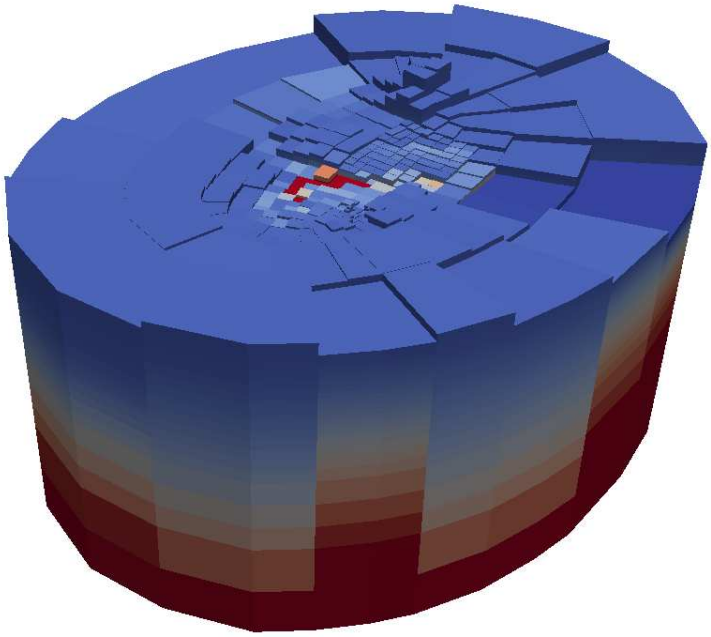
PyTOUGH user's guide



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Introduction

1.1 What is PyTOUGH?

PyTOUGH (**Py**thon **TOUGH**) is a set of Python software routines for making it easier to use the TOUGH2 geothermal reservoir simulator. Using PyTOUGH, it is possible to automate the creation and editing of TOUGH2 model grids and data files, and the analysis and display of model simulation results.

1.2 What are TOUGH2 and AUTOUGH2?

TOUGH2 (Pruess et al., 1999) is a general-purpose simulator for modelling subsurface fluid and heat flow, often used for simulating geothermal reservoirs.

AUTOUGH2 is the University of Auckland version of TOUGH2. The main differences between AUTOUGH2 and TOUGH2 are:

- **EOS handling**: AUTOUGH2 includes all different equations of state (EOSes) in a single executable program, whereas TOUGH2 uses different executables for each EOS. As a result, the main input data file for an AUTOUGH2 simulation also includes extra data blocks to specify which EOS is to be used.
- **Generator types**: AUTOUGH2 includes a variety of extra generator types developed for geothermal reservoir simulation (e.g. makeup and reinjection wells).

TOUGH2_MP (Zhang et al., 2008) is a multi-processor version of TOUGH2. TOUGH+ is a redeveloped version of TOUGH2, with a more modular code structure implemented in Fortran-95.

1.2.1 TOUGH2 data files

TOUGH2 takes its main input from a **data file**, which contains information about the model grid, simulation parameters, time stepping, sources of heat and mass etc. The data file formats for TOUGH2 and AUTOUGH2 are almost identical, with minor differences. TOUGH2_MP can read TOUGH2 data files, but also supports some extensions (e.g. for 8-character instead of 5-character block names) to this format. PyTOUGH does not currently support the TOUGH2_MP extensions. TOUGH+ data files can also have some extensions, which PyTOUGH does not support as yet.

Because TOUGH2 uses a finite volume formulation, the only model grid data it needs are the volumes of the grid blocks and the distances and areas associated with the connections between blocks. Hence, the TOUGH2 data file need not contain any information about the specific locations of the blocks in space, and it contains no information about the locations of the vertices or edges of the blocks. This makes it easy to use TOUGH2 to simulate one-, two- or three-dimensional models, all with the same format of data file. However, this lack of reference to any coordinate system also makes it more difficult to generate model grids, and to visualise simulation results in space.

1.2.2 MULgraph geometry files

For this reason, a separate **geometry file** can be used to create grids for TOUGH2 simulations and visualise simulation results. The geometry file contains information about the locations of the grid block vertices. The geometry file can be used to visualise results using the **MULgraph** graphical post-processor for TOUGH2 and AUTOUGH2 (O'Sullivan and Bullivant, 1995), developed at the University of Auckland in the 1990s.

The MULgraph geometry file assumes the grid has a layered structure, with blocks arranged in layers and columns, and the same arrangement of columns on each layer. (At the top of the model grid, blocks in some columns may be missing, to allow the grid to follow the surface topography.)

If you do not have a MULgraph geometry file for your model, it is easy to create one for a rectangular grid. In fact, PyTOUGH is able to reverse-engineer a MULgraph geometry from a TOUGH2 data file containing a rectangular grid.

A specification of the MULgraph geometry file format can be found in Appendix A.

1.2.3 TOUGH2 listing files

The output from TOUGH2 is written to a **listing file**, which is a text file containing tables of results for each time step (or only selected time steps, if preferred). At each time step there is an 'element table', containing results for block properties (e.g. pressure, temperature etc.). There may also be a 'connection table', containing results for flows between blocks, and a 'generation table', containing results (e.g. flow rates) at the generators in the model (e.g. wells).

The formats of the listing files produced by TOUGH2, AUTOUGH2, TOUGH2_MP and TOUGH+ are all slightly different, and also vary depending on the EOS used. However, PyTOUGH attempts to detect and read all of these formats.

1.3 What is Python?

Python is a general-purpose programming language. It is free and open-source, and runs on many different computer operating systems (Linux, Windows, Mac OS X and others). Python can be downloaded from the Python website (`http://www.python.org`), which also contains detailed reference material about the Python language. If you are using Linux you probably already have Python, as it is included in most Linux distributions.

PyTOUGH should run on any version of Python 2.x newer than 2.4 (though version 2.6 or newer is recommended). PyTOUGH version 1.5 or later should also run on Python 3.x.

If you are unfamiliar with Python (even if you have used another programming language before), it is highly recommended that you do one of the many Python tutorials available online, e.g.

- http://docs.python.org/tutorial/
- http://wiki.python.org/moin/BeginnersGuide

1.3.1 Python basics

Objects

Python is what is known as an **object-oriented** language, which means that it is possible to create special customised data types, or 'classes', to encapsulate all the properties and behaviour of the things (objects) we are dealing with in a program. This is a very useful way of simplifying complex programs. (In fact, in Python, everything is treated as an object, even simple things like integers and strings.)

For example, in a TOUGH2 model grid we have collections of grid blocks, and we need to store the names of these blocks and their volumes and rock types. In a non-object-oriented language, these could be stored in three separate arrays: a string array for the names, a real (or 'float') array for the volumes and another string array for the rock types. In an object-oriented language like Python, we can define a new data type (or 'class') for blocks, which holds the name, volume and rock type of the block. If we declare an object called `blk` of this block class, we can access or edit its volume by referring to `blk.volume`. In this way, we can store our blocks in one single array of block objects. When we add or delete blocks from our grid, we can just add or delete block objects from the array, rather than having to keep track of three separate arrays.

In general, an object not only has **properties** (like `blk.volume`) but also **methods**, which are functions the object can carry out. For example, if we wanted to rotate a MULgraph geometry file by 30°, we could do this in PyTOUGH by declaring a MULgraph geometry file object called `geo`, and calling its `rotate` method: `geo.rotate(30)`. The methods of an object are accessed in the same way that its properties are accessed: by adding a dot (.) after the object's name and then adding the name of the property or method. Any arguments of the method (e.g. the angle in the `rotate` function above) are added in parentheses afterwards.

Lists, dictionaries, tuples and sets

Most programming languages have simple data types built in, e.g. float, double precision or integer numbers, strings, and arrays of these. Python has some other data types which are very useful and are used a lot.

The first of these is the **list**. A list can contain any ordered collection of objects, of any type, or even of different types, and is delimited by square brackets. So for example we can declare a list `things = [1, 'two',3.0]` containing an integer, a string and a float. We can access the list's elements in much the same way as we access the elements of an array, for example `things[1]` would return the value `'two'` (note that in Python, as in most other languages besides Fortran, the indices of arrays and lists start at 0, not 1). Additional elements can be added to a list at any time, without having to re-declare the size of the list: for example, `things.append('IV')` would add an extra element to the end of the list, giving it the value `[1, 'two', 3.0, 'IV']`. It is also possible to remove elements from a list, e.g. `things.remove(3.0)`, which would give our list the value `[1, 'two', 'IV']`.

Another useful Python data type is the **dictionary**. Dictionaries are mainly used to store collections of objects (again, of any type or of different types) that are referenced by

name rather than by index (as in an array or list). A dictionary is delimited by curly brackets. So for example we can declare a dictionary `phone = {'Eric':8155, 'Fred':2350, 'Wilma':4667}` and then find Fred's phone number from `phone['Fred']`, which would return `2350`. For TOUGH2 models, blocks, generators, rock types and other objects are often referred to by name rather than index, so dictionaries are an appropriate way to store them.

A third Python data type, similar to a list, is the **tuple**. A tuple is essentially a list that cannot be changed, and is often used just for grouping objects together. A tuple is delimited by parentheses. For example, `things = (1, 'two', 3.0)` declares a tuple with three elements. We can still refer to the elements of a tuple using e.g. `a[1]`, but we cannot assign new values to these elements or add or remove elements from the tuple once it has been declared.

Python also has a **set** data type, which represents a mathematical set - an unordered collection of objects. One of the useful aspects of sets is that they cannot contain duplicate items. As a result, for example, duplicate items can be removed from a list `x` simply by converting it to a set, and then back to a list: `x = list(set(x))`.

1.3.2 How to run Python

Python can be run either interactively or via scripts.

Running Python interactively

The simplest way to run Python interactively is just by typing `python` at the command line. (On Windows the directory that Python was installed into may have to be added to your `PATH` environment variable first.) The command line then becomes an interactive Python environment in which you can type Python commands at the Python command prompt `>>>`, e.g. in Windows:

```
C:\>python
Python 2.6.4 (r264:75708, Oct 26 2009, 08:23:19) [MSC v.1500 32 bit (Intel)]
on win32
Type "help", "copyright", "credits" or "license" for more information.
>>> things = [1, 'two', 3.0]
>>> print things[1]
two
>>> exit()

C:\>
```

In the interactive Python environment, you can view help on the properties and methods of any Python object by typing `help(`*`objectname`*`)`, where *`objectname`* is the name of an object that has been declared. This will list the properties and methods of the object and a description of each one.

You can exit the interactive Python environment by typing `exit()` or `Ctrl-Z` on Windows, or `Ctrl-D` on Linux.

Python scripts

The real power of Python, however, lies in using it to write **scripts** to automate repetitive or complex tasks. You can just type Python commands into a text file, save it with the file

extension `.py`, and execute it by typing `python` *`filename.py`*, where *`filename.py`* is the name of the file. (Once again, on Windows the directory that Python was installed into may have to be added to your `PATH` environment variable first.)

You can also debug a Python script using the 'pdb' command-line debugger. Typing `python -m pdb` *`filename.py`* will start debugging the script *filename.py*.

It is also possible to run a Python script from within the interactive Python environment. From the Python environment command line, typing `execfile('`*`filename.py`*`')` will execute the script *filename.py*.

1.3.3 Python libraries

Python comes with a large number of features already built in, but for specialised tasks, additional **libraries** of Python software can be imported into Python as you need them. PyTOUGH itself is a set of such libraries, and it in turn makes use of some other third-party Python libraries.

Numerical Python

The most important of these is Numerical Python ('numpy'), which you will need to have installed on your computer before you can use PyTOUGH at all [1]. Numerical Python adds a special `numpy.array` class for fast multi-dimensional arrays, which PyTOUGH makes heavy use of, and a whole range of other features, e.g. linear algebra routines, Fourier transforms and statistics.

Other libraries

Some parts of PyTOUGH use other Python libraries. You do not need these libraries unless you are using the parts of PyTOUGH that depend on them.

- **Scientific Python** (`http://www.scipy.org/`), a library of advanced mathematical functions (e.g. interpolation, calculus, optimisation)
- **matplotlib** (`http://matplotlib.sourceforge.net/`), a library of graphical plotting routines
- **VTK**, a Python interface to the Visualization Tool Kit (`http://www.vtk.org/`), a library for 3D visualisation of data via VTK itself, or software such as ParaView, Mayavi etc.

1.3.4 Installing third-party Python libraries

Linux

On Linux you can install third-party Python libraries via your package manager, e.g. on Debian or Debian-based distributions like Ubuntu:

```
apt-get install python-numpy python-scipy python-matplotlib python-vtk
```

[1] PyTOUGH will run using Numeric, a now-obsolete predecessor of Numerical Python, though the PyTOUGH plotting functions will not work. In general it is recommended to use Numerical Python if possible.

MS Windows

On MS Windows systems, the easiest way to install these libraries is by using the **pip** tool. This is a Python package management tool which allows the user to install Python packages and also manages dependencies (when one package depends on other packages).

If you have Python version 2.7.9 or a more recent one then you should have pip already available on your system. If not, the best thing is probably to upgrade to a newer version of Python. If that is not possible for some reason, you can install pip separately by following the instructions at https://pip.pypa.io/en/stable/installing/.

It is recommended to download libraries to use with PyTOUGH (as *.whl files) from Christoph Gohlke's Python package site:

http://www.lfd.uci.edu/~gohlke/pythonlibs/

Here you can find Windows Python packages for numpy, scipy, matplotlib and VTK (and lots of others as well). Be sure to choose the version of each package appropriate for your version of Python. For example, if you are using 64-bit Python 2.7, then choose *.whl files with names including "cp27", and "amd64".

