.1.1 main()

```
int main (
            int argc,
            char * argv[] )
```

Definition at line 21 of file plot-overlaps.cpp.

References AtomProbe::RangeFile::addIon(), AtomProbe::findOverlaps(), AtomProbe::RangeFile::getErrString(), AtomProbe::RangeFile::getName(), AtomProbe::RangeFile::getNumIons(), AtomProbe::AbundanceData::open(), and AtomProbe::RangeFile::open().

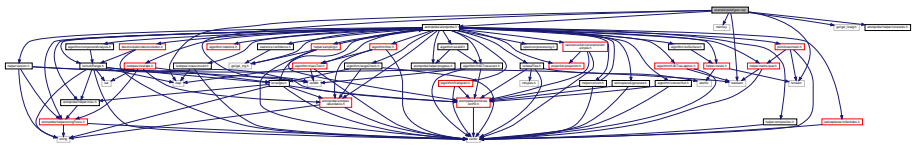
Here is the call graph for this function:



7.10 example/polefigure.cpp File Reference

```
#include <iostream>
#include <cstdlib>
#include <fstream>
#include <memory>
#include <map>
#include "atomprobe/atomprobe.h"
#include <gsl/gsl_linalg.h>
#include "atomprobe/helper/constants.h"
```

Include dependency graph for polefigure.cpp:



Functions

- void gsl_print_matrix (gsl_matrix ∗m)
- int main (int argc, char ∗argv[ ])

7.10.1 Function Documentation

7.10.1.1 gsl_print_matrix()

```
void gsl_print_matrix (
             gsl_matrix * m )
```

Definition at line 15 of file polefigure.cpp.

Referenced by main().

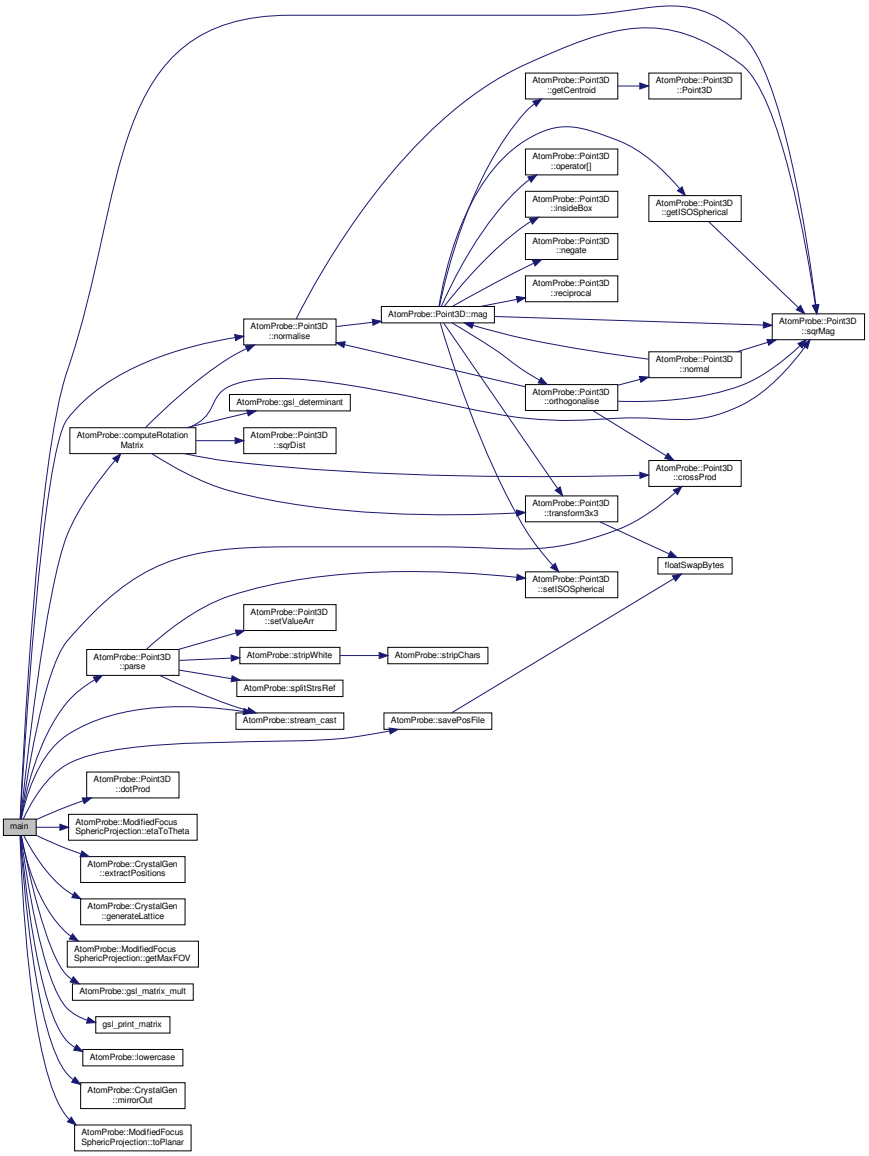
7.10.1.2 main()

```
int main (
             int argc,
             char * argv[] )
```

Definition at line 34 of file polefigure.cpp.

References AtomProbe::computeRotationMatrix(), AtomProbe::Point3D::crossProd(), AtomProbe::Point3D::dot↩Prod(), AtomProbe::ModifiedFocusSphericProjection::etaToTheta(), AtomProbe::CrystalGen::extractPositions(), AtomProbe::CrystalGen::generateLattice(), AtomProbe::ModifiedFocusSphericProjection::getMaxFOV(), Atom↩Probe::gsl_matrix_mult(), gsl_print_matrix(), AtomProbe::LATTICE_BCC, AtomProbe::LATTICE_FCC, Atom↩Probe::lowercase(), M_PI, AtomProbe::CrystalGen::mirrorOut(), AtomProbe::Point3D::normalise(), AtomProbe↩::Point3D::parse(), AtomProbe::savePosFile(), AtomProbe::Point3D::sqrMag(), AtomProbe::stream_cast(), and AtomProbe::ModifiedFocusSphericProjection::toPlanar().

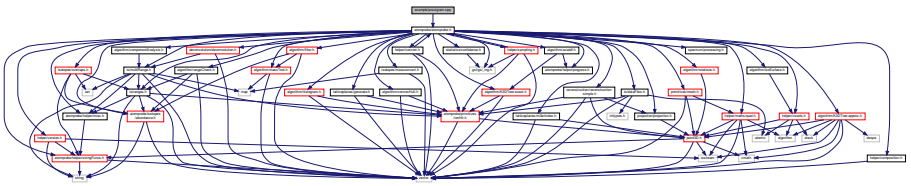
Here is the call graph for this function:



7.11 example/proxigram.cpp File Reference

```
#include "atomprobe/atomprobe.h"
```

Include dependency graph for proxigram.cpp:



Functions

- int main (int argc, char ∗argv[ ])

7.11.1 Function Documentation

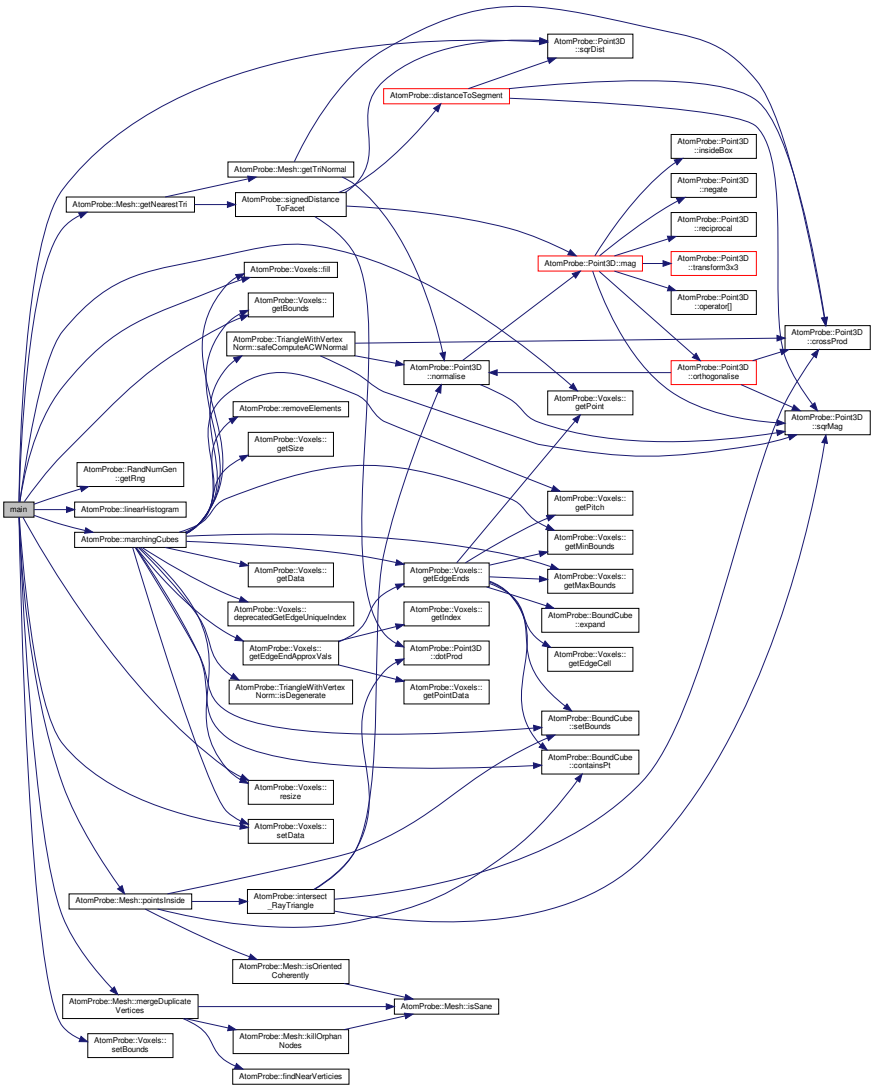
7.11.1.1 main()

```
int main (
            int argc,
            char * argv[] )
```

Definition at line 7 of file proxigram.cpp.

References AtomProbe::Voxels< T >::fill(), AtomProbe::Voxels< T >::getBounds(), AtomProbe::Mesh::get↩NearestTri(), AtomProbe::Voxels< T >::getPoint(), AtomProbe::RandNumGen::getRng(), AtomProbe::linear↩Histogram(), AtomProbe::marchingCubes(), AtomProbe::Mesh::mergeDuplicateVertices(), AtomProbe::Mesh↩::nodes, AtomProbe::Mesh::pointsInside(), progress, AtomProbe::randGen, AtomProbe::Voxels< T >::resize(), AtomProbe::Voxels< T >::setBounds(), AtomProbe::Voxels< T >::setData(), AtomProbe::Point3D::sqrDist(), and AtomProbe::Mesh::triangles.

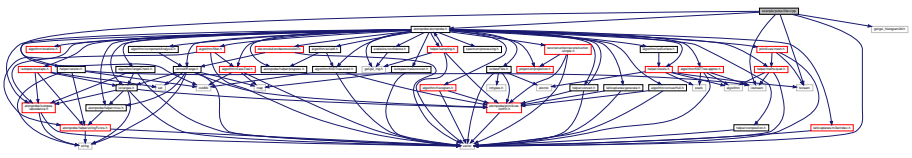
Here is the call graph for this function:



7.12 example/pulse-filter.cpp File Reference

```
#include <atomprobe/atomprobe.h>
#include <gsl/gsl_histogram2d.h>
#include <iostream>
#include <cstdlib>
#include <vector>
#include <fstream>
```

Include dependency graph for pulse-filter.cpp:



Enumerations

- enum { ERR_BAD_ARGS, ERR_BAD_EPOS_READ, ERR_BAD_NUMSAMPLES, ERR_NOMEM }

Functions

- bool convertToPos (const vector< EPOS_ENTRY > &epos, vector< IonHit > &pos)
- bool dumpHistogram (gsl_histogram2d *h, const char *outFile)
- void filterEposByPulse (const vector< EPOS_ENTRY > &input, unsigned int filterCount, vector< EPOS_↩ ENTRY > &output)
- int main (int argc, const char *argv[])

7.12.1 Enumeration Type Documentation

7.12.1.1 anonymous enum

```
anonymous enum
```

Enumerator

ERR_BAD_ARGS	
ERR_BAD_EPOS_READ	
ERR_BAD_NUMSAMPLES	
ERR_NOMEM	

Definition at line 33 of file pulse-filter.cpp.

7.12.2 Function Documentation

7.12.2.1 convertToPos()

```
bool convertToPos (
            const vector< EPOS_ENTRY > & epos,
            vector< IonHit > & pos )
```

Definition at line 42 of file pulse-filter.cpp.

7.12.2.2 dumpHistogram()

```
bool dumpHistogram (
            gsl_histogram2d * h,
            const char * outFile )
```

Definition at line 64 of file pulse-filter.cpp.

7.12.2.3 filterEposByPulse()

```
void filterEposByPulse (
            const vector< EPOS_ENTRY > & input,
            unsigned int filterCount,
            vector< EPOS_ENTRY > & output )
```

Definition at line 84 of file pulse-filter.cpp.

Referenced by main().

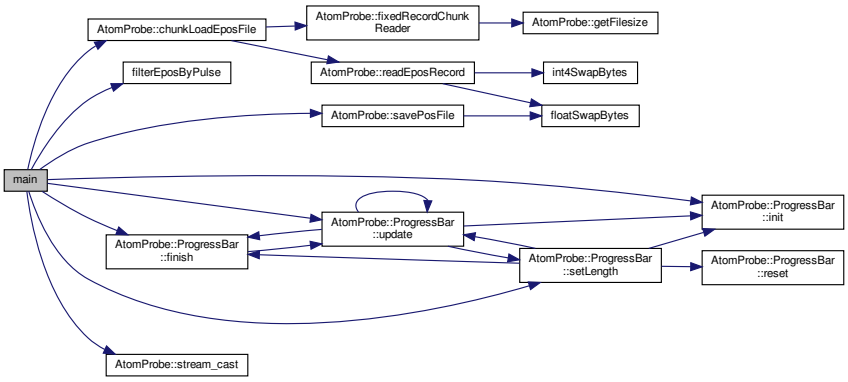
7.12.2.4 main()

```
int main (
            int argc,
            const char * argv[] )
```

Definition at line 102 of file pulse-filter.cpp.

References AtomProbe::chunkLoadEposFile(), ERR_BAD_ARGS, ERR_BAD_EPOS_READ, filterEposByPulse(), AtomProbe::ProgressBar::finish(), AtomProbe::ProgressBar::init(), AtomProbe::RECORDREAD_ERR_STRINGS, AtomProbe::savePosFile(), AtomProbe::ProgressBar::setLength(), AtomProbe::stream_cast(), and AtomProbe::↩ ProgressBar::update().

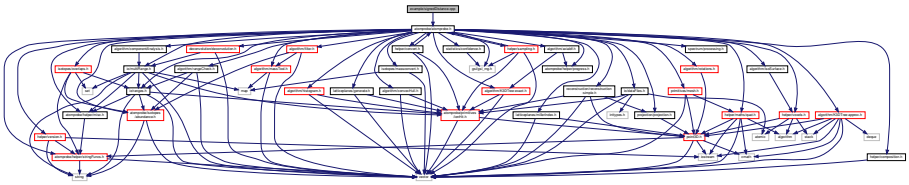
Here is the call graph for this function:



7.13 example/signedDistance.cpp File Reference

```
#include "atomprobe/atomprobe.h"
```

Include dependency graph for signedDistance.cpp:



Functions

- int main ()

7.13.1 Function Documentation

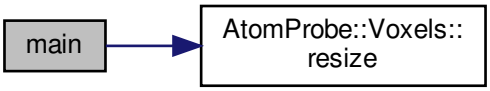
7.13.1.1 main()

```
int main ( )
```

Definition at line 8 of file signedDistance.cpp.

References AtomProbe::Voxels< T >::resize().

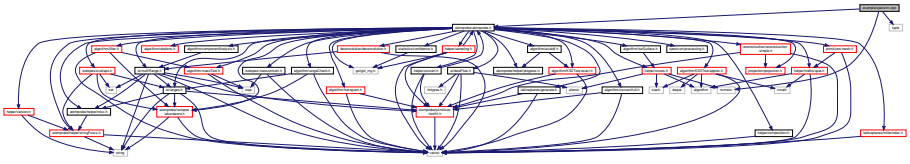
Here is the call graph for this function:



7.14 example/specsim.cpp File Reference

```
#include "atomprobe/atomprobe.h"
#include <tuple>
#include <numeric>
```

Include dependency graph for specsim.cpp:



Typedefs

- typedef vector< pair< string, size_t > > FRAGMENT

Functions

- void getMassDistributions (const vector< FRAGMENT > &fragmentVec, const vector< string > &parentSpecies, const AbundanceData &natTable, vector< vector< pair< float, float > > > &massDistVec)
- void normaliseVec (vector< float > &v)
- int main (int argc, char *argv[])

Variables

- const float MASS_TOL =0.05

7.14.1 Typedef Documentation

7.14.1.1 FRAGMENT

```
typedef vector<pair<string,size_t> > FRAGMENT
```

Definition at line 11 of file specsim.cpp.

7.14.2 Function Documentation

7.14.2.1 getMassDistributions()

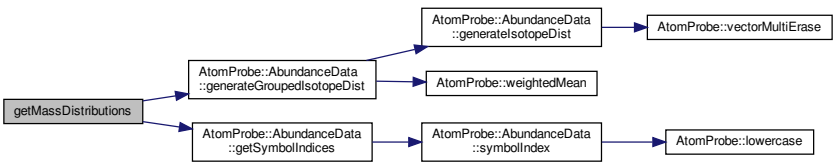
```
void getMassDistributions (
            const vector< FRAGMENT > & fragmentVec,
            const vector< string > & parentSpecies,
            const AbundanceData & natTable,
            vector< vector< pair< float, float > > > & massDistVec )
```

Definition at line 358 of file specsim.cpp.

References AtomProbe::AbundanceData::generateGroupedIsotopeDist(), AtomProbe::AbundanceData::getSymbolIndices(), and MASS_TOL.

Referenced by main().

Here is the call graph for this function:



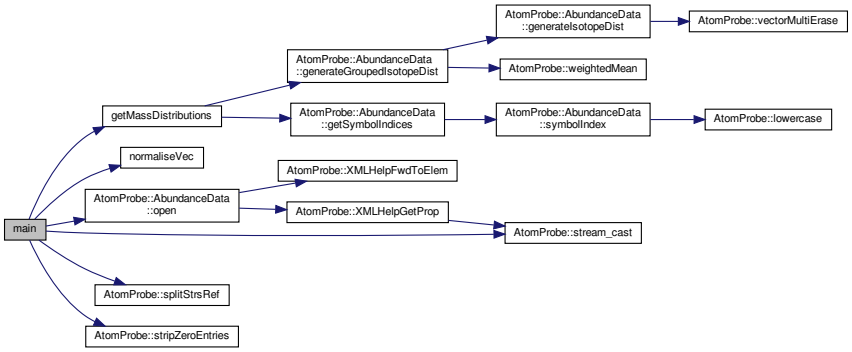
7.14.2.2 main()

```
int main (
            int argc,
            char * argv[] )
```

Definition at line 26 of file specsim.cpp.

References getMassDistributions(), MASS_TOL, normaliseVec(), AtomProbe::AbundanceData::open(), AtomProbe::splitStrsRef(), AtomProbe::stream_cast(), and AtomProbe::stripZeroEntries().

Here is the call graph for this function:



7.14.2.3 normaliseVec()

```
void normaliseVec (
            vector< float > & v )
```

Definition at line 18 of file specsim.cpp.

Referenced by main().

7.14.3 Variable Documentation

7.14.3.1 MASS_TOL

```
const float MASS_TOL =0.05
```

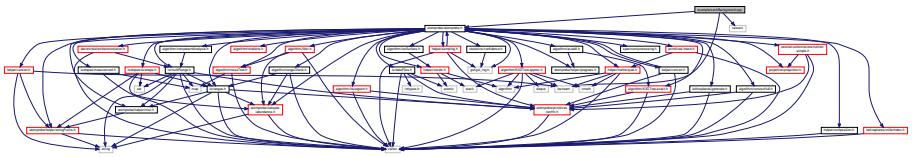
Definition at line 9 of file specsim.cpp.

Referenced by AtomProbe::MultiRange::copyDataFromRange(), getMassDistributions(), and main().

7.15 example/zechBackground.cpp File Reference

```
#include <iostream>
#include "atomprobe/atomprobe.h"
#include <cassert>
```

Include dependency graph for zechBackground.cpp:



Macros

- #define ASSERT(f) assert(f)

Functions

- template<class T >
  bool dumpHistogramToFile (std::vector< std::vector< T > > &hist, const char *filename)
- void zechCorrect (vector< float > &background, vector< float > &observation, float alpha, vector< float > &corrected)
- int main (int argc, char *argv[])

7.15.1 Macro Definition Documentation

7.15.1.1 ASSERT

```
#define ASSERT(
              f ) assert(f)
```

Definition at line 26 of file zechBackground.cpp.

Referenced by AtomProbe::AbundanceData::abundanceBetweenLimits(), AtomProbe::MultiRange::addIon(), AtomProbe::RangeFile::addIon(), AtomProbe::MultiRange::addRange(), AtomProbe::RangeFile::addRange(), AtomProbe::Voxels< T >::applyMask(), AtomProbe::K3DTreeExact::build(), AtomProbe::buildFrequencyTable(), AtomProbe::K3DTreeExact::clearAllTags(), AtomProbe::computeIonDistAdjacency(), AtomProbe::computeRangeAdjacency(), AtomProbe::computeRotationMatrix(), AtomProbe::BoundCube::containsPt(), AtomProbe::convertMolToMass(), AtomProbe::MultiRange::copyDataFromRange(), AtomProbe::Point3D::copyValueArr(),

AtomProbe::countDataDistanceWeight(), AtomProbe::cumTrapezoid(), AtomProbe::Determinant(), AtomProbe::Mesh::divideMeshSurface(), AtomProbe::doFitBackground(), AtomProbe::edgeIdx(), AtomProbe::TRIANGLE::edgesMismatch(), AtomProbe::AbundanceData::elementNames(), AtomProbe::RangeFile::eraseIon(), AtomProbe::RangeFile::eraseRange(), AtomProbe::ModifiedFocusSphericProjection::etaToTheta(), AtomProbe::Point3D::extend(), AtomProbe::filterPeakNeedBiggerObs(), AtomProbe::findMaxLessThanOrEq(), AtomProbe::K3DTreeApprox::findNearest(), AtomProbe::K3DTreeExact::findNearestUntagged(), AtomProbe::findNearVerticies(), AtomProbe::findOverlaps(), AtomProbe::findPeaks(), AtomProbe::K3DTreeExact::findUntaggedInRadius(), AtomProbe::MultiRange::flattenToMassAxis(), AtomProbe::generate1DAxialDistHist(), AtomProbe::generate1DAxialDistHistSweep(), AtomProbe::AbundanceData::generateIsotopeDist(), AtomProbe::RangeFile::getAllExts(), AtomProbe::AbundanceData::getAtomicNumber(), AtomProbe::BoundCube::getBound(), AtomProbe::IonHit::getBoundCube(), AtomProbe::K3DTreeExact::getBoundCube(), AtomProbe::BoundCube::getBounds(), AtomProbe::Mesh::getBounds(), AtomProbe::BoundCube::getCentroid(), AtomProbe::MultiRange::getColour(), AtomProbe::RangeFile::getColour(), AtomProbe::Mesh::getContainedNodes(), AtomProbe::Voxels< T >::getData(), AtomProbe::Voxels< T >::getEdgeCell(), AtomProbe::Voxels< T >::getEdgeEnds(), AtomProbe::AbundanceData::getErrorText(), AtomProbe::MultiRange::getErrString(), AtomProbe::getFitErrorMsg(), AtomProbe::Voxels< T >::getIndex(), AtomProbe::Voxels< T >::getInterpolatedData(), AtomProbe::Voxels< T >::getInterpSlice(), AtomProbe::Mesh::getIntersectingPrimitives(), AtomProbe::IonHit::getIonDataLimits(), AtomProbe::MultiRange::getIonID(), AtomProbe::RangeFile::getIonID(), AtomProbe::MultiRange::getIonName(), AtomProbe::AbundanceData::getMajorIsotopeFromElemIdx(), AtomProbe::Voxels< T >::getMaxBounds(), AtomProbe::BoundCube::getMaxDistanceToBox(), AtomProbe::Voxels< T >::getMinBounds(), AtomProbe::MultiRange::getMolecule(), AtomProbe::RangeFile::getName(), AtomProbe::AbundanceData::getNearestCharge(), AtomProbe::MultiRange::getNumRanges(), AtomProbe::K3DTreeExact::getOrigIndex(), AtomProbe::Voxels< T >::getPointData(), AtomProbe::K3DTreeExact::getPt(), AtomProbe::K3DTreeExact::getPtRef(), AtomProbe::MultiRange::getRange(), AtomProbe::RangeFile::getRangeVolume(), AtomProbe::GetReducedHullPts(), AtomProbe::BoundCube::getSize(), AtomProbe::Voxels< T >::getSize(), AtomProbe::Voxels< T >::getSlice(), AtomProbe::Voxels< T >::getSum(), AtomProbe::K3DTreeExact::getTag(), AtomProbe::Mesh::getTriNormal(), AtomProbe::Mesh::getVolume(), AtomProbe::gsl_determinant(), AtomProbe::hexStrToUChar(), AtomProbe::Mesh::isOrientedCoherently(), AtomProbe::AbundanceData::isotope(), AtomProbe::AbundanceData::isotopeIndex(), AtomProbe::AbundanceData::isotopes(), AtomProbe::RangeFile::isSelfConsistent(), AtomProbe::Mesh::killOrphanNodes(), AtomProbe::leastSquaresDeconvolve(), AtomProbe::linearHistogram(), AtomProbe::loadATOFile(), AtomProbe::loadPosFile(), main(), AtomProbe::makeHistogram(), AtomProbe::marchingCubes(), AtomProbe::BoundCube::max(), AtomProbe::Voxels< T >::max(), AtomProbe::maxExplainedFraction(), AtomProbe::Mesh::mergeDuplicateVertices(), AtomProbe::BoundCube::min(), AtomProbe::Voxels< T >::min(), AtomProbe::Voxels< T >::minMax(), AtomProbe::MultiRange::MultiRange(), AtomProbe::Mesh::numDupTris(), AtomProbe::numericalEstimateGaussRatioConf(), AtomProbe::numericalEstimatePoissRatioConf(), AtomProbe::numericalEstimateSkellamConf(), AtomProbe::RangeFile::open(), AtomProbe::RangeFile::openFormat(), AtomProbe::Voxels< T >::operator/=(), AtomProbe::IonHit::operator[](), AtomProbe::Point3D::operator[](), AtomProbe::pairContains(), AtomProbe::pairOverlaps(), AtomProbe::Mesh::pointsInside(), AtomProbe::poissonConfidenceObservation(), FixedStack< T >::pop(), AtomProbe::Mesh::print(), AtomProbe::K3DTreeExact::ptsInSphere(), AtomProbe::pushLocale(), AtomProbe::pyramidVol(), AtomProbe::quat_get_rot_quat(), AtomProbe::quat_rot(), AtomProbe::quat_rot_array(), AtomProbe::RangeFile::rangeTypeString(), AtomProbe::readPosapOps(), AtomProbe::ReconstructionSphereOnCone::reconstruct(), AtomProbe::Mesh::removeDuplicateTris(), AtomProbe::removeElements(), AtomProbe::Voxels< T >::resizeKeepData(), AtomProbe::Mesh::saveGmshMesh(), AtomProbe::saveTapsimBin(), AtomProbe::GnomonicProjection::scaleDown(), AtomProbe::StereographicProjection::scaleDown(), AtomProbe::ModifiedFocusSphericProjection::scaleDown(), AtomProbe::GnomonicProjection::scaleUp(), AtomProbe::StereographicProjection::scaleUp(), AtomProbe::ModifiedFocusSphericProjection::scaleUp(), AtomProbe::BoundCube::segmentTriple(), AtomProbe::BoundCube::setBound(), AtomProbe::Voxels< T >::setBounds(), AtomProbe::RangeFile::setColour(), AtomProbe::Voxels< T >::setData(), AtomProbe::ReconstructionSphereOnCone::setDetectorEfficiency(), AtomProbe::ReconstructionSphereOnCone::setFlightPath(), AtomProbe::ReconstructionSphereOnCone::setInitialRadius(), AtomProbe::MultiRange::setIonID(), AtomProbe::RangeFile::setIonID(), AtomProbe::LinearFeedbackShiftReg::setMaskPeriod(), AtomProbe::Voxels< T >::setPoint(), AtomProbe::IonHit::setPos(), AtomProbe::RangeFile::setRangeEnd(), AtomProbe::RangeFile::setRangeStart(), AtomProbe::RangeFile::setRangeVolume(), AtomProbe::ReconstructionSphereOnCone::setReconFOV(), AtomProbe::ReconstructionSphereOnCone::setShankAngle(), AtomProbe::Mesh::setTriangleMesh(), AtomProbe::signedDistanceToFacet(), AtomProbe::K3DTreeExact::size(), AtomProbe::MultiRange::splitOverlapping(), AtomProbe::AbundanceData::symbolIndex(), AtomProbe::K3DTreeExact::tag(), AtomProbe::GnomonicProjection::toPlanar(), AtomProbe::vectorPointDir(), AtomProbe::LinearFeedbackShiftReg::verifyTable(), AtomProbe::MultiRange::write(), AtomProbe::RangeFile::write(), AtomProbe::Voxels< T >::writeFile(), Atom

Probe::zechConfidenceLimits(), and zechCorrect().

