CHEMTABLE

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Contents

Chapter 1

CHEMTABLE GENERATOR - Beta Version

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1.1 INTRODUCTION

This file includes instructions for building and running the chemtable generator software. This software processes .kg data files produced by FlameMaster to create a table of chemical source terms (chemtable) and various plots for visualizing the data. The program is run by executing a single Python script (chemtable_io.py) as described below.

1.2 BETA DIRECTORY CONTENTS

This directory contains the following files:

- README
- Makefile - generates C++ code
- Makefile.in - called by Makefile
- Doxyfile - generates documentation
- chemtable_io.py - Python script which executes the program
- chemtable_inputs - stores user inputs for chemtable_io.py

The contents of the subdirectories are:

- src - all C++ source code including .cc, .h and .i (SWIG) files

- python - contains Python files with helper functions for chemtable_io.py
- obj - object files are stored here after building
- mod - SWIG-generated Python modules are stored here after building
- alglib - source code for the external library, AlgLib v. 3.9cpp
- test - tests for classes and functions used in the program
- data - sample data sets to be processed by the program
- profiling - results of profiling studies
- output - generated when chemtable_io.py is run, stores program outputs
- doc - contains Doxygen generated documentation

1.3 INSTALLATION

The user interface for this version of the software (and a few helper functions) is written in Python and is ready to use. However, the Python code also contains calls to C++ functions (connected through SWIG) which must be compiled and wrapped before the software can be run, as described below. Building the program generates a variety of shared libraries containing the C++ functions which can be called from Python.

NOTE: when building the program the compiler may issue warnings due to AlgLib and SWIG, but the original code does not generate warnings.

Building the program (compiling and wrapping C++ functions):

- From the current (home) directory, type "make".
- "make cleanall" removes all files generated by make.
- "make cleanlib" removes all external library object files.
- "make clean" removes all compiled source code/modules.

External libraries/Modules/Files needed (∗denotes files included with this software):

- Python v. 2.6
- ∗AlgLib v. 3.9.0 C++ version (for glquad.cc and hermiteinterp.cc)
- SWIG
- MatPlotLib
- Numpy
- ∗Numpy.i for SWIG

Generated shared libraries:

- _convolute.so

- _fittogrid.so
- _integrator.so
- _interpolator.so
- _leastnonmono.so
- _matrix3d.so
- _matrix4d.so
- _matrix.so
- _maxslope.so
- _monocheck.so
- _pdf.so
- _sorting.so

Capabilities of shared library functions:

- Monotonicity checks and slope tests
- Sorting
- Probability Density Functions (PDFs)
- Convolution with delta or beta PDFs
- Grid fitting
- Interpolation

1.4 RUNNING THE PROGRAM

After building, the chemtable generation program is run by executing a single Python script (chemtable_-io.py) as described below. The program (fittogrid function) has been parallelized using OpenMP and can be run on multiple cores by changing the appropriate value in the input file.

Command: ./chemtable_io.py OR python chemtable_io.py

Inputs:

- 'chemtable_inputs' text file (must be in same directory as chemtable_io.py)
- '∗.kg' datafiles (in directory as specified in chemtable_inputs file)

Outputs (written to /output/ directory):

- text data file (name specified in chemtable_inputs file) containing tabulated source terms as a function of Cmean, Zmean, and Zvar (4 columns of data)
- 'CvsTemp.pdf' plot of the chosen progress variable vs. temperature to verify monotonicity

- 'contour_zvar_XXX.pdf' contour plots of the chemical source term vs. Cmean and Zmean for up to 10 values of Zvar
- Several status messages, including the identity of the best progress variable, are printed to the terminal

DETAILED INPUT FILE DESCRIPTION:

Inputs are specified with the following syntax: <inputname:><inputvalue1><inputvalue2><inputvalue3>...

Each input name must appear on only one line. A value for every input must be specified unless it has a DEFAULT value specified. The table below lists the possible inputs and indicates which have default values. Setting 'extrapolate in fittogrid' to 'yes' populates all elements of the final chemtable, but may greatly increase run time. If this option is set to 'no' then values which would require extrapolation are set to -1.

INPUT: DEFAULT <NOTES>

- data file directory: data <can specify a path, eg data/C2H4>
- test species: Y-H2O Y-H2 Y-CO2
- output file name: data_output
- plot all progress variables: yes <options: yes, no>
- skip progress variable optimization: no <options: yes, no>
- extrapolate in fittogrid: no <options: yes, no>
- number of threads: 1 <integer>
- Zpdf: [none] <options: delta, beta>
- sort method: bubble <other options: standard, brute>
- interp method: linear <other options: hermite, cubic>
- least nonmonotonic check: simple <other options: advanced>
- max slope test: linear regression <other options: endpointslope>
- integrator: trapezoid <other options: glquad, simpson>
- StoichMassFrac: 0.055
- glq Number of Nodes: 50 <integer, only required when using glquad inter.>
- length Cgrid: 20 <integer>
- Zvar_max: [none] <integer, only required for beta PDF>
- Zvar_grid: [none] <integer, only required for beta PDF>
- Zmean_grid: Z <if Z, set to be same as the Zgrid in Flamelet files, otherwise, an integer>

DETAILED DATAFILE DESCRIPTION:

The program is designed specifically to run on .kg datafiles. The first line of each datafile is expected to be blank and is ignored. The following requirements exist for processing the datafiles:

- All files in the data file directory specified by the user must be .kg files

- No file may be repeated
- All files must have the same column headers and the same number of rows of data
- 2nd line contains column headers, 3rd line and on contain data
- Column headers for production rate should be: 'ProdRate<SPECIES> [kg/m^3s]'

Two sets of sample data files are included:

- data/C2H4: full output from FlameMaster for a C2H4 flame
- data/C2H4truncated: a subset of the above selected to be a well-behaved test case

----

1.5 TESTING

Several test functions for both the Python and C++ portions of the code are available in the /test/ directory. All tests are run using Python unites (C++ functions are tested through their SWIG wrappers). The following test functions are available:

combinations_test.py findprogvar_test.py iofuncs_test.py sorting_test.py maxslope_test.py convolute_-test.py integrator_test.py pdf_test.py monotonic_test.py leastnonmono_test.py interpolator_test.py fittogrid_test.py

Command: python XXXX_test.py (runs individual tests)

In addition, there is a Bash script "test_all" which can be used to run all tests with one command.