Once you have downloaded them, you can install them by opening a command prompt in the download directory and typing `pip install` followed by the exact name of the *.whl file.

Importing libraries

To use any Python library, you just need to **import** it first. For example, once you have installed Numerical Python, you can make it available (in the interactive Python environment or in a Python script) by typing the command `import numpy`, or alternatively `from numpy import *`. This imports all classes and commands from Numerical Python and makes them available for use. (You can also import only parts of a library rather than the whole thing, e.g. `from numpy import linalg` just imports the linear algebra routines from Numerical Python.)

When you import a library, you can also change its name. For example, PyTOUGH imports Numerical Python using the command `import numpy as np`, which renames `numpy` as the abbreviated `np`. This means it can, for example, access the Numerical Python `numpy.array` data type as `np.array`. It also means you have access to Numerical Python as `np` in your own scripts and in the interactive Python environment, without having to import it yourself.

1.4 Installing and accessing PyTOUGH

The latest version of PyTOUGH can always be downloaded from the PyTOUGH website:

https://github.com/acroucher/PyTOUGH/

First, make sure you have Python, and the Numerical Python library (see section 1.3.3) installed. On Windows, you may have to add the directory where Python has installed (e.g. `C:\Python27` or similar, depending on which version you have) to your PATH environment variable, before you can access Python from the command line.

On the PyTOUGH website, click the 'Download ZIP' button at the right of the page:

https://github.com/acroucher/PyTOUGH/archive/master.zip

to download PyTOUGH as a .zip file. Unzip this to any directory on your computer. This will create a directory containing a file called `setup.py`.

To install PyTOUGH, you will need administrator ('root' on Linux) privileges on your computer. As administrator, open a command prompt, navigate to this new directory and type:

```
python setup.py install
```

You should now be able to import the PyTOUGH libraries into the Python interactive environment or your Python scripts, from any directory on your computer. For example, you can import the MULgraph geometry library using `from mulgrids import *` (see chapter 2).

1.5 Testing PyTOUGH

PyTOUGH includes a suite of "unit tests" which can be used to verify that it is working correctly. These are located in the `tests/` directory, which includes a number of Python scripts for testing individual PyTOUGH modules.

These unit test modules may be run individually, the same way as any other Python script would be run. If the tests in the script all pass, the last message printed out to the console will read `OK`. If not, details will be output regarding which tests did not pass.

It is also possible to run the unit tests for all modules by running the following command in the `tests/` directory:

```
python -m unittest discover
```

or with the `-v` (verbose) flag to output more detail on which tests are being run:

```
python -m unittest discover -v
```

1.6 Licensing

PyTOUGH is free software, distributed under the GNU Lesser General Public License (LGPL). For more information, see http://www.gnu.org/licenses/.

Chapter 2

MULgraph geometry files

2.1 Introduction

The `mulgrids` library in PyTOUGH contains classes and routines for creating, editing and saving MULgraph geometry files. It can be imported using the command:

```
from mulgrids import *
```

2.2 `mulgrid` objects

The `mulgrids` library defines a `mulgrid` class, used for representing MULgraph geometry files.

Example:

```
geo = mulgrid()
```

creates an empty `mulgrid` object called `geo`.

```
geo = mulgrid('geom.dat')
```

creates a `mulgrid` object called `geo` and reads its contents from a file named `'geom.dat'`.

Printing a `mulgrid` object (e.g. `print geo`) displays a summary of information about the grid: how many nodes, columns, layers, blocks and wells it contains, as well as its naming convention and atmosphere type.

A specification of the MULgraph geometry file format can be found in Appendix A.

2.2.1 Properties

The main properties of a `mulgrid` object are listed in Table 2.1. Some of these properties are 'header' information, corresponding to the data at the start of a MULgraph geometry file (`type`, `convention`, `atmosphere_type`, `atmosphere_volume`, `atmosphere_connection` and `unit_type`).

The most important properties of a `mulgrid` object are `node`, `column`, `connection`, `layer` and `well`, which are dictionaries of the grid nodes, columns, connections, layers and wells, accessed by name. For example, grid layer 'AA' of a `mulgrid` object `geo` can be accessed by `geo.layer['AA']`. (The `nodelist`, `columnlist`, `connectionlist`, `layerlist`

and `welllist` properties offer access to the nodes, columns, connections, layers and wells by index, which is sometimes useful e.g. for looping over all columns in the grid.)

Connections are slightly different from nodes, columns etc. in that they are not named individually. However, they can be accessed by the names of the columns connected by the connection. For example, the connection between columns ' 10' and ' 11' in a `mulgrid` called `geo` is given by `geo.connection[' 10',' 11']`.

The elements of these lists and dictionaries are of type `node`, `column`, `connection`, `layer` and `well` respectively. These are additional object classes to represent nodes, columns, connections, layers and wells, defined in the `mulgrids` library (see section 2.3).

Grid diagnostics

A `mulgrid` object has some properties (and methods) for evaluating its integrity. The property `column_angle_ratio` returns an `np.array` of the 'angle ratio' for each column (the ratio of largest to smallest interior angles - see section 2.3.2), a measure of skewness. The `column_side_ratio` returns an `np.array` of the 'side ratio' for each column (the ratio of largest to smallest side length), a measure of elongation. These array properties can be plotted using the `layer_plot` method (see section 2.2.2) for a graphical overview of grid quality.

There is also a `connection_angle_cosine` property, which returns an `np.array` of the angle cosine for each connection (the cosine of the angle between a line joining the nodes in the connection and a line joining the centres of the blocks in the connection). In general it is desirable for these lines to be as close to perpendicular as possible, making the cosines close to zero.

The `bad_columns`, `bad_layers`, `missing_connections`, `extra_connections` and `orphans` properties return actual problems with the grid which should be fixed. A summary of all these problems is given by the `check` method (see section 2.2.2).

Blocks at the ground surface that have very small vertical thickness can sometimes cause problems. The `min_surface_block_thickness` property gives a tuple containing the minimum surface block thickness and the name of the column in which it occurs. Thin surface blocks of this type can be eliminated using the `snap_columns_to_layers()` method.

Functions for reading data from file

A `mulgrid` object has a `read_function` property which controls how data are read from file. This property is a dictionary with six keys: 'd', 'f', 'e', 'g', 's' and 'x', denoting respectively integer, float, exponential, general, string and blank. Each item in the dictionary is a function which converts a string from the file on disk into the appropriate value. For example, `read_function['f']` converts a string to a floating point value. By default, the built-in Python `float` function is used for this (although it is modified slightly so that it returns `None` if the input string is blank). There is a dictionary of default reading functions included in PyTOUGH, called `default_read_function`.

However, the user can specify other functions if needed. In particular, files produced from Fortran programs sometimes have formatting that is not readable by the default functions, if some more exotic Fortran formatting options have been used. For example, a 'd' can also be used to represent an exponent (like 'e'), or spaces can be included within a number, or the exponent identifier (e.g. 'e') can be omitted. PyTOUGH includes a second set of reading functions, called `fortran_read_function`, for handling Fortran formatting. These are slightly slower than the default reading functions.

The reading functions for a `mulgrid` object can be specified when the object is being created, e.g.:

```
geo = mulgrid('geom.dat', read_function = fortran_read_function)
```

Block ordering schemes

By default, the blocks in a TOUGH2 grid created from a `mulgrid` geometry are ordered by layer, from the atmosphere down to the bottom of the model, with the blocks within each layer ordered by column (following the ordering of the `columnlist` property, which is the same as the column order specified in the geometry file).

It is also possible to sort the blocks according to their geometrical type (8-node hexahedrons and 6-node wedges, corresponding to 4-node or 3-node columns respectively). This is useful for exporting the model to Waiwera, which uses the PETSc DMPlex mesh representation, which sorts cells by cell type in this way.

This can be done by setting the `block_order` property of the geometry. This can be set when the `mulgrid` object is created or read from file, as an optional parameter, e.g.:

```
geo = mulgrid('geom.dat', block_order = 'dmplex')
```

It can also be specified after creation. The `block_order` property is a string which can take the value **'layer_column'** for layer/column block ordering, or **'dmplex'** if the blocks are to be sorted by geometrical type. It can also take the value `None` which gives the default layer/column ordering.

```
geo.block_order = 'layer_column'
```

The block ordering scheme can be stored in the MULgraph geometry file, via an integer flag in the header (see Appendix A). This flag is an extension to the original MULgraph geometry file format. If a `mulgrid` object is created by reading a file in which this flag is not present, its `block_order` property will be `None`, in which case the default layer/column ordering will be used. When a geometry file is read in, and a block ordering is specified via the `block_order` parameter, this will override any block ordering stored in the file.

Tilted geometries

Non-horizontal (i.e. tilted) geometries can be constructed by setting the `mulgrid` properties `gdcx` and `gdcy` non-zero. These properties represent the cosines of the angles the x- and y-axes make with the gravity vector. By default they are both zero, giving a horizontal grid. A geometry with `gdcx` = 1 can be used to construct a 2-D vertical slice grid with a non-layered structure. When a `t2grid` object is created from a tilted geometry, e.g. using the `t2grid` fromgeo() method, only the gravity cosines of the connections are affected (the `dircos` property of each connection).

Rotating permeability directions

It is possible to rotate the permeability principal directions of a `mulgrid` object with respect to the coordinate axes- for example, to align permeabilities with a dominant fault direction- by specifying the `permeability_angle` property. When a `t2grid` object is created, e.g. using the `t2grid` fromgeo() method, this can change the `direction` property of each connection.

Conversion to Layermesh

A `mulgrid` geometry may be converted to a Layermesh (https://github.com/acroucher/layermesh) mesh simply by accessing its `layermesh` property. Layermesh is a dedicated library for general layer/column meshes. Its mesh objects have capabilities similar to those of a `mulgrid` object, but it has advantages such as higher efficiency and a simpler interface. The Layermesh library must be installed before this property can be used.

Example:

```
geo = mulgrid('gmymesh.dat')
m = geo.layermesh # m is a Layermesh mesh object
```

Property	Type	Description
`area`	float	total horizontal area covered by the grid
`atmosphere_connection`	float	connection distance to atmosphere blocks
`atmosphere_type`	integer	type of atmosphere
`atmosphere_volume`	float	volume of atmosphere blocks
`bad_columns`	set	columns that do not contain their own centres
`bad_layers`	set	layers that do not contain their own centres
`block_connection_name_index`	dictionary	indices of block connections (by name)
`block_connection_name_list`	list	names of block connections (by index)
`block_name_index`	dictionary	indices of blocks (by name)
`block_name_list`	list	names of blocks (by index)
`block_order`	string	block ordering scheme
`boundary_columns`	set	set of columns on the outer boundary of the grid
`boundary_nodes`	list	ordered list of nodes on the outer boundary of the grid
`boundary_polygon`	list	list of points representing grid boundary (extra colinear points removed)
`bounds`	list	[bottom left, top right] horizontal bounds of grid
`centre`	`np.array`	position of horizontal centre of the grid
`columnlist`	list	columns (by index, e.g. `columnlist[23]`)
`column_angle_ratio`	`np.array`	angle ratio for each column
`column_side_ratio`	`np.array`	side ratio for each column
`column`	dictionary	columns (by name, e.g. `column['AA']`)
`connectionlist`	list	connections between columns (by index)
`connection_angle_cosine`	`np.array`	angle cosines for all connections
`convention`	integer	naming convention for columns and layers
`default_surface`	Boolean	`True` if all columns have default surface elevation
`extra_connections`	set	connections defined between columns that are not against each other
`filename`	string	file name on disk
`gdcx`, `gdcy`	float	cosines of angles x- and y-axes make with gravity vector
`node_kdtree`	`cKDTree`	tree structure for fast searching for nodes
`layerlist`	list	layers (by index)
`layermesh`	`layermesh` mesh	Layermesh library mesh object
`layer`	dictionary	layers (by name)

min_surface_block_thickness	(float, string)	thickness of thinnest surface block (and associated column name)
missing_connections	set	missing connections between columns
nodelist	list	nodes (by index)
node	dictionary	nodes (by name)
num_atmosphere_blocks	integer	number of atmosphere blocks
num_blocks	integer	total number of blocks in the grid
num_block_connections	integer	total number of block connections in the grid
num_columns	integer	number of columns
num_connections	integer	number of connections between columns
num_layers	integer	number of layers
num_nodes	integer	number of nodes
num_underground_blocks	integer	number of non-atmosphere blocks
num_wells	integer	number of wells
orphans	set	orphaned nodes (nodes not belonging to any column)
permeability_angle	float	rotation angle (degrees anticlockwise) of first horizontal permeability direction
read_function	dictionary	dictionary of functions used to read data from file
type	string	type of geometry (currently only 'GENER' supported)
unit_type	string	distance unit (blank for metres, 'FEET' for ft)
welllist	list	wells (by index)
well	dictionary	wells (by name)

Table 2.1: Properties of a `mulgrid` object

2.2.2 Methods

The main methods of a `mulgrid` object are listed in Table 2.2. Details of these methods are given below.