7.15.2 Function Documentation

7.15.2.1 dumpHistogramToFile()

```
template<class T >
bool dumpHistogramToFile (
            std::vector< std::vector< T > > & hist,
            const char * filename )
```

Definition at line 30 of file zechBackground.cpp.

Referenced by main().

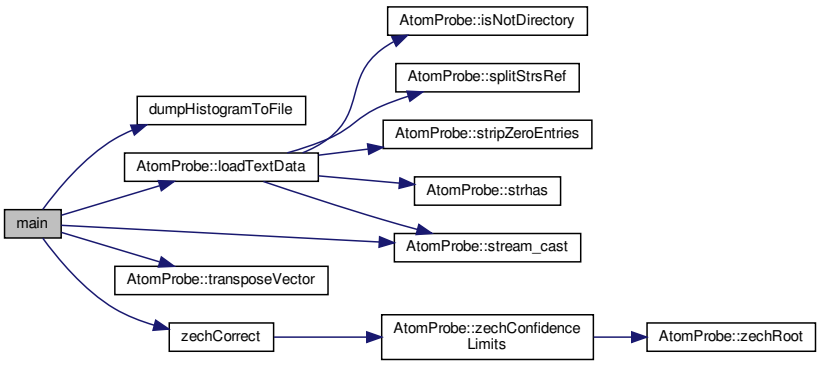
7.15.2.2 main()

```
int main (
            int argc,
            char * argv[] )
```

Definition at line 80 of file zechBackground.cpp.

References ASSERT, dumpHistogramToFile(), AtomProbe::loadTextData(), AtomProbe::stream_cast(), AtomProbe::transposeVector(), and zechCorrect().

Here is the call graph for this function:



7.15.2.3 zechCorrect()

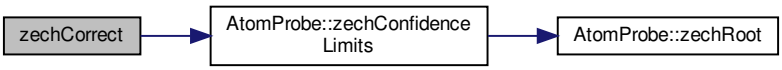
```
void zechCorrect (
            vector< float > & background,
            vector< float > & observation,
            float alpha,
            vector< float > & corrected )
```

Definition at line 49 of file zechBackground.cpp.

References ASSERT, and AtomProbe::zechConfidenceLimits().

Referenced by main().

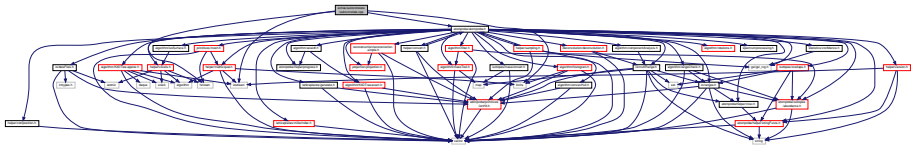
Here is the call graph for this function:



7.16 extras/autocorrelate/autocorrelate.cpp File Reference

```
#include <iostream>
#include <fstream>
#include <limits>
#include "atomprobe/atomprobe.h"
```

Include dependency graph for autocorrelate.cpp:



Macros

- #define ASSERT(f) {}

Functions

- bool callback ()
- template<class T >
  void dumpAutocorrelation (const vector< vector< T > > &autoCorrelateFunc, const RangeFile &rangeFile, float binStep, std::ostream &strm)
- int main (int argc, char *argv[])

Variables

- const unsigned int PROGRESS_BAR_SIZE =50
- ProgressBar * treeProgressBar =0
- unsigned int treeProgressValue =0

7.16.1 Macro Definition Documentation

7.16.1.1 ASSERT

```
#define ASSERT(
               f ) {}
```

Definition at line 35 of file autocorrelate.cpp.

Referenced by dumpAutocorrelation(), and main().

7.16.2 Function Documentation

7.16.2.1 callback()

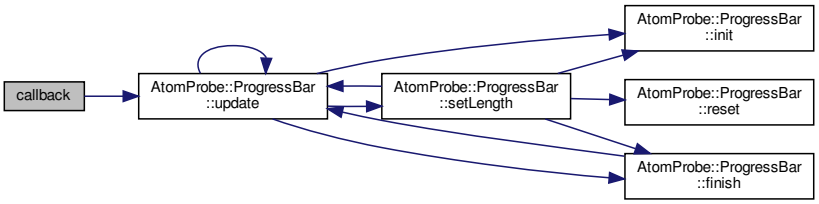
```
bool callback ( )
```

Definition at line 43 of file autocorrelate.cpp.

References treeProgressValue, and AtomProbe::ProgressBar::update().

Referenced by main().

Here is the call graph for this function:



7.16.2.2 dumpAutocorrelation()

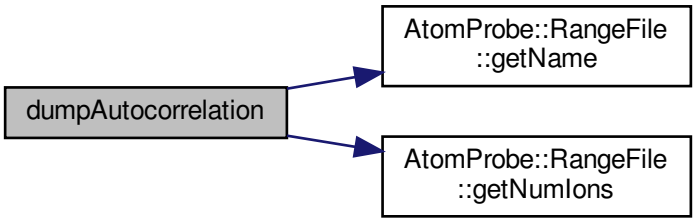
```
template<class T >
void dumpAutocorrelation (
            const vector< vector< T > > & autoCorrelateFunc,
            const RangeFile & rangeFile,
            float binStep,
            std::ostream & strm )
```

Definition at line 59 of file autocorrelate.cpp.

References ASSERT, AtomProbe::RangeFile::getName(), and AtomProbe::RangeFile::getNumIons().

Referenced by main().

Here is the call graph for this function:



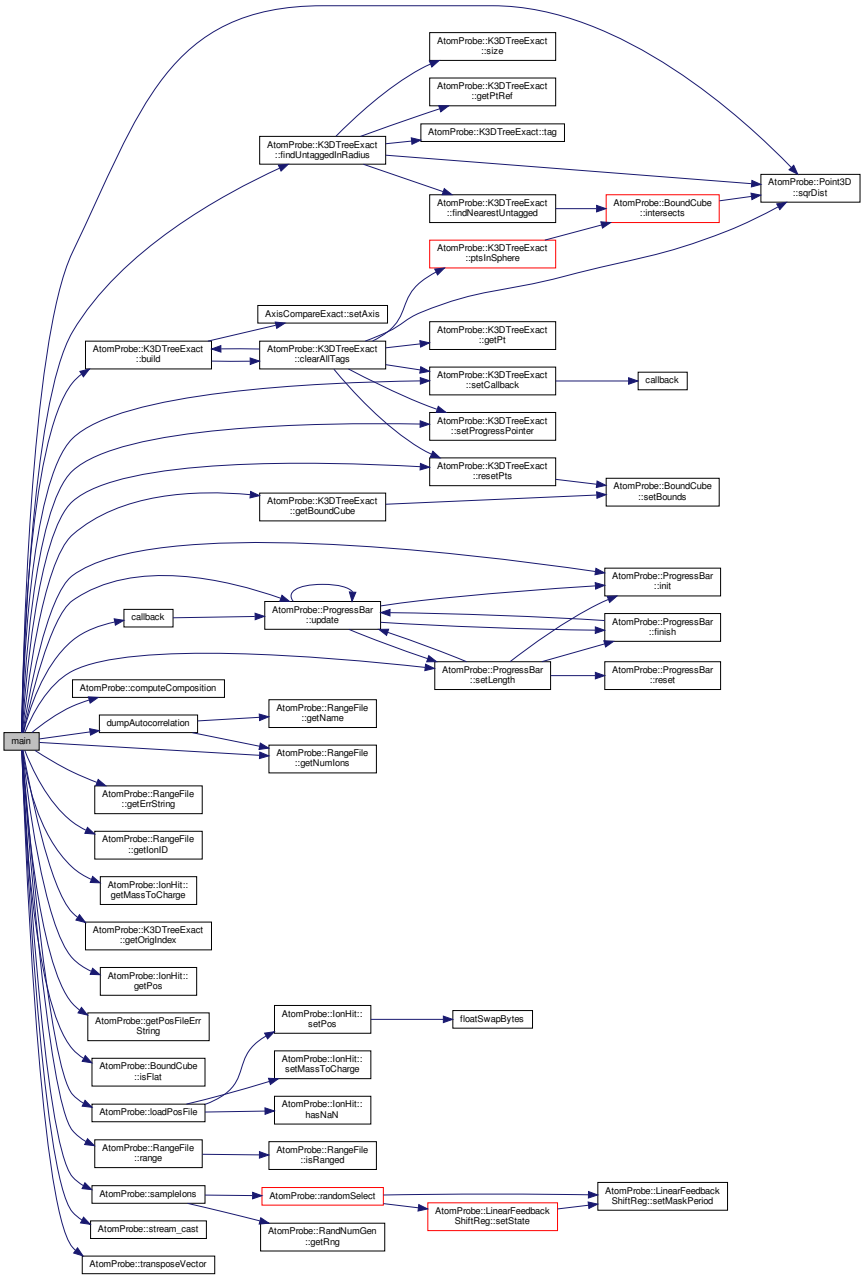
7.16.2.3 main()

```
int main (
            int argc,
            char * argv[] )
```

Definition at line 86 of file autocorrelate.cpp.

References ASSERT, AtomProbe::K3DTreeExact::build(), callback(), AtomProbe::computeComposition(), dumpAutocorrelation(), AtomProbe::K3DTreeExact::findUntaggedInRadius(), AtomProbe::K3DTreeExact::getBoundCube(), AtomProbe::RangeFile::getErrString(), AtomProbe::RangeFile::getIonID(), AtomProbe::IonHit::getMassToCharge(), AtomProbe::RangeFile::getNumIons(), AtomProbe::K3DTreeExact::getOrigIndex(), AtomProbe::IonHit::getPos(), AtomProbe::getPosFileErrString(), AtomProbe::ProgressBar::init(), AtomProbe::BoundCube::isFlat(), AtomProbe::loadPosFile(), PROGRESS_BAR_SIZE, AtomProbe::RangeFile::range(), AtomProbe::K3DTreeExact::resetPts(), AtomProbe::sampleIons(), AtomProbe::K3DTreeExact::setCallback(), AtomProbe::ProgressBar::setLength(), AtomProbe::K3DTreeExact::setProgressPointer(), AtomProbe::Point3D::sqrDist(), AtomProbe::stream_cast(), AtomProbe::transposeVector(), treeProgressBar, treeProgressValue, and AtomProbe::ProgressBar::update().

Here is the call graph for this function:



7.16.3 Variable Documentation

7.16.3.1 PROGRESS_BAR_SIZE

```
const unsigned int PROGRESS_BAR_SIZE =50
```

Definition at line 38 of file autocorrelate.cpp.

Referenced by main().

7.16.3.2 treeProgressBar

```
ProgressBar* treeProgressBar =0
```

Definition at line 40 of file autocorrelate.cpp.

Referenced by main().

7.16.3.3 treeProgressValue

```
unsigned int treeProgressValue =0
```

Definition at line 41 of file autocorrelate.cpp.

Referenced by callback(), and main().

7.17 extras/readpos_c/readpos.h File Reference

Functions

- unsigned int readPos (const char *filename, float **x, float **y, float **z, float **m, unsigned int *nPts)

7.17.1 Function Documentation

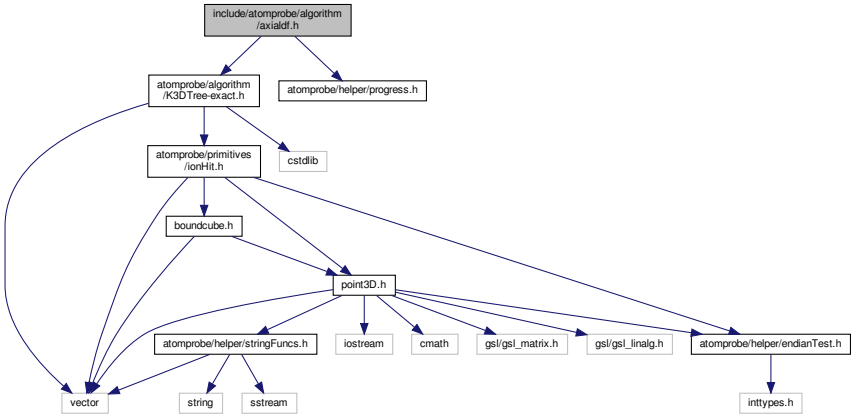
7.17.1.1 readPos()

```
unsigned int readPos (
            const char * filename,
            float ** x,
            float ** y,
            float ** z,
            float ** m,
            unsigned int * nPts )
```

7.18 include/atomprobe/algorithm/axialdf.h File Reference

```
#include "atomprobe/algorithm/K3DTree-exact.h"
#include "atomprobe/helper/progress.h"
```

Include dependency graph for axialdf.h:



This graph shows which files directly or indirectly include this file:

Namespaces

- AtomProbe

Functions

- unsigned int AtomProbe::generate1DAxialDistHist (const std::vector< Point3D > &pointList, K3DTreeExact &tree, const Point3D &axisDir, float distMax, std::vector< unsigned int > &histogram)

  Generate a 1D axial distribution function,.

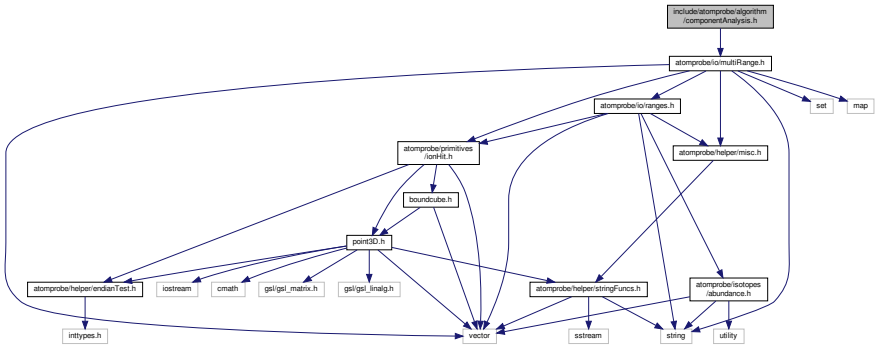
- unsigned int AtomProbe::generate1DAxialDistHistSweep (const std::vector< Point3D > &pointList, K3D↩ TreeExact &tree, float distMax, float dTheta, float dPhi, ProgressBar &prog, std::vector< std::vector< std↩ ::vector< unsigned int > > > &histogram)

  Generate a series of 1D distribution functions, one per pixel in a 2D grid of spherical coordinate directions.

7.19 include/atomprobe/algorithm/componentAnalysis.h File Reference

```
#include "atomprobe/io/multiRange.h"
```

Include dependency graph for componentAnalysis.h:



This graph shows which files directly or indirectly include this file:

Classes

- struct AtomProbe::OVERLAP_PROBLEM_SETTINGS

Namespaces

- AtomProbe

Functions

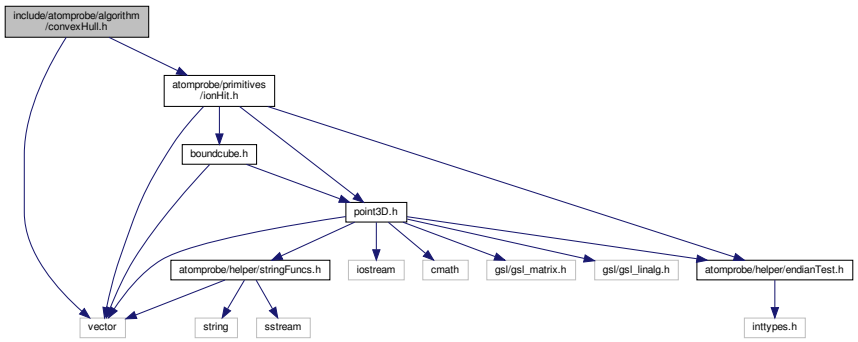
- void AtomProbe::computeIonDistAdjacency (const MultiRange &mrf, const AbundanceData &abundance, const OVERLAP_PROBLEM_SETTINGS &settings, gsl_matrix ∗&m, gsl_vector ∗&vOwnership, gsl_vector ∗&vMass)

  Calculate the adjacency matrix for the ions in a multirange.

7.20 include/atomprobe/algorithm/convexHull.h File Reference

```
#include <vector>
#include "atomprobe/primitives/ionHit.h"
```

Include dependency graph for convexHull.h:



This graph shows which files directly or indirectly include this file:

Namespaces

- AtomProbe

Enumerations

- enum { AtomProbe::HULL_SURFREDUCE_NEGATIVE_SCALE_FACT =1, AtomProbe::HULL_ERR_USE↩ R_ABORT, AtomProbe::HULL_ERR_NO_MEM }

Functions

- unsigned int AtomProbe::GetReducedHullPts (const std::vector< IonHit > &points, float reductionDim, unsigned int *progress, bool(*callback)(bool), std::vector< IonHit > &pointResult)

  Obtain a set of points that are a subset of points the convex hull that are at least "reductionDim" away from the hull itself.

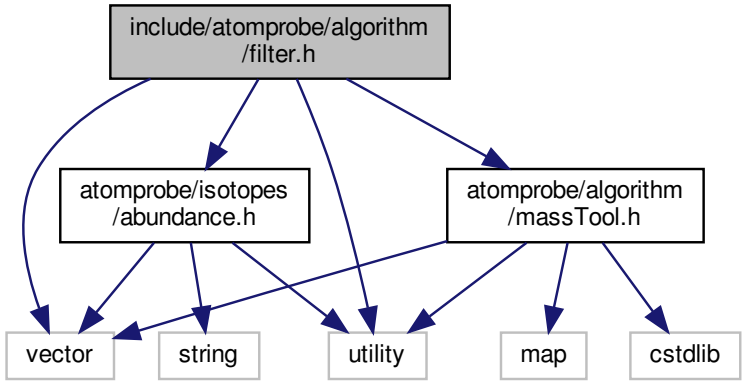
- unsigned int AtomProbe::computeConvexHull (const std::vector< IonHit > &data, unsigned int *progress, bool(*callback)(bool), std::vector< Point3D > &curHull, bool freeHull)

  Obtain the convex hull of a set of ions.

7.21 include/atomprobe/algorithm/filter.h File Reference

```
#include <vector>
#include <utility>
#include "atomprobe/isotopes/abundance.h"
#include "atomprobe/algorithm/massTool.h"
```

Include dependency graph for filter.h:



This graph shows which files directly or indirectly include this file:

Namespaces

- AtomProbe

Functions

- void AtomProbe::filterPeakNeedBiggerObs (const AbundanceData &massTable, const std::vector< float > &peakData, float tolerance, size_t solutionCharge, std::vector< std::vector< ISOTOPE_ENTRY > > &solutions)
- void AtomProbe::filterBySolutionPPM (const AbundanceData &massTable, float minPpm, std::vector< std::vector< ISOTOPE_ENTRY > > &solutions)

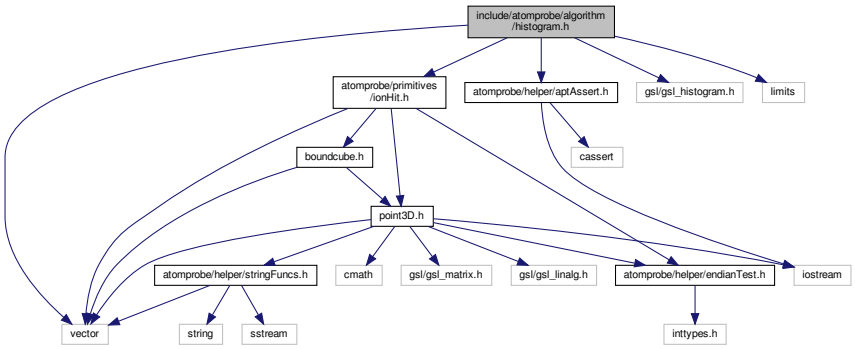
  Use the maximum possible PPM for each isotopic combination to filter possible solutions.
- std::vector< float > AtomProbe::maxExplainedFraction (const std::vector< std::pair< float, float > > &massData, float peakMass, float massWidth, const std::vector< std::vector< ISOTOPE_ENTRY > > &solutions, const AbundanceData &massTable, float massDistTol, unsigned int solutionCharge)

  Compute the fraction of the data that has been explained, using the natural abundance information, and intensity data.

7.22 include/atomprobe/algorithm/histogram.h File Reference

```
#include <vector>
#include "atomprobe/primitives/ionHit.h"
#include "atomprobe/helper/aptAssert.h"
#include <gsl/gsl_histogram.h>
#include <limits>
```

Include dependency graph for histogram.h:



This graph shows which files directly or indirectly include this file:

Namespaces

- AtomProbe

Functions

- bool AtomProbe::correlationHistogram (const std::vector< EPOS_ENTRY > &eposIons, std::vector< std::vector< unsigned int > > &histogram, float stepMass, float endMass, bool lowerTriangular=false)

  Generates an ion "correlation histogram" from a vector of EPOS ions. The input vector MUST

- bool AtomProbe::accumulateCorrelationHistogram (const std::vector< EPOS_ENTRY > &eposIons, std::vector< std::vector< unsigned int > > &histogram, float stepMass, float endMass, bool lowerTriangular=true)

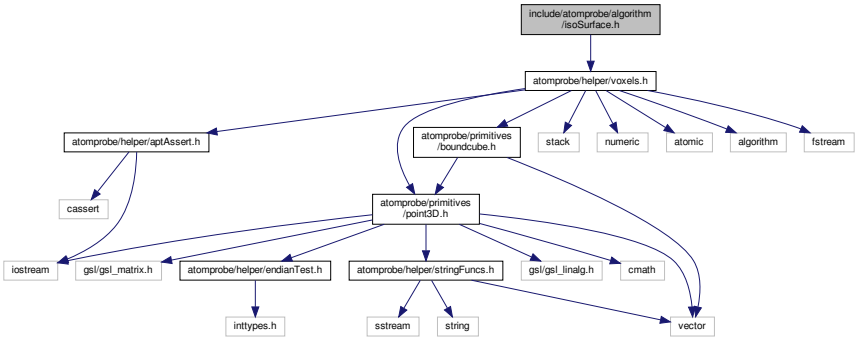
  Increments a correlation histogram, as per correlationHistogram,.

- template<class T >
  void AtomProbe::linearHistogram (const std::vector< T > &data, T start, T end, T step, std::vector< T > &histVals)

7.23 include/atomprobe/algorithm/isoSurface.h File Reference

```
#include "atomprobe/helper/voxels.h"
```

Include dependency graph for isoSurface.h:



This graph shows which files directly or indirectly include this file:

Classes

- class AtomProbe::TriangleWithVertexNorm
- struct AtomProbe::TriangleWithIndexedVertices

Namespaces

- AtomProbe

Functions

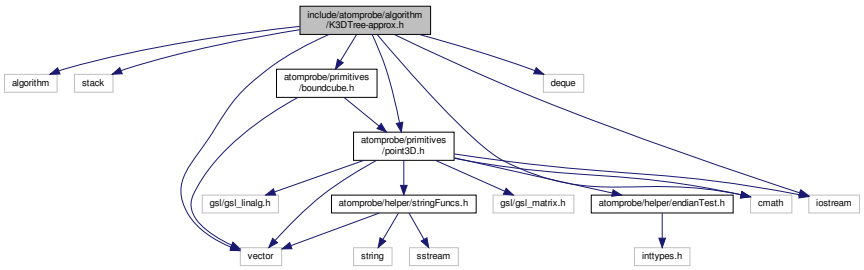
- void AtomProbe::marchingCubes (const Voxels< float > &v, float isoValue, std::vector< TriangleWithVertex↩ Norm > &tVec)

7.24 include/atomprobe/algorithm/K3DTree-approx.h File Reference

```
#include <algorithm>
#include <stack>
#include <vector>
#include <deque>
#include <cmath>
#include <iostream>
#include "atomprobe/primitives/point3D.h"
```

```
#include "atomprobe/primitives/boundcube.h"
```

Include dependency graph for K3DTree-approx.h:



This graph shows which files directly or indirectly include this file:

Classes

- class AtomProbe::AxisCompare

  Functor allowing for sorting of points in 3D.
- class AtomProbe::K3DNodeApprox

  Node Class for storing point.
- class AtomProbe::K3DTreeApprox

  3D specific KD tree

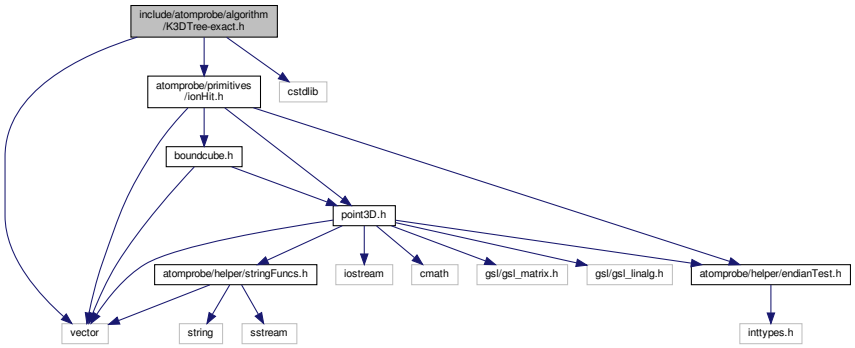
Namespaces

- AtomProbe

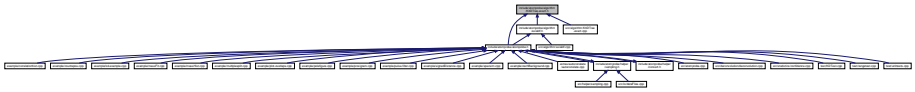
7.25 include/atomprobe/algorithm/K3DTree-exact.h File Reference

```
#include <vector>
#include <cstdlib>
#include "atomprobe/primitives/ionHit.h"
```

Include dependency graph for K3DTree-exact.h:



This graph shows which files directly or indirectly include this file:



Classes

- class AtomProbe::K3DNodeExact

  Node Class for storing point.
- class AtomProbe::K3DTreeExact

  3D specific KD tree

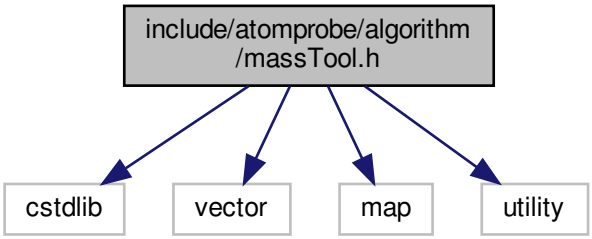
Namespaces

- AtomProbe

7.26 include/atomprobe/algorithm/massTool.h File Reference

```
#include <cstdlib>
#include <vector>
#include <map>
#include <utility>
```

Include dependency graph for massTool.h:



This graph shows which files directly or indirectly include this file:

Classes

- class AtomProbe::Weight

  Placeholder class for containing input weights for MassTool.
- class AtomProbe::MassTool

  Class that brute-force solves the knapsack problem.