Command: ./test_all (runs all tests)

1.6 DETAILED DOCUMENTATION

For detailed documentation of all classes and functions used by this program, see the Doxygen-generated HTML documentation.

Chapter 2

Namespace Index

2.1 Namespace List

Here is a list of all documented namespaces with brief descriptions:

Chapter 3

Class Index

3.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

Chapter 4

Class Index

4.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

Chapter 5

File Index

5.1 File List

Here is a list of all documented files with brief descriptions:

Chapter 6

Namespace Documentation

6.1 chemtable_io Namespace Reference

Executable Python script for chemtable generation, including calling findprogvar to determine the best progress variable.

Variables

- tuple **fin1** = open('chemtable_inputs')
- list **inputs** = [line.strip().split('\t') for line in fin1]
- tuple **datafiledir** = iof.read_input("data file directory:", inputs, default=['data'])
- tuple **datafiles** = glob.glob("".join(["".join(datafiledir), "/∗.kg"]))
- tuple **testspecies** = iof.read_input("test species:", inputs, minargs=0, default=["Y-CO2","Y-CO","Y-H2O"])
- dictionary **options** = { }
- list **bestC** = [ ]
- tuple **nofiles** = len(datafiles)
- tuple **filesmatC** = fpv.findC(datafiles, testspecies, bestC, options)
- tuple **sorter** = sorting.BubbleSort(filesmatC)
- tuple **Z** = np.genfromtxt(datafiles[0], unpack=False, skip_header=2, delimiter = "\t", usecols = 0)
- **Zmean** = Z
- list **Zpdf** = options["Zpdf"]
- list **Zvar_grid** = [1]
- list **Zvar_max** = [0]
- tuple **Zvar** = np.linspace(0, float(Zvar_max[0]), int(Zvar_grid[0]))
- tuple **d** = pdf.DeltaPDF(Zmean)
- tuple **ZPoints** = len(Z)
- tuple **ZvarPoints** = len(Zvar)
- tuple **ZmeanPoints** = len(Zmean)
- tuple **pdfValM** = matrix3d.Matrix3D(ZvarPoints, ZmeanPoints, ZPoints)
- tuple **pdfValReturn** = d.pdfVal(Z, pdfValM)
- tuple **dataobj** = iof.ProcFile(datafiles[0])
- tuple **titles** = dataobj.gettitles()
- tuple **rxn_rate_locs** = range(len(bestC[0]))
- int **locflag** = 0

- tuple **species** = list(bestC[1][ii])
- list **speciesprodrate** = species[2:]
- list **integ** = options["Integrator"]
- tuple **Intgr** = integrator.Trapz()
- tuple **NumberNodes** = iof.read_input("glq Number of Nodes:", inputs, minargs=0, default=[50])
- list **convolutedC** = [0]
- list **convolutedST** = [0]
- int **maxC** = 0
- int **maxRate** = 0
- list **file** = datafiles[int(filesmatC.GetVal(kk,1))]
- tuple **massfracs** = np.genfromtxt(file, unpack=False, skip_header=2, delimiter = "\t", usecols = bestC[0])
- tuple **rxnrates** = np.genfromtxt(file, unpack=False, skip_header=2, delimiter = "\t", usecols = rxn_-rate_locs)
- tuple **progvar** = np.zeros(ZPoints)
- tuple **rxnRates** = np.zeros(ZPoints)
- tuple **ConvReturn** = convolute.convVal_func(Z, progvar, pdfValM, convolutedC[kk], Intgr)
- int **dim1** = 2
- **dim2** = ZmeanPoints
- **dim3** = ZvarPoints
- **dim4** = nofiles
- tuple **lcgrid** = int(options["LCgrid"][0])
- tuple **cgrid** = np.linspace(0.0, maxC∗1.5, lcgrid)
- list **interpmethod** = options["InterpMethod"]
- tuple **interp** = interpolator.LinInterp()
- tuple **datain** = matrix4d.Matrix4D(dim1, dim2, dim3, dim4)
- tuple **dataout** = matrix3d.Matrix3D(dim2, dim3, lcgrid)
- int **extrap** = 1
- tuple **f2gflag** = fittogrid.fittogrid_func(datain, cgrid, interp, dataout, int(options["nothreads"][0]), ex-trap)
- tuple **FinalData** = np.zeros((lcgrid, dim2, dim3))
- tuple **f** = open("".join(["output/",options["OutputFile"][0]]),'w')
- int **noplots** = 10
- tuple **plots** = range(noplots)
- tuple **i** = int((j+1)∗ZvarPoints/(noplots+2))
- tuple **levels** = np.linspace(-1, maxRate, 50)
- tuple **CS** = plt.contourf(X, Y, FinalData[:,:,i], levels)
- tuple **grid** = pow(10,np.floor(np.log10(maxRate))-1)

6.1.1 Detailed Description

Executable Python script for chemtable generation, including calling findprogvar to determine the best progress variable. Inputs:

- chemtable_inputs: text file containing user options. Each option is written on it's own line, and if multiple values are required they should be seperated by tabs. Details of the chemtable_inputs file and it's required contents can be found in the README.

- .kg (FlameMaster output) data files: in a directory specified by the user in chemtable_inputs. All files must be unique.

Outputs:

- /output/textfile (name specified by user in chemtable_inputs): 4 columns of data, representing Cmean, Zmean, Zvar, and the Chemical Source Term
- /output/contour_zvar_XXX.pdf $*10$: 10 contour plots of chemical source term vs. Zmean and Cmean at the values of Zvar specified in the filenames. If the user specifies taht less than 10 values of Zvar should be calculated, then that number of contour plots is generates
- /output/CvsTemp.pdf: plot of the best progress variable (and others if the user desries) vs. Temperature

Note: this Python script relies on C++ functions connected through SWIG, which must generate the following modules:

- matrix, matrix3D, matrix4D
- pdf
- integrator
- convolute
- sorting
- interpolator
- fittogrid

6.2 combinations Namespace Reference

Module containing functions necessary for creating matrices for calculating all possible combinations of elements of a vector/matrix.

Functions

- def numcoms
- def totnumcoms
- def combos
- def combination_mat

6.2.1 Detailed Description

Module containing functions necessary for creating matrices for calculating all possible combinations of elements of a vector/matrix.