Method	Type	Description
add_column	–	adds a column to the grid
add_connection	–	adds a connection to the grid
add_layer	–	adds a layer to the grid
add_node	–	adds a node to the grid
add_well	–	adds a well to the grid
block_centre	np.array	block centre
block_contains_point	Boolean	whether a block contains a 3D point
block_mapping	dictionary	mapping from the blocks of another `mulgrid` object
block_name	string	name of block at given layer and column
block_name_containing_point	string	name of block containing specified point
block_surface	float	block top elevation
block_volume	float	block volume

check	Boolean	checks grid for errors (and optionally fixes them)
column_boundary_nodes	list	nodes around the outer boundary of a group of columns
column_bounds	list	bounding rectangle around a list of columns
column_containing_point	column	column containing specified horizontal point
column_mapping	dictionary	mapping from the columns of another `mulgrid` object
column_name	string	column name of a block name
column_neighbour_groups	list	groups connected columns
column_quadtree	quadtree	quadtree structure for searching columns
column_surface_layer	layer	surface layer for a specified column
column_values	tuple	values of a variable down a column
columns_in_polygon	list	columns inside a specified polygon (or rectangle)
connects	Boolean	whether the grid has a connection between two specified columns
copy_layers_from	–	copies layer structure from another geometry
copy_wells_from	–	copies wells from another geometry
decompose_columns	–	decomposes columns into triangles and quadrilaterals
delete_column	–	deletes a column from the grid
delete_connection	–	deletes a connection from the grid
delete_layer	–	deletes a layer from the grid
delete_node	–	deletes a node from the grid
delete_orphans	–	deletes any orphaned nodes from the grid
delete_orphan_wells	–	deletes any orphaned wells from the grid
delete_well	–	deletes a well from the grid
empty	–	empties contents of grid
export_surfer	–	exports to various files on disk for visualization in Surfer
fit_columns	`np.array` or dictionary	fits scattered data to column centres
fit_surface	–	fits column surface elevations from data
from_amesh	(mulgrid, dict)	creates Voronoi geometry from AMESH grid
from_gmsh	mulgrid	creates geometry from a `gmsh` grid
layer_containing_elevation	layer	layer containing specified vertical elevation
layer_mapping	dictionary	mapping from the layers of another `mulgrid` object
layer_name	string	layer name of a block name
layer_plot	–	plots a variable over a layer of the grid
line_plot	–	plots a variable along an arbitrary line through the grid
line_values	tuple	values of a variable along an arbitrary line through the grid
meshio_grid	tuple	mesh in `meshio` format
minc_array	array	values for a particular level in a MINC grid
nodes_in_columns	list	nodes in a specified list of columns
nodes_in_polygon	list	nodes inside a specified polygon (or rectangle)
node_nearest_to	node	node nearest to a specified point

optimize	–	adjusts node positions to optimize grid quality
polyline_values	tuple	values of a variable along an arbitrary polyline through the grid
read	mulgrid	reads geometry file from disk
rectangular	mulgrid	creates rectangular grid
reduce	–	reduces a grid to contain only specified columns
refine	–	refines specified columns in the grid
refine_layers	–	refines specified layers in the grid
rename_column	Boolean	renames a column
rename_layer	Boolean	renames a layer
rotate	–	rotates a grid in the horizontal plane
slice_plot	–	plots a variable over a vertical slice through the grid
snap_columns_to_layers	–	snaps column surfaces to layer bottoms
snap_columns_to_nearest_layers	–	snaps column surfaces to nearest layer elevations
split_column	Boolean	splits a quadrilateral column into two triangles
translate	–	moves a grid by simple translation in 3D
well_values	tuple	values of a variable down a well
write	–	writes to geometry file on disk
write_bna	–	writes to Atlas BNA file on disk
write_exodusii	–	writes to ExodusII file on disk
write_mesh	–	writes to mesh file (various formats) on disk
write_vtk	–	writes to VTK file on disk

Table 2.2: Methods of a `mulgrid` object

`add_column(col)`

Adds a `column` object `col` to the grid. If a column with the same name already exists, no new column is added.

`add_connection(con)`

Adds a `connection` object `con` to the grid. If a connection with the same name already exists, no new connection is added.

`add_layer(lay)`

Adds a `layer` object `lay` to the grid. If a layer with the same name already exists, no new layer is added.

`add_node(n)`

Adds a `node` object `n` to the grid. If a node with the same name already exists, no new node is added.

`add_well(w)`

Adds a `well` object `w` to the grid. If a well with the same name already exists, no new well is added.

`block_contains_point(blockname, pos)`

Returns `True` if the grid block with the given name contains the 3D point `pos`.

Parameters:

- **blockname**: string
  The name of the block.
- **pos**: `np.array`
  3-element array representing the 3D point.

`block_centre(lay, col)`

Returns the centre of the block corresponding to the given layer and column.

The horizontal centre is given by the column centre. The vertical centre is given by the layer centre, except for surface blocks with column surface lower than the layer top, in which case it is the midpoint between the column surface and the layer bottom. (For surface blocks with column surface higher than the layer top, the vertical centre is still the layer centre, to give a uniform pressure reference.)

Parameters:

- **lay**: `layer` or string
  The specified layer or layer name.
- **col**: `column` or string
  The specified column or column name.

`block_mapping(geo, column_mapping=False)`

Returns a dictionary mapping each block name in the `mulgrid` object `geo` to the name of the nearest block in the object's own geometry. Can optionally also return the associated column mapping.

Parameters:

- **geo**: `mulgrid`
  The `mulgrid` object to create a block mapping from.
- **column_mapping**: Boolean
  If `True`, the column mapping will also be returned (i.e. the function will return a tuple containing the block mapping and the column mapping). Default value is `False`.

`block_name(layer_name, column_name, blockmap = {})`

Gives the name of the block corresponding to the specified layer and column names, according to the naming convention of the grid.

An optional block name mapping can be applied.

Parameters:

- **layer_name**, **column_name**: string
  Name of layer and column (the widths of these strings are determined by the grid's naming convention).

- **blockmap**: dictionary
  Dictionary mapping the block names in the geometry to another block naming system. This dictionary need not contain entries for all blocks in the geometry- those not included in the mapping will not be altered.

`block_name_containing_point(pos, qtree=None, blockmap={})`

Gives the name of the block containing a specified 3-D position in the grid (returns `None` if the point lies outside the grid).

Parameters:

- **pos**: `np.array`
  Position of point in 3-D
- **qtree**: `quadtree`
  Quadtree object for fast searching of grid columns (can be constructed using the `column_quadtree()` method).
- **blockmap**: dictionary
  Dictionary mapping the block names in the geometry to another block naming system.

`block_surface(lay, col)`

Returns the elevation of the top surface of the block corresponding to the given layer and column.

Parameters:

- **lay**: `layer`
  The specified layer.
- **col**: `column`
  The specified column.

`block_volume(lay, col)`

Returns the volume of the block corresponding to the given layer and column.

Parameters:

- **lay**: `layer`
  The specified layer.
- **col**: `column`
  The specified column.

`check(fix=False,silent=False)`

Checks a grid for errors and optionally fixes them. Errors checked for are: missing connections, extra connections, orphaned nodes, and columns and layers that do not contain their own centres. Returns `True` if no errors were found, and `False` otherwise. If `fix` is `True`, any identified problems will be fixed. If `silent` is `True`, there is no printout (only really useful if `fix` is `True`).

Parameters:

- **fix**: Boolean
  Whether to fix any problems identified.

- **silent**: Boolean
  Whether to print out feedback or not.

`column_boundary_nodes(columns)`

Returns the nodes around the outer boundary of a list of columns. The list is ordered, in a counter-clockwise direction.

Parameters:

- **columns**: list
  The list of columns for which the boundary is required.

`column_bounds(columns)`

Returns a bounding rectangle around a list of columns.

Parameters:

- **columns**: list
  The list of columns for which the bounds are required.

`column_containing_point(pos, columns=None, guess=None, bounds=None, qtree=None)`

Returns the grid column containing the specified horizontal point. If `columns` is specified, only columns in the given list will be searched. An initial `guess` column can optionally be specified. If `bounds` is specified, points outside the given polygon will always return `None`. A quadtree structure can also be specified to speed up searching.

Parameters:

- **pos**: `np.array`
  Horizontal position (x, y)

- **columns**: list of `column` (or `None`)
  List of columns to search. If `None`, the entire grid will be searched.

- **guess**: `column` (or `None`)
  Guess of required column. If specified, this column will be tested first, followed (if necessary) by its neighbours; only if none of these contain the point will the remaining columns be searched. This can speed up the process if data follow a sequential pattern in space, e.g. a grid or lines.

- **bounds**: list of `np.array` (or `None`)
  Polygon or rectangle representing e.g. the boundary of the grid: points outside this polygon will always return `None`. If the polygon has only two points, it will be interpreted as a rectangle [bottom left, top right].

- **qtree**: `quadtree`
  A quadtree object for searching the columns of the grid. If many points are to be located, this option can speed up the search. The quadtree can be constructed before searching using the `column_quadtree()` method.

`column_mapping(geo)`

Returns a dictionary mapping each column name in the `mulgrid` object `geo` to the name of the nearest column in the object's own geometry. If the SciPy library is available, a KDTree structure is used to speed searching.

Parameters:

- **geo**: `mulgrid`
  The `mulgrid` object to create a column mapping from.

`column_name(block_name)`

Gives the name of the column corresponding to the specified block name, according to the naming convention of the grid.

Parameters:

- **block_name**: string
  Block name.

`column_neighbour_groups(columns)`

From the given list or set of columns, finds sets of columns that are connected together, and returns a list of them.

Parameters:

- **columns**: list or set
  List or set of columns to group.

`column_quadtree(columns=None)`

Returns a quadtree structure for fast searching of grid columns, to find which column a given point lies in. This can then be passed into various other `mulgrid` methods that do such searching, e.g. `block_name_containing_point()` or `well_values()`, to speed them up (useful for large grids).

The quadtree is an instance of a `quadtree` class, defined in the `mulgrids` module.

Parameters:

- **columns**: list (or `None`)
  A list of columns in the grid, specifying the search area. This parameter can be used to further speed searching if it is only necessary to search columns in a defined area. If `None`, the search area is the whole grid (all columns).

`column_surface_layer(col)`

Returns the layer containing the surface elevation of a specified column.

Parameters:

- **col**: `column`
  The column for which the surface layer is to be found.

`column_values(col, variable, depth = False)`

Returns values of a specified variable down a specified column. The variable can be a list or `np.array` containing a value for every block in the grid.

The routine returns a tuple of two arrays (`d`,`v`), the first (`d`) containing the elevation (or depth from surface if the `depth` parameter is set to `True`), and the second (`v`) containing the value of the variable at each block in the column.

Parameters:

- **col**: column or string
  The column for which values are to be found.

- **variable**: list (or np.array)
  Values of variable, of length equal to the number of blocks in the grid.

- **depth**: Boolean
  Set to True to give depths from surface, instead of elevations, as the first returned array.

`columns_in_polygon(polygon)`

Returns a list of all columns with centres inside the specified polygon or rectangle.
Parameters:

- **polygon**: list (of np.array)
  List of points defining the polygon (each point is a two-element np.array). If the list has only two points, it will be interpreted as a rectangle [bottom left, top right].

`connects(column1, column2)`

Returns True if the geometry contains a connection connecting the two specified columns.
Parameters:

- **column1, column2**: column
  Two columns in the geometry.

`copy_layers_from(geo)`

Copies the layer structure from the geometry geo (deleting any existing layers first).
Parameters:

- **geo**: mulgrid
  The geometry to copy layers from.

`copy_wells_from(geo)`

Copies the wells from the geometry geo (deleting any existing wells first).
Parameters:

- **geo**: mulgrid
  The geometry to copy wells from.

`decompose_columns(columns = [], mapping = False, chars = ascii_lowercase)`

Decomposes columns with more than four sides into triangular and quadrilateral columns. This can be useful when carrying out calculations on the geometry that rely on finite element methods (e.g. the fit_columns() method uses it).

In general, columns are decomposed by adding a node at the column centroid and forming triangles around it. However, there are special cases for columns with lower numbers of sides (less than 9) and 'straight' nodes, i.e. nodes on a straight line between their neighbouring nodes in the column). These make use of simpler decompositions.

Parameters:

- **columns**: list
  List of columns to be decomposed. If the list is empty (the default), all columns are decomposed.

- **mapping**: Boolean
  If `True`, return a dictionary mapping each original column name to a list of decomposed columns that replace it.

- **chars**: string
  Specifies a string of characters to use when forming new node and column names. Default is lowercase letters.

`delete_column(`*`colname`*`)`

Deletes the column with the specified name from the grid.
Parameters:
- **colname**: string
  Name of the column to be deleted.

`delete_connection(`*`colnames`*`)`

Deletes the connection between the specified columns from the grid.
Parameters:
- **colnames**: tuple of string
  Tuple of two column names.

`delete_layer(`*`layername`*`)`

Deletes the layer with the specified name from the grid.
Parameters:
- **layername**: string
  Name of the layer to be deleted.

`delete_node(`*`nodename`*`)`

Deletes the node with the specified name from the grid.
Parameters:
- **nodename**: string
  Name of the node to be deleted.

`delete_orphans()`

Deletes any orphaned nodes (those not belonging to any column) from the grid.

`delete_orphan_wells()`

Deletes any orphaned wells (those with wellheads outside the grid).

`delete_well(wellname)`

Deletes the well with the specified name from the grid.
Parameters:
- **layername**: string
  Name of the layer to be deleted.

`empty()`

Empties the grid of all its nodes, columns, layers, wells and connections. Other properties are unaffected.

`export_surfer(filename='', aspect=8.0, left=0.0)`

Exports the grid to files on disk useful for visualization in Surfer. Six files are written out:
- an Atlas BNA file (`filename.bna`) representing the grid columns
- a CSV file (`filename_column_names.csv`) containing the column names
- a Golden Software blanking file (`filename_layers.bln`) file representing the grid layers
- a CSV file (`filename_layer_bottom_elevations.csv`) containing the bottom elevations of the layers
- a CSV file (`filename_layer_centres.csv`) containing the elevations of the centres of the layers
- a CSV file (`filename_layer_names.csv`) containing the names of the layers

Parameters:
- **filename**: string
  Base name for the exported files. If it is not specified, the `filename` property of the `mulgrid` object itself is used (unless this is also blank, in which case a default name is used), with its extension removed.
- **aspect**: float
  Aspect ratio for the layer plot, so that the width is the total height of the grid divided by `aspect` (default 8.0).
- **left**: float
  Coordinate value of the left hand side of the layer plot (default zero).