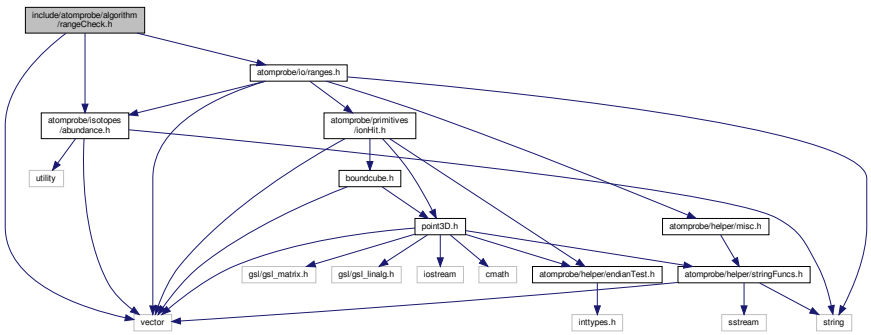
Namespaces

- AtomProbe

7.27 include/atomprobe/algorithm/rangeCheck.h File Reference

```
#include "atomprobe/isotopes/abundance.h"
#include "atomprobe/io/ranges.h"
#include <vector>
```

Include dependency graph for rangeCheck.h:



This graph shows which files directly or indirectly include this file:

Namespaces

- AtomProbe

Functions

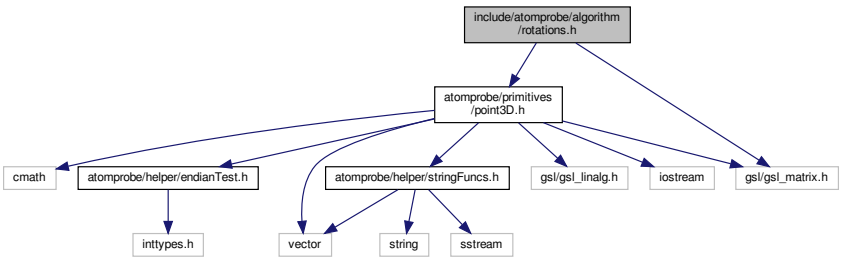
- void AtomProbe::checkMassRangingCorrectness (const RangeFile &rng, AbundanceData &massTable, float massTolerance, unsigned int maxChargeState, unsigned int maxComponents, std::vector< bool > &badRanges)

  Ensure that each mass given spans a peak that should exist.

7.28 include/atomprobe/algorithm/rotations.h File Reference

```
#include "atomprobe/primitives/point3D.h"
#include <gsl/gsl_matrix.h>
```

Include dependency graph for rotations.h:



This graph shows which files directly or indirectly include this file:

Namespaces

- AtomProbe

Functions

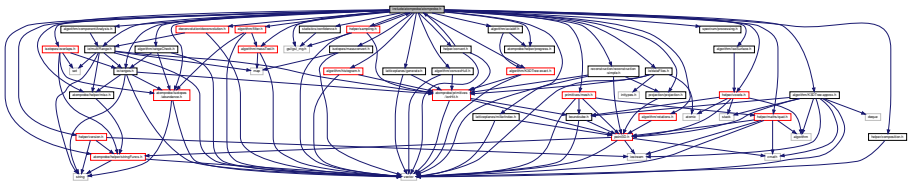
- void AtomProbe::computeRotationMatrix (const Point3D &ur1, const Point3D &ur2, const Point3D &r1, const Point3D &r2, gsl_matrix ∗m)

7.29 include/atomprobe/atomprobe.h File Reference

```
#include "io/ranges.h"
#include "io/multiRange.h"
#include "io/dataFiles.h"
#include "algorithm/K3DTree-approx.h"
#include "algorithm/K3DTree-exact.h"
#include "algorithm/rotations.h"
#include "algorithm/convexHull.h"
#include "algorithm/axialdf.h"
#include "algorithm/histogram.h"
#include "algorithm/massTool.h"
#include "algorithm/filter.h"
#include "algorithm/rangeCheck.h"
#include "algorithm/componentAnalysis.h"
#include "helper/progress.h"
```

```
#include "helper/misc.h"
#include "helper/stringFuncs.h"
#include "helper/sampling.h"
#include "helper/composition.h"
#include "helper/convert.h"
#include "helper/maths/quat.h"
#include "helper/version.h"
#include "isotopes/abundance.h"
#include "isotopes/overlaps.h"
#include "isotopes/massconvert.h"
#include "projection/projection.h"
#include "latticeplanes/millerIndex.h"
#include "latticeplanes/generate.h"
#include "reconstruction/reconstruction-simple.h"
#include "spectrum/processing.h"
#include "primitives/mesh.h"
#include "statistics/confidence.h"
#include "deconvolution/deconvolution.h"
#include "helper/voxels.h"
#include "algorithm/isoSurface.h"
#include <gsl/gsl_rng.h>
```

Include dependency graph for atomprobe.h:



This graph shows which files directly or indirectly include this file:

Classes

- class AtomProbe::RandNumGen

Namespaces

- AtomProbe

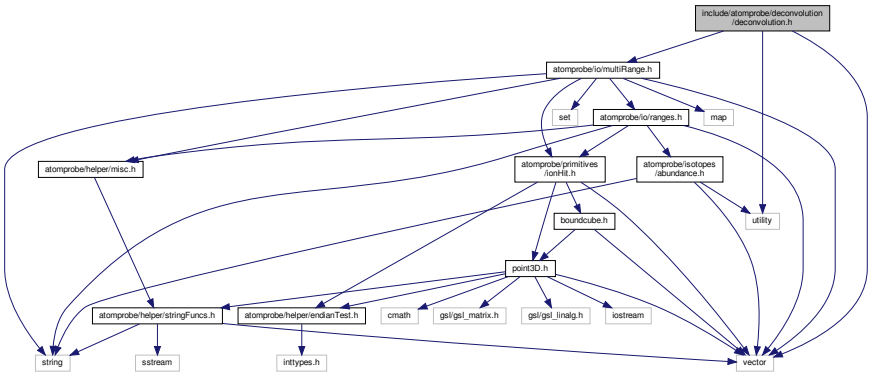
Variables

- LibVersion AtomProbe::libVersion
- RandNumGen AtomProbe::randGen

7.30 include/atomprobe/deconvolution/deconvolution.h File Reference

```
#include <vector>
#include <utility>
#include "atomprobe/io/multiRange.h"
```

Include dependency graph for deconvolution.h:



This graph shows which files directly or indirectly include this file:

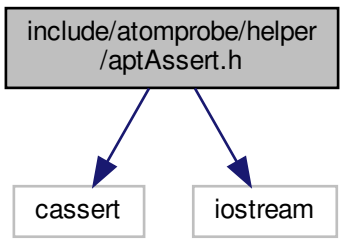
Namespaces

- AtomProbe

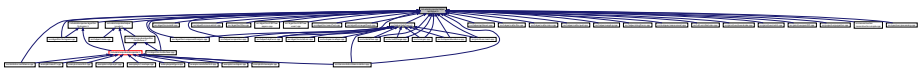
7.31 include/atomprobe/helper/aptAssert.h File Reference

```
#include <cassert>
#include <iostream>
```

Include dependency graph for aptAssert.h:



This graph shows which files directly or indirectly include this file:



Namespaces

- AtomProbe

Macros

- #define ASSERT(f)
- #define WARN(f, g)
- #define TEST(f, g)

Functions

- void AtomProbe::setHardAssert (bool enabled)

  Do assertions cause a straight up crash (enabled), or write a mesage to stderr (disabled)? By default, hard crash.
- void AtomProbe::askAssert (const char *, unsigned int)

  Either abort program, or ask the user what to do for an assertion. depending on hardAssert setting.

7.31.1 Macro Definition Documentation

7.31.1.1 ASSERT

```
#define ASSERT(
               f )
```

Definition at line 47 of file aptAssert.h.

7.31.1.2 TEST

```
#define TEST(
               f,
               g )
```

Definition at line 49 of file aptAssert.h.

Referenced by AtomProbe::MassTool::bruteKnapsack(), AtomProbe::checkMassRangingCorrectness(), AtomProbe::K3DTreeExact::clearAllTags(), AtomProbe::computeRangeAdjacency(), AtomProbe::computeRotationMatrix(), AtomProbe::MultiRange::copyDataFromRange(), AtomProbe::countDataDistanceWeight(), AtomProbe::TRIANGLE::edgesMismatch(), AtomProbe::K3DTreeApprox::findKNearest(), AtomProbe::findOverlaps(), AtomProbe::BodyCentredCubicGen::generateLattice(), AtomProbe::AbundanceData::getNearestCharge(), AtomProbe::RangeFile::guessChargeState(), main(), AtomProbe::marchingCubes(), AtomProbe::maxExplainedFraction(), AtomProbe::MILLER_TRIPLET::operator==(), AtomProbe::EPOS_ENTRY::operator==(), AtomProbe::parseCompositionData(), AtomProbe::poissonConfidenceObservation(), AtomProbe::ReconstructionSphereOnCone::reconstruct(), runTests(), AtomProbe::sampleIons(), and AtomProbe::ModifiedFocusSphericProjection::scaleUp().

7.31.1.3 WARN

```
#define WARN(
              f,
              g )
```

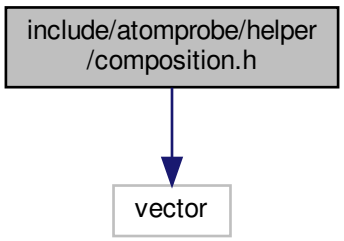
Definition at line 48 of file aptAssert.h.

Referenced by AtomProbe::computeRangeAdjacency(), and AtomProbe::leastSquaresDeconvolve().

7.32 include/atomprobe/helper/composition.h File Reference

```
#include <vector>
```

Include dependency graph for composition.h:



This graph shows which files directly or indirectly include this file:

Namespaces

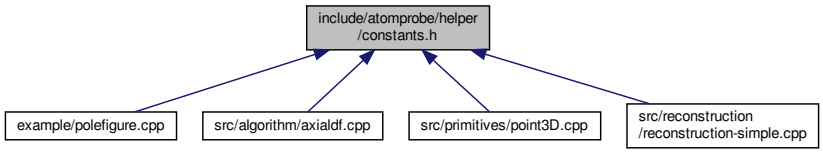
- AtomProbe

Functions

- void AtomProbe::computeComposition (const std::vector< unsigned int > &countData, std::vector< float > &compositionData)

7.33 include/atomprobe/helper/constants.h File Reference

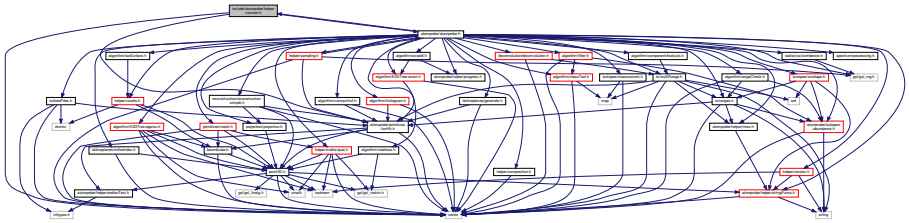
This graph shows which files directly or indirectly include this file:



7.34 include/atomprobe/helper/convert.h File Reference

```
#include <vector>
#include "atomprobe/primitives/ionHit.h"
#include "atomprobe/atomprobe.h"
```

Include dependency graph for convert.h:



This graph shows which files directly or indirectly include this file:

Namespaces

- AtomProbe

Functions

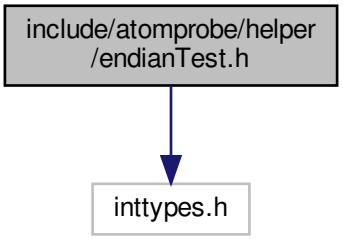
- void AtomProbe::convertEPOStoPos (const std::vector< EPOS_ENTRY > &eposEntry, std::vector< IonHit > &posFile)

  Convert an incoming entry of EPOS files to pos, and the append this to the pos vector given.

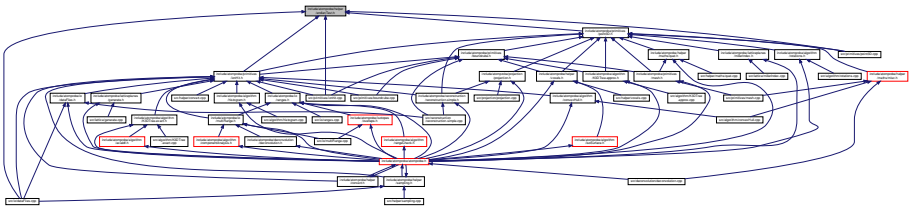
7.35 include/atomprobe/helper/endianTest.h File Reference

```
#include <inttypes.h>
```

Include dependency graph for endianTest.h:



This graph shows which files directly or indirectly include this file:



Functions

- int is_bigendian ()
- int is_littleendian ()
- void floatSwapBytes (float *inFloat)
- void int4SwapBytes (int32_t *inInt)

Variables

- const int ENDIAN_TEST =1

7.35.1 Function Documentation

7.35.1.1 floatSwapBytes()

```
void floatSwapBytes (
            float * inFloat )  [inline]
```

Definition at line 58 of file endianTest.h.

Referenced by AtomProbe::loadATOFile(), AtomProbe::readEposRecord(), AtomProbe::savePosFile(), AtomProbe::saveTapsimBin(), AtomProbe::IonHit::setPos(), and AtomProbe::Point3D::transform3x3().

7.35.1.2 int4SwapBytes()

```
void int4SwapBytes (
            int32_t * inInt )  [inline]
```

Definition at line 76 of file endianTest.h.

Referenced by AtomProbe::readEposRecord().

7.35.1.3 is_bigendian()

```
int is_bigendian ( )  [inline]
```

Definition at line 52 of file endianTest.h.

References ENDIAN_TEST.

7.35.1.4 is_littleendian()

```
int is_littleendian ( )  [inline]
```

Definition at line 54 of file endianTest.h.

References ENDIAN_TEST.

7.35.2 Variable Documentation

7.35.2.1 ENDIAN_TEST

```
const int ENDIAN_TEST =1
```

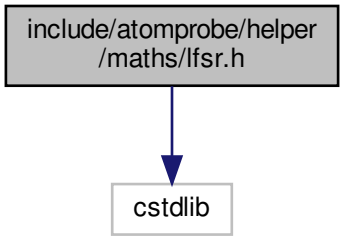
Definition at line 50 of file endianTest.h.

Referenced by is_bigendian(), and is_littleendian().

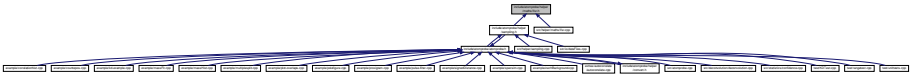
7.36 include/atomprobe/helper/maths/lfsr.h File Reference

```
#include <cstdlib>
```

Include dependency graph for lfsr.h:



This graph shows which files directly or indirectly include this file:



Classes

- class AtomProbe::LinearFeedbackShiftReg

  This class implements a Linear Feedback Shift Register (in software)

Namespaces

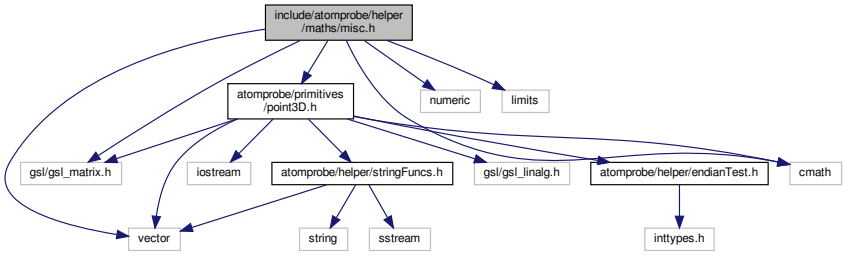
- AtomProbe

7.37 include/atomprobe/helper/maths/misc.h File Reference

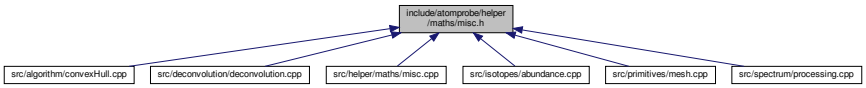
```
#include "gsl/gsl_matrix.h"
#include <numeric>
#include <vector>
#include <limits>
#include <cmath>
```

```
#include "atomprobe/primitives/point3D.h"
```

Include dependency graph for misc.h:



This graph shows which files directly or indirectly include this file:



Namespaces

- AtomProbe

Enumerations

- enum AtomProbe::PointDir { AtomProbe::POINTDIR_TOGETHER =0, AtomProbe::POINTDIR_IN_COMM↩ ON, AtomProbe::POINTDIR_APART }

Functions

- unsigned int AtomProbe::estimateRank (const gsl_matrix ∗m, float tolerance=sqrt(std::numeric_limits< float >::epsilon()))

  Estimate the rank of the given matrix.
- bool AtomProbe::solveLeastSquares (gsl_matrix ∗m, gsl_vector ∗b, gsl_vector ∗&x)

  Use an SVD based least-squares solver to solve Mx=b (for x).
- template<class T >
  T AtomProbe::weightedMean (const std::vector< T > &values, const std::vector< T > &weight)
- template<typename T >
  void AtomProbe::meanAndStdev (const std::vector< T > &f, float &meanVal, float &stdevVal, bool normal↩ Correction=true)
- unsigned int AtomProbe::vectorPointDir (const Point3D &pA, const Point3D &pB, const Point3D &vC, const Point3D &vD)

  Check which way vectors attached to two 3D points "point",.
- float AtomProbe::distanceToSegment (const Point3D &fA, const Point3D &fB, const Point3D &p)
- float AtomProbe::signedDistanceToFacet (const Point3D &fA, const Point3D &fB, const Point3D &fC, const Point3D &normal, const Point3D &p)

Find the distance between a point, and a triangular facet – may be positive or negative.

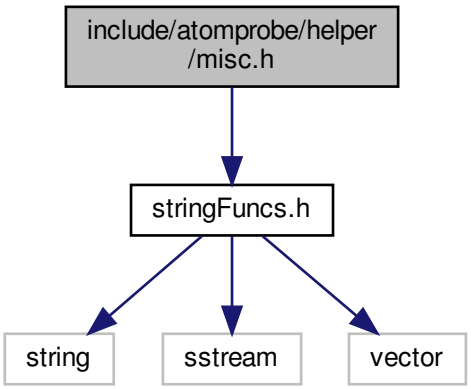
- float AtomProbe::distanceToFacet (const Point3D &fA, const Point3D &fB, const Point3D &fC, const Point3D &normal, const Point3D &p)
- float AtomProbe::dotProduct (float a1, float a2, float a3, float b1, float b2, float b3)

  Inline func for calculating a(dot)b.
- double AtomProbe::det3by3 (const double *ptArray)
- double AtomProbe::pyramidVol (const Point3D *planarPts, const Point3D &apex)
- bool AtomProbe::triIsDegenerate (const Point3D &fA, const Point3D &fB, const Point3D &fC)

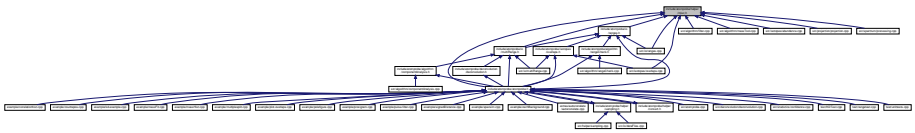
7.38 include/atomprobe/helper/misc.h File Reference

```
#include "stringFuncs.h"
```

Include dependency graph for misc.h:



This graph shows which files directly or indirectly include this file:



Classes

- class AtomProbe::RGBf

  Data holder for colour as float.

Namespaces

- AtomProbe

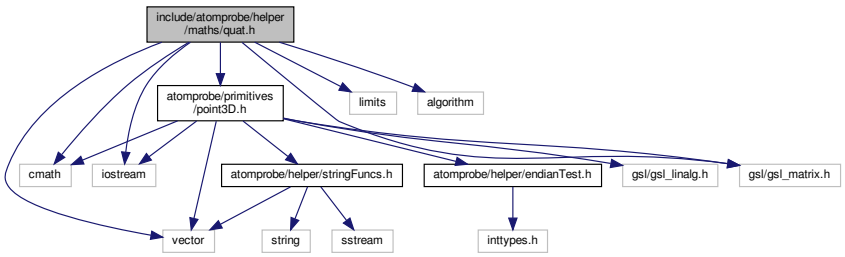
Functions

- template<class T >
  bool AtomProbe::tolEqual (const T &a, const T &b, const T &f)
- template<class T >
  void AtomProbe::selectElements (const std::vector< T > &in, const std::vector< unsigned int > &indices, std::vector< T > &out)
- template<class T >
  void AtomProbe::transposeVector (std::vector< std::vector< T > > &v)
- template<class T >
  void AtomProbe::vectorMultiErase (std::vector< T > &vec, const std::vector< bool > &wantKill)

7.39 include/atomprobe/helper/maths/quat.h File Reference

```
#include <cmath>
#include <limits>
#include <iostream>
#include <vector>
#include <algorithm>
#include <gsl/gsl_matrix.h>
#include "atomprobe/primitives/point3D.h"
```

Include dependency graph for quat.h:



This graph shows which files directly or indirectly include this file:

Classes

- struct AtomProbe::Quaternion

  Data storage structure for quaternions.
- struct AtomProbe::Point3f

  Data storage structure for points.

Namespaces

- AtomProbe

Functions

- void AtomProbe::quat_rot (Point3D &p, const Point3D &r, float angle)

  Rotate a point around a given rotation axis by a specified angle.
- void AtomProbe::quat_rot (Point3f ∗point, const Point3f ∗rotVec, float angle)

  Rotate a point around a given vector, with specified angle.
- void AtomProbe::quat_rot_array (Point3f ∗point, unsigned int n, const Point3f ∗rotVec, float angle)

  Rotate each point in array of size n around a given vector, with specified angle.
- void AtomProbe::quat_rot_array (Point3D ∗point, unsigned int n, const Point3f ∗rotVec, float angle)

  Rotate each point in array of size n around a given vector, with specified angle.
- void AtomProbe::quat_get_rot_quat (const Point3f ∗rotVec, float angle, Quaternion ∗rotQuat)

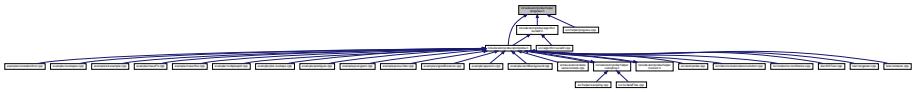
  Compute the quaternion for specified rotation.
- void AtomProbe::quat_rot_apply_quat (Point3f ∗point, const Quaternion ∗rotQuat)

  Use previously generated quats from quat_get_rot_quats to rotate a point.
- void AtomProbe::applyQuaternionRotation (std::vector< Point3D > &pts, const Quaternion &q)

  Apply the given quaternion rotation to the input points.

7.40 include/atomprobe/helper/progress.h File Reference

This graph shows which files directly or indirectly include this file:



Classes

- class AtomProbe::ProgressBar

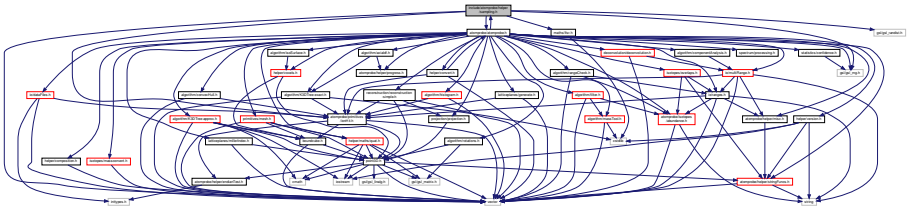
Namespaces

- AtomProbe

7.41 include/atomprobe/helper/sampling.h File Reference

```
#include <vector>
#include "atomprobe/primitives/ionHit.h"
#include "atomprobe/atomprobe.h"
#include "maths/lfsr.h"
#include <gsl/gsl_randist.h>
```

```
#include <gsl/gsl_rng.h>
```
Include dependency graph for sampling.h:



This graph shows which files directly or indirectly include this file:

Namespaces

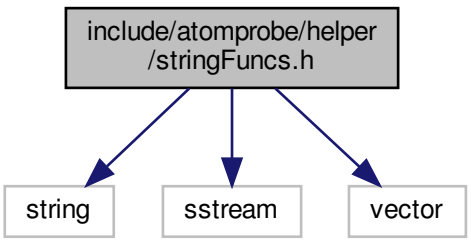
- AtomProbe

Functions

- void AtomProbe::sampleIons (const std::vector< IonHit > &ions, float sampleFactor, std::vector< IonHit > &sampled, bool strongRandom=true)
- template<class T >
  size_t AtomProbe::randomSelect (std::vector< T > &result, const std::vector< T > &source, size_t num, gsl_rng *rng)
- template<class T >
  void AtomProbe::randomIndices (std::vector< T > &res, size_t num, size_t nMax, gsl_rng *rng)

7.42 include/atomprobe/helper/stringFuncs.h File Reference

```
#include <string>
#include <sstream>
#include <vector>
```
Include dependency graph for stringFuncs.h:



This graph shows which files directly or indirectly include this file:

Namespaces

- AtomProbe

Functions

- template<class T1 , class T2 >
  bool AtomProbe::stream_cast (T1 &result, const T2 &obj)

  Template function to cast and object to another by the stringstream.
- template<class T >
  void AtomProbe::strAppend (std::string s, const T &a)
- void AtomProbe::genColString (unsigned char r, unsigned char g, unsigned char b, unsigned char a, std::string &s)
- void AtomProbe::genColString (unsigned char r, unsigned char g, unsigned char b, std::string &s)
- bool AtomProbe::parseColString (const std::string &str, unsigned char &r, unsigned char &g, unsigned char &b, unsigned char &a)

  Parse a colour string containing rgb[a]; hex for with leading #.
- std::string AtomProbe::digitString (unsigned int thisDigit, unsigned int maxDigit)

  Generate a string with leading digits up to maxDigit (eg, if maxDigit is 424, and thisDigit is 1.
- std::string AtomProbe::stripWhite (const std::string &str)

  Strip whitespace, (eg tab,space) from either side of a string.
- std::string AtomProbe::stripChars (const std::string &Str, const char *chars)
- std::string AtomProbe::lowercase (std::string s)

  Return a lowercase version for a given string.
- std::string AtomProbe::uppercase (std::string s)

  Return a uppercase version for a given string.
- void AtomProbe::stripZeroEntries (std::vector< std::string > &s)
- void AtomProbe::splitStrsRef (const char *cpStr, const char delim, std::vector< std::string > &v)

  Split string references using a single delimiter.
- void AtomProbe::splitStrsRef (const char *cpStr, const char *delim, std::vector< std::string > &v)

  Split string references using any of a given string of delimiters.
- std::string AtomProbe::onlyFilename (const std::string &path)

  Return only the filename component.
- std::string AtomProbe::onlyDir (const std::string &path)

  Return only the directory name component of the full path.
- std::string AtomProbe::convertFileStringToNative (const std::string &s)

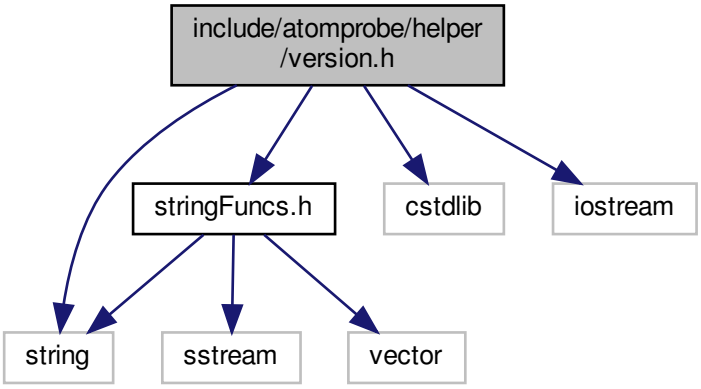
  Convert a path format into a native path from unix format.
- std::string AtomProbe::convertFileStringToCanonical (const std::string &s)

  Convert a path format into a unix path from native format.
- std::string AtomProbe::tabs (unsigned int nTabs)
- std::string AtomProbe::stlWStrToStlStr (const std::wstring &s)
- std::wstring AtomProbe::stlStrToStlWStr (const std::string &s)
- void AtomProbe::nullifyMarker (char *buffer, char marker)

7.43 include/atomprobe/helper/version.h File Reference

```
#include "stringFuncs.h"
#include <string>
#include <cstdlib>
#include <iostream>
```

Include dependency graph for version.h:



This graph shows which files directly or indirectly include this file:

Classes

- class AtomProbe::LibVersion

  Class to hold the library version data.

Namespaces

- AtomProbe

Macros

- #define LIBATOMPROBE_MAJOR 0
- #define LIBATOMPROBE_MINOR 0
- #define LIBATOMPROBE_REVISION 1

7.43.1 Macro Definition Documentation

7.43.1.1 LIBATOMPROBE_MAJOR

```
#define LIBATOMPROBE_MAJOR 0
```

Definition at line 7 of file version.h.