6.2.2 Function Documentation

6.2.2.1 def combinations::combination_mat (*matrix*)

```
returns a combinations matrix A such that for a row vector x:

x*A gives a row vector y which contains all possible combinations of
the elements of x. For example, for x = [x1 x2 x3], then x*A gives:
[x1 x2 x3 x1+x2 x1+x3 x2+x3 x1+x2+x3]
```

6.2.2.2 def combinations::combos (*k*, *matrix*)

```
returns a combinations matrix A such that for a row vector x:

x*A gives a row vector y which contains all possible combinations of
k elements of x. For example, for x = [x1 x2 x3], k=2, then
x*A gives: [x1+x2 x1+x3 x2+x3]
```

6.2.2.3 def combinations::numcoms (*n*, *k*)

```
Returns the number of ways k elements can be selected from a
set of size n
```

6.2.2.4 def combinations::totnumcoms (*n*)

```
Returns the number of ways elements can be selected from a set of size n
in any group size from 1 to n.
```

6.3 findprogvar Namespace Reference

Package containing findC, a function which selects the best progress variable based on the given data files.

Functions

- def findC

  Determines the best progress variable for the given data files.

6.3.1 Detailed Description

Package containing findC, a function which selects the best progress variable based on the given data files.

6.3.2 Function Documentation

6.3.2.1 def findprogvar::findC (*datafiles*, *testspecies*, *bestC*, *options*)

Determines the best progress variable for the given data files. This function returns a matrix containing the following: (row1) stoich prog var (row2) file indices (row3) stoich Temps, sorted by row1

This function also produces plots of the progress variables: output/CvsTemp.pdf. Note that a directory "output" must exist in the directory from which this function is called.

The user can skip optimization by specifying options["SkipProgVar"] = 'yes'

Note: this Python script relies on C++ functions connected through SWIG, which must generate the following modules:

- matrix
- sorting
- interpolator
- monocheck
- maxslope
- least nonmono

Parameters:

datafiles vector of strings specifying file names or paths for the desired data files. Note that the data files should be .kg files produced by FlameMaster

testspecies vector of strings specifying the species to be considered in the progress variable

bestC vector containing information about the best progress variable (output)

options Python dictionary filled with user specified options for the program. Requires options["sort method"], options["StoichMassFrac"], options["InterpMethod"], options["MaxSlopeTest"], options["PlotAllC"], options["lnmcheck"], and options["SkipProgVar"] to be specified

6.4 iofuncs Namespace Reference

Module containing text file processing functions used by other python scripts.

Classes

- class ProcFile

Functions

- def read_input

  Function that extracts input options from a text file.

- def get_progvar

  Function that creates a vector containing information about a progress variable.

6.4.1 Detailed Description

Module containing text file processing functions used by other python scripts.

6.4.2 Function Documentation

6.4.2.1 def iofuncs::get_progvar (*progvarvec*, *testspecies*, *locs*, *index* = `1`)

Function that creates a vector containing information about a progress variable. returns [progvarlocsFULL, progvarnames, index]

progvarnames: strings of species for a given PROGVARVEC, eg [0, 1, 0, 0, 1] --> ['Y-CH4', 'Y-O2'] for TESTSPECIES = ['Y-CO', 'Y-CH4', 'Y-H2', 'Y-CO2', 'Y-O2']

progvarlocsFull: a vector containing all elements of LOCS corresponding to non-zero elements of PROGVARVEC, eg [2, 5] for LOCS = [1 2 3 4 5] in the above example.

index: INDEX unchanged

6.4.2.2 def iofuncs::read_input (*inputname*, *inputsarray*, *minargs* = `1`, *default* = `None`)

Function that extracts input options from a text file. Searches for a row in the text file beginning with the string specified by INPUTNAME. Raises an error if this string appears on multiple lines.

Writes the rest of that line (delimited by tabs) as a vector of strings into INPUTSARRAY.

Raises an error if fewer than MINARGS tab delimited elements are found on the input line.

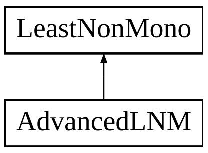
If INPUTNAME is not found, writes returns DEFAULT to INPUTSARRAY, otherwise raises an error.

Chapter 7

Class Documentation

7.1 AdvancedLNM Class Reference

Inheritance diagram for AdvancedLNM::



Public Member Functions

- AdvancedLNM (const Matrix &progVar)

    Constructor.

- ∼AdvancedLNM ()

    Destructor.

- int LeastNonMonotonic (int ∗monoAry, const int ncols, const int col)

    Method to find least monotonic progress variable.

7.1.1 Constructor & Destructor Documentation

7.1.1.1 AdvancedLNM::AdvancedLNM (const Matrix & *progVar*)

Constructor. AdvancedLNM is a class that determines the least non-monotonic progress variable with respect to temperature (or another specified column). It determines the progress variable with the smallest percentage of non-unique (one-to-one) points and selects it as the least non-monotonic progress variable.

If two or more progress variables share the smallest percentage, then the progress variable with the greatest magnitude slope (by endpoints) is selected.

7.1.2 Member Function Documentation

7.1.2.1 int AdvancedLNM::LeastNonMonotonic (int * *monoAry*, const int *ncols*, const int *col*) `[virtual]`

Method to find least monotonic progress variable. LeastNonMonotonic calculates the percentage of non-unique points. The input array monoAry will initially be filled with 0s since all progress variables are non-monotonic. This method will select the least non-monotonic and change its value in monoAry to 1. col is the reference column.

```
INPUTS:

int *monoAry     array containing integer flags that denote the monotonicity of candidate progress variabl

const int ncols  number of columns of monoAry

const int col    the reference column

OUTPUT:

int              flag specifying whether or not the function succeeded
                  = 0: success
 != 0: something went wrong
```

Implements LeastNonMono.

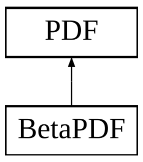
The documentation for this class was generated from the following files:

- src/advancedlnm.h
- src/advancedlnm.cc

7.2 BetaPDF Class Reference

Evaluates beta PDF and stores values in a Matrix3D object.

`#include <betaPDF.h>`Inheritance diagram for BetaPDF::



Public Member Functions

- BetaPDF (const double ∗Zmean, const int ZmeanPoints, const double ∗Zvar, const int ZvarPoints)

  Constructor.