`fit_columns(data, alpha=0.1, beta=0.1, columns=[], min_columns=[], grid_boundary=False, silent=False, output_dict=False)`

Fits scattered data to column centres, using bilinear least-squares finite element fitting with Sobolev smoothing. Smoothing is useful when data density is low in some areas of the grid, in which case least-squares fitting without smoothing can fail (e.g. if there are any columns which do not contain any data points).

By default, this method returns an `np.array` with length given by the number of columns to be fitted. Each value in the array represents the fitted data value at the centre of the corresponding column. If the `output_dict` parameter is set to `True`, a dictionary is returned, with fitted values indexed by column names.

Parameters:

- **data**: `np.array`
  Two-dimensional array of data to fit. Each row of the array should contain the x,y co-ordinates for each data point, followed by the corresponding data value. Such an array can be conveniently read from a text file using the `np.loadtxt()` method.

- **alpha**: float
  Smoothing parameter for first derivatives - increasing its value results in solutions with lower gradients (but may result in extrema being smoothed out).

- **beta**: float
  Smoothing parameter for second derivatives - increasing its value results in solutions with lower curvature.

- **columns**: list of string or `column`
  Columns, or names of columns to be fitted. If empty (the default), then all columns will be fitted.

- **min_columns**: list of string or `column`
  Columns, or names of columns for which fitted data will be determined from the minimum of the fitted nodal values (fitted values at all other columns are determined from the average of the fitted nodal values).

- **grid_boundary**: Boolean
  If `True`, test each data point first to see if it lies inside the boundary polygon of the grid. This can speed up the fitting process if there are many data points outside the grid, and the grid has a simple boundary (e.g. a rectangle). In general if there are many data points outside the grid, it is best to clip the data set before fitting, particularly if it is to be used more than once.

- **silent**: Boolean
  Set to `True` to suppress printing fitting progress.

- **output_dict**: Boolean
  Set `True` to return results as a dictionary of fitted values indexed by column names, instead of an array.

```
fit_surface(data, alpha=0.1, beta=0.1, columns=[], min_columns=[],
grid_boundary=False, layer_snap=0.0, silent=False)
```

Fits column surface elevations from data, using bilinear least-squares finite element fitting with Sobolev smoothing (using the `fit_columns()` method). Smoothing is useful when data density is low in some areas of the grid, in which case least-squares fitting without smoothing can fail (e.g. if there are any columns which do not contain any data points). Use the `layer_snap` parameter to eliminate surface blocks with very small thickness.

Parameters:

- **data**: `np.array`
  Two-dimensional array of data to fit. Each row of the array should contain the x,y,z

values for each data point. Such an array can be conveniently read from a text file using the `np.loadtxt()` method.

- **alpha**: float
  Smoothing parameter for first derivatives - increasing its value results in solutions with lower gradients (but may result in extrema being smoothed out).

- **beta**: float
  Smoothing parameter for second derivatives - increasing its value results in solutions with lower curvature.

- **columns**: list of string or `column`
  Columns, or names of columns to be fitted. If empty (the default), then all columns will be fitted.

- **min_columns**: list of string or `column`
  Columns, or names of columns for which elevations will be determined from the minimum of the fitted nodal elevations (elevations at all other columns are determined from the average of the fitted nodal elevations).

- **grid_boundary**: Boolean
  If `True`, test each data point first to see if it lies inside the boundary polygon of the grid. This can speed up the fitting process if there are many data points outside the grid, and the grid has a simple boundary (e.g. a rectangle). In general if there are many data points outside the grid, it is best to clip the data set before fitting, particularly if it is to be used more than once.

- **layer_snap**: float
  Smallest desired surface block thickness. Set to a positive value to prevent columns being assigned surface elevations that are very close to the bottom of a layer (resulting in very thin surface blocks). Default value is zero (i.e. no layer snapping).

- **silent**: Boolean
  Set to `True` to suppress printing fitting progress.

```
from_amesh(input_filename='in', segment_filename='segmt', convention=0,
node_tolerance=None, justify='r', chars=ascii_lowercase, spaces=True,
block_order=None)
```

Returns a `mulgrid` object (and a block mapping dictionary) from a Voronoi mesh previously created by the AMESH utility (Haukwa, 1998), or by other software that uses AMESH (e.g. WinGridder or Steinar).

The block naming convention for the output `mulgrid` object can be specified via the `convention` parameter. Note that in general this may not be the same as the block naming convention of the original mesh created by AMESH. In fact, AMESH can create meshes with block naming conventions that do not correspond to any of the MULgraph conventions. This is why the `from_amesh()` method also returns a block mapping dictionary, which maps block names in the `mulgrid` geometry to the block names in the original AMESH grid.

The optional `justify` and `case` parameters control the formatting of the character part of the block names. Additionally, the characters used to form node/column or layer names can be specified using the `chars` parameter. (This can be useful for example for grids

with large numbers of nodes and/or columns, for which lowercase letters alone may not be enough.)

The `from_amesh()` method assumes the original AMESH grid has layers of constant thickness (i.e. all blocks in each layer of the AMESH input file have the same specified thickness). Grids with layers of non-constant thickness cannot be represented by a `mulgrid` object and will cause an exception to be raised.

Parameters:

- **input_filename**: string
  Filename for AMESH input file. Default is 'in'.
- **segment_filename**: string
  Filename for AMESH output segment file. Default is 'segmt'.
- **convention**: integer
  Naming convention for grid columns and layers.
- **node_tolerance**: float or `None`
  Horizontal tolerance for identifying distinct nodes in the segment file. If a node is read in with horizontal distance from an existing node less than the tolerance, then the two nodes are assumed to be identical. If `None` (the default), then the tolerance is set to 90% of the smallest segment length. If errors are encountered in identifying nodes belonging to the grid columns, it may be worth adjusting this parameter.
- **justify**: string
  Specify 'r' for the character part of the block names (first three characters) to be right-justified, 'l' for left-justified.
- **chars**: string
  Specify a string of characters to be used to form the character part of block names. For example, to use both lowercase and uppercase characters, set `chars` to `ascii_lowercase + ascii_uppercase`, or to use uppercase letters only, specify `ascii_uppercase`.
- **spaces**: Boolean
  Specify `False` to disallow spaces in character part of block names. In this case, the first element of the `chars` parameter functions like a 'zero' and replaces spaces.
- **block_order**: string or `None`
  Specify `None` or 'layer_column' for default block ordering by layer and column, starting from the atmosphere. Specify 'dmplex' to order blocks by geometrical type (8-node hexahedrons first followed by 6-node wedges) as in PETSc DMPlex meshes.

```
from_gmsh(filename, layers, convention=0, atmosphere_type=2,
top_elevation=0, justify = 'r', chars = ascii_lowercase, spaces=True,
block_order=None)
```

Imports a 2-D `gmsh` mesh into a geometry object. `gmsh` is a grid generation program (see http://geuz.org/gmsh/). The horizontal structure of the geometry object is created from the `gmsh` mesh, while the layer structure is specified via the `layers` parameter, a list of layer thicknesses. The elevation of the top surface can also be specified, as well as the naming convention and atmosphere type.

Parameters:

- **filename**: string
  Name of the `gmsh` mesh file.

- **layers**: list
  List of floats containing the desired layer thicknesses.
- **convention**: integer
  Naming convention for grid columns and layers.
- **atmosphere_type**: integer
  Type of atmosphere.
- **top_elevation**: float
  Elevation of the top surface of the model (default is zero).
- **justify**: string
  Specify 'r' for the character part of the block names (first three characters) to be right-justified, 'l' for left-justified.
- **chars**: string
  Specifies a string of characters to use when forming the character part of block names. Default is lowercase letters.
- **spaces**: Boolean
  Specify `False` to disallow spaces in character part of block names. In this case, the first element of the `chars` parameter functions like a 'zero' and replaces spaces.
- **block_order**: string or `None`
  Specify `None` or 'layer_column' for default block ordering by layer and column, starting from the atmosphere. Specify 'dmplex' to order blocks by geometrical type (8-node hexahedrons first followed by 6-node wedges) as in PETSc DMPlex meshes.

`layer_containing_elevation(`*`elevation`*`)`

Returns the grid layer containing the specified vertical elevation.

Parameters:

- **elevation**: float
  Vertical elevation.

`layer_mapping(`*`geo`*`)`

Returns a dictionary mapping each layer name in the `mulgrid` object `geo` to the name of the nearest layer in the object's own geometry. (Note: this mapping takes no account of the grid surface, which may alter which layer is nearest in a given column.)

Parameters:

- **geo**: `mulgrid`
  The `mulgrid` object to create a layer mapping from.

`layer_name(`*`block_name`*`)`

Gives the name of the layer corresponding to the specified block name, according to the naming convention of the grid.

Parameters:

- **block_name**: string
  Block name.

```
layer_plot(layer, variable=None, variable_name=None, unit=None,
column_names=None, node_names=None, column_centres=None, nodes=None,
colourmap=None, linewidth=0.2, linecolour='black', aspect='equal', plt=None,
subplot=111, title=None, xlabel='x (m)', ylabel='y (m)', contours=False,
contour_label_format='%3.0f', contour_grid_divisions=(100,100),
connections=None, colourbar_limits=None, plot_limits=None, wells=None,
well_names=True, hide_wells_outside=True, wellcolour='blue',
welllinewidth=1.0, wellname_bottom=True, rocktypes=None, allrocks=False,
rockgroup=None, flow=None, grid=None, flux_matrix=None,
flow_variable_name=None, flow_unit=None, flow_scale=None,
flow_scale_pos=(0.5, 0.02), flow_arrow_width=None, connection_flows=False,
blockmap = {}, block_names=None)
```

Plots a variable over a layer of the grid, using the `matplotlib` plotting library. The required layer can be specified by name or as an elevation (in which case the routine will find the corresponding layer). Specifying the layer as `None` gives a plot over the ground surface of the geometry (i.e. the surface layer for each column).

The variable can be a list or `np.array` containing a value for every block (or column) in the grid, in the order given by the `block_name_list` property of the geometry. If no variable is specified, only the grid in the layer is plotted, without shading. If the variable contains a value for each column in the grid, these values are extended down each column to fill the entire grid.

The name and units of the variable can optionally be specified, and the names of the columns and nodes can also optionally be displayed on the plot, as well as the column centres (represented by crosses). The colour map and limits of the variable shading, the line width of the grid columns and the aspect ratio of the plot can also be set, as can the title and x- and y-axis labels, and the plot limits.

When a variable is plotted over the grid, contours at specified levels can also be drawn, and optionally labelled with their values.

Well tracks can also optionally be plotted. Each well is drawn as a line following the well track, with the well name at the bottom (or optionally the top) of the well. For surface plots (`layer = None`), wells are drawn with solid lines; otherwise, wells are drawn with dotted lines except where they pass through the specified layer, where they are drawn with solid lines.

Rock types can be shown on the layer plot by specifying a `t2grid` object as the `rocktypes` parameter. It is possible to group similar rock types (e.g. those in the same geological formation but with slightly different permeabilities) to simplify the plot if there are a lot of rock types.

Flows can be shown on the layer by specifying an array of connection flow values (e.g mass flow) as the `flow` parameter. Flows will then be drawn on the slice by arrows at the block centres, each representing the average flux (flow per unit area) over the block, projected onto the layer. (For example, connection values of mass flow in kg/s will be represented as block-average mass fluxes in kg/m^2/s.) Alternatively, flows through the connection faces can be plotted by setting the `connection_flows` parameter to `True`.

Parameters:

- **layer**: `layer`, string, integer, float or `None`
  Layer or name (string) of layer to plot, or elevation (float or integer). Specifying `None` gives a surface plot.

- **variable**: list (or `np.array`)
  Variable to be plotted, of length equal to the number of blocks or columns in the grid (or `None` just to plot the grid).
- **variable_name**: string
  Name of the variable (as it will appear on the scale of the plot).
- **unit**: string
  Units of the variable (as it will appear on the scale of the plot).
- **column_names**: Boolean or list
  Set to `True` if column names are to be indicated on the plot, or to a list of names of columns to be named.
- **node_names**: Boolean or list
  Set to `True` if node names are to be indicated on the plot, or to a list of names of nodes to be named.
- **column_centres**: Boolean or list
  Set to `True` if column centres are to be indicated on the plot (as crosses), or to a list of names of columns to be indicated.
- **nodes**: Boolean or list
  Set to `True` if nodes are to be indicated on the plot (as crosses), or to a list of names of nodes to be indicated.
- **colourmap**: string
  Name of `matplotlib` colour map to use for shading the variable.
- **linewidth**: float
  Line width to use for drawing the grid.
- **linecolour**: string
  Line colour to use for drawing the grid.
- **aspect**: string
  Aspect ratio to use for drawing the grid (default is 'equal' (i.e. 1:1).
- **plt**: `matplotlib.pyplot` instance
  An instance of the `matplotlib.pyplot` library, imported in the calling script using e.g. `import matplotlib.pyplot as plt`.
- **subplot**: integer
  Subplot number for multi-plots, e.g. set 223 to draw the third plot in a 2-by-2 multiplot (default is 111).
- **title**: string
  Plot title. If set to `None` (the default value), a title will be constructed from the other plot parameters. Set to '' for no title.
- **xlabel**: string
  x axis label (default is 'x (m)').
- **ylabel**: string
  y axis label (default is 'y (m)').