Referenced by AtomProbe::LibVersion::getMajor(), and AtomProbe::LibVersion::LibVersion().

7.43.1.2 LIBATOMPROBE_MINOR

```
#define LIBATOMPROBE_MINOR 0
```

Definition at line 8 of file version.h.

Referenced by AtomProbe::LibVersion::getMinor(), and AtomProbe::LibVersion::LibVersion().

7.43.1.3 LIBATOMPROBE_REVISION

```
#define LIBATOMPROBE_REVISION 1
```

Definition at line 9 of file version.h.

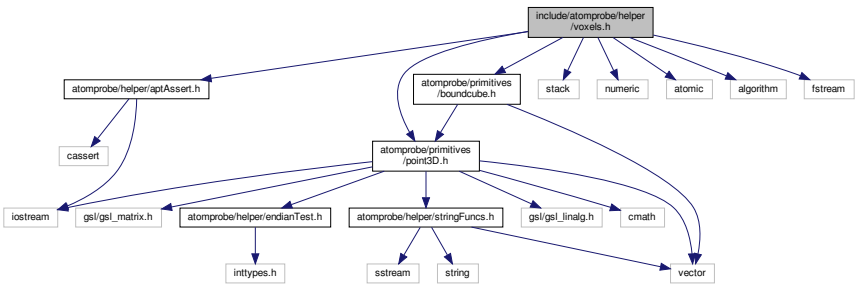
Referenced by AtomProbe::LibVersion::getRevision(), and AtomProbe::LibVersion::LibVersion().

7.44 include/atomprobe/helper/voxels.h File Reference

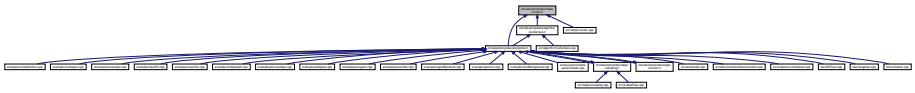
```
#include "atomprobe/helper/aptAssert.h"
#include "atomprobe/primitives/boundcube.h"
#include "atomprobe/primitives/point3D.h"
#include <stack>
#include <numeric>
#include <atomic>
#include <algorithm>
```

```
#include <fstream>
```

Include dependency graph for voxels.h:



This graph shows which files directly or indirectly include this file:



Classes

- class AtomProbe::Voxels< T >

  Template class that stores 3D voxel data.

Namespaces

- AtomProbe

Macros

- #define XOR(a, b) ((!(a)) ^ (!(b)))

Enumerations

- enum { AtomProbe::BOUND_CLIP =1, AtomProbe::BOUND_HOLD, AtomProbe::BOUND_DERIV_HOLD, AtomProbe::BOUND_MIRROR, AtomProbe::BOUND_ZERO, AtomProbe::BOUND_ENUM_END }

  Boundary clipping mode.
- enum { AtomProbe::VOX_INTERP_NONE, AtomProbe::VOX_INTERP_LINEAR, AtomProbe::VOX_INTERP_ENUM_END }
- enum { AtomProbe::ADJ_ALL, AtomProbe::ADJ_PLUS }
- enum { AtomProbe::VOXELS_BAD_FILE_READ =1, AtomProbe::VOXELS_BAD_FILE_OPEN, AtomProbe::VOXELS_BAD_FILE_SIZE, AtomProbe::VOXELS_OUT_OF_MEMORY }
- enum { AtomProbe::CLIP_NONE =0, AtomProbe::CLIP_LOWER_SOUTH_WEST, AtomProbe::CLIP_UPPER_NORTH_EAST }

  Clipping direction constants.
- enum { AtomProbe::VOXEL_ABORT_ERR, AtomProbe::VOXEL_MEMORY_ERR, AtomProbe::VOXEL_BOUNDS_INVALID_ERR }

Functions

- template<class T , class U >
  void AtomProbe::castVoxels (const Voxels< T > &src, Voxels< U > &dest)

  Convert one type of voxel into another by assignment operator.
- template<class T , class U >
  void AtomProbe::sumVoxels (const Voxels< T > &src, U &counter)

  Use one counting type to sum counts in a voxel of given type.

7.44.1 Macro Definition Documentation

7.44.1.1 XOR

```
#define XOR(
             a,
             b ) ((!(a)) ^ (!(b)))
```

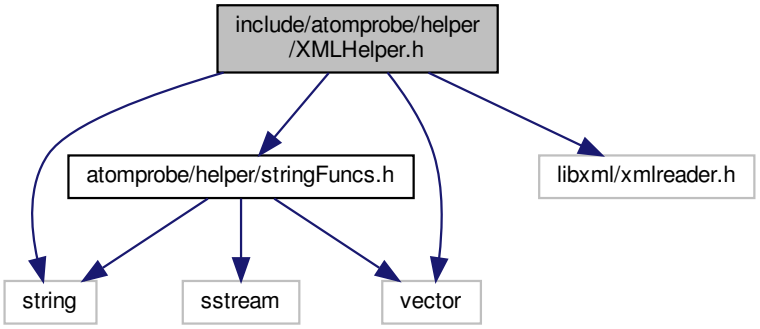
Definition at line 38 of file voxels.h.

Referenced by AtomProbe::RangeFile::rangeInvertable(), and AtomProbe::Voxels< T >::thresholdToBoolMask().

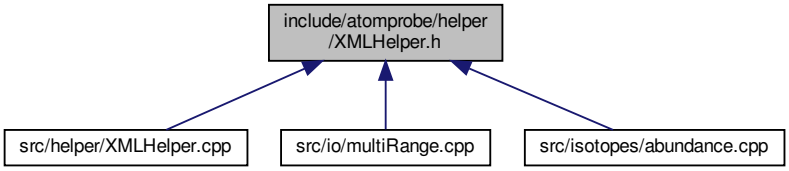
7.45 include/atomprobe/helper/XMLHelper.h File Reference

```
#include "atomprobe/helper/stringFuncs.h"
#include <libxml/xmlreader.h>
#include <string>
#include <vector>
```

Include dependency graph for XMLHelper.h:



This graph shows which files directly or indirectly include this file:



Namespaces

- AtomProbe

Enumerations

- enum { AtomProbe::PROP_PARSE_ERR = 1, AtomProbe::PROP_BAD_ATT }

Functions

- unsigned int AtomProbe::XMLHelpNextType (xmlNodePtr &node, int)
- unsigned int AtomProbe::XMLHelpFwdToElem (xmlNodePtr &node, const char *nodeName)
- unsigned int AtomProbe::XMLHelpFwdNotElem (xmlNodePtr &node, const char *nodeName)
- unsigned int AtomProbe::XMLHelpFwdToList (xmlNodePtr &node, const std::vector< std::string > &nodeList)
- std::string AtomProbe::XMLHelpGetText (xmlNodePtr &node)
- void AtomProbe::XMLFreeDoc (void *data)

  Free a xmlDoc pointer. For use in conjunction with std::unique_ptr for auto-deallocation.
- template<class T >
  unsigned int AtomProbe::XMLHelpGetProp (T &prop, xmlNodePtr node, std::string propName)
- template<class T >
  bool AtomProbe::XMLGetNextElemAttrib (xmlNodePtr &nodePtr, T &v, const char *nodeName, const char *attrib)

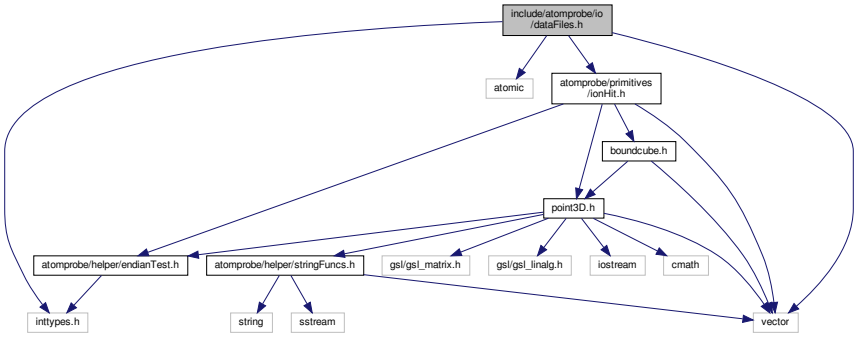
  Grab the specified attribute from the next element, then stream_cast() it into the passed-in object. Returns true on success, false on error.

7.46 include/atomprobe/io/dataFiles.h File Reference

```
#include <vector>
#include <atomic>
#include <inttypes.h>
```

```
#include "atomprobe/primitives/ionHit.h"
```

Include dependency graph for dataFiles.h:



This graph shows which files directly or indirectly include this file:

Classes

- struct AtomProbe::ATO_ENTRY
- struct AtomProbe::SINGLE_HIT

  Single 3DAP hit event.
- struct AtomProbe::VOLTAGE_DATA

  Voltage data structure – these updates occur periodically during the experiment.
- struct AtomProbe::THREEDAP_DATA

  experimental setup data
- struct AtomProbe::THREEDAP_EXPERIMENT

  Data structure that contains the experiment information present in a 3Dap file.

Namespaces

- AtomProbe

Typedefs

- typedef struct AtomProbe::ATO_ENTRY AtomProbe::ATO_ENTRY

Enumerations

- enum {
  AtomProbe::RECORDREAD_ERR_GET_FILESIZE =1, AtomProbe::RECORDREAD_ERR_FILESIZE_M↩
  ODULO, AtomProbe::RECORDREAD_ERR_FILE_OPEN, AtomProbe::RECORDREAD_ERR_NOMEM,
  AtomProbe::RECORDREAD_BAD_FILEREAD, AtomProbe::RECORDREAD_ERR_CHUNKOFFSET,
  AtomProbe::RECORDREAD_BAD_RECORD }
- enum {
  AtomProbe::ATO_OPEN_FAIL =1, AtomProbe::ATO_EMPTY_FAIL, AtomProbe::ATO_SIZE_ERR, Atom↩
  Probe::ATO_VERSIONCHECK_ERR,
  AtomProbe::ATO_MEM_ERR, AtomProbe::ATO_BAD_ENDIAN_DETECT, AtomProbe::ATO_ENUM_END }
- enum { AtomProbe::TEXT_ERR_FILE_OPEN =1, AtomProbe::TEXT_ERR_FILE_NUM_FIELDS, Atom↩
  Probe::TEXT_ERR_FILE_FORMAT }
- enum {
  AtomProbe::OPSREADER_FORMAT_CLINE_ERR =1, AtomProbe::OPSREADER_FORMAT_DETECTO↩
  RLINE_ERR, AtomProbe::OPSREADER_FORMAT_LINE_DASH_ERR, AtomProbe::OPSREADER_FOR↩
  MAT_LINE_VOLTAGE_ERR,
  AtomProbe::OPSREADER_FORMAT_LINE_VOLTAGE_NOBETA, AtomProbe::OPSREADER_FORMAT↩
  _LINE_VOLTAGE_DATA_ERR, AtomProbe::OPSREADER_FORMAT_LINE_VOLTAGE_DATACOUNT_↩
  ERR, AtomProbe::OPSREADER_FORMAT_LINETYPE_ERR,
  AtomProbe::OPSREADER_FORMAT_CHANNELS_ERR, AtomProbe::OPSREADER_CHANNELS_DAT↩
  A_ERR, AtomProbe::OPSREADER_FORMAT_SLINE_EVENTCOUNT_ERR, AtomProbe::OPSREADER↩
  _FORMAT_SLINE_EVENTDATA_ERR,
  AtomProbe::OPSREADER_FORMAT_SLINE_FORMAT_ERR, AtomProbe::OPSREADER_FORMAT_SL↩
  INE_PREFIX_ERR, AtomProbe::OPSREADER_FORMAT_DUPLICATE_SYSDATA, AtomProbe::OPSRE↩
  ADER_FORMAT_DUPLICATE_DETECTORSIZE,
  AtomProbe::OPSREADER_FORMAT_TRAILING_DASH_ERR, AtomProbe::OPSREADER_FORMAT_D↩
  OUBLEDASH, AtomProbe::OPSREADER_OPEN_ERR, AtomProbe::OPSREADER_READ_ERR,
  AtomProbe::OPSREADER_ABORT_ERR, AtomProbe::OPSREADER_ENUM_END }

  Error codes for OPS file loading.

Functions

- const char * AtomProbe::getRecordReadErrString (unsigned int errCode)
- const char * AtomProbe::getAtoErrString (unsigned int errCode)
- unsigned int AtomProbe::loadPosFile (std::vector< IonHit > &posIons, const char *posFile)

  Load a pos file directly into a single ion list.
- unsigned int AtomProbe::loadPosFile (std::vector< IonHit > &posIons, const char *posFile, unsigned int nSamplesMax)

  As per loadPosFile, but with an additional setting for the maximum number of ions to load.
- const char * AtomProbe::getPosFileErrString (unsigned int errMesg)
- unsigned int AtomProbe::savePosFile (const std::vector< Point3D > &points, float mass, const char *name, bool append=false)

  Save a vector of Point3Ds into a pos file, using a fixed mass, return nonzero on error.
- unsigned int AtomProbe::savePosFile (const std::vector< IonHit > &data, const char *name, bool append=false)

  Save a vector of IonHits into a "pos" file, return nonzero on error.
- unsigned int AtomProbe::saveTapsimBin (std::ostream &f, std::vector< IonHit > &posIons)

  Write a tapsim file from a bunch of IonHits.
- size_t AtomProbe::loadEposFile (std::vector< EPOS_ENTRY > &outData, const char *filename)

  Load an entire "EPOS" File.
- size_t AtomProbe::chunkLoadEposFile (std::vector< EPOS_ENTRY > &outData, const char *filename, unsigned int chunkSize, unsigned int chunkOffset, unsigned int &nEntriesLeft)

  Load an "EPOS" file, with a maximum chunk size.

- unsigned int AtomProbe::loadTextData (const char *cpFilename, std::vector< std::vector< float > > &data↩ Vec, std::vector< std::string > &headerVec, const char *delim, bool allowNan=true)

  Load a CSV, TSV or similar text file. Assumes "C" Locale for input (ie "." as decimal separator).
- unsigned int AtomProbe::readPosapOps (const char *file, THREEDAP_EXPERIMENT &data, unsigned int &badLine, unsigned int &progress, std::atomic< bool > &wantAbort, unsigned int nDelayLines=2, bool strictMode=false)

  Function to read POSAP "OPS" files.
- unsigned int AtomProbe::loadATOFile (const char *fileName, std::vector< ATO_ENTRY > &ions, unsigned int forceEndian=0)

  Load a LAWATAP "ATO" file.

Variables

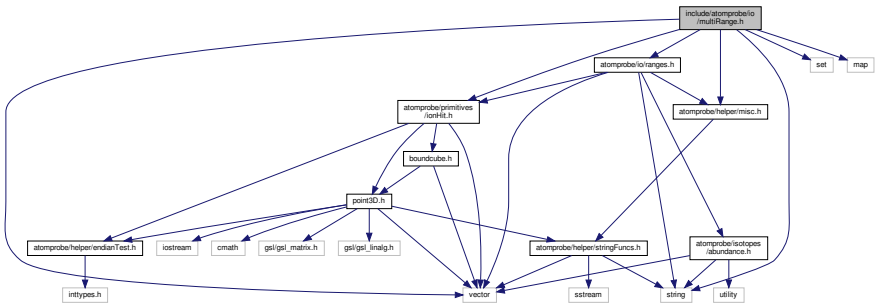
- const char * AtomProbe::RECORDREAD_ERR_STRINGS [ ]
- const char * AtomProbe::ATO_ERR_STRINGS [ ]

  Human readable error messages for use with ATO reader return values.
- const char * AtomProbe::OPS_ENUM_ERRSTRINGS [ ]

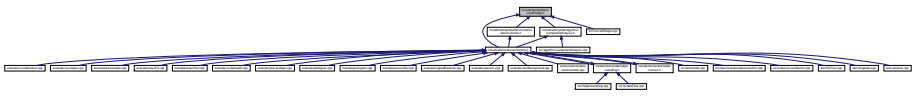
7.47 include/atomprobe/io/multiRange.h File Reference

```
#include <vector>
#include <set>
#include <string>
#include <map>
#include "atomprobe/io/ranges.h"
#include "atomprobe/helper/misc.h"
#include "atomprobe/primitives/ionHit.h"
```

Include dependency graph for multiRange.h:



This graph shows which files directly or indirectly include this file:



Classes

- struct AtomProbe::SIMPLE_SPECIES
- struct AtomProbe::FLATTENED_RANGE

  Structure that allows for the multirange data to be mapped into.
- class AtomProbe::MultiRange

  Data storage and retrieval class for "ranging" a spectra, where overlapping ranges are permitted.

Namespaces

- AtomProbe

Enumerations

- enum { AtomProbe::MULTIRANGE_FORMAT_XML }

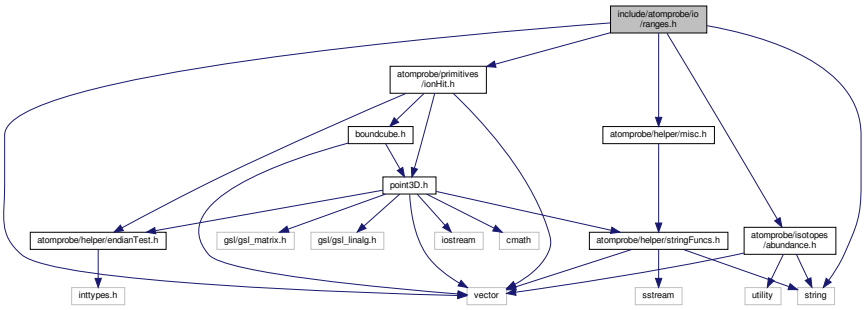
Functions

- bool AtomProbe::operator< (const SIMPLE_SPECIES &a, const SIMPLE_SPECIES &b)

7.48 include/atomprobe/io/ranges.h File Reference

```
#include <vector>
#include <string>
#include "atomprobe/primitives/ionHit.h"
#include "atomprobe/isotopes/abundance.h"
#include "atomprobe/helper/misc.h"
```

Include dependency graph for ranges.h:



This graph shows which files directly or indirectly include this file:

Classes

- class AtomProbe::RangeFile

  Data storage and retrieval class for various range files.

Namespaces

- AtomProbe

Enumerations

- enum {
  AtomProbe::RANGE_FORMAT_ORNL, AtomProbe::RANGE_FORMAT_DBL_ORNL, AtomProbe::RANGE_FORMAT_ENV, AtomProbe::RANGE_FORMAT_RRNG,
  AtomProbe::RANGE_FORMAT_END_OF_ENUM }
- enum {
  AtomProbe::RANGE_ERR_FORMAT =1, AtomProbe::RANGE_ERR_FORMAT_HEADER, AtomProbe::RANGE_ERR_EMPTY, AtomProbe::RANGE_ERR_FORMAT_LONGNAME,
  AtomProbe::RANGE_ERR_FORMAT_SHORTNAME, AtomProbe::RANGE_ERR_FORMAT_COLOUR,
  AtomProbe::RANGE_ERR_FORMAT_TABLESEPARATOR, AtomProbe::RANGE_ERR_FORMAT_MASS_PAIR,
  AtomProbe::RANGE_ERR_FORMAT_TABLE_ENTRY, AtomProbe::PARSE_RANGE_FORMAT_GENERIC_FAIL, AtomProbe::RANGE_ERR_DATA_TOO_MANY_USELESS_RANGES, AtomProbe::RANGE_ERR_DATA_FLIPPED,
  AtomProbe::RANGE_ERR_DATA_INCONSISTENT, AtomProbe::RANGE_ERR_DATA_NOMAPPED_IONNAME, AtomProbe::RANGE_ERR_OPEN, AtomProbe::RANGE_ERR_FORMAT_RANGETABLE,
  AtomProbe::RANGE_ERR_FORMAT_TABLEHEADER_NUMIONS, AtomProbe::RANGE_ERR_NONUNIQUE_POLYATOMIC, AtomProbe::RANGE_ERR_TOO_LARGE, AtomProbe::RANGE_ERR_DASHHEADER,
  AtomProbe::RANGE_ERR_IONBLOCK_CONTENT, AtomProbe::RANGE_ERR_NUMIONS, AtomProbe::RANGE_ERR_NUMIONS_DUPLICATED, AtomProbe::RANGE_ERR_TOO_MANYIONS,
  AtomProbe::RANGE_ERR_ION_BLOCK_NOT_PRESENT, AtomProbe::RANGE_ERR_DUPLICATE_NUMRANGES, AtomProbe::RANGE_ERR_NUMRANGE_PARSE, AtomProbe::RANGE_ERR_RRNG_IONS_TOOSHORT,
  AtomProbe::RANGE_ERR_RRNG_COLON_SEPARATOR, AtomProbe::RANGE_ERR_BADCOLOUR, AtomProbe::RANGE_ERR_ION_NOT_MAPPED, AtomProbe::RANGE_ERR_BADSTART,
  AtomProbe::RANGE_ERR_BADEND, AtomProbe::RANGE_ERR_NAME_EMPTY, AtomProbe::RANGE_ERR_BAD_LINE_RANGEBLOCK, AtomProbe::RANGE_ERR_MISSING_IONBLOCK,
  AtomProbe::RANGE_ERR_NO_RANGES, AtomProbe::RANGE_ERR_NO_BASIC_IONS, AtomProbe::RANGE_ERR_MISMATCHED_NUMRANGES, AtomProbe::RANGE_ERR_RANGEBLOCK_FORMAT,
  AtomProbe::RANGE_ERR_BAD_MULTIPLICITY, AtomProbe::RANGE_ERR_FORMAT_EMPTY_RANGEROW, AtomProbe::RANGE_ERR_FILESIZE, AtomProbe::RANGE_ERR_ENUM_END }

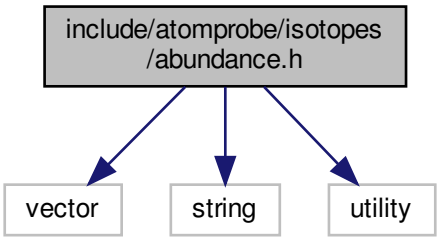
Variables

- const unsigned int AtomProbe::NUM_ELEMENTS =119

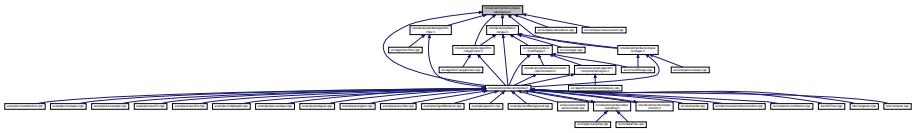
7.49 include/atomprobe/isotopes/abundance.h File Reference

```
#include <vector>
#include <string>
#include <utility>
```

Include dependency graph for abundance.h:



This graph shows which files directly or indirectly include this file:



Classes

- struct AtomProbe::ISOTOPE_ENTRY
- class AtomProbe::AbundanceData

  Class to load abundance information for natural isotopes.

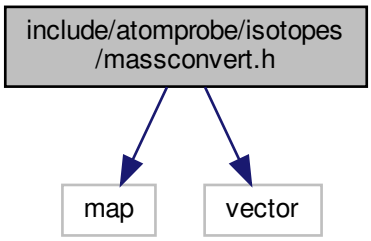
Namespaces

- AtomProbe

7.50 include/atomprobe/isotopes/massconvert.h File Reference

```
#include <map>
#include <vector>
```

Include dependency graph for massconvert.h:



This graph shows which files directly or indirectly include this file:

Namespaces

- AtomProbe

Enumerations

- enum {
  AtomProbe::COMPPARSE_BAD_INPUT_FORMAT =1, AtomProbe::COMPPARSE_BAD_COMP_VALUE,
  AtomProbe::COMPPARSE_BAD_BAL_USAGE, AtomProbe::COMPPARSE_BAD_SYMBOL,
  AtomProbe::COMPPARSE_DUPLICATE_SYMBOL, AtomProbe::COMPPARSE_BAD_TOTAL_COMP }

  composition parsing error messages

Functions

- unsigned int AtomProbe::parseCompositionData (const std::vector< std::string > &s, const AbundanceData &atomTable, std::map< unsigned int, double > &atomData)

  Convert atomic string label data, in the form "Fe 0.81" to fraction map.
- void AtomProbe::convertMolToMass (const AbundanceData &atomTable, const std::map< unsigned int, double > &compositionMols, std::map< unsigned int, double > &compositionMass)

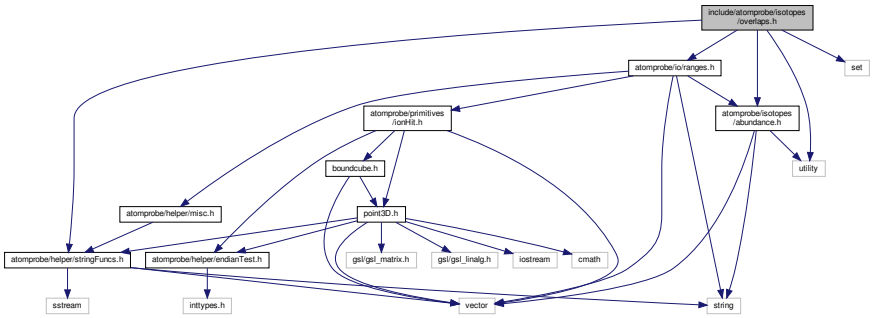
  Convert the given composition from molar fraction data to mass fraction.
- void AtomProbe::convertMassToMol (const AbundanceData &atomTable, const std::map< unsigned int, double > &compositionMass, std::map< unsigned int, double > &compositionMols)

  Convert the given composition from mass fraction data to molar fraction.

7.51 include/atomprobe/isotopes/overlaps.h File Reference

```
#include "atomprobe/isotopes/abundance.h"
#include "atomprobe/helper/stringFuncs.h"
#include "atomprobe/io/ranges.h"
#include <utility>
#include <set>
```

Include dependency graph for overlaps.h:



This graph shows which files directly or indirectly include this file:

Namespaces

- AtomProbe

Functions

- void AtomProbe::findOverlaps (const AbundanceData &natData, const RangeFile &rng, float massDelta, unsigned int maxCharge, std::vector< std::pair< size_t, size_t > > &overlapIdx, std::vector< std::pair< float, float > > &overlapMasses)

  Find the overlaps stemming from a given rangefile.

- void AtomProbe::findOverlaps (const AbundanceData &natData, const std::vector< std::string > &ions, float massDelta, unsigned int maxCharge, std::vector< std::pair< size_t, size_t > > &overlapIdx, std::vector< std::pair< float, float > > &overlapMasses)

  As per findOverlaps(...Rangefile ...) , but uses a vector of ions instead.

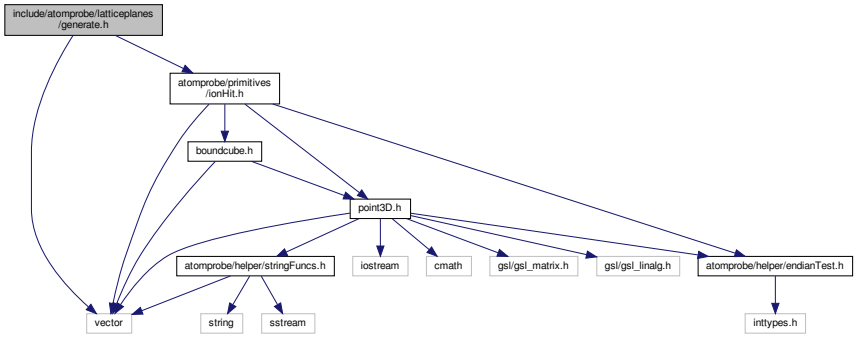
- void AtomProbe::findOverlapsFromSpectra (const std::vector< std::vector< std::pair< float, float > > > &massDistributions, float massDelta, const std::set< unsigned int > &skipIDs, std::vector< std::pair< size_t, size_t > > &overlapIdx, std::vector< std::pair< float, float > > &overlapMasses)

  Find overlaps in the given mass distributions, as per findOverlaps(...Rangefile...)