- ∼BetaPDF ()

  Destructor.

- int pdfVal (const double ∗Z, const int ZPoints, Matrix3D ∗pdfValM)

  Main routine that generates the PDF values.

7.2.1 Detailed Description

Evaluates beta PDF and stores values in a Matrix3D object.

7.2.2 Member Function Documentation

7.2.2.1 int BetaPDF::pdfVal (const double ∗ *Z*, const int *ZPoints*, Matrix3D ∗ *pdfValM*) `[virtual]`

Main routine that generates the PDF values. The Beta PDF uses statistics (means and variances) to generate a PDF. The PDF values are stored in a Matrix3D object: dim1 is the variance, dim2 is the mean, and dim3 are the data points.

```
 INPUTS:
 const double* Z        double array containing mixture fraction values coming from the files

 const int ZPoints      number of mixture fraction values in the Z array

 Matrix3D* pdfValM      the Matrix3D type container that stores the PDF values


 OUTPUT:

 int                    flag specifying whether or not the function succeeded
                         = 0: success
!= 0: something went wrong
```

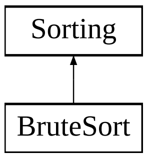
Implements PDF.

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

- src/betaPDF.h
- src/betaPDF.cc

7.3 BruteSort Class Reference

Inheritance diagram for BruteSort::



Public Member Functions

- BruteSort (Matrix ∗data)

  Constructor.

- ∼BruteSort ()

  Destructor.

- int sort_data ()

  Main function that sorts the given data.

- void SetRefColNum (int num)

  Set the reference column number.

7.3.1 Constructor & Destructor Documentation

7.3.1.1 BruteSort::BruteSort (Matrix ∗ *data*)

Constructor. This algorithm goes over the each entry (rows times) at the selected column, finds the maximum entry, records its index. This is repeated rows times until the indices of the entries are obtained in order. Then each column of the matrix is reordered using these indices.

7.3.2 Member Function Documentation

7.3.2.1 int BruteSort::sort_data () `[virtual]`

Main function that sorts the given data. The algortihm processes the reference column and sorts it using the brute sort approach.

```
INPUT:

There are no inputs. The data to be sorted is already passed via the constructor


OUTPUT:

int           flag specifying whether or not the function succeeded
               = 0: success
     != 0: something went wrong
```

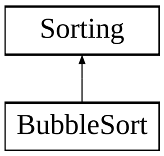
Implements Sorting.

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

- src/brutesort.h
- src/brutesort.cc

7.4 BubbleSort Class Reference

Inheritance diagram for BubbleSort::



Public Member Functions

- BubbleSort (Matrix ∗data)
- ~BubbleSort ()

  Destructor.
- int sort_data ()

  Main sorting body.
- void SetRefColNum (int num)

  Set the reference column number and extract the data of the reference column to the container refColumn_.

7.4.1 Constructor & Destructor Documentation

7.4.1.1 BubbleSort::BubbleSort (Matrix ∗ *data*)

The constructor duplicates the data from the matrix pointer to datacopy_ object. It also generates the array containing the indices to be used during sorting.

7.4.2 Member Function Documentation

7.4.2.1 int BubbleSort::sort_data () `[virtual]`

Main sorting body. This function processes the reference column with the bubble sorting algorithm.

Details of the bubble sort algortihm can be found from the following link: http://en.wikipedia.org/wiki/Bubble_sort

```
INPUT

There are no inputs. The data to be sorted is already passed via the constructor

OUTPUT:

int         flag specifying whether or not the function succeeded
             = 0: success
    != 0: something went wrong
```

Implements Sorting.

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

- src/bubblesort.h
- src/bubblesort.cc

7.5 CompVec Class Reference

Comparator for the standard sorting algorithm.

Public Member Functions

- **CompVec** (double ∗arr)
- bool **operator()** (size_t i, size_t j)

7.5.1 Detailed Description

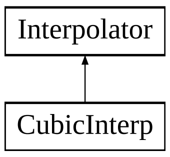
Comparator for the standard sorting algorithm.

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

- src/standardsort.cc

7.6 CubicInterp Class Reference

Inheritance diagram for CubicInterp::



Public Member Functions

- CubicInterp ()

  Constructor.

- ∼CubicInterp ()

  Destructor.

- int Interp (const Matrix ∗matin, int col, double ival, double ∗vecout, int cols)

  Cubic spline interpolation function.

7.6.1 Member Function Documentation

7.6.1.1 int CubicInterp::Interp (const Matrix ∗ *matin*, int *col*, double *ival*, double ∗ *vecout*, int *cols*) `[virtual]`

Cubic spline interpolation function. This function takes in a 2D matrix of data and interpolates an entire row from it using a cubic spline interpolator. Each column of the matrix is treated as a variable, with a specified column being the independent variable. The input data is assumed to be sorted by the independent variable.

```
  INPUTS:

  const Matrix *matin    pointer to a Matrix object. This is the input data.

  int col                integer specifying which column of the input Matrix is the independent
                         variable

  double ival            value at which to interpolate

  double *vecout         pointer to an array which contains the interpolated row. This array has
                         the same number of columns as the input Matrix.

  int cols               number of columns of matin/vecout

  OUTPUTS:

  int                    flag specifying whether or not the function succeeded
                         = 0: success
 = 1: extrapolation attempted
```

Implements Interpolator.

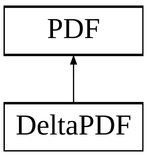
The documentation for this class was generated from the following files:

- src/cubicinterp.h
- src/cubicinterp.cc

7.7 DeltaPDF Class Reference

Evaluates delta PDF and stores values in a Matrix3D object.

`#include <deltaPDF.h>`Inheritance diagram for DeltaPDF::



Public Member Functions

- DeltaPDF (const double ∗Zmean, const int ZmeanPoints)

  Constructor.

- ∼DeltaPDF ()

  Destructor.

- int pdfVal (const double ∗Z, const int ZPoints, Matrix3D ∗pdfValM)

7.7.1 Detailed Description

Evaluates delta PDF and stores values in a Matrix3D object.