- **contours**: Boolean, list or `np.array`
  Set to `True` or to a list or array of contour values to draw contours on the plot (default `False`).

- **contour_label_format**: string
  Format string for contour labels (default '%3.0f').

- **contour_grid_divisions**: tuple (of integer)
  Number of divisions in the x- and y-directions in the regular grid superimposed on the model grid, and used to produce the contours (default (100,100)).

- **connections**: float (or `None`)
  Set non-zero to plot connections in the grid, shaded by absolute value of the connection angle cosine. The value specifies the lower cut-off value, above which connections will be plotted. Connections are shaded in greyscale from white (0.0) to black (1.0). This can be used to check orthogonality of grid connections, as less orthogonal connections (with larger angle cosine) will show up darker on the plot. If set to `None`, no connections will be plotted.

- **colourbar_limits**: tuple, list, `np.array` (or `None`)
  Specify a two-element tuple, list or `np.array` to set the limits of the colour scale. Default (`None`) will auto-scale.

- **plot_limits**: tuple or list (or `None`)
  Specify a two-element tuple (or list) of plot axis ranges, each itself being a tuple (or list) of minimum and maximum values, i.e. ((xmin,xmax),(ymin,ymax)). Default is `False` which will auto-scale.

- **wells**: Boolean or list (or `None`)
  Specify `True` to plot all well tracks, `False` or `None` not to plot them, or a list of wells or well names to specify only particular wells.

- **well_names**: Boolean or list (or `None`)
  Specify `True` to label each well with its name , `False` or `None` not to label them, or a list of wells or well names to label only particular wells.

- **hide_wells_outside**: Boolean
  Set to `True` if wells that do not intersect the specified layer are to be hidden.

- **wellcolour**: string
  Colour to use for drawing the wells.

- **welllinewidth**: float
  Line width for drawing the wells.

- **wellname_bottom**: Boolean
  Set to `False` to label wells at the wellhead rather than the bottom.

- **rocktypes**: `t2grid` (or `None`)
  To plot rock types, specify a `t2grid` object containing rock types for the grid. If `None`, no rock types will be plotted.

- **allrocks**: Boolean
  If `False` (the default), only rock types present on the specified layer will be shown in the colour bar; others will be omitted. If `True`, all rocks present in the model grid will be shown on the colour bar, regardless of whether they appear in the specified layer.

- **rockgroup**: tuple, list, string (or `None`)
  To group similar rock types into one colour, specify a tuple or list of integers, representing the significant characters of the rock type names. For example, to group rock types having the same first two characters, specify (0,1). Alternatively, specify a 5-character string mask containing asterisks in positions that are not significant, and any other characters in the significant positions (e.g. '++***').

- **flow**: `np.array` (or `None`)
  To plot flows, specify an array of connection flow values (one floating point value for each connection in the grid). These may for example be extracted from the columns of the connection table in a `t2listing` object.

- **grid**: `t2grid` (or `None`)
  Specify a `t2grid` object associated with the grid, to be used to calculate the 'flux matrix' which converts the connection flow values to block-average fluxes. If this is not specified (and neither is the `flux_matrix` parameter), then a `t2grid` object will be created internally.

- **flux_matrix**: `scipy.sparse.lil_matrix` (or `None`)
  A sparse matrix used to convert the connection flow values to block-average fluxes. Such a matrix can be created using the `flux_matrix()` method of a `t2grid` object and an appropriate `mulgrid` object. If no flux matrix is specified, one will be created internally. This can be time-consuming for large grids, so for multiple flow plots it is faster to pre-calculate a flux matrix in your script and pass it via this parameter. If this parameter is specified, there is no need also to specify the `grid` parameter.

- **flow_variable_name**: string (or `None`)
  Name of the flow variable (as it will appear on the scale of the plot).

- **flow_unit**: string (or `None`)
  Units of the flow variable (as it will appear on the scale of the plot, divided by area).

- **flow_scale**: string (or `None`)
  Length of flow scale arrow. If not specified, this will be calculated.

- **flow_scale_pos**: tuple
  Position of the flow scale on the plot, in units of dimensionless plot size. The default (0.5, 0.02) draws the flow scale in the horizontal centre of the plot, slightly above the bottom axis. If you want the flow scale below the bottom axis (so it doesn't get mixed up with the actual flow arrows), specify this parameter with a small negative second component, e.g. (0.8, -0.1).

- **flow_arrow_width**: float (or `None`)
  Width of the flow arrows, in units of dimensionless plot width. If not specified, this will be calculated internally.

- **connection_flows**: Boolean
  Set to `True` to plot flows through connection faces, rather than block-averaged fluxes.

In this case, usually the `grid` parameter should also be specified (but not `flux_matrix`), otherwise a grid will be calculated internally.

- **blockmap**: dictionary
  Dictionary mapping the block names in the geometry to another block naming system. This has an effect only on the block names displayed on the plot via the `block_names` parameter, and on the rock types displayed. Note that if a mapping is used, then the `block_names` list should contain mapped block names.

- **block_names**: Boolean or list
  Set to `True` if block names are to be indicated on the plot, or to a list of names of blocks to be named.

Example:

```
geo.layer_plot(-500., t, 'Temperature', '$\degree$C', contours =
    np.arange(100,200,25))
```

plots the variable `t` at elevation -500 m over the grid, with the values as Temperature (°C), and with contours drawn from 100°C to 200°C with a contour interval of 25°C.

```
line_plot(start=None, end=None, variable, variable_name=None,
unit=None, divisions=100, plt=None, subplot=111, title='',
xlabel='distance (m)', coordinate=False)
```

Plots a variable along a line through the grid, using the `matplotlib` plotting library. The line is specified by its start and end points in 3D. The variable can be a list or `np.array` containing a value for every block (or column) in the grid. If the variable contains a value for each column in the grid, these values are extended down each column to fill the entire grid. The name and units of the variable can optionally be specified, as well as the number of divisions the line is divided into (default 100), the plot title and the axis labels.

Parameters:

- **start**, **end**: list, tuple or `np.array`
  Start and end point of the line, each of length 3 (`None` to plot across the bounds of the grid).

- **variable**: list (or `np.array`)
  Variable to be plotted, of length equal to the number of blocks (or columns) in the grid.

- **variable_name**: string
  Name of the variable (as it will appear on the scale of the plot).

- **unit**: string
  Units of the variable (as it will appear on the scale of the plot).

- **divisions**: integer
  Number of divisions to divide the line into (default 100).

- **plt**: `matplotlib.pyplot` instance
  An instance of the `matplotlib.pyplot` library, imported in the calling script using e.g. `import matplotlib.pyplot as plt`.

- **subplot**: integer
  Subplot number for multi-plots, e.g. set 223 to draw the third plot in a 2-by-2 multiplot (default is 111).

- **title**: string
  Plot title. If set to `None` (the default value), a title will be constructed from the other plot parameters. Set to '' for no title.

- **xlabel**: string
  x axis label (default is 'distance (m)').

- **coordinate**: integer or Boolean
  If `False`, plot against distance along the line, otherwise plot against specified coordinate (0,1 or 2) values.

Example:

```
geo.line_plot([0.,0.,500.], [1000.,0.,500.], t, 'Temperature',
    '$\degree$C')
```

plots the variable `t` along a line from (0,0,500) to (1000,0,500) through the grid, with the values as Temperature (°C).

`line_values(`*`start`*`, `*`end`*`, `*`variable`*`, `*`divisions`*`=100, `*`coordinate`*`=False, `*`qtree`*`=None)`

Returns values of a specified variable along an arbitrary line through the grid. The start and end points of the line (`start` and `end`) are 3-element lists, tuples or `np.arrays` specifying points in 3D. The variable can be a list or `np.array` containing a value for every block in the grid. The number of divisions along the line (default 100) can be optionally specified.

The routine returns a tuple of two arrays (l,v), the first (l) containing the distance from the start (or the appropriate coordinate (0,1, or 2) if `coordinate` is specified) for each point along the line, and the second (v) containing the value of the variable at that point. The value of the variable at any point is the (block average) value at the block containing the point.

Parameters:

- **start**, **end**: list, tuple or `np.array` (of length 3)
  Start and end points of the line in 3D.

- **variable**: list (or `np.array`)
  Variable to be plotted, of length equal to the number of blocks in the grid.

- **divisions**: integer
  Number of segments the line is divided up into (default 100).

- **coordinate**: integer or Boolean
  If `False`, return distance along the line in first array, otherwise return specified coordinate (0,1 or 2) values.

- **qtree**: `quadtree`
  Quadtree object for fast searching of grid columns (can be constructed using the `column_quadtree()` method).

`meshio_grid(surface_snap = 0.1, dimension = 3, slice = None)`

Returns mesh corresponding to the geometry, in the format used by the `meshio` library (https://pypi.python.org/pypi/meshio). This consists of a two-element tuple: firstly, an `np.array` of nodal coordinates, and secondly a dictionary of element definitions, indexed by number of nodes in the elements.

The primary use of this is as an interchange format for input/output of meshes in different formats. Note that exporting the geometry directly to a mesh file can also be done using the `write_mesh()` method (which is just a wrapper for this one).

Parameters:

- **surface_snap**: float
  Tolerance for eliminating elements with very small vertical thickness at the top of the mesh.

- **dimension**: integer
  Dimension of the mesh: when set to 3, return the full 3-D mesh. When set to 2, return a 2-D mesh, corresponding either to the horizontal mesh only (the default), or a vertical slice mesh if the `slice` parameter is used.

- **slice**: list, string, float or `None`
  Horizontal line defining the slice for vertical 2-D meshes. This can be a list of two horizontal (x,y) points (`np.arrays`) defining the endpoints of the slice line, or string 'x' or 'y' to specify the x- or y-axis, or northing (float) through grid centre. If set to `None` (the default) then the horizontal 2-D mesh is returned.

`minc_array(vals, minc_indices, level=0, outside=0.0)`

Returns an array for all blocks in the geometry, with values taken from the input `vals` array, for the specified MINC level. Indexing of MINC blocks is specified by the `minc_indices` array (returned by the `t2grid` `minc()` method).

Parameters:

- **vals**: `np.array`
  Array of values over the entire MINC grid, with values for all MINC levels, obtained e.g. from a column of the element table of a `t2listing` object.

- **minc_indices**: `np.array` (of integer)
  Rank-2 array containing integer indices for each MINC level, obtained from the output of the `t2grid` `minc()` method.

- **level**: integer
  MINC level, 0 being the fracture level and higher levels being the matrix levels.

- **outside**: Boolean or float
  Determines how blocks outside the MINC part of the grid are handled. If `True`, include porous medium values outside the MINC part of the grid. If a float value is given, assign that value instead. If `False`, the value zero will be assigned.

`nodes_in_columns(columns)`

Returns a list of all nodes in a specified list of columns.

Parameters:

- **columns**: list (of column)
  List of columns in which to find nodes.

`nodes_in_polygon(polygon)`

Returns a list of all nodes inside the specified polygon or rectangle.

Parameters:

- **polygon**: list (of `np.array`)
  List of points defining the polygon (each point is a two-element `np.array`). If the list has only two points, it will be interpreted as a rectangle [bottom left, top right].

`node_nearest_to(point, kdtree=None)`

Returns the node nearest to a specified point. An optional kd-tree structure can be specified to speed searching - useful if searching for many points.

Parameters:

- **point**: `np.array`, list or tuple
  Array or list of length 2, specifying the required point in 2-D.

- **kdtree**: `cKDTree`
  kd-tree structure for searching for nodes. Such a tree can be constructed using the `node_kdtree` property of a `mulgrid` object. You will need the `scipy` library installed before you can use this property.

`optimize(nodenames=None, connection_angle_weight=1.0, column_aspect_weight=0.0, column_skewness_weight=0.0, pest=False)`

Adjusts positions of the specified nodes to optimize grid quality. If no nodes are specified, all node positions are optimized. Grid quality can be defined as a combination of connection angle cosine, column aspect ratio and column skewness. Increasing the weight for any of these increases its importance in the evaluation of grid quality.

Note that an error will result if the connection angle weight and either of the other two weights is set to zero - in this case there are not enough constraints to fit the parameters.

If the `pest` parameter is set to `True`, the PEST parameter estimation software is used to carry out the optimzation (this obviously requires that PEST is installed on your machine). Otherwise, the `leastsq` routine in the `scipy` Python library is used. PEST seems to be more robust in some cases, and often gives better results when nodes on the boundary of the grid are included in the optimization. However, when `leastsq` does work satisfactorily, it is generally faster (mainly because PEST has to read the geometry from disk and write it out again each time the grid quality is evaluated during the optimization). PEST is free software and may be downloaded from http://www.pesthomepage.org/. If PEST is used, a variety of intermediate files (named `pestmesh.*`) will be written to the working directory, including the PEST run record file (`pestmesh.rec`) which contains a detailed record of the optimization process.

Parameters:

- **nodenames**: list of string
  List of names of nodes to optimize. If not specified, all nodes in the grid are optimized.

- **connection_angle_weight**: float
  Weighting to be given to connection angle cosines. A higher value will place greater priority on making connections perpendicular to the column sides.

- **column_aspect_weight**: float
  Weighting to be given to column aspect ratios. A higher value will place greater priority on making column side ratios closer to 1.0.

- **column_skewness_weight**: float
  Weighting to be given to column skewness. A higher value will place greater priority on making column angle ratios closer to 1.0.

- **pest**: Boolean
  Set `True` to use the PEST parameter estimation software to perform the optimization.