7.52 include/atomprobe/latticeplanes/generate.h File Reference

```
#include <vector>
#include "atomprobe/primitives/ionHit.h"
```

Include dependency graph for generate.h:



This graph shows which files directly or indirectly include this file:

Classes

- class AtomProbe::CrystalGen
- class AtomProbe::SimpleCubicGen
- class AtomProbe::FaceCentredCubicGen
- class AtomProbe::BodyCentredCubicGen

Namespaces

- AtomProbe

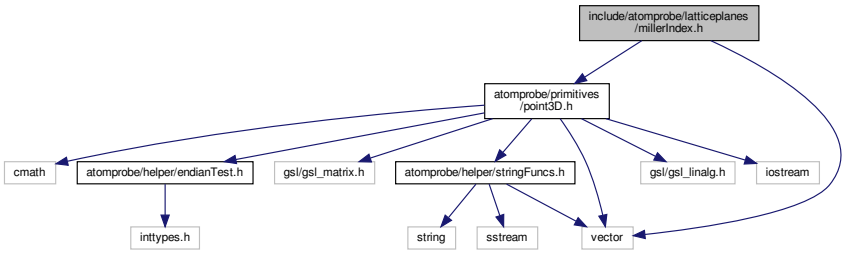
Enumerations

- enum { AtomProbe::CRYSTAL_BAD_UNIT_CELL, AtomProbe::CRYSTAL_ENUM_END }

7.53 include/atomprobe/latticeplanes/millerIndex.h File Reference

```
#include "atomprobe/primitives/point3D.h"
#include <vector>
```

Include dependency graph for millerIndex.h:



This graph shows which files directly or indirectly include this file:

Classes

- class AtomProbe::MILLER_TRIPLET

Namespaces

- AtomProbe

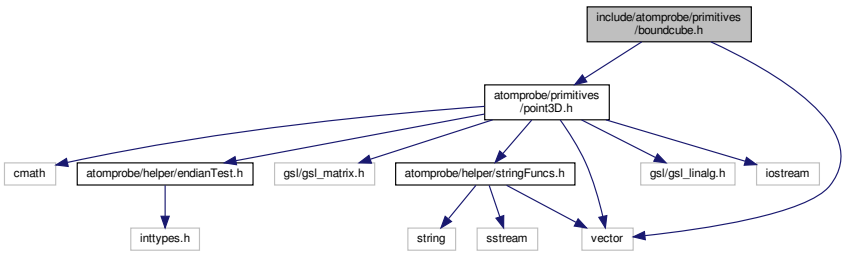
Enumerations

- enum { AtomProbe::LATTICE_FCC, AtomProbe::LATTICE_BCC, AtomProbe::LATTICE_HCP, AtomProbe::LATTICE_END_OF_ENUM }

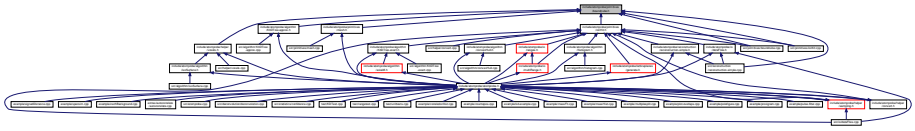
7.54 include/atomprobe/primitives/boundcube.h File Reference

```
#include "atomprobe/primitives/point3D.h"
#include <vector>
```

Include dependency graph for boundcube.h:



This graph shows which files directly or indirectly include this file:



Classes

- class AtomProbe::BoundCube

  Helper class to define a bounding cube.

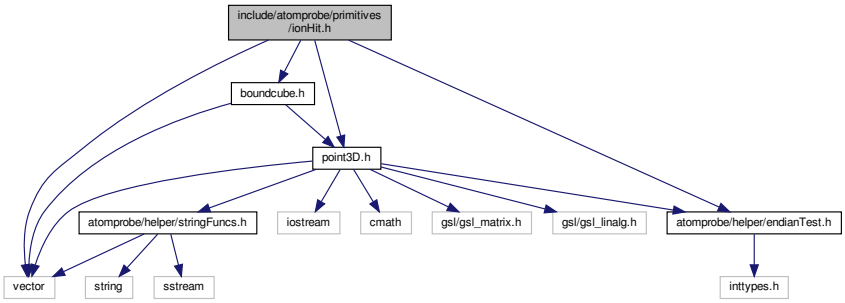
Namespaces

- AtomProbe

7.55 include/atomprobe/primitives/ionHit.h File Reference

```
#include <vector>
#include "atomprobe/helper/endianTest.h"
#include "point3D.h"
#include "boundcube.h"
```

Include dependency graph for ionHit.h:



This graph shows which files directly or indirectly include this file:

Classes

- class AtomProbe::IonHit

  This is a data holding class for POS file ions, from.
- class AtomProbe::EPOS_ENTRY

Namespaces

- AtomProbe

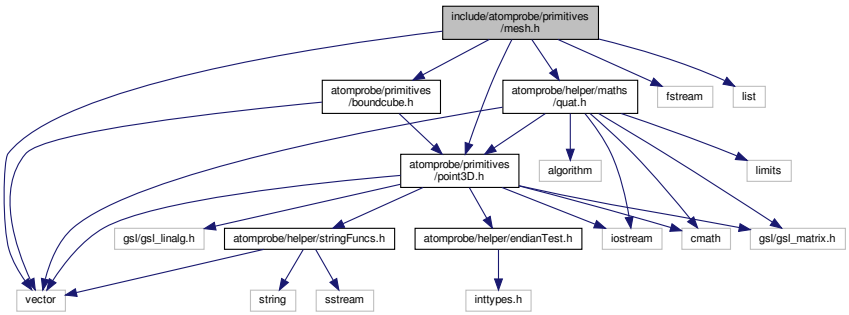
Variables

- const size_t AtomProbe::EPOS_RECORD_SIZE = 11∗4

7.56 include/atomprobe/primitives/mesh.h File Reference

```
#include "atomprobe/primitives/point3D.h"
#include "atomprobe/primitives/boundcube.h"
#include "atomprobe/helper/maths/quat.h"
#include <vector>
#include <fstream>
#include <list>
```

Include dependency graph for mesh.h:



This graph shows which files directly or indirectly include this file:

Classes

- class AtomProbe::TETRAHEDRON
- class AtomProbe::TRIANGLE
- class AtomProbe::LINE
- class AtomProbe::Mesh

  Simple mesh class for storing and manipulating meshes consisting of 2 and 3D simplexes (triangles or tetrahedra)

Namespaces

- AtomProbe

Enumerations

- enum { AtomProbe::ELEMENT_TRIANGLE =1, AtomProbe::ELEMENT_TETRAHEDRON =2, AtomProbe::ELEMENT_LINE =4 }

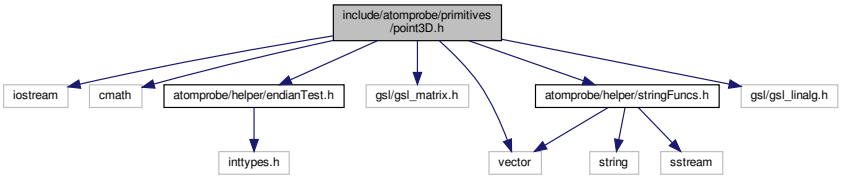
Variables

- const unsigned int AtomProbe::ELEM_SINGLE_NODE_POINT =15
- const unsigned int AtomProbe::ELEM_TWO_NODE_LINE =1
- const unsigned int AtomProbe::ELEM_THREE_NODE_TRIANGLE =2
- const unsigned int AtomProbe::ELEM_FOUR_NODE_TETRAHEDRON =4
- const char * AtomProbe::MESH_LOAD_ERRS [ ]

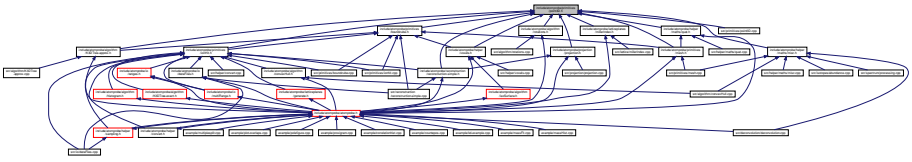
7.57 include/atomprobe/primitives/point3D.h File Reference

```
#include <iostream>
#include <cmath>
#include <vector>
#include <gsl/gsl_matrix.h>
#include "atomprobe/helper/endianTest.h"
#include "atomprobe/helper/stringFuncs.h"
#include <gsl/gsl_linalg.h>
```

Include dependency graph for point3D.h:



This graph shows which files directly or indirectly include this file:



Classes

- class AtomProbe::Point3D

  A 3D point data class storage.

Namespaces

- AtomProbe

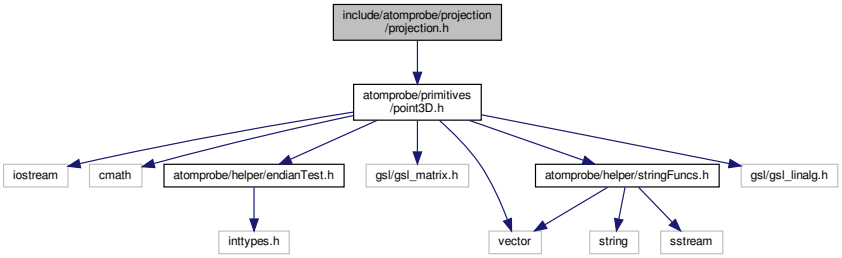
Functions

- void AtomProbe::gsl_matrix_mult (const gsl_matrix *a, const gsl_matrix *b, gsl_matrix *&res)

7.58 include/atomprobe/projection/projection.h File Reference

```
#include "atomprobe/primitives/point3D.h"
```

Include dependency graph for projection.h:



This graph shows which files directly or indirectly include this file:

Classes

- class AtomProbe::SphericPlaneProjection
- class AtomProbe::GnomonicProjection
- class AtomProbe::StereographicProjection
- class AtomProbe::ModifiedFocusSphericProjection

Namespaces

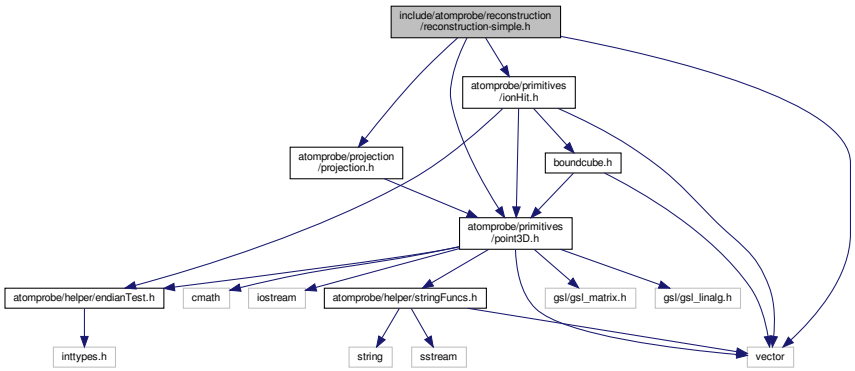
- AtomProbe

7.59 include/atomprobe/reconstruction/reconstruction-simple.h File Reference

```
#include "atomprobe/primitives/point3D.h"
#include "atomprobe/primitives/ionHit.h"
#include "atomprobe/projection/projection.h"
```

```
#include <vector>
```

Include dependency graph for reconstruction-simple.h:



This graph shows which files directly or indirectly include this file:

Classes

- class AtomProbe::ReconstructionSphereOnCone

Namespaces

- AtomProbe

Enumerations

- enum { AtomProbe::EVOLUTION_MODE_SHANKANGLE }

Functions

- bool AtomProbe::reconstructTest ()

7.60 include/atomprobe/spectrum/processing.h File Reference

This graph shows which files directly or indirectly include this file:

Classes

- struct AtomProbe::BACKGROUND_PARAMS

Namespaces

- AtomProbe

Enumerations

- enum { AtomProbe::BACK_FIT_MODE_CONST_TOF, AtomProbe::BACK_FIT_MODE_ENUM_END }
  Background fitting modes.

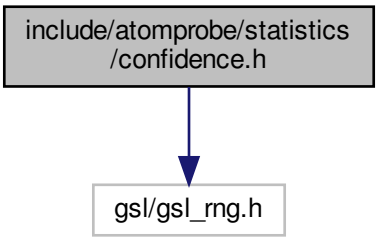
Functions

- unsigned int AtomProbe::doFitBackground (const std::vector< float > &massData, BACKGROUND_PAR↩ AMS &params)
  Perform a background fit, assuming constant TOF noise, from 0->inf time.
- std::string AtomProbe::getFitErrorMsg (unsigned int errCode)
- void AtomProbe::createMassBackground (float massStart, float massEnd, unsigned int nBinsMass, float tof↩ BackIntensity, std::vector< float > &histogram)
  Build a histogram of the background counts.
- void AtomProbe::findPeaks (const std::vector< float > &x0, std::vector< unsigned int > &peakInds, float sel, bool autoSel=true, bool includeEndpoints=true)
  Simple peak-finding algorithm.

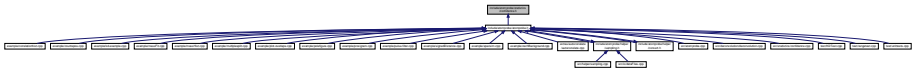
7.61 include/atomprobe/statistics/confidence.h File Reference

```
#include <gsl/gsl_rng.h>
```

Include dependency graph for confidence.h:



This graph shows which files directly or indirectly include this file:



Namespaces

- AtomProbe

Functions

- void AtomProbe::poissonConfidenceObservation (float counts, float alpha, float &lBound, float &uBound)

  Obtain poisson confidence limits for the mean of a poisson distribution.
- bool AtomProbe::numericalEstimatePoissRatioConf (float lambda1, float lambda2, float alpha, unsigned int nTrials, gsl_rng *r, float &lBound, float &uBound)

  Brute-force poisson ratio confidence estimator. Returns the confidence interval in the estimate of the mean, at the given rates.
- bool AtomProbe::numericalEstimateGaussRatioConf (float mu1, float mu2, float var1, float var2, float alpha, unsigned int nTrials, gsl_rng *r, float &lBound, float &uBound)

  Brute-force guassian ratio confidence estimator.
- bool AtomProbe::numericalEstimateSkellamConf (float lambda1, float lambda2, float alpha, unsigned int n↩ Trials, gsl_rng *r, float &lBound, float &uBound)

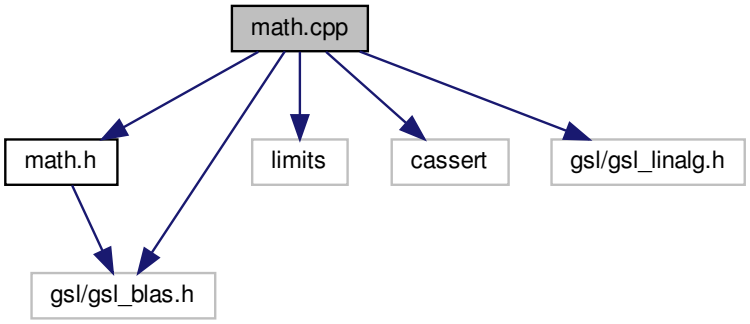
  Brute-force the confidence bounds of a skellam distribution.
- bool AtomProbe::zechConfidenceLimits (float lambdaBack, unsigned int observation, float alpha, float &estimate)

  Provides a best estimate for true signal when true signal, background.

7.62 math.cpp File Reference

```
#include "math.h"
#include <limits>
#include <cassert>
#include <gsl/gsl_blas.h>
#include <gsl/gsl_linalg.h>
```

Include dependency graph for math.cpp:



Macros

- #define ASSERT(f) assert((f))

Functions

- void psuedoInverseFromSVD (const gsl_matrix ∗U, const gsl_vector ∗S, const gsl_matrix ∗V, gsl_matrix ∗P)
- void gsl_matrix_mult (const gsl_matrix ∗A, const gsl_matrix ∗B, gsl_matrix ∗&res, bool alloc)
- void gsl_pseudo_inverse (gsl_matrix ∗A, gsl_matrix ∗&res)

7.62.1 Macro Definition Documentation

7.62.1.1 ASSERT

```
#define ASSERT(
               f ) assert((f))
```

Definition at line 6 of file math.cpp.

Referenced by gsl_matrix_mult().

7.62.2 Function Documentation

7.62.2.1 gsl_matrix_mult()

```
void gsl_matrix_mult (
             const gsl_matrix * A,
             const gsl_matrix * B,
             gsl_matrix *& res,
             bool alloc )
```

Definition at line 16 of file math.cpp.

Referenced by psuedoInverseFromSVD().

7.62.2.2 gsl_pseudo_inverse()

```
void gsl_pseudo_inverse (
             gsl_matrix * A,
             gsl_matrix *& res )
```

Definition at line 56 of file math.cpp.

7.62.2.3 psuedoInverseFromSVD()

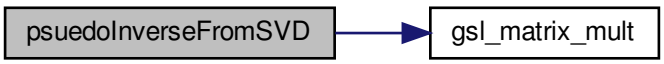
```
void psuedoInverseFromSVD (
             const gsl_matrix * U,
             const gsl_vector * S,
             const gsl_matrix * V,
             gsl_matrix * P )
```

Definition at line 78 of file math.cpp.

References gsl_matrix_mult().

Referenced by gsl_pseudo_inverse().

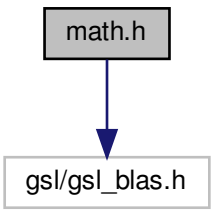
Here is the call graph for this function:



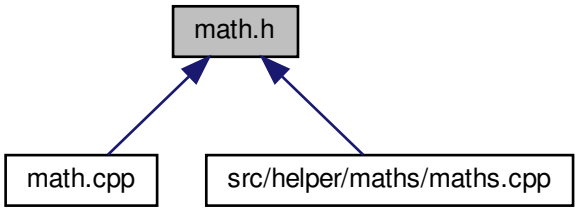
7.63 math.h File Reference

```
#include <gsl/gsl_blas.h>
```

Include dependency graph for math.h:



This graph shows which files directly or indirectly include this file:



Functions

- void gsl_pseudo_inverse (gsl_matrix ∗A, gsl_matrix ∗&res)
- void gsl_matrix_mult (const gsl_matrix ∗A, const gsl_matrix ∗B, gsl_matrix ∗&res, bool alloc=true)
- template<class T >
  void computeMeanAndVariance (const T ∗data, unsigned int n, T &mean, T &var)

7.63.1 Function Documentation

7.63.1.1 computeMeanAndVariance()

```
template<class T >
void computeMeanAndVariance (
             const T * data,
             unsigned int n,
             T & mean,
             T & var )
```

Definition at line 16 of file math.h.

7.63.1.2 gsl_matrix_mult()

```
void gsl_matrix_mult (
             const gsl_matrix * A,
             const gsl_matrix * B,
             gsl_matrix *& res,
             bool alloc = true )
```

Definition at line 16 of file math.cpp.

References ASSERT.

Referenced by psuedoInverseFromSVD().

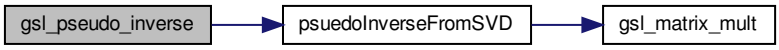
7.63.1.3 gsl_pseudo_inverse()

```
void gsl_pseudo_inverse (
            gsl_matrix * A,
            gsl_matrix *& res )
```

Definition at line 56 of file math.cpp.

References psuedoInverseFromSVD().

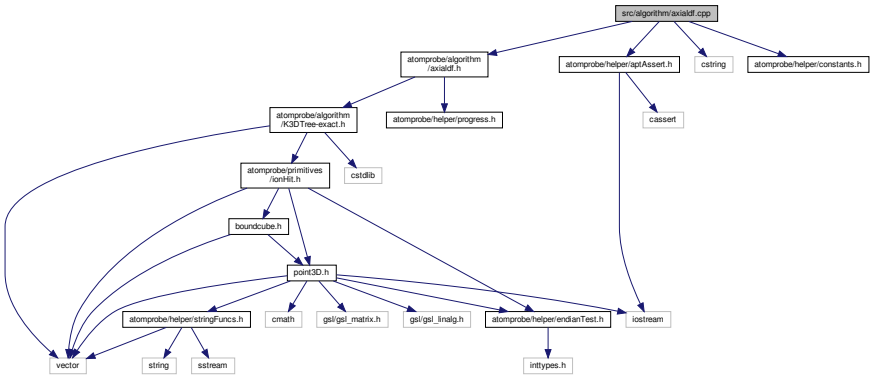
Here is the call graph for this function:



7.64 src/algorithm/axialdf.cpp File Reference

```
#include "atomprobe/algorithm/axialdf.h"
#include "atomprobe/helper/aptAssert.h"
#include <cstring>
#include "atomprobe/helper/constants.h"
```

Include dependency graph for axialdf.cpp:



Namespaces

- AtomProbe

Functions

- unsigned int AtomProbe::generate1DAxialDistHist (const std::vector< Point3D > &pointList, K3DTreeExact &tree, const Point3D &axisDir, float distMax, std::vector< unsigned int > &histogram)

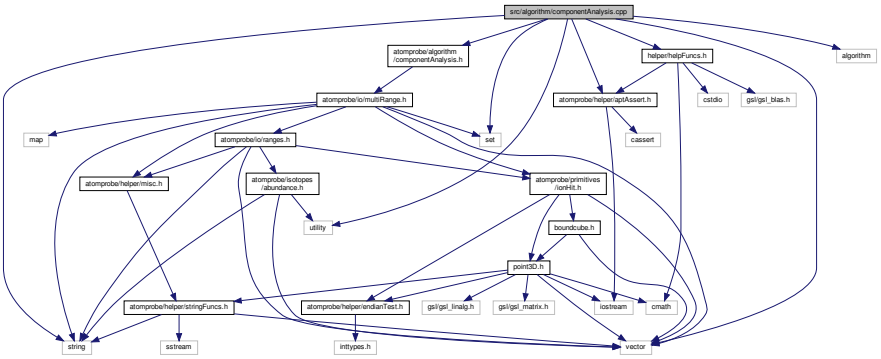
  Generate a 1D axial distribution function,.
- unsigned int AtomProbe::generate1DAxialDistHistSweep (const std::vector< Point3D > &pointList, K3D↩ TreeExact &tree, float distMax, float dTheta, float dPhi, ProgressBar &prog, std::vector< std::vector< std↩ ::vector< unsigned int > > > &histogram)

  Generate a series of 1D distribution functions, one per pixel in a 2D grid of spherical coordinate directions.

7.65 src/algorithm/componentAnalysis.cpp File Reference

```
#include "atomprobe/algorithm/componentAnalysis.h"
#include "atomprobe/helper/aptAssert.h"
#include "helper/helpFuncs.h"
#include <string>
#include <utility>
#include <vector>
#include <set>
#include <algorithm>
```

Include dependency graph for componentAnalysis.cpp:



Namespaces

- AtomProbe

Functions

- void AtomProbe::computeIonDistAdjacency (const MultiRange &mrf, const AbundanceData &abundance, const OVERLAP_PROBLEM_SETTINGS &settings, gsl_matrix ∗&m, gsl_vector ∗&vOwnership, gsl_vector ∗&vMass)

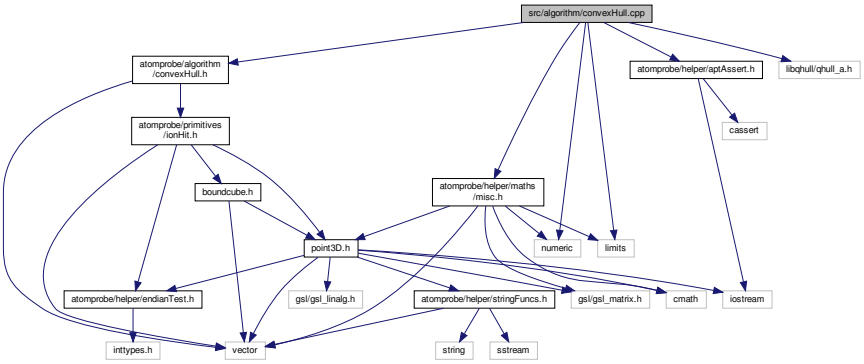
  Calculate the adjacency matrix for the ions in a multirange.
- bool AtomProbe::rangeOverlaps (const pair< float, float > &r1, const pair< float, float > &r2)
- void AtomProbe::computeRangeAdjacency (const MultiRange &mrf, const OVERLAP_PROBLEM_SETTI↩ NGS &settings, gsl_matrix ∗&m)

7.66 src/algorithm/convexHull.cpp File Reference

```
#include "atomprobe/algorithm/convexHull.h"
#include "atomprobe/helper/maths/misc.h"
#include <libqhull/qhull_a.h>
#include <numeric>
#include <limits>
```

```
#include "atomprobe/helper/aptAssert.h"
```

Include dependency graph for convexHull.cpp:



Namespaces

- AtomProbe

Functions

- void AtomProbe::freeConvexHull ()
- unsigned int AtomProbe::doHull (unsigned int bufferSize, double *buffer, vector< Point3D > &resHull, Point3D &midPoint, bool freeHullOnExit)
- unsigned int AtomProbe::computeConvexHull (const std::vector< IonHit > &data, unsigned int *progress, bool(*callback)(bool), std::vector< Point3D > &curHull, bool freeHull)

  Obtain the convex hull of a set of ions.
- unsigned int AtomProbe::GetReducedHullPts (const std::vector< IonHit > &points, float reductionDim, unsigned int *progress, bool(*callback)(bool), std::vector< IonHit > &pointResult)

  Obtain a set of points that are a subset of points the convex hull that are at least "reductionDim" away from the hull itself.

Variables

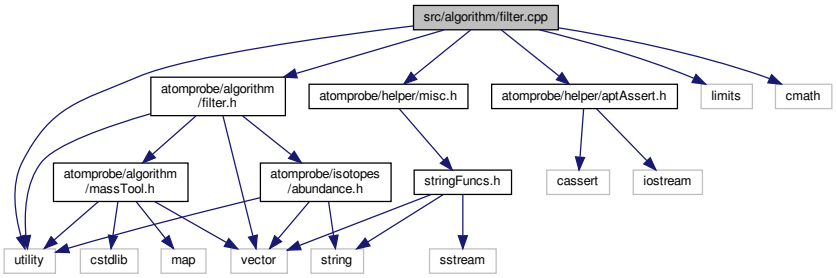
- bool AtomProbe::qhullInited =false
- const unsigned int AtomProbe::HULL_GRAB_SIZE =4096

7.67 src/algorithm/filter.cpp File Reference

```
#include "atomprobe/algorithm/filter.h"
#include "atomprobe/helper/aptAssert.h"
#include "atomprobe/helper/misc.h"
#include <limits>
#include <cmath>
```

```
#include <utility>
```

Include dependency graph for filter.cpp:



Namespaces

- AtomProbe

Functions

- unsigned int AtomProbe::countIntensityEvents (const vector< pair< float, float > > &data, float minV, float maxV)
- void AtomProbe::buildFrequencyTable (const vector< ISOTOPE_ENTRY > &solutionVec, vector< size_t > &solutionElements, vector< size_t > &solutionFrequency)
- void AtomProbe::filterBySolutionPPM (const AbundanceData &massTable, float minPpm, std::vector< std::vector< ISOTOPE_ENTRY > > &solutions)

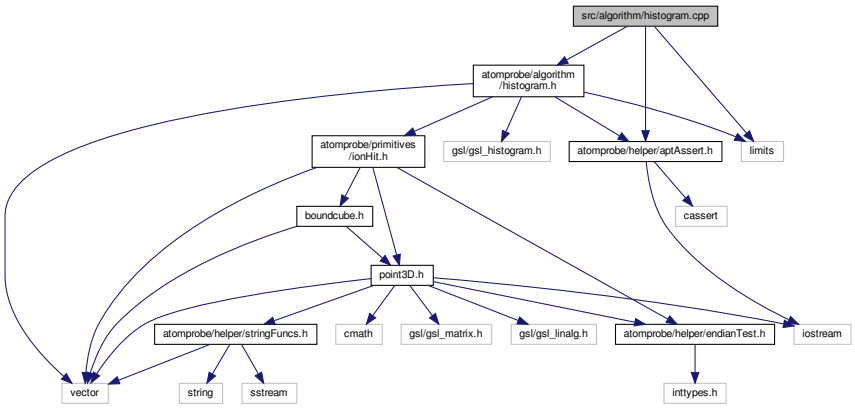
  Use the maximum possible PPM for each isotopic combination to filter possible solutions.
- void AtomProbe::filterPeakNeedBiggerObs (const AbundanceData &massTable, const std::vector< float > &peakData, float tolerance, size_t solutionCharge, std::vector< std::vector< ISOTOPE_ENTRY > > &solutions)
- vector< float > AtomProbe::maxExplainedFraction (const vector< pair< float, float > > &intensityData, float peakMass, float massWidth, const vector< vector< ISOTOPE_ENTRY > > &solutions, const AbundanceData &massTable, float massDistTol, unsigned int solutionCharge)

7.68 src/algorithm/histogram.cpp File Reference

```
#include "atomprobe/algorithm/histogram.h"
#include "atomprobe/helper/aptAssert.h"
```

```
#include <limits>
```

Include dependency graph for histogram.cpp:



Namespaces

- AtomProbe

Functions

- bool AtomProbe::incrementCorrelationHist (const std::vector< EPOS_ENTRY > &eposIons, std::vector< std::vector< unsigned int > > &histogram, float stepMass, float endMass)
- bool AtomProbe::correlationHistogram (const std::vector< EPOS_ENTRY > &eposIons, std::vector< std::vector< unsigned int > > &histogram, float stepMass, float endMass, bool lowerTriangular=false)

  Generates an ion "correlation histogram" from a vector of EPOS ions. The input vector MUST
- bool AtomProbe::accumulateCorrelationHistogram (const std::vector< EPOS_ENTRY > &eposIons, std::vector< std::vector< unsigned int > > &histogram, float stepMass, float endMass, bool lowerTriangular=true)

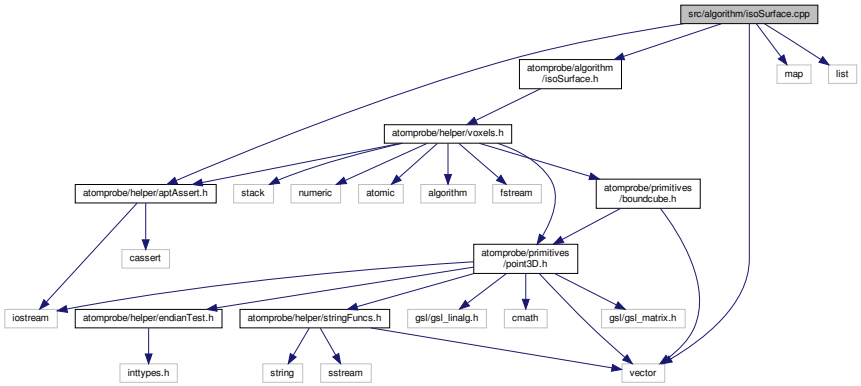
  Increments a correlation histogram, as per correlationHistogram,.