7.7.2 Member Function Documentation

7.7.2.1 int DeltaPDF::pdfVal (const double ∗ *Z*, const int *ZPoints*, Matrix3D ∗ *pdfValM*) `[virtual]`

The Delta PDF uses statistics (means) to generate a PDF. The PDF values are stored in a Matrix3D object: dim1 is the variance, dim2 is the mean, and dim3 are the data points.

```
INPUTS:

const double *Z           double arrray containing mixture fraction values coming from the files

const int ZPoints         number of mixture fraction values in the Z array

Matrix3D* pdfValm         the Matrix3D type container that stores the PDF values


OUTPUT:

int                       flag specifying whether or not the function succeeded
                           = 0: success
  != 0: something went wrong
```

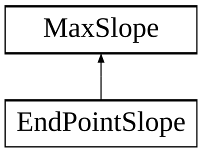
Implements PDF.

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

- src/deltaPDF.h
- src/deltaPDF.cc

7.8 EndPointSlope Class Reference

Inheritance diagram for EndPointSlope::



Public Member Functions

- EndPointSlope (const Matrix &progVar)

  Constructor.

- ∼EndPointSlope ()

  Destructor.

- int MostMonotonic (int ∗monoAry, const int ncols, const int col)

  Method to find the most monotonic progress variable.

7.8.1 Constructor & Destructor Documentation

7.8.1.1 EndPointSlope::EndPointSlope (const Matrix & *progVar*)

Constructor. EndPointSlope is a class that determines the most monotonic progress variable with respect to temperature (or another specified column). It calculates the slope from the first and last endpoints of each progress variable column and selects the progress variable with the largest magnitude slope.

The slope is given by $\frac{C_i(N)-C_i(1)}{N}$

7.8.2 Member Function Documentation

7.8.2.1 int EndPointSlope::MostMonotonic (int ∗ *monoAry*, const int *ncols*, const int *col*) `[virtual]`

Method to find the most monotonic progress variable. MostMonotonic calculates the slope of the best linear approximation for each progress variable which is strictly increasing or strictly decreasing. The output array monoAry must be of length ncols, where each cell holds a value of 3 if C is strictly monotonic and has the largest slope, 2 if C is strictly monotonic but does not have the largest slope, and 0 for non-monotonic C. col is the reference column.

```
INPUTS:

int *monoAry       array containing integer flags that denote the monotonicity of candidate progress varia

const int ncols    number of columns of monoAry

const int col      the reference column
```

```
OUTPUT:

int                 flag specifying whether or not the function succeeded
                     = 0: success
   != 0: something went wrong
```

Implements MaxSlope.

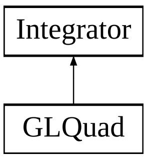
The documentation for this class was generated from the following files:

- src/endpointslope.h
- src/endpointslope.cc

7.9 GLQuad Class Reference

Calculates integral using Gauss-Legendre quadrature.

`#include <glquad.h>`Inheritance diagram for GLQuad::



Public Member Functions

- GLQuad (int Nodes)

    Constructor.

- ∼GLQuad ()

    Destructor.

- double integrate (const double ∗integrand, const double ∗Z, const int ZPoints)

    Integration using Gauss-Legendre quadrature.

7.9.1 Detailed Description

Calculates integral using Gauss-Legendre quadrature. GLQuad takes in an array (the integrand) and returns the integral of that array using Gauss-Legendre quadrature. Abscissa are calculated using the external library AlgLib.

7.9.2 Constructor & Destructor Documentation

7.9.2.1 GLQuad::GLQuad (int *Nodes*)

Constructor. Coordinates of abcissas are calculated in this function.

INPUTS:

const int Nodes number of abcissa

OUTPUT:

No particular output objects. Abcissas and weights are stored in x_ and w_ objects, respectively.

7.9.3 Member Function Documentation

7.9.3.1 double GLQuad::integrate (const double ∗ *integrand*, const double ∗ *Z*, const int *ZPoints*) `[virtual]`

Integration using Gauss-Legendre quadrature. Gauss-Legendre quadrature is applied to integrate a given integrand over a given double array, Z. Abcissas and weights are created during the execution of the constructor. The default number of nodes is 20, the number of nodes for the quadrature can be modified from the input file

```
INPUTS:

const double *integrand            array that contains function values to be integrated

const double *Z                    array that contains the mixture fraction values which the integrand w

const int ZPoints                  number of values, size of the integrand and Z containers

OUTPUT:

double                             result of the integration
```

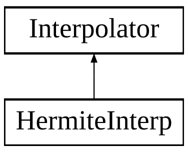
Implements Integrator.

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

- src/glquad.h
- src/glquad.cc

7.10 HermiteInterp Class Reference

Inheritance diagram for HermiteInterp::



Public Member Functions

- HermiteInterp ()
  Constructor.
- ∼HermiteInterp ()
  Destructor.
- int Interp (const Matrix ∗matin, int col, double ival, double ∗vecout, int cols)
  Hermite spline interpolation function.

7.10.1 Member Function Documentation

7.10.1.1 int HermiteInterp::Interp (const Matrix ∗ *matin*, int *col*, double *ival*, double ∗ *vecout*, int *cols*) `[virtual]`

Hermite spline interpolation function. This function takes in a 2D matrix of data and interpolates an entire row from it using a hermite spline interpolator. Each column of the matrix is treated as a variable, with a specified column being the independent variable. The input data is assumed to be sorted

```
  INPUTS:

  const Matrix *matin     pointer to a Matrix object. This is the input data.

  int col                 integer specifying which column of the input Matrix is the independent
                          variable

  double ival             value at which to interpolate

  double *vecout          pointer to an array which contains the interpolated row. This array has
                          the same number of columns as the input Matrix.

  int cols                number of columns of matin/vecout


  OUTPUTS:

  int                     flag specifying whether or not the function succeeded
                          = 0: success
 = 1: extrapolation attempted
```

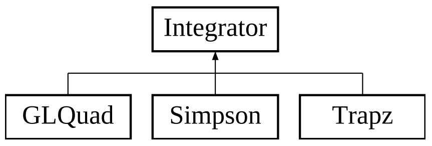
Implements Interpolator.