`polyline_values(`*`polyline`*`, `*`variable`*`, `*`divisions`*`=100, `*`coordinate`*`=False, `*`qtree`*`=None)`

Returns values of a specified variable along an arbitrary polyline through the grid, defined as a list of 3-element lists or `np.arrays` specifying points in 3D. The variable can be a list or `np.array` containing a value for every block in the grid. The number of divisions along the line (default 100) can be optionally specified.

The routine returns a tuple of two arrays (`l`,`v`), the first (`l`) containing the distance from the start (or the appropriate coordinate (0, 1, or 2) if `coordinate` is specified) for each point along the polyline, and the second (`v`) containing the value of the variable at that point. The value of the variable at any point is the (block average) value at the block containing the point.

Parameters:

- **polyline**: list of 3-element lists or `np.arrays`
  Polyline points in 3D.

- **variable**: list (or `np.array`)
  Variable to be plotted, of length equal to the number of blocks in the grid.

- **divisions**: integer
  Number of segments the line is divided up into (default 100).

- **coordinate**: integer or Boolean
  If `False`, return distance along the line in first array, otherwise return specified coordinate (0, 1 or 2) values.

- **qtree**: `quadtree`
  Quadtree object for fast searching of grid columns (can be constructed using the `column_quadtree()` method).

`read(`*`filename`*`)`

Reads a `mulgrid` object from a MULgraph geometry file on disk.

Parameters:

- **filename**: string
  Name of the MULgraph geometry file to be read.

Example:

```
geo = mulgrid().read(filename)
```

creates a `mulgrid` object and reads its contents from file `filename`. This can be done more simply just by passing the filename into the `mulgrid` creation command:

```
geo = mulgrid(filename)
```

```
rectangular(xblocks, yblocks, zblocks, convention=0, atmos_type=2,
origin=[0,0,0], justify='r', case=None, chars=ascii_lowercase,
spaces=True, block_order=None)
```

Gives a `mulgrid` geometry object a rectangular grid structure. The grid sizes in the x, y and z directions can be non-uniform, and the grid column and layer naming convention, atmosphere type and origin can be specified. The optional `justify` and `case` parameters control the formatting of the character part of the block names. Additionally, the characters used to form node/column or layer names can be specified using the `chars` parameter. (This can be useful for example for grids with large numbers of nodes and/or columns, for which lowercase letters alone may not be enough.)

Note that it is also possible to reverse-engineer a rectangular geometry from an existing TOUGH2 data file or `t2grid` object, using the `rectgeo()` method.

Parameters:

- **xblocks**, **yblocks**, **zblocks**: list, tuple or `np.array`
  Lists (or arrays) of block sizes (float) in the x, y and z directions.
- **convention**: integer
  Naming convention for grid columns and layers.
- **atmos_type**: integer
  Type of atmosphere.
- **origin**: list (or `np.array`)
  Origin of the grid (of length 3).
- **justify**: string
  Specify 'r' for the character part of the block names (first three characters) to be right-justified, 'l' for left-justified.
- **case**: string
  Specify 'l' for the character part of the block names (first three characters) to be lower case, 'u' for upper case. Now deprecated - using the `chars` parameter is more flexible.
- **chars**: string
  Specify a string of characters to be used to form the character part of block names. For example, to use both lowercase and uppercase characters, set `chars` to `ascii_lowercase + ascii_uppercase`, or to use uppercase letters only, specify `ascii_uppercase`.
- **spaces**: Boolean
  Specify `False` to disallow spaces in character part of block names. In this case, the first element of the `chars` parameter functions like a 'zero' and replaces spaces.
- **block_order**: string or `None`
  Specify `None` or 'layer_column' for default block ordering by layer and column, starting from the atmosphere. Specify 'dmplex' to order blocks by geometrical type (8-node hexahedrons first followed by 6-node wedges) as in PETSc DMPlex meshes.

Example:

```
geo = mulgrid().rectangular([1000]*10, [500]*20, [100]*5+[200]*10,
    origin=[0,0,2500])
```

creates a `mulgrid` object called `geo`, and fills it with a rectangular grid of 10 blocks of size 1000 m in the x-direction, 20 blocks of size 500 m in the x-direction, 5 layers at the top of thickness 100 m and 10 layers underneath of thickness 200 m, and with origin (0,0,2500) m. The grid will have the default naming convention (0) and atmosphere type (2).

`reduce(`*`columns`*`)`

Reduces a grid so that it contains only the specified list of columns (or columns with specified names).

Parameters:

- **columns**: list
  List of required columns or column names.

`refine(`*`columns`*`=[], `*`bisect`*`=False, `*`bisect_edge_columns`*`=[],`
`chars` `= ascii_lowercase, `*`spaces`*`=True)`

Refines the specified columns in the grid. Appropriate transition columns are created around the refined region. If no columns are specified, all columns are refined. All columns in the region to be refined (and in the transition region) must be either triangular or quadrilateral. Each column in split into four, unless the `bisect` parameter is `True`, in which case each column in split into two. If `bisect` is 'x' or 'y', columns are split in the closest direction to the axis specified; or if `bisect` is `True`, between its longest sides.

The `bisect_edge_columns` parameter can be used to give more desirable column shapes in the transition region, if the original columns occupying the transition region have large aspect ratios. By default, these will become even worse when they are triangulated to form the transition columns, if they are connected to the refinement region by their shorter sides. Including them in `bisect_edge_columns` means they will be bisected (parallel to the edge of the refinement region) before the refinement is carried out, which should improve the aspect ratios of the transition columns.

Note: TOUGH2 implicitly assumes that the connections in its finite volume grids are orthogonal, i.e. the line joining the centres of two connected blocks should be perpendicular to the connecting face. The triangular transition columns generated by the `refine()` method generally give rise to connections that are not orthogonal. However, they can be modified and made as orthogonal as possible using the `optimize()` method.

Parameters:

- **columns**: list
  List of columns or column names to be refined.

- **bisect**: Boolean or string
  Set to `True` if columns are to be split into two, between their longest sides, instead of four (the default). Set to 'x' or 'y' to split columns along the specified axis.

- **bisect_edge_columns**: list
  List of columns or column names in the transition region (just outside the refinement area) to be bisected prior to the refinement, to improve the aspect ratios of the transition columns.

- **chars**: string
  Specifies a string of characters to use when forming the character part of block names. Default is lowercase letters.

- **spaces**: Boolean
  Specify `False` to disallow spaces in character part of block names. In this case, the first element of the `chars` parameter functions like a 'zero' and replaces spaces.

`refine_layers(layers=[], factor=2, chars = ascii_lowercase, spaces=True)`

Refines the specified layers in the grid. If no layers are specified, all layers are refined. Each layer is refined by the specified integer factor.

Parameters:

- **layers**: list
  List of layers or layer names to be refined.

- **factor**: integer
  Refinement factor: default is 2, which bisects each layer.

- **chars**: string
  Specifies a string of characters to use when forming the character part of block names. Default is lowercase letters.

- **spaces**: Boolean
  Specify `False` to disallow spaces in character part of block names. In this case, the first element of the `chars` parameter functions like a 'zero' and replaces spaces.

`rename_column(oldcolname, newcolname)`

Renames a grid column. Returns `True` if the column was found and renamed, or `False` if the specified column does not exist. Multiple columns can be renamed at once by specifying lists of old and new column names - this is faster than calling the method multiple times, and the block and connection name lists are updated only once.

Parameters:

- **oldcolname**: string or list of strings
  Name(s) of the column(s) to rename.

- **newcolname**: string or list of strings
  New name(s) of the column(s).

`rename_layer(oldlayername, newlayername)`

Renames a grid layer. Returns `True` if the layer was found and renamed, or `False` if the specified layer does not exist. Multiple layers can be renamed at once by specifying lists of old and new layer names - this is faster than calling the method multiple times, and the block and connection name lists are updated only once.

Parameters:

- **oldlayername**: string or list of strings
  Name(s) of the layer(s) to rename.

- **newlayername**: string or list of strings
  New name(s) of the layer(s).

```
rotate(angle, centre=None, wells=False)
```

Rotates a grid by a specified angle (in degrees) clockwise in the horizontal plane. Any wells in the grid are also rotated. The centre of rotation can be optionally specified. If it is not specified, the centre of the grid is used as the centre of rotation. If the `wells` parameter is `True`, any wells in the grid are also rotated.

Parameters:

- **angle**: float
  Angle (in degrees) to rotate the grid, positive for clockwise, negative for anti-clockwise.
- **centre**: list, tuple or `np.array`
  Centre of rotation in the horizontal x,y plane (of length 2).
- **wells**: Boolean
  Set `True` to rotate wells.

Example:

```
geo.rotate(30)
```

rotates the grid `geo` clockwise by 30° about its centre in the horizontal plane.

```
slice_plot(line=None, variable=None, variable_name=None, unit=None,
block_names=None, colourmap=None, linewidth=0.2, linecolour='black',
aspect='auto', plt=None, subplot=111, title=None, xlabel="",
ylabel='elevation (m)', contours=False, contour_label_format='%3.0f',
contour_grid_divisions=(100,100), colourbar_limits=None, plot_limits=None,
column_axis=False, layer_axis=False, wells=None, well_names=True,
hide_wells_outside=False, wellcolour='blue', welllinewidth=1.0,
wellname_bottom=False, rocktypes=None, allrocks=False, rockgroup=None,
flow=None, grid=None, flux_matrix=None, flow_variable_name=None,
flow_unit=None, flow_scale=None, flow_scale_pos=(0.5, 0.02),
flow_arrow_width=None, connection_flows=False, blockmap = {})
```

Plots a variable over a vertical slice through the grid, using the `matplotlib` plotting library. The required slice is specified by a horizontal line through the grid, defined as either a two-element list of (x,y) points (`np.arrays`), or as a string 'x' or 'y' which defines the x- or y-axes respectively, or as a northing (in degrees) through the centre of the grid. If no line is specified, the line is taken to be across the bounds of the grid. For slice plots along the x- or y-axis, the horizontal coordinate represents the x- or y-coordinate; for other slice directions it represents distance along the slice line.

The variable can be a list or `np.array` containing a value for every block (or column) in the grid, in the order given by the `block_name_list` property of the geometry. If no variable is specified, only the grid is plotted, without shading. If the variable contains a value for each column in the grid, these values are extended down each column to fill the entire grid.

The name and units of the variable can optionally be specified, and the name of each block can also optionally be displayed on the plot. The colour map and limits of the variable shading, the line width of the grid columns and the aspect ratio of the plot can also be set, as can the plot title and x- and z-axis labels, and the plot limits.

When a variable is plotted over the grid, contours at specified levels can also be drawn, and optionally labelled with their values.

Well tracks can also optionally be plotted. Each well is drawn as a line following the well track, with the well name at the top (or optionally the bottom) of the well. If `hide_wells_outside` is specified as a floating point number, wells that do not pass within the specified distance from the slice line are not shown. Well tracks are shown as solid lines over sections within the specified distance from the slice line, and dotted lines otherwise.

Rock types can be shown on the slice plot by specifying a `t2grid` object as the `rocktypes` parameter. It is possible to group similar rock types (e.g. those in the same geological formation but with slightly different permeabilities) to simplify the plot if there are a lot of rock types.

Flows can be shown on the slice by specifying an array of connection flow values (e.g mass flow) as the `flow` parameter. Flows will then be drawn on the slice by arrows at the block centres, each representing the average flux (flow per unit area) over the block, projected onto the slice. (For example, connection values of mass flow in kg/s will be represented as block-average mass fluxes in kg/m^2/s.) Alternatively, flows through the connection faces can be plotted by setting the `connection_flows` parameter to `True`.

Parameters:

- **line**: list, string or float
  List of two horizontal (x,y) points (`np.arrays`) defining the endpoints of the line, or string 'x' or 'y' to specify the x- or y-axis, or northing (float) through grid centre.

- **variable**: list (or `np.array`)
  Variable to be plotted, of length equal to the number of blocks (or columns) in the grid (or `None` just to plot the grid).

- **variable_name**: string
  Name of the variable (as it will appear on the scale of the plot).

- **unit**: string
  Units of the variable (as it will appear on the scale of the plot).

- **block_names**: Boolean or list
  Set to `True` if block names are to be indicated on the plot, or to a list of names of blocks to be named.

- **colourmap**: string
  Name of `matplotlib` colour map to use for shading the variable.

- **linewidth**: float
  Line width to use for drawing the grid.

- **linecolour**: string
  Line colour to use for drawing the grid.

- **aspect**: string
  Aspect ratio to use for drawing the grid (default is 'auto').

- **plt**: `matplotlib.pyplot` instance
  An instance of the `matplotlib.pyplot` library, imported in the calling script using e.g. `import matplotlib.pyplot as plt`.

- **subplot**: integer
  Subplot number for multi-plots, e.g. set 223 to draw the third plot in a 2-by-2 multiplot (default is 111).

- **title**: string
  Plot title. If set to `None` (the default value), a title will be constructed from the other plot parameters. Set to '' for no title.

- **xlabel**: string
  x axis label. If set to `None` (the default value), a label will be constructed according to the slice orientation- either 'x (m)', 'y (m)' or 'distance (m)' as appropriate.

- **ylabel**: string
  y axis label (default is 'elevation (m)').

- **contours**: Boolean, list or `np.array`
  Set to `True` or to a list or array of contour values to draw contours on the plot (default `False`).

- **contour_label_format**: string
  Format string for contour labels (default '%3.0f').

- **contour_grid_divisions**: tuple (of integer)
  Number of divisions in the x- and z-directions in the regular grid superimposed on the slice, and used to produce the contours (default (100,100)).