7.69 src/algorithm/isoSurface.cpp File Reference

```
#include "atomprobe/algorithm/isoSurface.h"
#include "atomprobe/helper/aptAssert.h"
#include <map>
#include <list>
```

```
#include <vector>
```

Include dependency graph for isoSurface.cpp:



Namespaces

- AtomProbe

Functions

- template<class T >
  void AtomProbe::removeElements (const std::vector< size_t > &elems, std::vector< T > &vec)
- void AtomProbe::marchingCubes (const Voxels< float > &v, float isoValue, std::vector< TriangleWithVertex↩ Norm > &tVec)

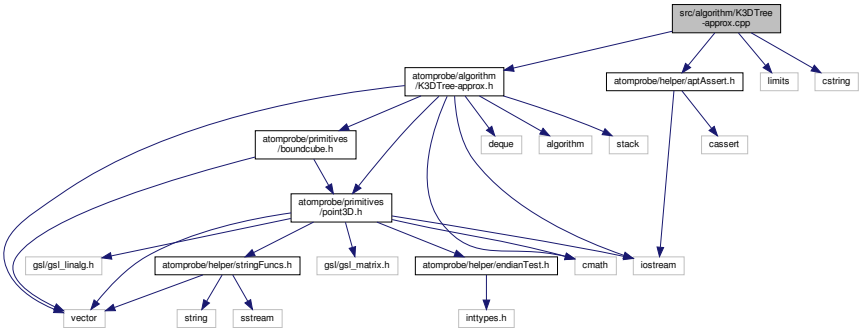
Variables

- int AtomProbe::aiCubeEdgeFlags [256]
- int AtomProbe::a2iTriangleConnectionTable [256][16]
- const unsigned int AtomProbe::VERTEX_OFFSET [8][3]
- int AtomProbe::edgeRemap [12]

7.70 src/algorithm/K3DTree-approx.cpp File Reference

```
#include "atomprobe/algorithm/K3DTree-approx.h"
#include "atomprobe/helper/aptAssert.h"
#include <limits>
```

```
#include <cstring>
```
Include dependency graph for K3DTree-approx.cpp:

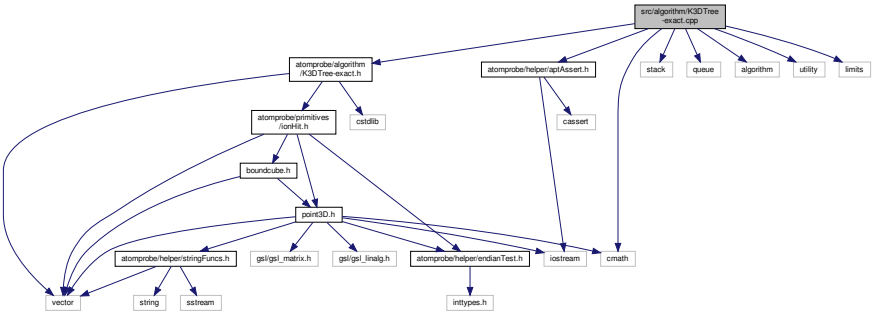


Namespaces

- AtomProbe

7.71 src/algorithm/K3DTree-exact.cpp File Reference

```
#include "atomprobe/algorithm/K3DTree-exact.h"
#include <stack>
#include <queue>
#include <algorithm>
#include <cmath>
#include <utility>
#include <limits>
#include "atomprobe/helper/aptAssert.h"
```
Include dependency graph for K3DTree-exact.cpp:



Classes

- class AxisCompareExact

  Functor allowing for sorting of points in 3D.
- class NodeWalk

Variables

- const int PROGRESS_REDUCE =5000

7.71.1 Variable Documentation

7.71.1.1 PROGRESS_REDUCE

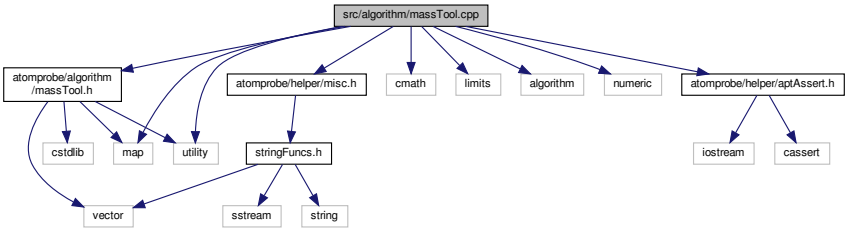
```
const int PROGRESS_REDUCE =5000
```

Definition at line 38 of file K3DTree-exact.cpp.

7.72 src/algorithm/massTool.cpp File Reference

```
#include "atomprobe/algorithm/massTool.h"
#include <cmath>
#include <limits>
#include <algorithm>
#include <numeric>
#include <utility>
#include <map>
#include "atomprobe/helper/misc.h"
#include "atomprobe/helper/aptAssert.h"
```

Include dependency graph for massTool.cpp:



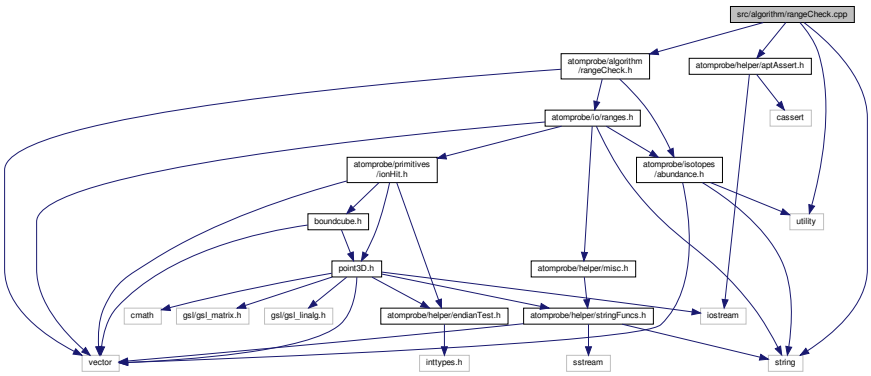
Classes

- class WEIGHT_SEARCH_ENTRY
- class FixedStack< T >

7.73 src/algorithm/rangeCheck.cpp File Reference

```
#include "atomprobe/algorithm/rangeCheck.h"
#include "atomprobe/helper/aptAssert.h"
#include <string>
#include <utility>
```

Include dependency graph for rangeCheck.cpp:



Classes

- struct AtomProbe::RANGE_MOLECULE

Namespaces

- AtomProbe

Functions

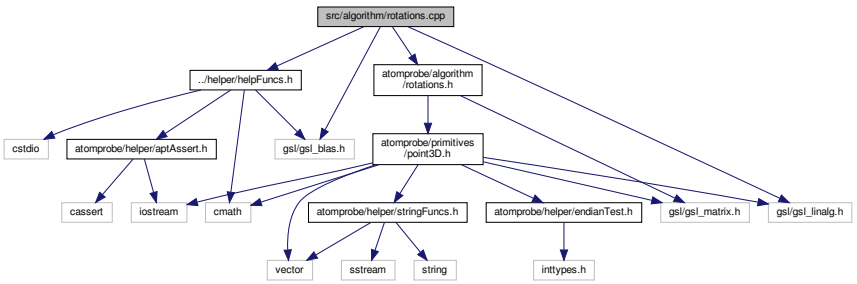
- bool AtomProbe::pairContains (const pair< float, float > &p, float m)
- RANGE_MOLECULE AtomProbe::getRangeMolecule (const AbundanceData &massTable, const RangeFile &rng, unsigned int rangeId)
- void AtomProbe::checkMassRangingCorrectness (const RangeFile &rng, AbundanceData &massTable, float massTolerance, unsigned int maxChargeState, unsigned int maxComponents, std::vector< bool > &badRanges)

  Ensure that each mass given spans a peak that should exist.

7.74 src/algorithm/rotations.cpp File Reference

```
#include "atomprobe/algorithm/rotations.h"
#include "../helper/helpFuncs.h"
#include <gsl/gsl_blas.h>
```

```
#include <gsl/gsl_linalg.h>
```
Include dependency graph for rotations.cpp:



Namespaces

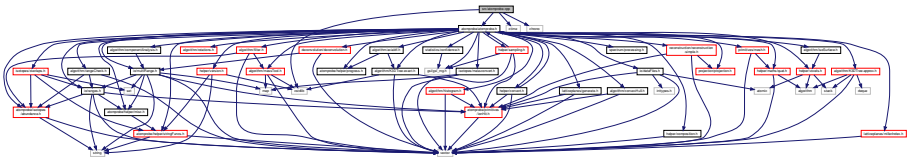
- AtomProbe

Functions

- void AtomProbe::computeRotationMatrix (const Point3D &ur1, const Point3D &ur2, const Point3D &r1, const Point3D &r2, gsl_matrix ∗m)

7.75 src/atomprobe.cpp File Reference

```
#include "atomprobe/atomprobe.h"
#include <cstdlib>
#include <ctime>
#include <chrono>
```
Include dependency graph for atomprobe.cpp:



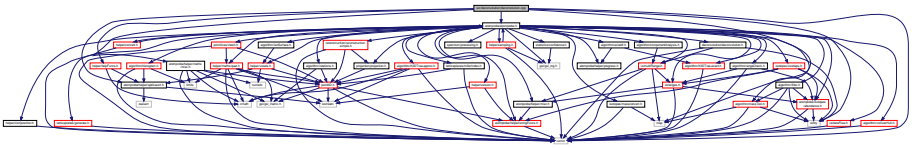
Namespaces

- AtomProbe

7.76 src/deconvolution/deconvolution.cpp File Reference

```
#include "atomprobe/atomprobe.h"
#include "atomprobe/helper/maths/misc.h"
#include "atomprobe/helper/aptAssert.h"
#include "helper/helpFuncs.h"
#include <utility>
#include <vector>
#include <map>
```

Include dependency graph for deconvolution.cpp:



Namespaces

- AtomProbe

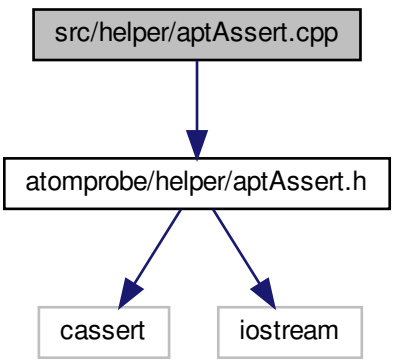
Functions

- float AtomProbe::nullBackground (float rangeStart, float rangeEnd)
- bool AtomProbe::leastSquaresDeconvolve (const MultiRange &rangeData, const AbundanceData &abundance, const float massTol, const vector< IonHit > &hits, float(*backgroundEstimator)(float, float), vector< pair< unsigned int, float > > &decomposedHits)

7.77 src/helper/aptAssert.cpp File Reference

```
#include <atomprobe/helper/aptAssert.h>
```

Include dependency graph for aptAssert.cpp:



Namespaces

- AtomProbe

Functions

- bool AtomProbe::getHardAssert ()
- void AtomProbe::setHardAssert (bool enabled)

  Do assertions cause a straight up crash (enabled), or write a mesage to stderr (disabled)? By default, hard crash.
- void AtomProbe::askAssert (const char *, unsigned int)

  Either abort program, or ask the user what to do for an assertion. depending on hardAssert setting.

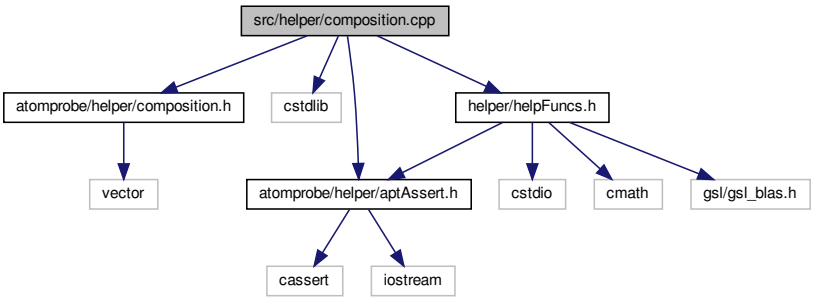
Variables

- bool AtomProbe::hardAssert =true

7.78 src/helper/composition.cpp File Reference

```
#include "atomprobe/helper/composition.h"
#include <cstdlib>
#include "atomprobe/helper/aptAssert.h"
#include "helper/helpFuncs.h"
```

Include dependency graph for composition.cpp:



Namespaces

- AtomProbe

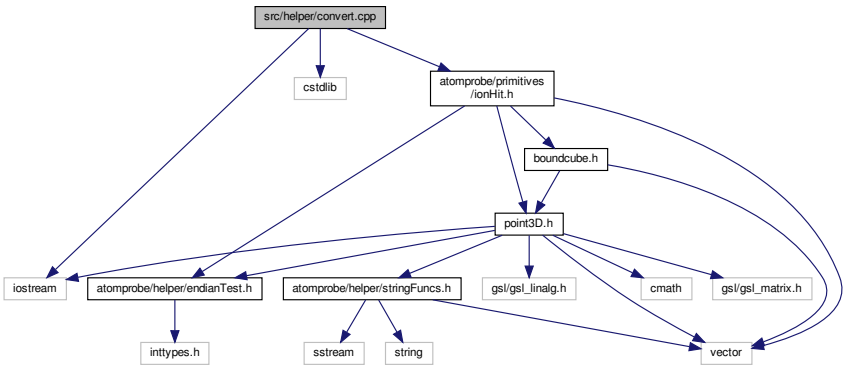
Functions

- void AtomProbe::computeComposition (const std::vector< unsigned int > &countData, std::vector< float > &compositionData)

7.79 src/helper/convert.cpp File Reference

```
#include <iostream>
#include <cstdlib>
#include "atomprobe/primitives/ionHit.h"
```

Include dependency graph for convert.cpp:



Functions

- void convertEPOStoPos (const std::vector< EPOS_ENTRY > &eposEntry, std::vector< IonHit > &posFile)

  Convert an incoming entry of EPOS files to pos, and the append this to the pos vector given.

7.79.1 Function Documentation

7.79.1.1 convertEPOStoPos()

```
void convertEPOStoPos (
            const std::vector< EPOS_ENTRY > & eposEntry,
            std::vector< IonHit > & posFile )
```

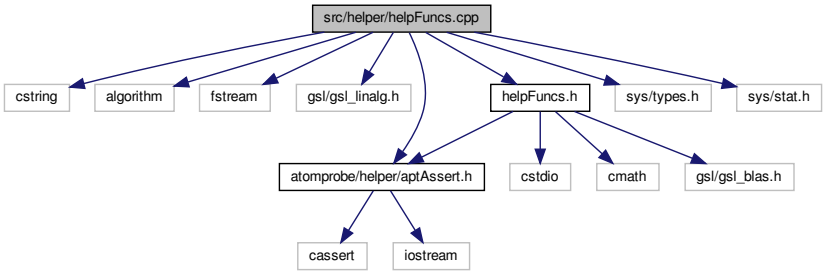
Convert an incoming entry of EPOS files to pos, and the append this to the pos vector given.

Definition at line 29 of file convert.cpp.

7.80 src/helper/helpFuncs.cpp File Reference

```
#include <cstring>
#include <algorithm>
#include <fstream>
#include <gsl/gsl_linalg.h>
#include "atomprobe/helper/aptAssert.h"
#include "helpFuncs.h"
#include <sys/types.h>
#include <sys/stat.h>
```

Include dependency graph for helpFuncs.cpp:



Namespaces

- AtomProbe

Functions

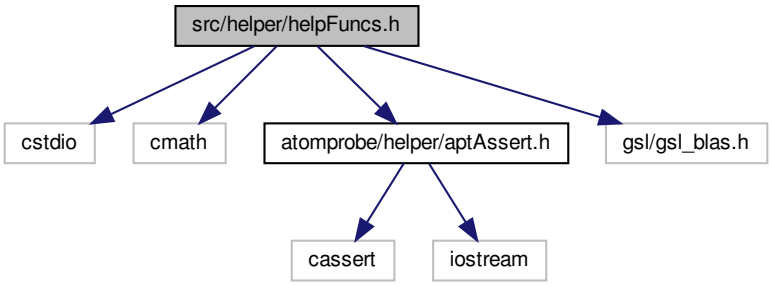
- char * AtomProbe::myStrDup (const char *s)
- void AtomProbe::pushLocale (const char *newLocale, int type)
- void AtomProbe::popLocale ()
- bool AtomProbe::getFilesize (const char *fname, size_t &size)
- void AtomProbe::gsl_print_matrix (const gsl_matrix *m)
- void AtomProbe::gsl_print_vector (const gsl_vector *v)
- float AtomProbe::gsl_determinant (const gsl_matrix *m)
- bool AtomProbe::isNotDirectory (const char *filename)

7.81 src/helper/helpFuncs.h File Reference

```
#include <cstdio>
#include <cmath>
#include "atomprobe/helper/aptAssert.h"
```

```
#include <gsl/gsl_blas.h>
```

Include dependency graph for helpFuncs.h:



This graph shows which files directly or indirectly include this file:

Classes

- class AtomProbe::ComparePairFirst
- class AtomProbe::ComparePairSecond
- class AtomProbe::ComparePairFirstReverse

Namespaces

- AtomProbe

Macros

- #define XOR(a, b) ((!(a)) ^ (!(b)))
- #define ARRAYSIZE(f) (sizeof (f) / sizeof(*f))

Functions

- void AtomProbe::pushLocale (const char *newLocale, int type)
- void AtomProbe::popLocale ()
- int AtomProbe::fpeek (FILE *stream)
- bool AtomProbe::getFilesize (const char *fname, size_t &size)
- void AtomProbe::gsl_print_matrix (const gsl_matrix *m)
- void AtomProbe::gsl_print_vector (const gsl_vector *v)
- float AtomProbe::gsl_determinant (const gsl_matrix *m)
- bool AtomProbe::isNotDirectory (const char *filename)

7.81.1 Macro Definition Documentation

7.81.1.1 ARRAYSIZE

```
#define ARRAYSIZE(
              f ) (sizeof (f) / sizeof(*f))
```

Definition at line 34 of file helpFuncs.h.

Referenced by AtomProbe::RangeFile::getAllExts(), AtomProbe::RangeFile::getErrString(), AtomProbe::getPos↩FileErrString(), AtomProbe::Mesh::loadGmshMesh(), AtomProbe::RangeFile::RangeFile(), AtomProbe::Range↩File::rangeTypeString(), and AtomProbe::readPosapOps().

7.81.1.2 XOR

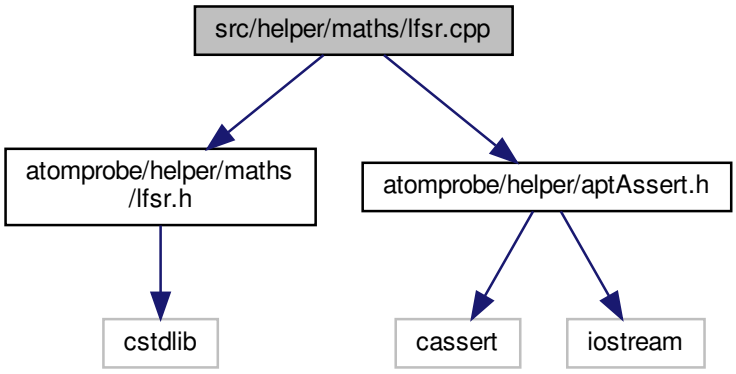
```
#define XOR(
              a,
              b ) ((!(a)) ^ (!(b)))
```

Definition at line 30 of file helpFuncs.h.

7.82 src/helper/maths/lfsr.cpp File Reference

```
#include "atomprobe/helper/maths/lfsr.h"
#include "atomprobe/helper/aptAssert.h"
```

Include dependency graph for lfsr.cpp:



Namespaces

- AtomProbe

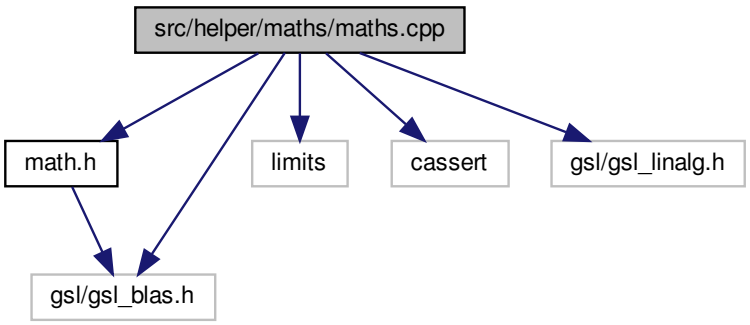
Variables

- const size_t AtomProbe::maximumLinearTable [ ]

7.83 src/helper/maths/maths.cpp File Reference

```
#include "math.h"
#include <limits>
#include <cassert>
#include <gsl/gsl_blas.h>
#include <gsl/gsl_linalg.h>
```

Include dependency graph for maths.cpp:



Macros

- #define ASSERT(f) assert((f))

Functions

- void psuedoInverseFromSVD (const gsl_matrix ∗U, const gsl_vector ∗S, const gsl_matrix ∗V, gsl_matrix ∗P)
- void gsl_matrix_mult (const gsl_matrix ∗A, const gsl_matrix ∗B, gsl_matrix ∗&res, bool alloc)
- void gsl_pseudo_inverse (gsl_matrix ∗A, gsl_matrix ∗&res)

7.83.1 Macro Definition Documentation

7.83.1.1 ASSERT

```
#define ASSERT(
              f ) assert((f))
```

Definition at line 6 of file maths.cpp.

Referenced by gsl_matrix_mult().

7.83.2 Function Documentation

7.83.2.1 gsl_matrix_mult()

```
void gsl_matrix_mult (
             const gsl_matrix * A,
             const gsl_matrix * B,
             gsl_matrix *& res,
             bool alloc )
```

Definition at line 16 of file maths.cpp.

References ASSERT.

Referenced by psuedoInverseFromSVD().

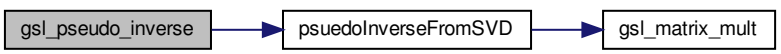
7.83.2.2 gsl_pseudo_inverse()

```
void gsl_pseudo_inverse (
             gsl_matrix * A,
             gsl_matrix *& res )
```

Definition at line 56 of file maths.cpp.

References psuedoInverseFromSVD().

Here is the call graph for this function:



7.83.2.3 psuedoInverseFromSVD()

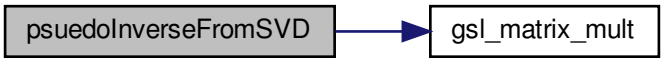
```
void psuedoInverseFromSVD (
            const gsl_matrix * U,
            const gsl_vector * S,
            const gsl_matrix * V,
            gsl_matrix * P )
```

Definition at line 78 of file maths.cpp.

References gsl_matrix_mult().

Referenced by gsl_pseudo_inverse().