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

- src/hermiteinterp.h
- src/hermiteinterp.cc

7.11 Integrator Class Reference

Inheritance diagram for Integrator::



Public Member Functions

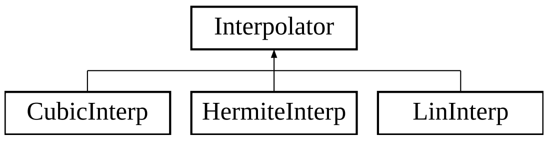
- virtual double integrate (const double ∗integrand, const double ∗Z, const int ZPoints)=0
  Virtual function to be inherited by each integration algorithm to integrate the given data set.

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

- src/integrator.h

7.12 Interpolator Class Reference

Inheritance diagram for Interpolator::



Public Member Functions

- virtual int Interp (const Matrix ∗matin, int col, double ival, double ∗vecout, int cols)=0

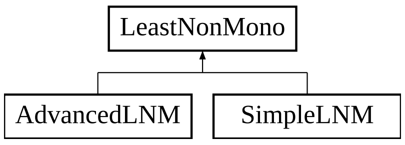
    Virtual function to be inherited by each interpolation algorithm to interpolate the given data.

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

- src/interpolator.h

7.13 LeastNonMono Class Reference

Inheritance diagram for LeastNonMono::



Public Member Functions

- virtual int LeastNonMonotonic (int ∗monoAry, const int ncols, const int col)=0

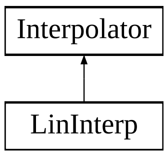
  Virtual function to be inherited by each monotonicity cheking algorithm to determine the least non-monotonic progress variable.

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

- src/leastnonmono.h

7.14 LinInterp Class Reference

Inheritance diagram for LinInterp::



Public Member Functions

- LinInterp ()

  Constructor.

- ~LinInterp ()

  Destructor.

- int Interp (const Matrix ∗matin, int col, double ival, double ∗vecout, int cols)

  Linear interpolation function.

7.14.1 Member Function Documentation

7.14.1.1 int LinInterp::Interp (const Matrix ∗ *matin*, int *col*, double *ival*, double ∗ *vecout*, int *cols*) `[virtual]`

Linear interpolation function. This function takes in a 2D matrix of data and interpolates an entire row from it using a linear interpolator. Each column of the matrix is treated as a variable, with a specified column being the independent variable. The input data is not assumed to be sorted.

```
  INPUTS:

  const Matrix *matin     pointer to a Matrix object. This is the input data.

  int col                 integer specifying which column of the input Matrix is the independent
                          variable

  double ival             value at which to interpolate

  double *vecout          pointer to an array which contains the interpolated row. This array has
                          the same number of columns as the input Matrix.

  int cols                number of columns of matin/vecout


  OUTPUTS:

  int                     flag specifying whether or not the function succeeded
                          = 0: success
= 1: extrapolation attempted
```

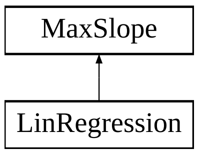
Implements Interpolator.

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

- src/lininterp.h
- src/lininterp.cc

7.15 LinRegression Class Reference

Inheritance diagram for LinRegression::



Public Member Functions

- LinRegression (const Matrix &progVar)

  Constructor.

- ∼LinRegression ()

  Destructor.

- int MostMonotonic (int ∗monoAry, const int ncols, const int col)

  Method to find the most monotonic progress variable.

7.15.1 Constructor & Destructor Documentation

7.15.1.1 LinRegression::LinRegression (const Matrix & *progVar*)

Constructor. LinRegression is a class that determines the most monotonic progress variable with respect to temperature (or another specified column). It calculates the slope of the best linear approximation for each progress variable and selects the largest magnitude.

The slope is given by {sum_i=1_i=N (C_i-C_ave)(T_i-T_ave)}/{sum_i=1_i=N (T_i-T_ave)^2}

7.15.2 Member Function Documentation

7.15.2.1 int LinRegression::MostMonotonic (int ∗ *monoAry*, const int *ncols*, const int *col*) `[virtual]`

Method to find the most monotonic progress variable. MostMonotonic calculates the slope of the best linear approximation for each progress variable which is strictly increasing or strictly decreasing. The output array monoAry must be of length ncols, where each cell holds a value of 3 if C is strictly monotonic and has the largest slope, 2 if C is strictly monotonic but does not have the largest slope, and 0 for non-monotonic C. col is the reference column.

Implements MaxSlope.

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

- src/linregression.h
- src/linregression.cc

7.16 Matrix Class Reference

Public Member Functions

- Matrix (int rows, int cols)

  Constructor.

- ∼Matrix ()

  Destructor.

- double GetVal (int i, int j) const

  Get the value at a specified index.

- void SetVal (int i, int j, double val)

  Set the value at a specific location.

- int GetNumRows () const

  Return the number of rows.

- int GetNumCols () const

  Return the number of columns.

- int GetCol (int j, double ∗colAry) const

  Return an array containing column j.

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

- src/matrix.h
- src/matrix.cc

7.17 Matrix3D Class Reference

Public Member Functions

- Matrix3D (int dim1, int dim2, int dim3)

  Constructor.

- ~Matrix3D ()

  Destructor.

- double GetVal (int i, int j, int k) const

  Get the value at a specified index.

- void SetVal (int i, int j, int k, double vol)

  Set the value at a specified index.

- int GetNumDim1 () const

  Return dim1.

- int GetNumDim2 () const

  Return dim2.

- int GetNumDim3 () const

  Return dim3.

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

- src/matrix3d.h
- src/matrix3d.cc

7.18 Matrix4D Class Reference

Public Member Functions

- Matrix4D (int dim1, int dim2, int dim3, int dim4)

  Constructor.

- ∼Matrix4D ()

  Destructor.

- double GetVal (int i, int j, int k, int l) const

  Get the value at a specified index.

- void SetVal (int i, int j, int k, int l, double val)

  Set the value at a specified index.

- int GetNumDim1 () const

  Return dim1.

- int GetNumDim2 () const

  Return dim2.

- int GetNumDim3 () const

  Return dim3.

- int GetNumDim4 () const

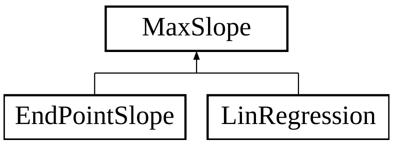
  Return dim4.

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

- src/matrix4d.h
- src/matrix4d.cc

7.19 MaxSlope Class Reference

Inheritance diagram for MaxSlope::



Public Member Functions

- virtual int MostMonotonic (int ∗monoAry, const int ncols, const int col)=0

  Virtual function to be inherited by each monotonicity checking algorithm to determine the most monotonic progress variable.