- **colourbar_limits**: tuple, list, `np.array` (or `None`)
  Specify a two-element tuple, list or `np.array` to set the limits of the colour scale. Default (`None`) will auto-scale.

- **plot_limits**: tuple or list (or `None`)
  Specify a two-element tuple (or list) of plot axis ranges, each itself being a tuple (or list) of minimum and maximum values, i.e. ((xmin,xmax),(zmin,zmax)). Default is `False` which will auto-scale.

- **column_axis**: Boolean
  If `True`, show column names instead of coordinates on the horizontal axis.

- **layer_axis**: Boolean
  If `True`, show layer names instead of coordinates on the vertical axis.

- **wells**: Boolean or list (or `None`)
  Specify `True` to plot all well tracks, `False` or `None` not to plot them, or a list of wells or well names to specify only particular wells.

- **well_names**: Boolean or list (or `None`)
  Specify `True` to label each well with its name , `False` or `None` not to label them, or a list of wells or well names to label only particular wells.

- **hide_wells_outside**: `False` or float
  Specify distance as a floating point number to hide wells further from the slice line than the specified distance.

- **wellcolour**: string
  Colour to use for drawing the wells.

- **welllinewidth**: float
  Line width for drawing the wells.

- **wellname_bottom**: Boolean
  Set to `True` to label wells at the bottom rather than the wellhead.

- **rocktypes**: `t2grid` (or `None`)
  To plot rock types, specify a `t2grid` object containing rock types for the grid. If `None`, no rock types will be plotted.

- **allrocks**: Boolean
  If `False` (the default), only rock types present on the specified slice will be shown in the colour bar; others will be omitted. If `True`, all rocks present in the model grid will be shown on the colour bar, regardless of whether they appear in the specified slice.

- **rockgroup**: tuple, list, string (or `None`)
  To group similar rock types into one colour, specify a tuple or list of integers, representing the significant characters of the rock type names. For example, to group rock types having the same first two characters, specify (0,1). Alternatively, specify a 5-character string mask containing asterisks in positions that are not significant, and any other characters in the significant positions (e.g. '++***').

- **flow**: `np.array` (or `None`)
  To plot flows, specify an array of connection flow values (one floating point value for each connection in the grid). These may for example be extracted from the columns of the connection table in a `t2listing` object.

- **grid**: `t2grid` (or `None`)
  Specify a `t2grid` object associated with the grid, to be used to calculate the 'flux matrix' which converts the connection flow values to block-average fluxes. If this is not specified (and neither is the `flux_matrix` parameter), then a `t2grid` object will be created internally.

- **flux_matrix**: `scipy.sparse.lil_matrix` (or `None`)
  A sparse matrix used to convert the connection flow values to block-average fluxes. Such a matrix can be created using the `flux_matrix()` method of a `t2grid` object and an appropriate `mulgrid` object. If no flux matrix is specified, one will be created internally. This can be time-consuming for large grids, so for multiple flow plots it is faster to pre-calculate a flux matrix in your script and pass it via this parameter. If this parameter is specified, there is no need also to specify the `grid` parameter.

- **flow_variable_name**: string (or `None`)
  Name of the flow variable (as it will appear on the scale of the plot).

- **flow_unit**: string (or `None`)
  Units of the flow variable (as it will appear on the scale of the plot, divided by area).

- **flow_scale**: string (or `None`)
  Length of flow scale arrow. If not specified, this will be calculated.

- **flow_scale_pos**: tuple
  Position of the flow scale on the plot, in units of dimensionless plot size. The default (0.5, 0.02) draws the flow scale in the horizontal centre of the plot, slightly above the

bottom axis. If you want the flow scale below the bottom axis (so it doesn't get mixed up with the actual flow arrows), specify this parameter with a small negative second component, e.g. (0.8, -0.1).

- **flow_arrow_width**: float (or `None`)
  Width of the flow arrows, in units of dimensionless plot width. If not specified, this will be calculated internally.

- **connection_flows**: Boolean
  Set to `True` to plot flows through connection faces, rather than block-averaged fluxes. In this case, usually the `grid` parameter should also be specified (but not `flux_matrix`), otherwise a grid will be calculated internally.

- **blockmap**: dictionary
  Dictionary mapping the block names in the geometry to another block naming system. This has an effect only on the block names displayed on the plot via the `block_names` parameter, and on the rock types displayed. Note that if a mapping is used, then the `block_names` list should contain mapped block names.

Example:

```
geo.slice_plot(45., t, 'Temperature', '$\degree$C', contours = [100,200])
```

plots the variable `t` through a SW–NE vertical slice (heading 45°) through the grid, with the values as Temperature (°C) and contours drawn at 100°C and 200°C.

```
from matplotlib import cm
cmap = cm.get_cmap('jet', 10)
geo.slice_plot(45., t, 'Temperature', '$\degree$C',
  colourbar_limits = (0., 250.), colourmap = cmap)
```

plots the variable `t` again, but with a specified discrete colour scale with 10 divisions from zero to 250°C.

`snap_columns_to_layers(`*`min_thickness`*`=1.0, `*`columns`*`=[])`

Snaps column surfaces to the bottom of their layers, if the surface block thickness is smaller than a given value. This can be carried out over an optional subset of columns in the grid, otherwise over all columns.

Parameters:

- **min_thickness**: float
  Minimum surface block thickness. Blocks with thickness less than this value will be eliminated by 'snapping' the column surface elevation to the bottom of the surface layer. Values of `min_thickness` less than or equal to zero will have no effect.

- **columns**: list (of `column` or string)
  List of columns to process. If empty (the default), process all columns.

`snap_columns_to_nearest_layers(`*`columns`*`=[])`

Snaps column surfaces to the nearest layer elevation (top or bottom). This can be carried out over an optional subset of columns in the grid, otherwise over all columns.

Parameters:

- **columns**: list (of column or string)
  List of columns to process. If empty (the default), process all columns.

`split_column(colname, nodename, chars = ascii_lowercase)`

Splits a quadrilateral column with specified name into two triangular columns. The direction of the split is determined by specifying the name of one of the splitting nodes. The method returns `True` if the split was carried out successfully.

Parameters:

- **colname**: string
  Name of the quadrilateral column to be split. If the column is not quadrilateral, the method returns `False` and nothing is done to the column.

- **nodename**: string
  Name of one of the splitting nodes. The column is split across this node and the one on the opposite side of the column. If the specified node is not in the column, the method returns `False` and nothing is done to the column.

- **chars**: string
  Specifies a string of characters to use when forming the character part of block names. Default is lowercase letters.

`translate(shift, wells=False)`

Translates a grid by a specified shift in the x, y and z directions. If the `wells` parameter is `True`, any wells in the grid are also translated.

Parameters:

- **shift**: list, tuple or `np.array`
  Distance to shift the grid in the x, y and z directions (of length 3).

- **wells**: Boolean
  Set `True` to translate wells.

Example:

```
geo.translate([10.e3, 0.0, -1000.0])
```

translates the grid `geo` by 10 km in the x direction and down 1 km in the z direction.

`well_values(well_name, variable, divisions=1, elevation=False, deviations=False, qtree=None, extend=False)`

Returns values of a specified variable down a specified well. The variable can be a list or `np.array` containing a value for every block in the grid. The number of divisions between layer centres or along each well deviation (default 1) can be optionally specified (this can be increased to capture detail along a deviation that passes through several blocks). If `deviations` is `True`, values will be returned at the nodes of the well track, instead of at grid layer centres. If `extend` is `True`, the well trace is artificially extended to the bottom of the model.

The routine returns a tuple of two arrays (`d`,`v`), the first (`d`) containing the measured depth down the well (or elevation if the `elevation` parameter is set to `True`), and the second

(v) containing the value of the variable at each point. The value of the variable at any point is the (block average) value at the block containing the point.

Parameters:

- **well_name**: string
  Name of the well.
- **variable**: list (or `np.array`)
  Variable to be plotted, of length equal to the number of blocks in the grid.
- **divisions**: integer
  Number of divisions each well deviation is divided up into (default 1).
- **elevation**: Boolean
  Set to `True` if elevation rather than measured depth is to be returned.
- **deviations**: Boolean
  Set to `True` to return values at deviation nodes, rather than intersections of layer centres with the well track.
- **qtree**: `quadtree`
  Quadtree object for fast searching of grid columns (can be constructed using the `column_quadtree()` method).
- **extend**: Boolean
  Set `True` to artificially extend the well trace to the bottom of the model.

```
write(filename='')
```

Writes a `mulgrid` object to a MULgraph geometry file on disk.

Parameters:

- **filename**: string
  Name of the MULgraph geometry file to be written. If no file name is specified, the object's own `filename` property is used.

```
write_bna(filename='')
```

Writes a geometry object to an Atlas BNA file on disk, for visualisation with Surfer or GIS tools.

Parameters:

- **filename**: string
  Name of the BNA file to be written. If no file name is specified, the object's own `filename` property is used, with the extension changed to *.bna. If the object's `filename` property is not set, the default name 'geometry.bna' is used.

```
write_exodusii(filename='', arrays=None, blockmap={})
```

Writes a `mulgrid` object to an ExodusII file on disk, for visualisation or export to other software.

This method uses the VTK-Python library, so you will need that installed on your machine before you can use it. An alternative is to use the `write_mesh` method instead, which can also write meshes to ExodusII format (as well as others), and does not need the VTK-Python library (though you will need the `meshio` library).

Parameters:

- **filename**: string
  Name of the ExodusII file to be written. If no file name is specified, the object's own `filename` property is used, with the extension changed to *.exo. If the object's `filename` property is not set, the default name 'geometry.exo' is used.

- **arrays**: dictionary or `None`
  Data arrays to be included in the ExodusII file. If set to `None`, default arrays (block name, layer index, column index, column area, column elevation, block number and volume) are included.

- **blockmap**: dictionary
  Dictionary mapping the block names in the geometry to another block naming system.

```
write_mesh(filename, surface_snap = 0.1, dimension = 3, slice = None,
file_format = None)
```

Writes a `mulgrid` object to a mesh file on disk, with the specific format determined by the file extension of the specified filename. This method uses the `meshio` library:
https://pypi.python.org/pypi/meshio
which must be installed on your machine, and supports various mesh output formats including Dolfin XML, ExodusII, MSH, VTK, XDMF and others. The `meshio` library may be installed from PyPI (using e.g. `pip install meshio`).
Note that many of these formats do not support columns with more than four sides.
Parameters:

- **filename**: string
  Name of the mesh file to be written.

- **surface_snap**: float
  Tolerance for eliminating elements with very small vertical thickness at the top of the mesh (3-D meshes only).

- **dimension**: integer
  Dimension of the mesh: when set to 3 (the default), write the full 3-D mesh. When set to 2, write a 2-D mesh, corresponding either to the horizontal mesh only (the default), or a vertical slice mesh if the `slice` parameter is used.

- **slice**: list, string, float or `None`
  Horizontal line defining the slice for vertical 2-D meshes. This can be a list of two horizontal (x,y) points (`np.arrays`) defining the endpoints of the slice line, or string 'x' or 'y' to specify the x- or y-axis, or northing (float) through grid centre. If set to `None` (the default) then the horizontal 2-D mesh is written.

- **file_format**: string or `None`
  File format for mesh output. If `None`, the file format will be decided from the filename extension (e.g. if the filename is 'mesh.exo' then the mesh will be written in ExodusII format). See the `meshio` documentation for details.

```
write_vtk(filename='', arrays=None, wells=False, blockmap={},
surface_snap=0.1)
```

Writes a `mulgrid` object to a VTK file on disk, for visualisation with VTK, Paraview, Mayavi etc. The grid is written as an 'unstructured grid' VTK object with optional data arrays defined on cells. A separate VTK file for the wells in the grid can optionally be written.

Parameters:

- **filename**: string
  Name of the VTK file to be written. If no file name is specified, the object's own `filename` property is used, with the extension changed to *.vtu. If the object's `filename` property is not set, the default name 'geometry.vtu' is used.

- **arrays**: dictionary or `None`
  Data arrays to be included in the VTK file. If set to `None`, default arrays (block name, layer index, column index, column area, column elevation, block number and volume) are included.

- **wells**: Boolean
  If set to `True`, a separate VTK file is written representing the wells in the grid.

- **blockmap**: dictionary
  Dictionary mapping the block names in the geometry to another block naming system.

- **surface_snap**: float
  Tolerance for specifying how close column surface elevations need to be before being considered "equal" when constructing surface nodes.

2.3 Other objects (`node`, `column`, `layer`, `connection` and `well`)

A `mulgrid` object contains lists of other types of objects: `node`, `column`, `layer`, `connection` and `well` objects. These classes are described below.

2.3.1 `node` objects

A `node` object represents a node (i.e. vertex) in a `mulgrid` object. A `node` object has three properties: `name`, which is a string property containing the name of the node, `pos` which is an `np.array` with three elements, containing the node's position in 3D, and `column` which is a set of the columns the node belongs to. A `node` object does not have any methods.

A `node` object `n` can be created for example using the command `n = node(name,pos)` where `name` is the node name and pos is an `np.array` (or list, or tuple) representing the node's position.

2.3.2 `column` objects

A `column` object represents a column in a `mulgrid` object. The properties of a `column` object are listed in Table 2.3.

The main properties defining a column are its `name` and `node` properties. The `name` is specified according to the naming convention of the `mulgrid` object that the column belongs to. The `node` property is a list of `node` objects (not node names) that belong to the column. A `column`'s `neighbour` property is a set of other `columns` connected to that column via a `connection` (see section 2.3.4), and its `connection` property is a set of connections the

column is part of. The `neighbourlist` property is a list of neighbouring columns, with each item corresponding to a column edge (`None` if the edge is on a grid boundary). A `column`'s `centroid` property returns the average of the positions of its vertices - which is what the `centre` property is set to, unless otherwise specified.