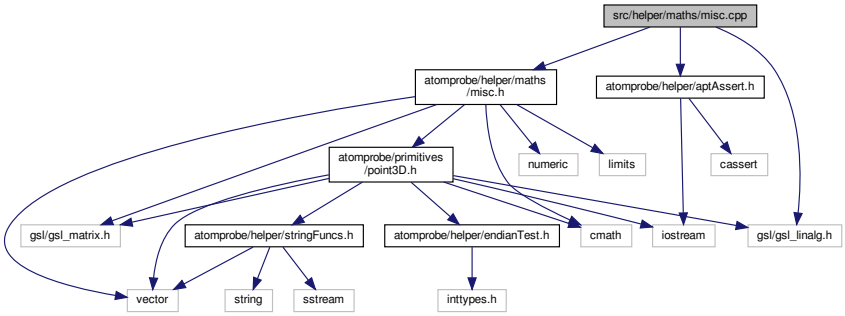
Here is the call graph for this function:



7.84 src/helper/maths/misc.cpp File Reference

```
#include "atomprobe/helper/maths/misc.h"
#include "gsl/gsl_linalg.h"
#include "atomprobe/helper/aptAssert.h"
```

Include dependency graph for misc.cpp:



Namespaces

- AtomProbe

Functions

- unsigned int AtomProbe::estimateRank (const gsl_matrix ∗m, float tolerance=sqrt(std::numeric_limits< float >::epsilon()))

  Estimate the rank of the given matrix.
- bool AtomProbe::solveLeastSquares (gsl_matrix ∗m, gsl_vector ∗b, gsl_vector ∗&x)

  Use an SVD based least-squares solver to solve Mx=b (for x).
- unsigned int AtomProbe::vectorPointDir (const Point3D &pA, const Point3D &pB, const Point3D &vC, const Point3D &vD)

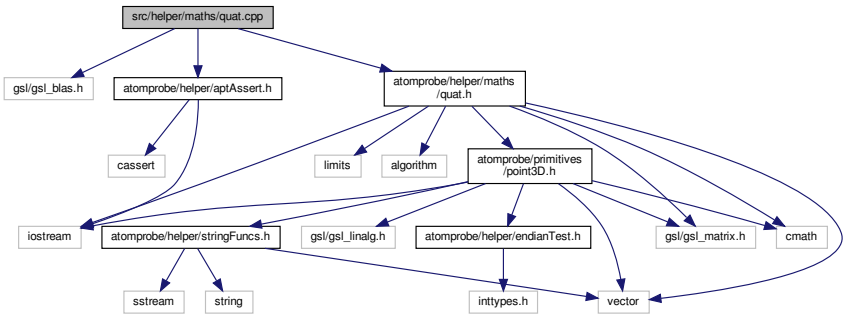
  Check which way vectors attached to two 3D points "point",.
- float AtomProbe::distanceToSegment (const Point3D &fA, const Point3D &fB, const Point3D &p)
- float AtomProbe::signedDistanceToFacet (const Point3D &fA, const Point3D &fB, const Point3D &fC, const Point3D &normal, const Point3D &p)

  Find the distance between a point, and a triangular facet – may be positive or negative.
- float AtomProbe::distanceToFacet (const Point3D &fA, const Point3D &fB, const Point3D &fC, const Point3D &normal, const Point3D &p)
- double AtomProbe::det3by3 (const double ∗ptArray)
- bool AtomProbe::triIsDegenerate (const Point3D &fA, const Point3D &fB, const Point3D &fC)
- double AtomProbe::pyramidVol (const Point3D ∗planarPts, const Point3D &apex)

7.85 src/helper/maths/quat.cpp File Reference

```
#include <gsl/gsl_blas.h>
#include <atomprobe/helper/maths/quat.h>
#include <atomprobe/helper/aptAssert.h>
```

Include dependency graph for quat.cpp:



Namespaces

- AtomProbe

Functions

- void AtomProbe::quat_mult_no_second_a (Quaternion *result, const Quaternion *q1, const Quaternion *q2)
- void AtomProbe::quat_pointmult (Point3f *result, const Quaternion *q1, const Quaternion *q2)
- void AtomProbe::quat_rot (Point3D &p, const Point3D &r, float angle)

  Rotate a point around a given rotation axis by a specified angle.
- void AtomProbe::quat_rot (Point3f *point, const Point3f *rotVec, float angle)

  Rotate a point around a given vector, with specified angle.
- void AtomProbe::quat_rot_array (Point3D *point, unsigned int n, const Point3f *rotVec, float angle)

  Rotate each point in array of size n around a given vector, with specified angle.
- void AtomProbe::quat_rot_array (Point3f *point, unsigned int n, const Point3f *rotVec, float angle)

  Rotate each point in array of size n around a given vector, with specified angle.
- void AtomProbe::quat_get_rot_quat (const Point3f *rotVec, float angle, Quaternion *rotQuat)

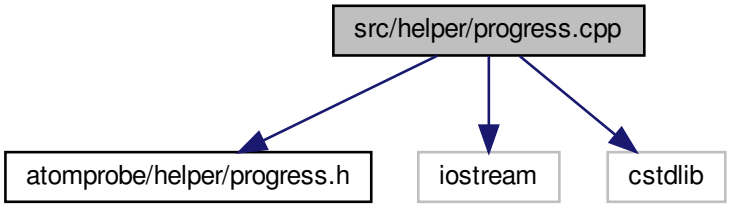
  Compute the quaternion for specified rotation.
- void AtomProbe::quat_rot_apply_quat (Point3f *point, const Quaternion *rotQuat)

  Use previously generated quats from quat_get_rot_quats to rotate a point.
- void AtomProbe::quat_invert (Quaternion *quat)

7.86 src/helper/progress.cpp File Reference

```
#include "atomprobe/helper/progress.h"
#include <iostream>
#include <cstdlib>
```

Include dependency graph for progress.cpp:



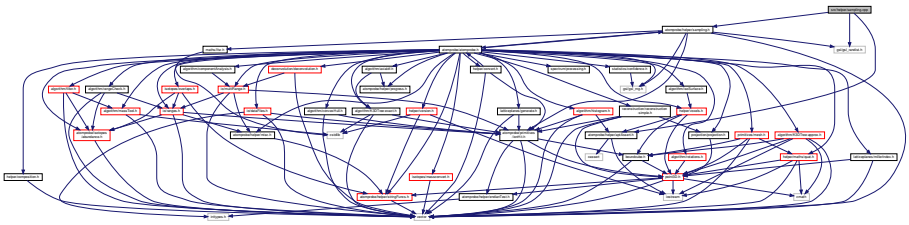
Namespaces

- AtomProbe

7.87 src/helper/sampling.cpp File Reference

```
#include "atomprobe/helper/aptAssert.h"
#include "atomprobe/helper/sampling.h"
#include "gsl/gsl_randist.h"
```

Include dependency graph for sampling.cpp:



Namespaces

- AtomProbe

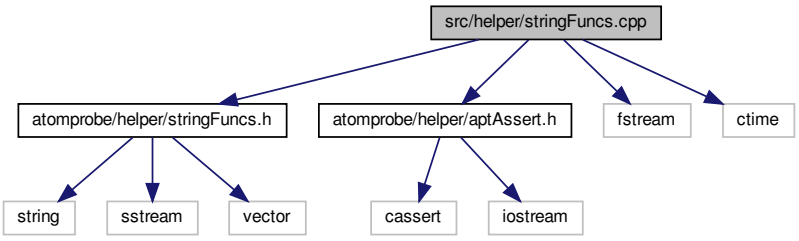
Functions

- void AtomProbe::sampleIons (const std::vector< IonHit > &ions, float sampleFactor, std::vector< IonHit > &sampled, bool strongRandom=true)

7.88 src/helper/stringFuncs.cpp File Reference

```
#include "atomprobe/helper/stringFuncs.h"
#include "atomprobe/helper/aptAssert.h"
#include <fstream>
#include <ctime>
```

Include dependency graph for stringFuncs.cpp:



Namespaces

- AtomProbe

Functions

- std::string AtomProbe::onlyFilename (const std::string &path)

  Return only the filename component.
- std::string AtomProbe::onlyDir (const std::string &path)

  Return only the directory name component of the full path.
- void AtomProbe::nullifyMarker (char ∗buffer, char marker)
- void AtomProbe::ucharToHexStr (unsigned char c, std::string &s)
- void AtomProbe::hexStrToUChar (const std::string &s, unsigned char &c)
- std::string AtomProbe::digitString (unsigned int thisDigit, unsigned int maxDigit)

  Generate a string with leading digits up to maxDigit (eg, if maxDigit is 424, and thisDigit is 1.
- std::string AtomProbe::stripWhite (const std::string &str)

  Strip whitespace, (eg tab,space) from either side of a string.
- std::string AtomProbe::stripChars (const std::string &Str, const char ∗chars)
- void AtomProbe::stripZeroEntries (std::vector< std::string > &s)
- std::string AtomProbe::lowercase (std::string s)

  Return a lowercase version for a given string.
- void AtomProbe::splitStrsRef (const char ∗cpStr, const char delim, std::vector< std::string > &v)

  Split string references using a single delimiter.
- void AtomProbe::splitStrsRef (const char ∗cpStr, const char ∗delim, std::vector< std::string > &v)

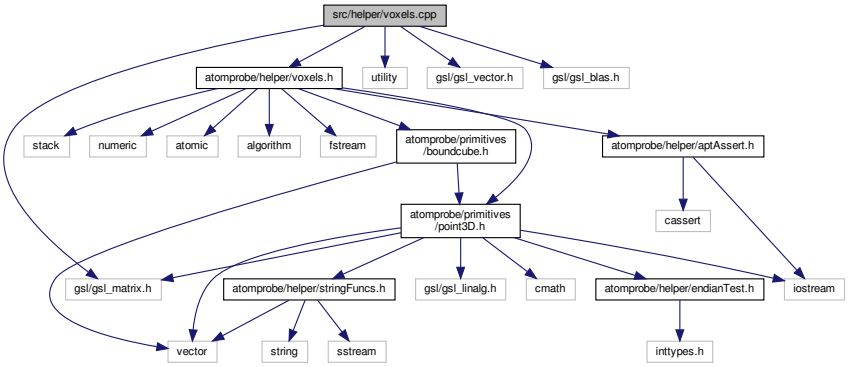
  Split string references using any of a given string of delimiters.
- bool AtomProbe::parseColString (const std::string &str, unsigned char &r, unsigned char &g, unsigned char &b, unsigned char &a)

  Parse a colour string containing rgb[a]; hex for with leading #.
- void AtomProbe::genColString (unsigned char r, unsigned char g, unsigned char b, std::string &s)

7.89 src/helper/voxels.cpp File Reference

```
#include "atomprobe/helper/voxels.h"
#include <utility>
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_vector.h>
#include <gsl/gsl_blas.h>
```

Include dependency graph for voxels.cpp:



Namespaces

- AtomProbe

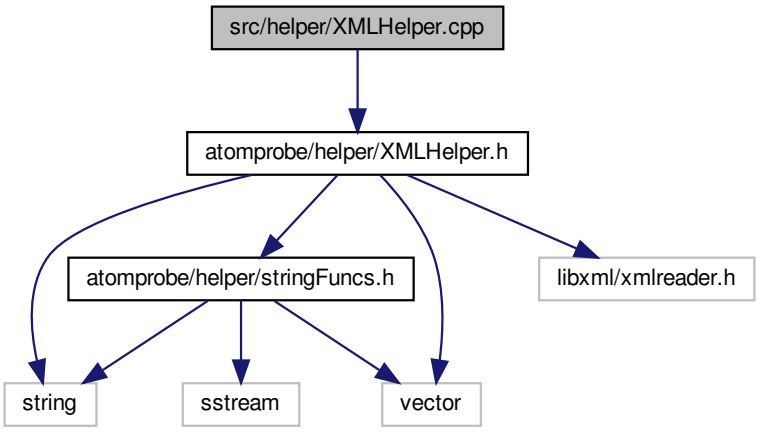
Functions

- void AtomProbe::incrementDataDistanceWeight (const Point3D &p, Voxels< float > &v)
- void AtomProbe::countDataDistanceWeight (const vector< Point3D > &pts, Voxels< float > &v)

7.90 src/helper/XMLHelper.cpp File Reference

```
#include "atomprobe/helper/XMLHelper.h"
```

Include dependency graph for XMLHelper.cpp:



Namespaces

- AtomProbe

Functions

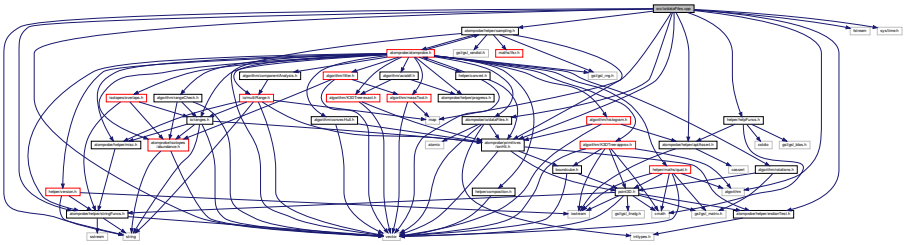
- void AtomProbe::XMLFreeDoc (void *data)

  Free a xmlDoc pointer. For use in conjunction with std::unique_ptr for auto-deallocation.
- unsigned int AtomProbe::XMLHelpNextType (xmlNodePtr &node, int)
- unsigned int AtomProbe::XMLHelpFwdToElem (xmlNodePtr &node, const char *nodeName)
- unsigned int AtomProbe::XMLHelpFwdNotElem (xmlNodePtr &node, const char *nodeName)
- string AtomProbe::XMLHelpGetText (xmlNodePtr node)

7.91 src/io/dataFiles.cpp File Reference

```
#include "atomprobe/io/dataFiles.h"
#include "atomprobe/primitives/ionHit.h"
#include "atomprobe/helper/stringFuncs.h"
#include "atomprobe/helper/endianTest.h"
#include "atomprobe/helper/sampling.h"
#include "helper/helpFuncs.h"
#include "atomprobe/helper/aptAssert.h"
#include <vector>
#include <string>
#include <fstream>
#include <map>
#include <algorithm>
#include <sys/time.h>
```

Include dependency graph for dataFiles.cpp:



Classes

- struct AtomProbe::IONHIT

  Record as stored in a .POS file.

Namespaces

- AtomProbe

Typedefs

- typedef struct AtomProbe::IONHIT AtomProbe::IONHIT

  Record as stored in a .POS file.

Enumerations

- enum { AtomProbe::POS_ALLOC_FAIL =1, AtomProbe::POS_OPEN_FAIL, AtomProbe::POS_SIZE_MODULUS↩_ERR, AtomProbe::POS_SIZE_EMPTY_ERR, AtomProbe::POS_READ_FAIL, AtomProbe::POS_NAN_LOAD_ERROR, AtomProbe::POS_FILE_ENUM↩_END }
- enum { AtomProbe::TAPSIM_FILE_FORMAT_FAIL =1, AtomProbe::TAPSIM_OPEN_FAIL }

Functions

- template<class T >
  unsigned int AtomProbe::fixedRecordReader (const char *filename, bool(*recordReader)(const char *buf↩
  Read, const char *destBuf), size_t recordSize, std::vector< T > &outputData)
- template<class T >
  unsigned int AtomProbe::fixedRecordChunkReader (const char *filename, bool(*recordReader)(const char *bufRead, const char *destBuf), size_t recordSize, std::vector< T > &outputData, unsigned int chunkSize, unsigned int chunkOffset, unsigned int &nEntriesLeft)
- const char * AtomProbe::getPosFileErrString (unsigned int errMesg)
- unsigned int AtomProbe::loadPosFile (std::vector< IonHit > &posIons, const char *posFile)

  Load a pos file directly into a single ion list.
- unsigned int AtomProbe::loadPosFile (std::vector< IonHit > &posIons, const char *posFile, unsigned int nSamplesMax)

  As per loadPosFile, but with an additional setting for the maximum number of ions to load.
- unsigned int AtomProbe::savePosFile (const std::vector< IonHit > &data, const char *name, bool append=false)

  Save a vector of IonHits into a "pos" file, return nonzero on error.
- unsigned int AtomProbe::savePosFile (const std::vector< Point3D > &points, float mass, const char *name, bool append=false)

  Save a vector of Point3Ds into a pos file, using a fixed mass, return nonzero on error.
- unsigned int AtomProbe::loadTapsimBinFile (vector< IonHit > &posIons, const char *posfile)
- unsigned int AtomProbe::saveTapsimBin (std::ostream &f, std::vector< IonHit > &posIons)

  Write a tapsim file from a bunch of IonHits.
- bool AtomProbe::readEposRecord (const char *src, const char *dest)
- size_t AtomProbe::loadEposFile (std::vector< EPOS_ENTRY > &outData, const char *filename)

  Load an entire "EPOS" File.
- size_t AtomProbe::chunkLoadEposFile (std::vector< EPOS_ENTRY > &outData, const char *filename, unsigned int chunkSize, unsigned int chunkOffset, unsigned int &nEntriesLeft)

  Load an "EPOS" file, with a maximum chunk size.
- unsigned int AtomProbe::readPosapOps (const char *file, THREEDAP_EXPERIMENT &data, unsigned int &badLine, unsigned int &progress, std::atomic< bool > &wantAbort, unsigned int nDelayLines=2, bool strictMode=false)

  Function to read POSAP "OPS" files.
- unsigned int AtomProbe::loadATOFile (const char *fileName, std::vector< ATO_ENTRY > &ions, unsigned int forceEndian=0)

  Load a LAWATAP "ATO" file.
- bool AtomProbe::strhas (const char *cpTest, const char *cpPossible)
- unsigned int AtomProbe::loadTextData (const char *cpFilename, std::vector< std::vector< float > > &data↩
  Vec, std::vector< std::string > &headerVec, const char *delim, bool allowNan=true)

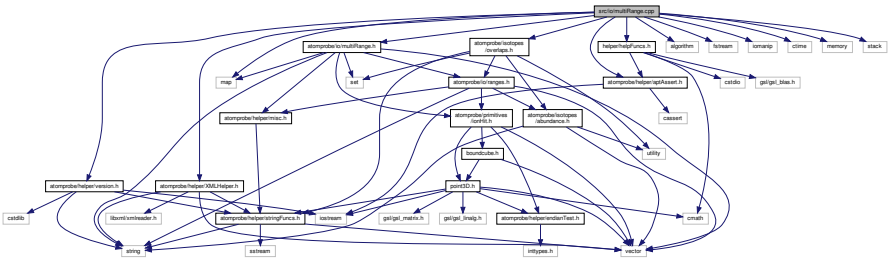
  Load a CSV, TSV or similar text file. Assumes "C" Locale for input (ie "." as decimal separator).

7.92 src/io/multiRange.cpp File Reference

```
#include "atomprobe/io/multiRange.h"
#include "atomprobe/helper/version.h"
#include "atomprobe/helper/XMLHelper.h"
#include "atomprobe/isotopes/overlaps.h"
#include "atomprobe/helper/aptAssert.h"
#include "helper/helpFuncs.h"
#include <algorithm>
#include <fstream>
```

```
#include <iomanip>
#include <ctime>
#include <memory>
#include <stack>
#include <map>
```

Include dependency graph for multiRange.cpp:



Namespaces

- AtomProbe

Enumerations

- enum {
  AtomProbe::MULTIRANGE_ERR_NO_PARSER =1, AtomProbe::MULTIRANGE_ERR_NO_XML_DOC,
  AtomProbe::MULTIRANGE_ERR_NO_XML_CONTEXT, AtomProbe::MULTIRANGE_ERR_NO_NODEP↩
  TR,
  AtomProbe::MULTIRANGE_NOT_VALID_ROOTNODE, AtomProbe::MULTIRANGE_ERR_NO_CONTENT,
  AtomProbe::MULTIRANGE_ERR_NO_TIMESTAMP, AtomProbe::MULTIRANGE_ERR_NO_MOLECULES,
  AtomProbe::MULTIRANGE_ERR_NO_MOLECULE_ENTRIES, AtomProbe::MULTIRANGE_ERR_MOL_↩
  MISSING_ENTRY, AtomProbe::MULTIRANGE_ERR_MOL_MISSING_NAME, AtomProbe::MULTIRANG↩
  E_ERR_MOL_MISSING_COMPONENTS,
  AtomProbe::MULTIRANGE_ERR_BAD_RANGE, AtomProbe::MULTIRANGE_ERR_BAD_RANGES,
  AtomProbe::MULTIRANGE_ERR_MOL_MISSING_COLOUR, AtomProbe::MULTIRANGE_ERR_MOL_↩
  BAD_COLOUR,
  AtomProbe::MULTIRANGE_ERR_NO_RANGES, AtomProbe::MULTIRANGE_ERR_BAD_GROUP, Atom↩
  Probe::MULTIRANGE_ERR_SELF_INCONSISTENT, AtomProbe::MULTIRANGE_ERR_RANGE_NOPA↩
  RENT,
  AtomProbe::MULTIRANGE_ERR_ENUM_END }

Functions

- template<class T >
  void AtomProbe::linkIdentifiers (vector< T > &link)
- bool AtomProbe::operator< (const SIMPLE_SPECIES &a, const SIMPLE_SPECIES &b)
- bool AtomProbe::pairOverlaps (float aStart, float aEnd, float bStart, float bEnd)

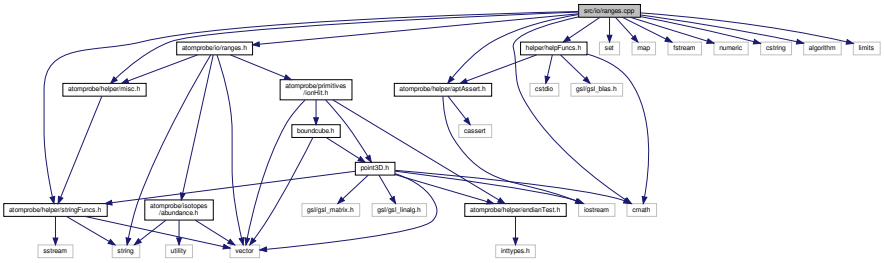
Variables

- const char AtomProbe::MULTIRANGE_FORMAT_VERSION [ ] = "0.0.1"

7.93 src/io/ranges.cpp File Reference

```
#include "atomprobe/io/ranges.h"
#include "atomprobe/helper/stringFuncs.h"
#include "atomprobe/helper/misc.h"
#include "atomprobe/helper/aptAssert.h"
#include "helper/helpFuncs.h"
#include <set>
#include <map>
#include <fstream>
#include <numeric>
#include <cstring>
#include <algorithm>
#include <limits>
#include <cmath>
```

Include dependency graph for ranges.cpp:



Namespaces

- AtomProbe

Functions

- string AtomProbe::rangeToStr (const pair< float, float > &rng)
- bool AtomProbe::matchComposedName (const std::map< string, size_t > &composedNames, const vector< pair< string, size_t > > &namesToFind, size_t &matchOffset)

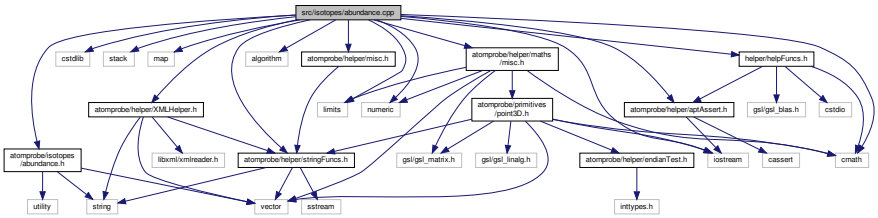
Variables

- const size_t AtomProbe::MAX_LINE_SIZE = 16536
- const size_t AtomProbe::MAX_RANGEFILE_SIZE = 50∗1024∗1024
- const char ∗ AtomProbe::RANGE_EXTS [ ]
- const char ∗ AtomProbe::elementList [ ]

7.94 src/isotopes/abundance.cpp File Reference

```
#include <iostream>
#include <cstdlib>
#include <stack>
#include <map>
#include <cmath>
#include <limits>
#include <algorithm>
#include <numeric>
#include "atomprobe/isotopes/abundance.h"
#include "atomprobe/helper/XMLHelper.h"
#include "atomprobe/helper/stringFuncs.h"
#include "atomprobe/helper/misc.h"
#include "atomprobe/helper/maths/misc.h"
#include "helper/helpFuncs.h"
#include "atomprobe/helper/aptAssert.h"
```

Include dependency graph for abundance.cpp:



Namespaces

- AtomProbe

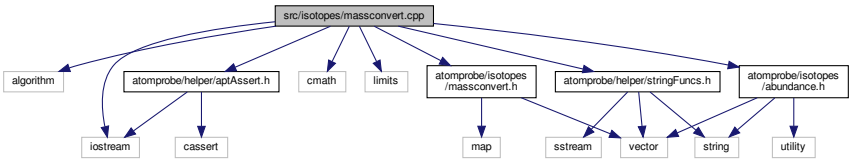
Variables

- const char * AtomProbe::ABUNDANCE_ERROR [ ]

7.95 src/isotopes/massconvert.cpp File Reference

```
#include <algorithm>
#include <iostream>
#include <cmath>
#include <limits>
#include "atomprobe/isotopes/abundance.h"
#include "atomprobe/helper/stringFuncs.h"
#include "atomprobe/helper/aptAssert.h"
```

```
#include "atomprobe/isotopes/massconvert.h"
```
Include dependency graph for massconvert.cpp:



Namespaces

- AtomProbe

Functions

- void AtomProbe::convertMolToMass (const AbundanceData &atomTable, const std::map< unsigned int, double > &compositionMols, std::map< unsigned int, double > &compositionMass)

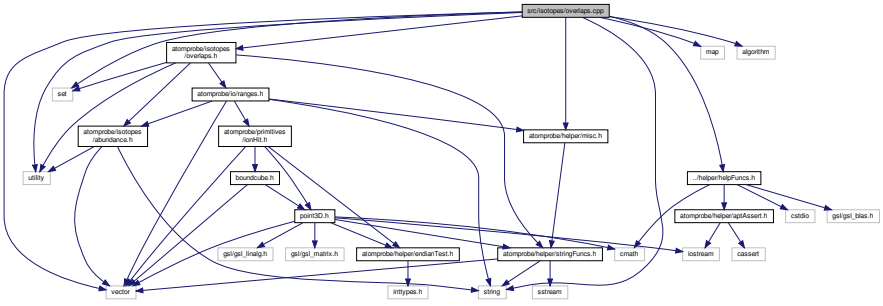
  Convert the given composition from molar fraction data to mass fraction.
- void AtomProbe::convertMassToMol (const AbundanceData &atomTable, const std::map< unsigned int, double > &compositionMass, std::map< unsigned int, double > &compositionMols)

  Convert the given composition from mass fraction data to molar fraction.
- unsigned int AtomProbe::parseCompositionData (const std::vector< std::string > &s, const AbundanceData &atomTable, std::map< unsigned int, double > &atomData)

  Convert atomic string label data, in the form "Fe 0.81" to fraction map.

7.96 src/isotopes/overlaps.cpp File Reference

```
#include "atomprobe/isotopes/overlaps.h"
#include "atomprobe/helper/misc.h"
#include "../helper/helpFuncs.h"
#include <vector>
#include <map>
#include <utility>
#include <string>
#include <algorithm>
#include <set>
```
Include dependency graph for overlaps.cpp:



Namespaces

- AtomProbe

Macros

- #define EQ_TOLV(f, g, h) (fabs((f) - (g)) < (h))

Functions

- void AtomProbe::findOverlapsFromSpectra (const vector< vector< pair< float, float > > > &massDistributions, float massDelta, const set< unsigned int > &skipIDs, vector< pair< size_t, size_t > > &overlapIdx, vector< pair< float, float > > &overlapMasses)
- void AtomProbe::findOverlaps (const AbundanceData &natData, const RangeFile &rng, float massDelta, unsigned int maxCharge, vector< pair< size_t, size_t > > &overlapIdx, vector< pair< float, float > > &overlapMasses)
- void AtomProbe::findOverlaps (const AbundanceData &natData, const vector< string > &ionNames, float massDelta, unsigned int maxCharge, vector< pair< size_t, size_t > > &overlapIdx, vector< pair< float, float > > &overlapMasses)

7.96.1 Macro Definition Documentation

7.96.1.1 EQ_TOLV

```
#define EQ_TOLV(
                f,
                g,
                h ) (fabs( (f) - (g)) < (h))
```

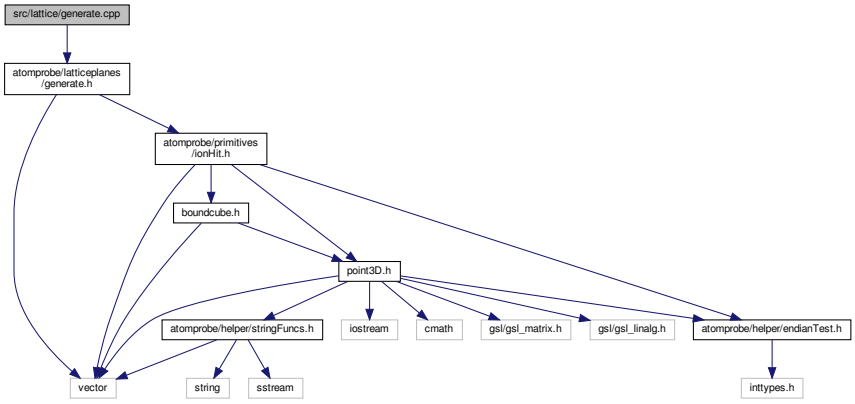
Definition at line 12 of file overlaps.cpp.

Referenced by AtomProbe::findOverlapsFromSpectra().