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

- src/maxslope.h

7.20 MonoCheck Class Reference

Public Member Functions

- MonoCheck (const Matrix &progVar)

  Constructor.
- ∼MonoCheck ()

  Destructor.
- int CheckStrictMonoticity (int ∗monoAry, const int ncols, int col)

  Method to check whether each progress variable is strictly monotonic.

7.20.1 Constructor & Destructor Documentation

7.20.1.1 MonoCheck::MonoCheck (const Matrix & *progVar*)

Constructor. monocheck is a class which checks whether a specified progress variable is strictly increasing or strictly decreasing with respect to temperature (or another specified column). That is, C(T1)<C(T2) or C(T1)>C(T2) for T1<T2, where T1 and T2 are any two temperatures and C is the progress variable.

7.20.2 Member Function Documentation

7.20.2.1 int MonoCheck::CheckStrictMonoticity (int ∗ *monoAry*, const int *ncols*, int *col*)

Method to check whether each progress variable is strictly monotonic. CheckStrictMonoticity checks the monotonicity of each column (AKA progress variable "C") in progVar with respect to column "col". The output array monoAry must be of length ncols_, where each cell holds a value of 3 if C is strictly increasing or strictly decreasing and 0 otherwise.

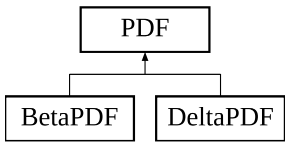
```
INPUTS:

int *monoAry        array containing integer flags that denote the monotonicity of candidate progress vari

const int ncols     number of columns of monoAry

const int col       the reference column


OUTPUT:

int                 flag specifying whether or not the function succeeded
                     = 0: success
    != 0: something went wrong
```

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

- src/monocheck.h
- src/monocheck.cc

7.21 PDF Class Reference

Inheritance diagram for PDF::



Public Member Functions

- virtual int **pdfVal** (const double ∗Z, const int ZPoints, Matrix3D ∗pdfValM)=0

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

- src/pdf.h

7.22 iofuncs::ProcFile Class Reference

Public Member Functions

- def __init__

  The Constructor.

- def gettitles

  Function that returns a vector containing the column headers in the 2nd row of the data file.

- def interpolate

  Interpolate function extracts/interpolates a row of data in the data file at the specified value in the first column.

7.22.1 Detailed Description

```
Class for processing .kg datafiles, including extracting column headers and interpolating a row of data.
```

7.22.2 Member Function Documentation

7.22.2.1 def iofuncs::ProcFile::__init__ (*self*, *sfile*)

The Constructor. SFILE: a string contiaining the name of the data file to be processed or path to that file

7.22.2.2 def iofuncs::ProcFile::gettitles (*self*)

Function that returns a vector containing the column headers in the 2nd row of the data file. Ignores 1st row, returns contents of 2nd row as elements of a vector (assuming datafile is tab delimited).

7.22.2.3 def iofuncs::ProcFile::interpolate (*self*, *inputvars*, *locs*, *datavec*, *interpval* = `0.27`, *interpmethod* = `'linear'`)

Interpolate function extracts/interpolates a row of data in the data file at the specified value in the first column. Read the columns of the data file with headers matching the strings in the INPUTVARS vector.

Write the column numbers corresponding to these column headers into LOCS vector.

Interpolate to find values of each column corresponding to INTERPVAL in the 1st column, using interpolation method specified by the INTERPMETHOD string.

Write interpolated values to DATAVEC.

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

- python/iofuncs.py

7.23 SequenceGen Class Reference

Sequence generator for the standard sorting algorithm.

Public Member Functions

- **SequenceGen** (int start=0)
- int **operator()** ()

7.23.1 Detailed Description

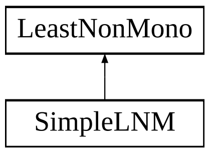
Sequence generator for the standard sorting algorithm.

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

- src/standardsort.cc

7.24 SimpleLNM Class Reference

Inheritance diagram for SimpleLNM::



Public Member Functions

- SimpleLNM (const Matrix &progVar)

  Constructor.

- ~SimpleLNM ()

  Destructor.

- int LeastNonMonotonic (int ∗monoAry, const int ncols, const int col)

  Method to find the least non monotonic progress variable.

7.24.1 Constructor & Destructor Documentation

7.24.1.1 SimpleLNM::SimpleLNM (const Matrix & *progVar*)

Constructor. SimpleLNM is a class that determines the least non-monotonic progress variable with respect to temperature (or another specified column). It determines the percentage which the progress variable is strictly increasing and the percentage which the progress variable is strictly decreasing. The larger percentage not only determines whether the progress variable is increasing or decreasing, but will also be compared with the percentages of other progress variables. The progress variable with the largest percentage of increasing or decreasing values is the least non-monotonic progress variable.

If two or more progress variables share the highest percentage, then the progress variable with the greatest magnitude slope (by endpoints) is selected. Progress variables with neither increasing nor decreasing data are considered strongly non-monotonic.

7.24.2 Member Function Documentation

7.24.2.1 int SimpleLNM::LeastNonMonotonic (int ∗ *monoAry*, const int *ncols*, const int *col*) `[virtual]`

Method to find the least non monotonic progress variable. LeastNonMonotonic calculates how much each progress variable is strictly increasing and strictly decreasing. The input array monoAry will initially be filled with 0s since all progress variables are non-monotonic. This method will select the least non-monotonic and change its value in monoAry to 1. col is the reference column.

```
INPUTS:

int *monoAry      array containing integer flags that denote the monotonicity of candidate slope variables
```

```
const int ncols   number of columns of monoAry

const int col     the reference column

OUTPUT:

int               flag specifying whether or not the function succeeded
                   = 0: success
  != 0: something went wrong
```

Implements LeastNonMono.

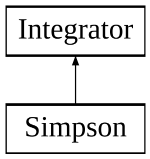
The documentation for this class was generated from the following files:

- src/simplelnm.h
- src/simplelnm.cc

7.25 Simpson Class Reference

Calculates integral using Simpson's rule.

`#include <simpson.h>`Inheritance diagram for Simpson::



Public Member Functions

- Simpson ()

  Constructor.

- ∼Simpson ()

  Destructor.

- double integrate (const double ∗integrand, const double ∗Z, const int ZPoints)

  Main function that integrates a given data set using Simpson's Rule.

7.25.1 Detailed Description

Calculates integral using Simpson's rule. Simpson takes in an array (the integrand) and returns the integral of that array using Simpson's rule.

7.25.2 Member Function Documentation

7.25.2.1 double Simpson::integrate (const double ∗ *integrand*, const double ∗ *Z*, const int *ZPoints*) `[virtual]`

Main function that integrates a given data set using Simpson's Rule. Simpson's rule is applied to integrate a given integrand over a given double array, Z.

```
INPUTS:

const double *integrand          array that contains function values to be integrated

const double *Z                  array that contains the mixture fraction values which the integrand wi

const int ZPoints                number of values, size of the integrand and Z arrays


OUTPUT:

double                           result of the integration
```

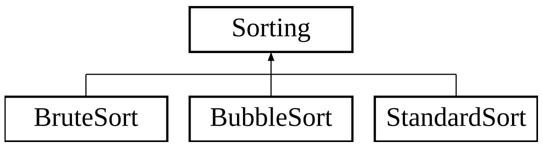
Implements Integrator.

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

- src/simpson.h
- src/simpson.cc

7.26 Sorting Class Reference

Inheritance diagram for Sorting::



Public Member Functions

- virtual int sort_data ()=0

  Virtual function to be inherited by each sorting algorithm to sort the give data.

- virtual void SetRefColNum (int num)

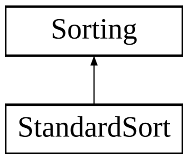
  Setting the reference column according to which the data will be sorted.

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

- src/sorting.h

7.27 StandardSort Class Reference

Inheritance diagram for StandardSort::



Public Member Functions

- StandardSort (Matrix ∗data)

  Constructor.

- ∼StandardSort ()

  Destructor.

- int sort_data ()

  Main function that sorts the given data.

- void SetRefColNum (int num)

  Set the reference column number.

7.27.1 Constructor & Destructor Documentation

7.27.1.1 StandardSort::StandardSort (Matrix ∗ *data*)

Constructor. The data to be sorted is passed to the constructor. A duplicate of the data is produced to be later at this stage

7.27.2 Member Function Documentation

7.27.2.1 int StandardSort::sort_data () `[virtual]`

Main function that sorts the given data. The algorithm sends the reference column to the standard sorting operator that is embedded into the C++ standard library

```
INPUT

There are no inputs. The data to be sorted is already passed via the constructor

OUTPUT:

int        flag specifying whether or not the function succeeded
            = 0: success
  != 0: something went wrong
```

Implements Sorting.

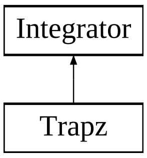
The documentation for this class was generated from the following files:

- src/standardsort.h
- src/standardsort.cc

7.28 Trapz Class Reference

Calculates integral using the trapezoidal method.

`#include <trapz.h>`Inheritance diagram for Trapz::



Public Member Functions

- Trapz ()

  Constructor.

- ~Trapz ()

  Destructor.

- double integrate (const double ∗integrand, const double ∗Z, const int ZPoints)

  Main function that integrates a given data set using Trapezoidal Rule.

7.28.1 Detailed Description

Calculates integral using the trapezoidal method. Trapz takes in an array (the integrand) and returns the integral of that array using the trapezoidal method.

7.28.2 Member Function Documentation

7.28.2.1 double Trapz::integrate (const double ∗ *integrand*, const double ∗ *Z*, const int *ZPoints*) `[virtual]`

Main function that integrates a given data set using Trapezoidal Rule. Trapezoidal rule is applied to integrate a given integrand over a given double array, Z.

```
INPUTS:

const double *integrand          array that contains function values to be integrated

const double *Z                  array that contains the mixture fraction values which the integrand wil

const int ZPoints                number of values, size of the integrand and Z containers


OUTPUT:

double                           result of the integration
```

Implements Integrator.

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

- src/trapz.h
- src/trapz.cc

Chapter 8

File Documentation

8.1 src/convolute.cc File Reference

```
#include "convolute.h"
#include "math.h"
```

Functions

- int convVal (double ∗Z, double ∗data, Matrix3D ∗pdfValues, Matrix ∗postConvVal, Integrator ∗intgr)

  Convolution function.

8.1.1 Detailed Description

8.1.2 Function Documentation

8.1.2.1 int convVal (double ∗ *Z*, double ∗ *data*, Matrix3D ∗ *pdfValues*, Matrix ∗ *postConvVal*, Integrator ∗ *intgr*)

Convolution function. Convolutes date and pdf.

8.2 src/fittogrid.cc File Reference

```
#include "fittogrid.h"
```

Functions

- int fittogrid (const Matrix4D ∗datain, const double ∗cgrid, Interpolator ∗interp, Matrix3D ∗dataout, int nthreads, int ex)

  Function which fits data to a grid.

8.2.1 Detailed Description

8.2.2 Function Documentation

8.2.2.1 int fittogrid (const Matrix4D ∗ *datain*, const double ∗ *cgrid*, Interpolator ∗ *interp*, Matrix3D ∗ *dataout*, int *nthreads*, int *ex*)

Function which fits data to a grid. This function takes in a 4D matrix and fits the data onto a specified grid.

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 INPUTS:

 Matrix4D *datain       input data stored as a 4D matrix. The structure is (mean, z~, z_v, file), where
                        mean has dimension 2 and contains w~ and c~. datain can be thought of as two 3D
                        matrices with structure (z~, z_v, file) containing values of w~ and c~,
                        respectively.

 const double *cgrid    pointer to an array which contains the values of c~ at which to interpolate

 Interpolator *interp   pointer to an Interpolator object

 Matrix3D *dataout      output data stored as a 3D matrix. The structure is (z~, z_v, cgrid), with the
                        numbers being interpolated values of w~

 int numthreads         integer specifying the number of threads to be used (1 = serial, >1 = parallel)

 int ex                 integer specifying whether or not to extrapolate (0 = no, 1 = yes)


 OUTPUTS:

 int                    flag specifying whether or not extrapolation was necessary:
                        = 0: no extrapolation
= 1: extrapolation performed
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