7.97 src/lattice/generate.cpp File Reference

```
#include "atomprobe/latticeplanes/generate.h"
```

Include dependency graph for generate.cpp:



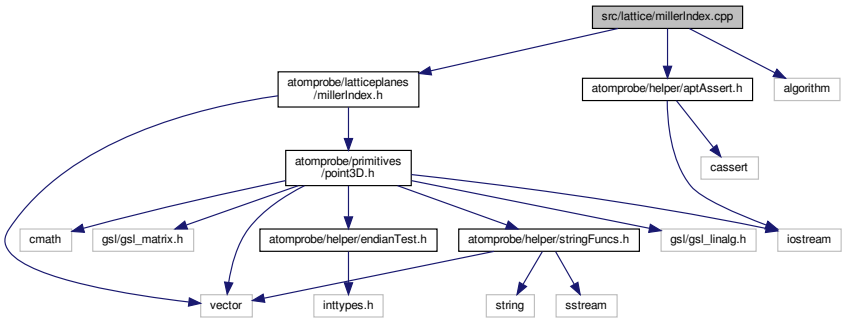
Namespaces

- AtomProbe

7.98 src/lattice/millerIndex.cpp File Reference

```
#include "atomprobe/latticeplanes/millerIndex.h"
#include "atomprobe/helper/aptAssert.h"
#include <algorithm>
```

Include dependency graph for millerIndex.cpp:



Namespaces

- AtomProbe

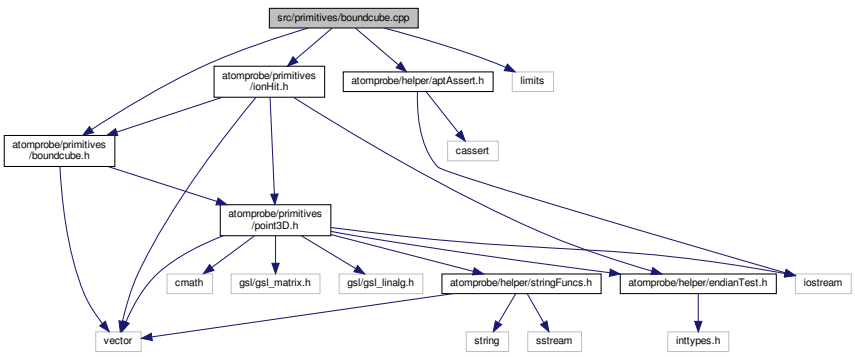
Functions

- int AtomProbe::gcd (int a, int b)

7.99 src/primitives/boundcube.cpp File Reference

```
#include "atomprobe/primitives/boundcube.h"
#include "atomprobe/primitives/ionHit.h"
#include "atomprobe/helper/aptAssert.h"
#include <limits>
```

Include dependency graph for boundcube.cpp:



Namespaces

- AtomProbe

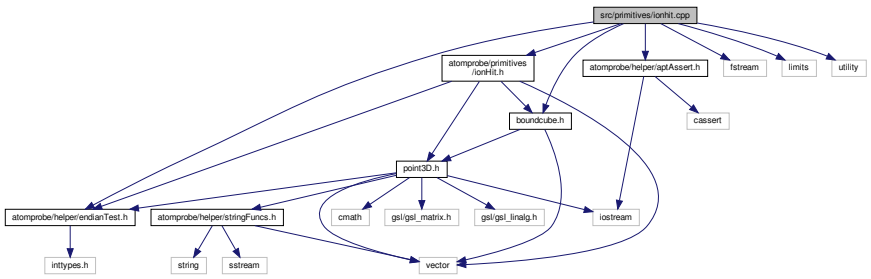
Functions

- std::ostream & AtomProbe::operator<< (std::ostream &stream, const BoundCube &b)

7.100 src/primitives/ionhit.cpp File Reference

```
#include "atomprobe/primitives/ionHit.h"
#include "atomprobe/primitives/boundcube.h"
#include "atomprobe/helper/aptAssert.h"
#include "atomprobe/helper/endianTest.h"
#include <fstream>
#include <limits>
#include <utility>
```

Include dependency graph for ionhit.cpp:



Namespaces

- AtomProbe

Functions

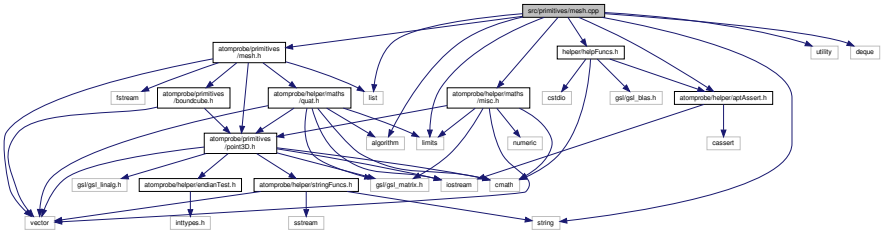
- std::ostream & AtomProbe::operator<< (std::ostream &stream, const IonHit &ion)

7.101 src/primitives/mesh.cpp File Reference

```
#include <atomprobe/primitives/mesh.h>
#include <atomprobe/helper/aptAssert.h>
#include <helper/helpFuncs.h>
#include "atomprobe/helper/maths/misc.h"
#include <string>
#include <algorithm>
#include <limits>
```

```
#include <list>
#include <utility>
#include <deque>
```

Include dependency graph for mesh.cpp:



Namespaces

- AtomProbe

Enumerations

- enum { AtomProbe::MESH_LOAD_UNSPECIFIED_ERROR =1, AtomProbe::MESH_LOAD_BAD_NODECOUNT, AtomProbe::MESH_LOAD_BAD_ELEMENTCOUNT, AtomProbe::MESH_LOAD_IS_INSANE, AtomProbe::MESH_LOAD_ENUM_END }

Functions

- bool AtomProbe::antiRotateMatch (const unsigned int *a, const unsigned int *b, size_t n)
- bool AtomProbe::rotateMatch (const unsigned int *a, const unsigned int *b, size_t n, bool directionForwards=true)
- float AtomProbe::signVal (unsigned int val)
- size_t AtomProbe::findMaxLessThanOrEq (const vector< std::pair< size_t, size_t > > &v, size_t value)
- float AtomProbe::Determinant (float **a, int n)
- float AtomProbe::fourDeterminant (const Point3D &a, const Point3D &b, const Point3D &c, const Point3D &d)
- unsigned int AtomProbe::edgeIdx (unsigned int i, unsigned int j)
- int AtomProbe::intersect_RayTriangle (const Point3D &rayStart, const Point3D &rayEnd, Point3D *tri, Point3D &I)
- void AtomProbe::findNearVerticies (float tolerance, const vector< Point3D > &ptVec, vector< std::pair< size_t, vector< size_t > > > &clusterList)
- void AtomProbe::findNearVerticies (float tolerance, const vector< Point3D > &ptVec, std::list< std::pair< size_t, vector< size_t > > > &clusterList)

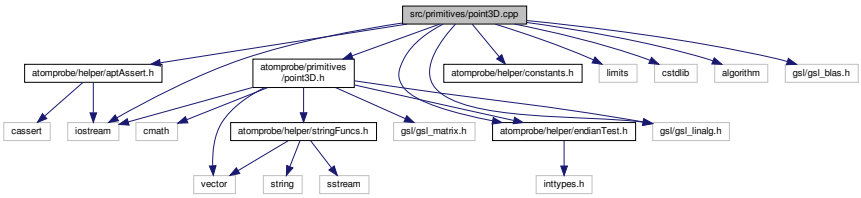
Variables

- const size_t AtomProbe::PROGRESS_REDUCE =500

7.102 src/primitives/point3D.cpp File Reference

```
#include "atomprobe/primitives/point3D.h"
#include "atomprobe/helper/endianTest.h"
#include "atomprobe/helper/aptAssert.h"
#include "atomprobe/helper/constants.h"
#include <limits>
#include <cstdlib>
#include <iostream>
#include <algorithm>
#include <gsl/gsl_linalg.h>
#include <gsl/gsl_blas.h>
```

Include dependency graph for point3D.cpp:



Namespaces

- AtomProbe

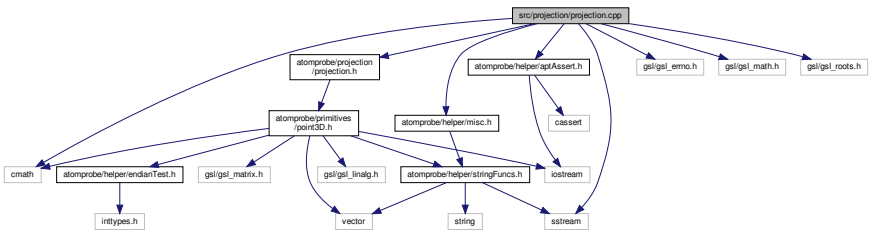
Functions

- void AtomProbe::gsl_matrix_mult (const gsl_matrix *a, const gsl_matrix *b, gsl_matrix *&res)
- std::ostream & AtomProbe::operator<< (std::ostream &stream, const Point3D &pt)

7.103 src/projection/projection.cpp File Reference

```
#include "atomprobe/projection/projection.h"
#include "atomprobe/helper/misc.h"
#include "atomprobe/helper/aptAssert.h"
#include <cmath>
#include <sstream>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_math.h>
#include <gsl/gsl_roots.h>
```

Include dependency graph for projection.cpp:



Classes

- struct AtomProbe::SphericProjectionParams

Namespaces

- AtomProbe

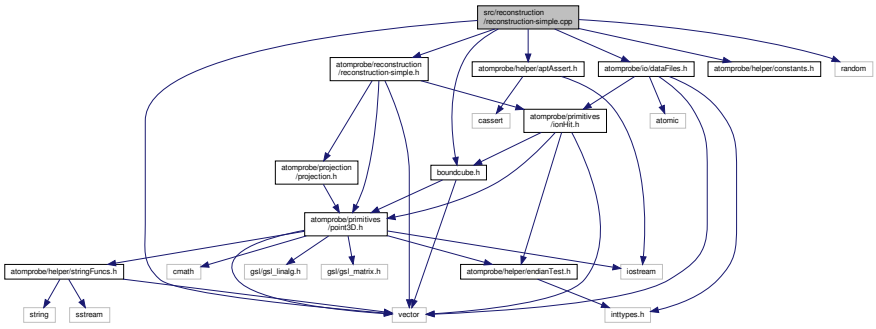
Functions

- double AtomProbe::SphericProjectionEqn (double eta, void *p)

7.104 src/reconstruction/reconstruction-simple.cpp File Reference

```
#include "atomprobe/reconstruction/reconstruction-simple.h"
#include "atomprobe/helper/aptAssert.h"
#include "atomprobe/primitives/boundcube.h"
#include "atomprobe/io/dataFiles.h"
#include "atomprobe/helper/constants.h"
#include <vector>
#include <random>
```

Include dependency graph for reconstruction-simple.cpp:



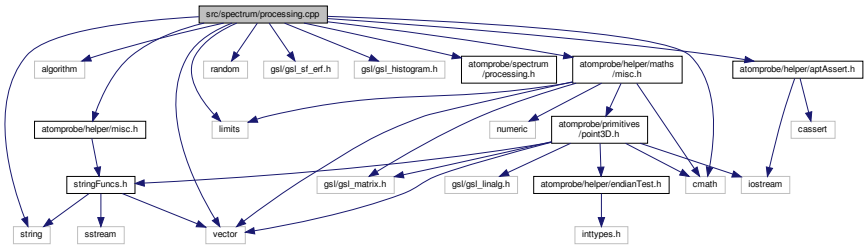
Namespaces

- AtomProbe

7.105 src/spectrum/processing.cpp File Reference

```
#include <vector>
#include <algorithm>
#include <cmath>
#include <limits>
#include <string>
#include <random>
#include <gsl/gsl_sf_erf.h>
#include <gsl/gsl_histogram.h>
#include "atomprobe/spectrum/processing.h"
#include "atomprobe/helper/misc.h"
#include "atomprobe/helper/maths/misc.h"
#include "atomprobe/helper/aptAssert.h"
```

Include dependency graph for processing.cpp:



Namespaces

- AtomProbe

Macros

- #define USE_CENTRAL

Functions

- template<class T >
  bool AtomProbe::andersonDarlingStatistic (std::vector< T > vals, float &meanV, float &stdevVal, float &statistic, size_t &undefCount, bool computeMeanAndStdev=true)
- void AtomProbe::makeHistogram (const vector< float > &data, float start, float end, float step, vector< float > &histVals)
- std::string AtomProbe::getFitErrorMsg (unsigned int errCode)
- unsigned int AtomProbe::doFitBackground (const std::vector< float > &massData, BACKGROUND_PARAMS &params)

  Perform a background fit, assuming constant TOF noise, from 0->inf time.
- void AtomProbe::createMassBackground (float massStart, float massEnd, unsigned int nBinsMass, float tofBackIntensity, std::vector< float > &histogram)

  Build a histogram of the background counts.
- void AtomProbe::diff (const vector< float > &in, vector< float > &out)
- void AtomProbe::findPeaks (const std::vector< float > &x0, std::vector< unsigned int > &peakInds, float sel, bool autoSel=true, bool includeEndpoints=true)

  Simple peak-finding algorithm.

7.105.1 Macro Definition Documentation

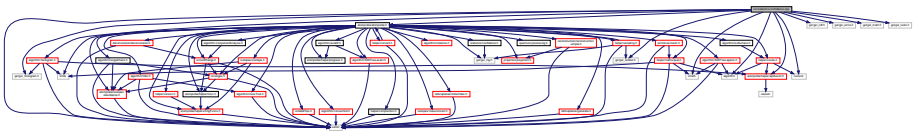
7.105.1.1 USE_CENTRAL

```
#define USE_CENTRAL
```

7.106 src/statistics/confidence.cpp File Reference

```
#include <algorithm>
#include <limits>
#include <cmath>
#include <vector>
#include <numeric>
#include "atomprobe/atomprobe.h"
#include "atomprobe/helper/aptAssert.h"
#include <gsl/gsl_cdf.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_histogram.h>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_math.h>
#include <gsl/gsl_roots.h>
```

Include dependency graph for confidence.cpp:



Classes

- struct AtomProbe::ZECH_ROOT

Namespaces

- AtomProbe

Functions

- template<class T , class T2 >
  std::iterator_traits< T >::value_type AtomProbe::kahansum (T begin, T end, T2 other)
- bool AtomProbe::numericalEstimatePoissRatioConf (float lambda1, float lambda2, float alpha, unsigned int nTrials, gsl_rng *r, float &lBound, float &uBound)

  Brute-force poisson ratio confidence estimator. Returns the confidence interval in the estimate of the mean, at the given rates.
- bool AtomProbe::numericalEstimateSkellamConf (float lambda1, float lambda2, float alpha, unsigned int n↩ Trials, gsl_rng *r, float &lBound, float &uBound)

  Brute-force the confidence bounds of a skellam distribution.
- bool AtomProbe::numericalEstimateGaussRatioConf (float mu1, float mu2, float var1, float var2, float alpha, unsigned int nTrials, gsl_rng *r, float &lBound, float &uBound)

  Brute-force guassian ratio confidence estimator.
- double AtomProbe::zechRoot (double sigGuess, void *params)
- bool AtomProbe::zechConfidenceLimits (float lambdaBack, unsigned int observation, float alpha, float &estimate)

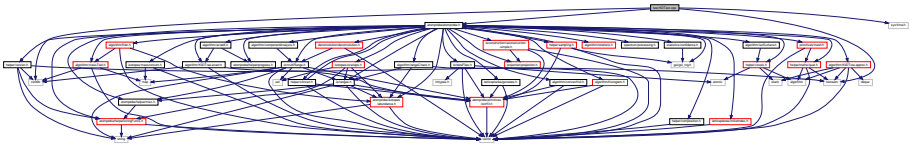
  Provides a best estimate for true signal when true signal, background.
- template<class T >
  void AtomProbe::cumTrapezoid (const vector< T > &x, const vector< T > &vals, vector< T > &res)
- double AtomProbe::gauss_ratio_pdf (double x, double muX, double muY, double varX, double varY)
- void AtomProbe::poissonConfidenceObservation (float counts, float alpha, float &lBound, float &uBound)

  Obtain poisson confidence limits for the mean of a poisson distribution.

7.107 test/KDTest.cpp File Reference

```
#include <iostream>
#include <cstdlib>
#include <sys/time.h>
#include "atomprobe/atomprobe.h"
```

Include dependency graph for KDTest.cpp:



Functions

- bool callback ()
- void kdExactFuzz ()
- bool testInexactKDTree ()
- int main ()

Variables

- const unsigned int NUM_IONS =1000
- const float SCALE =100
- const float SEARCH_RAD = 5
- unsigned int progress =0

7.107.1 Function Documentation

7.107.1.1 callback()

```
bool callback ( )
```

Definition at line 32 of file KDTest.cpp.

Referenced by kdExactFuzz().

7.107.1.2 kdExactFuzz()

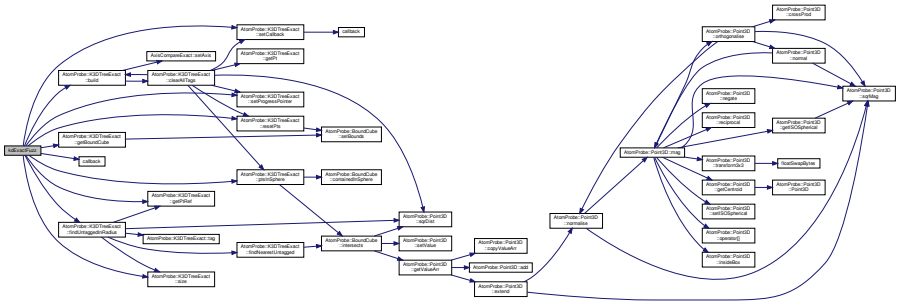
```
void kdExactFuzz ( )
```

Definition at line 37 of file KDTest.cpp.

References AtomProbe::K3DTreeExact::build(), callback(), AtomProbe::K3DTreeExact::findUntaggedInRadius(), AtomProbe::K3DTreeExact::getBoundCube(), AtomProbe::K3DTreeExact::getPtRef(), NUM_IONS, progress, AtomProbe::K3DTreeExact::ptsInSphere(), AtomProbe::K3DTreeExact::resetPts(), SCALE, SEARCH_RAD, AtomProbe::K3DTreeExact::setCallback(), AtomProbe::K3DTreeExact::setProgressPointer(), and AtomProbe↩ ::K3DTreeExact::size().

Referenced by main().

Here is the call graph for this function:



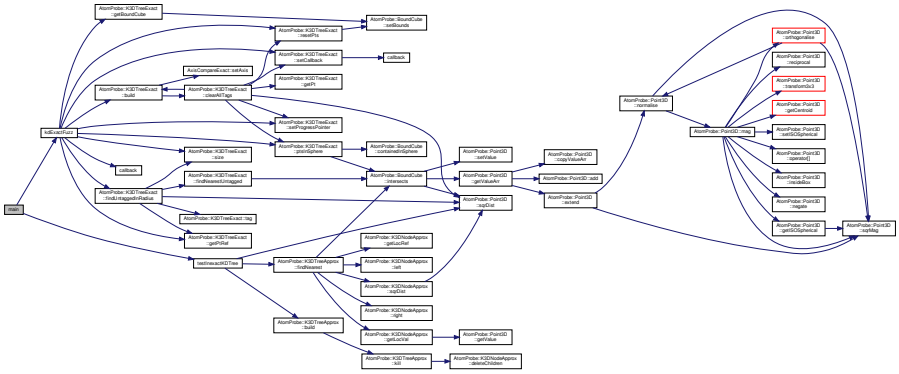
7.107.1.3 main()

```
int main ( )
```

Definition at line 125 of file KDTest.cpp.

References kdExactFuzz(), NUM_IONS, SCALE, SEARCH_RAD, and testInexactKDTree().

Here is the call graph for this function:



7.107.1.4 testInexactKDTree()

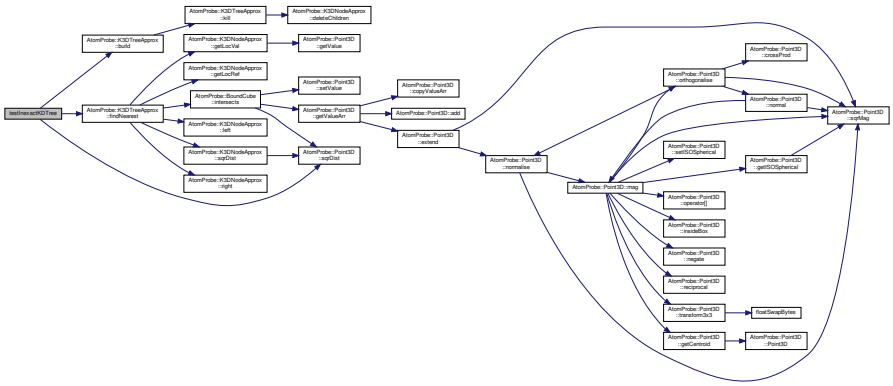
```
bool testInexactKDTree ( )
```

Definition at line 98 of file KDTest.cpp.

References AtomProbe::K3DTreeApprox::build(), AtomProbe::K3DTreeApprox::findNearest(), and AtomProbe::↩ Point3D::sqrDist().

Referenced by main().

Here is the call graph for this function:



7.107.2 Variable Documentation

7.107.2.1 NUM_IONS

```
const unsigned int NUM_IONS =1000
```

Definition at line 26 of file KDTest.cpp.

Referenced by AtomProbe::findPeaks(), AtomProbe::GetReducedHullPts(), kdExactFuzz(), and main().

7.107.2.2 progress

```
unsigned int progress =0
```

Definition at line 30 of file KDTest.cpp.

Referenced by kdExactFuzz().

7.107.2.3 SCALE

```
const float SCALE =100
```

Definition at line 27 of file KDTest.cpp.

Referenced by AtomProbe::GetReducedHullPts(), kdExactFuzz(), and main().

7.107.2.4 SEARCH_RAD

```
const float SEARCH_RAD = 5
```

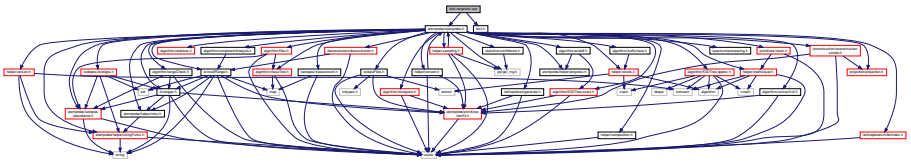
Definition at line 28 of file KDTest.cpp.

Referenced by kdExactFuzz(), and main().

7.108 test/rangetest.cpp File Reference

```
#include "atomprobe/atomprobe.h"
#include "test.h"
```

Include dependency graph for rangetest.cpp:



Functions

- int main ()

7.108.1 Function Documentation

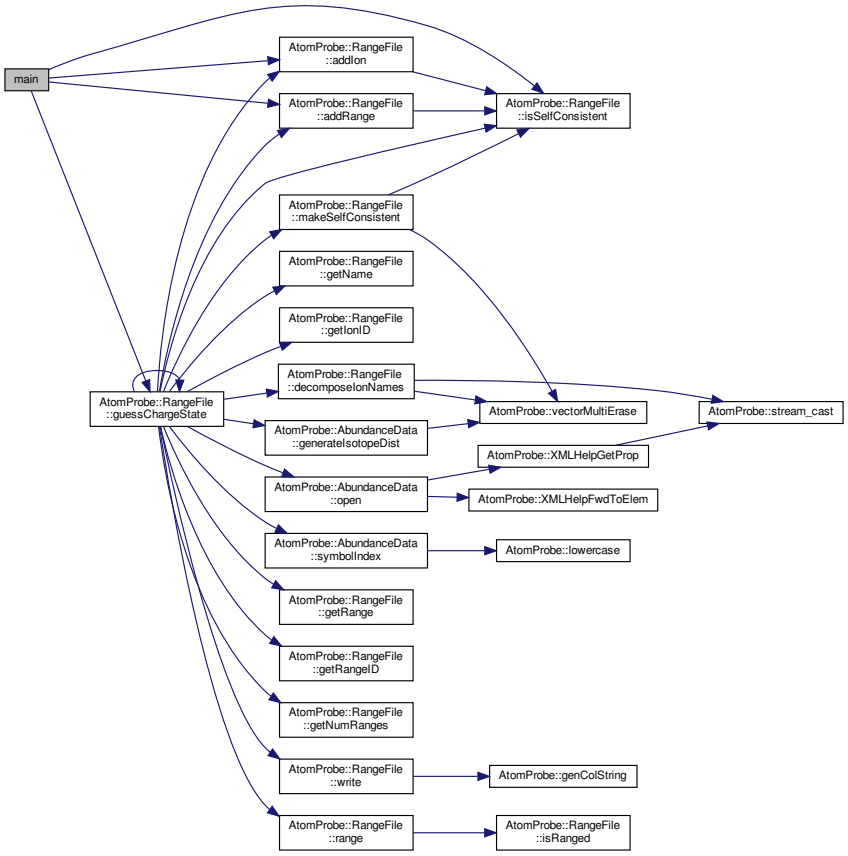
7.108.1.1 main()

```
int main ( )
```

Definition at line 9 of file rangetest.cpp.

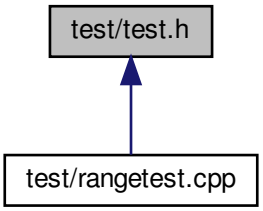
References AtomProbe::RangeFile::addIon(), AtomProbe::RangeFile::addRange(), AtomProbe::RGBf::blue, AtomProbe::RGBf::green, AtomProbe::RangeFile::guessChargeState(), AtomProbe::RangeFile::isSelfConsistent(), AtomProbe::RGBf::red, and TEST.

Here is the call graph for this function:



7.109 test/test.h File Reference

This graph shows which files directly or indirectly include this file:



Macros

- #define TEST(f, g) { if(!(f)) { cerr << "Test failed " << __FILE__ << ":" << __LINE__ << g << endl ; } } ;

7.109.1 Macro Definition Documentation

7.109.1.1 TEST

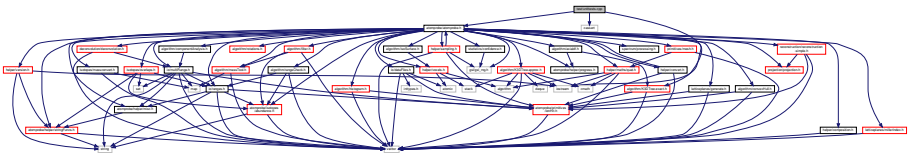
```
#define TEST(
              f,
              g ) { if(!(f)) { cerr << "Test failed " << __FILE__ << ":" << __LINE__ << g
<< endl ; } } ;
```

Definition at line 5 of file test.h.

7.110 test/unittests.cpp File Reference

```
#include <iostream>
#include <cassert>
#include "atomprobe/atomprobe.h"
```

Include dependency graph for unittests.cpp:



Macros

- #define ASSERT(f) assert((f));

Functions

- vector< string > rangePaths ()
- bool runTests ()
- int main ()

7.110.1 Macro Definition Documentation

7.110.1.1 ASSERT

```
#define ASSERT(
              f ) assert( (f) );
```

Definition at line 23 of file unittests.cpp.

Referenced by rangePaths().

7.110.2 Function Documentation

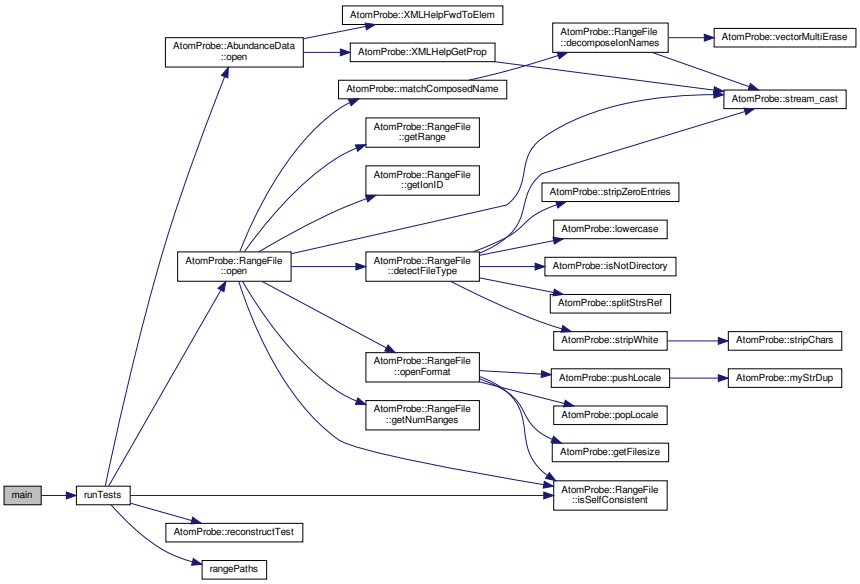
7.110.2.1 main()

```
int main ( )
```

Definition at line 203 of file unittests.cpp.

References runTests().

Here is the call graph for this function:



7.110.2.2 rangePaths()

```
vector<string> rangePaths ( )
```

Definition at line 34 of file unittests.cpp.

References ASSERT.

Referenced by runTests().

7.110.2.3 runTests()

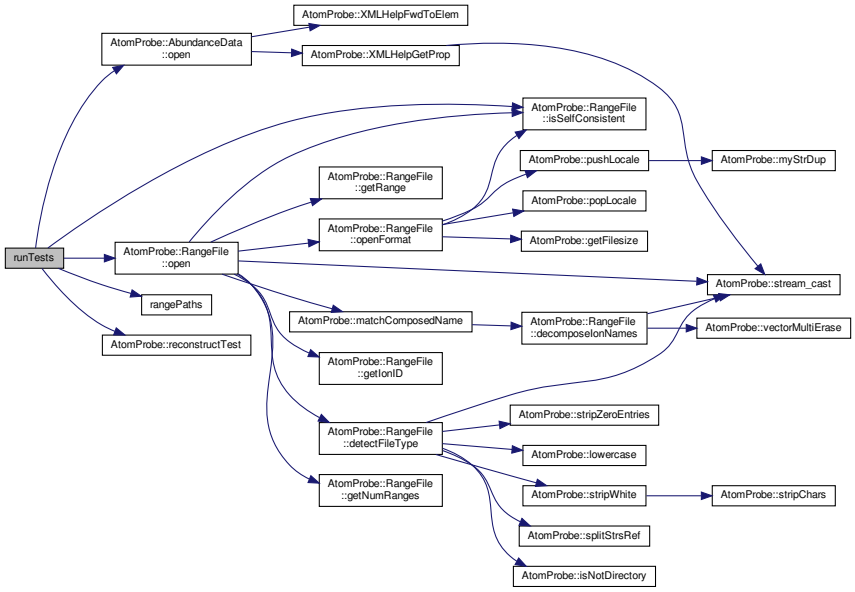
```
bool runTests ( )
```

Definition at line 70 of file unittests.cpp.

References AtomProbe::RangeFile::isSelfConsistent(), AtomProbe::AbundanceData::open(), AtomProbe::Range↩File::open(), rangePaths(), AtomProbe::reconstructTest(), and TEST.

Referenced by main().

Here is the call graph for this function:



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