A `column` object has two properties measuring 'grid quality'. The `angle_ratio` property returns the ratio of largest to smallest interior angles in the column. The `side_ratio` property returns the ratio of largest to smallest side lengths (a generalisation of 'aspect ratio' to columns with any number of sides). Values as close as possible to 1.0 for both these measures are desirable (their values are both exactly 1.0 for any regular polygon, e.g. an equilateral triangle or square). Columns with large angle ratios will be highly skewed, while those with large side ratios will be typically highly elongated in one direction.

A `column` object `col` can be created for example using the command:

```
col = column(name, nodes, centre, surface)
```

where `name` is the column name and `nodes` is a list of `node` objects defining the column. The `centre` and `surface` parameters are optional.

`column` objects have three methods, `contains_point`, `in_polygon` and `is_against`, as described below.

`contains_point(`*`pos`*`)`

Returns `True` if a 2D point lies inside the column, and `False` otherwise.

Parameters:

- **pos**: `np.array`
  Horizontal position of the point.

`in_polygon(`*`polygon`*`)`

Returns `true` if the column centre is inside the specified polygon or rectangle.

Parameters:

- **polygon**: list (of `np.array`)
  List of points defining the polygon (each point is a two-element `np.array`). If the list has only two points, it will be interpreted as a rectangle [bottom left, top right].

`is_against(`*`othercolumn`*`)`

Returns `true` if the column is 'against' `othercolumn` – that is, if it shares more than one node with it.

Parameters:

- **othercolumn**: `column`)
  Any other column in the geometry.

2.3.3 `layer` objects

A `layer` object represents a layer in a `mulgrid` object. The properties of a `layer` object are given in Table 2.4.

A `layer` object `lay` can be created for example using the command:

```
lay = layer(name, bottom, centre, top)
```

Property	Type	Description
`angle_ratio`	float	ratio of largest to smallest interior angles
`area`	float	horizontal area of the column
`centre`	`np.array`	horizontal centre of the column
`centroid`	`np.array`	average position of the column's vertices
`connection`	set	connections the column is in
`name`	string	name of the column
`neighbour`	set	set of neighbouring columns
`neighbourlist`	list	ordered list of neighbouring columns
`node`	list	list of nodes (vertices) belonging to the column
`num_neighbours`	integer	number of neighbouring columns
`num_nodes`	integer	number of nodes belonging to the column
`num_layers`	integer	number of layers in the column below the ground surface
`side_ratio`	float	ratio of largest to smallest side length
`surface`	float	surface elevation of the column (`None` if not specified)

Table 2.3: Properties of a `column` object

Property	Type	Description
`bottom`	float	elevation of the bottom of the layer
`centre`	float	elevation of the centre of the layer
`thickness`	float	layer thickness (top - bottom)
`top`	float	elevation of the top of the layer
`name`	string	name of the layer

Table 2.4: Properties of a `layer` object

where `name` is the layer name and `bottom`, `centre` and `top` specify the vertical position of the layer.

The methods of a `layer` object are as follows:

`contains_elevation(`*`z`*`)`

Returns `True` if a point at a given elevation lies inside the layer, and `False` otherwise.

Parameters:

- **z**: float
  Elevation of the point.

`translate(`*`shift`*`)`

Translates a layer up or down by a specified distance.

Parameters:

- **shift**: float
  Distance to shift the layer (positive for up, negative for down).

Property	Type	Description
bottom	np.array	well bottom position
deviated	Boolean	whether well is deviated
head	np.array	well head position
name	string	well name
num_deviations	integer	number of deviations
num_pos	integer	number of well track nodes
pos	list	positions (3-D arrays) of well track nodes
pos_depth	np.array	downhole depths along well track

Table 2.5: Properties of a well object

2.3.4 connection objects

A connection object represents a connection between columns in a mulgrid object. It has three properties: column, which contains a two-element list of the column objects making up the connection, node, which contains a two-element list of the nodes on the face joining the two columns in the connection, and angle_cosine, which gives the cosine of the angle between a line joining the nodes in the connection and a line joining the centres of the two columns. This is used as a measure of grid quality, these two lines should ideally be as close to perpendicular as possible, making the cosine of the angle zero. A connection has no methods.

A connection object con can be created for example using the command

```
con = connection(cols)
```

where cols is a two-element list of the column objects in the connection.

2.3.5 well objects

A well object represents a well in a mulgrid object. The properties of a well object are given in Table 2.5.

The well track can be deviated, and is defined as a list pos of (at least two) 3D positions (np.arrays). The num_deviations property returns the number of deviations in the track (one less than the num_pos property, which is the number of nodes in the pos list). The deviated property returns True if there is more than one deviation. The pos_depth property returns an array of the downhole depths at each node along the well track.

A well object w can be created simply with the command w = well(name,pos), where name is the well name and pos is a list of 3-element np.arrays (or lists, or tuples) representing the well trace (starting from the wellhead).

The methods of a well object are listed in Table 2.6 and described below.

depth_elevation(*depth*)

Returns the elevation corresponding to the specified downhole depth (or None if depth is above the wellhead or below the bottom).

Parameters:

- **depth**: float
  Downhole depth.

Method	Type	Description
depth_elevation	float	elevation for a given downhole depth
depth_pos	np.array	position on well track for a given downhole depth
elevation_depth	float	downhole depth for a given elevation
elevation_pos	np.array	position on well track for a given elevation
pos_coordinate	np.array	array of coordinates for a given index

Table 2.6: Methods of a `well` object

`depth_pos(`*`depth`*`)`

Returns the 3D position of the point in the well with specified downhole `depth` (or `None` if `depth` is above the wellhead or below the bottom). The position is interpolated between the deviation locations.

Parameters:

- **depth**: float
  Downhole depth of the required point.

`elevation_depth(`*`elevation`*`)`

Returns the downhole depth corresponding to the specified `elevation` (or `None` if `elevation` is above the wellhead or below the bottom).

Parameters:

- **elevation**: float
  Elevation.

`elevation_pos(`*`elevation`*`, `*`extend`*`=False)`

Returns the 3D position of the point in the well with specified `elevation` (or `None` if `elevation` is above the wellhead or below the bottom). The position is interpolated between the deviation locations. If `extend` is `True`, return extrapolated positions for elevations below the bottom of the well.

Parameters:

- **elevation**: float
  Elevation of the required point.

- **extend**: Boolean
  If `True`, extrapolated positions will be returned for elevations below the bottom of the well (otherwise `None` will be returned).

`pos_coordinate(`*`index`*`)`

Returns an `np.array` of the well track node coordinates for the given index (0, 1 or 2). For example, `pos_coordinate(2)` returns an array containing the elevations of all well track nodes.

Parameters:

- **index**: integer
  Index required (0, 1 or 2).

2.4 Other functions: block name conversions

The `mulgrids` library contains two other functions connected with working with geometry files and TOUGH2 grids:

`fix_blockname(`*`name`*`)`

TOUGH2 always assumes that the last two characters of a block name represent a two-digit number. However, if that number is less than 10, the fourth character is not padded with zeros, so for example 'AA101' becomes 'AA1 1' when processed by TOUGH2.

The `fix_blockname` function corrects this by padding the fourth character of a block name with a zero if necessary. This is only done if the third character is also a digit, e.g. when naming convention 2 is used (two characters for layer followed by three digits for column).

Parameters:

- **name**: string
  Block name.

`unfix_blockname(`*`name`*`)`

This function reverses the effect of `fix_blockname()`.

Parameters:

- **name**: string
  Block name.

2.5 Block mappings: handling other block naming conventions

The MULgraph geometry format names blocks according to one of its three naming conventions. All of these conventions use part of the block name to indicate the layer and part of it to indicate the column.

However, in PyTOUGH it is possible to make a `mulgrid` object handle other block naming conventions by means of a **block mapping**. This is simply a dictionary that maps the block names in a `mulgrid` to block names in a `t2grid` object. The block names in the `t2grid` can follow an arbitrary convention, not based on layers and columns. For example, blocks in TOUGH2 grids created by PetraSim may be simply numbered.

A block mapping dictionary can be passed in as an optional parameter to many PyTOUGH methods that involve both a MULgraph geometry and TOUGH2 grid, for example the `mulgrid` `block_name()`, `slice_plot()` and `write_vtk()` methods, and the `write_vtk()` methods of the `t2grid` and `t2listing` classes.

When the `rectgeo()` method is used to create a `mulgrid` object from a `t2grid`, a block mapping is also created, and may be used in the PyTOUGH methods that can accept a block mapping.

A block mapping need not contain entries for all blocks. If for example a model follows the naming convention of a MULgraph geometry in most blocks, and only a few are different, then only entries for the different block names need be present in the mapping dictionary.

Block mappings can be saved to and loaded from disk (like any other Python object) using the `pickle` library. This is part of the standard Python library collection. For example a block mapping called `blockmap` can be saved to a file called `'blockmap.pkl'` as follows:

```
import pickle
pickle.dump(blockmap, file('blockmap.pkl', 'w'))
```

It can be loaded back in again like this:

```
blockmap = pickle.load(file('blockmap.pkl'))
```

Chapter 3

TOUGH2 grids

3.1 Introduction

The `t2grids` library in PyTOUGH contains classes and routines for manipulating TOUGH2 grids. It can be imported using the command:

```
from t2grids import *
```

3.2 `t2grid` objects

The `t2grids` library defines a `t2grid` class, used for representing TOUGH2 grids. This gives access via Python to the grid's rock types, blocks, connections and other parameters.

Normally a TOUGH2 grid is not created directly, but is either read from a TOUGH2 data file, or constructed from a `mulgrid` geometry object (see chapter 2) using the `fromgeo()` method.

Printing a `t2grid` object (e.g. `print grid`) displays a summary of information about the grid: how many rock types, blocks and connections it contains.

3.2.1 Properties

The main properties of a `t2grid` object are listed in Table 3.1. Essentially a `t2grid` object contains collections of blocks, rock types and connections, each accessible either by name or by index. For example, block 'AB 20' in a `t2grid` called `grid` is given by `grid.block['AB 20']`.

Connections are slightly different from blocks or rock types, in that they are not named individually. However, they can be accessed by the names of the blocks connected by the connection. For example, the connection between blocks 'aa 10' and 'ab 10' in a `t2grid` called `grid` is given by `grid.connection['aa 10','ab 10']`.

The `rocktype_frequencies` property gives information about how frequently each rock type is used (i.e. how many blocks use that rock type). It returns a list of tuples, the first element of each tuple being the frequency of use, and the second element being a list of rock type names with that frequency. The list is given in order of increasing frequency.

The `rocktype_indices` property gives an `np.array` containing the index of the rocktype for each block in the grid. This can be used to give a plot of rock types, in conjunction with the `mulgrid` methods `layer_plot` or `slice_plot`.

Property	Type	Description
atmosphere_blocks	list	atmosphere blocks
blocklist	list	blocks (by index)
block	dictionary	blocks (by name)
block_centres_defined	Boolean	whether block centres have been calculated
connectionlist	list	connections (by index)
connection	dictionary	connections (by tuples of block names)
num_atmosphere_blocks	integer	number of atmosphere blocks
num_blocks	integer	number of blocks
num_connections	integer	number of connections
num_rocktypes	integer	number of rock types
num_underground_blocks	integer	number of non-atmosphere blocks
rocktypelist	list	rock types (by index)
rocktype	dictionary	rock types (by name)
rocktype_frequencies	list of tuples	frequencies of rock types
rocktype_indices	np.array	index of rock type for each block

Table 3.1: Properties of a t2grid object

3.2.2 Methods

The main methods of a t2grid object are listed in Table 3.2. Details of these methods are given below.

`+`

Adds two grids a and b together (i.e. amalgamates them) to form a new grid a+b. If any rock types, blocks or connections exist in both grids a and b, the value from b is used, so there are no duplicates. (Technically this is really an 'operator' rather than a method.)

Parameters:

- **a, b**: t2grid
  The two grids to be added together.

`add_block(block)`

Adds a block to the grid. If another block with the same name already exists, it is replaced.

Parameters:

- **block**: t2block
  Block to be added to the grid.

`add_connection(connection)`

Adds a connection to the grid. If another connection with the same column names already exists, it is replaced.

Parameters:

- **connection**: t2connection
  Connection to be added to the grid.

Method	Type	Description
+	t2grid	adds two grids together
add_block	–	adds a block to the grid
add_connection	–	adds a connection to the grid
add_rocktype	–	adds a rock type to the grid
blockmap	dictionary	returns block name mapping from a geometry
block_index	integer	returns index of a block with a specified name
calculate_block_centres	–	calculates geometrical centre of all blocks in the grid
check	Boolean	checks grid for errors and optionally fixes them
clean_rocktypes	–	deletes any unused rock types from the grid
connection_index	integer	returns index of a connection with a specified pair of names
copy_connection_directions	–	copies connection permeability directions from another grid
delete_block	–	deletes a block from the grid
delete_connection	–	deletes a connection from the grid
delete_rocktype	–	deletes a rock type from the grid
demote_block	–	shifts a block (or blocks) to the end of the blocklist
embed	t2grid	embeds a subgrid inside one block of another
empty	–	empties contents of grid
flux_matrix	scipy.sparse.lil_matrix	constructs a sparse matrix for calculating block-average flows
fromgeo	t2grid	constructs a TOUGH2 grid from a mulgrid object
incons	t2incon	constructs initial conditions for the grid
minc	list	creates MINC blocks and connections
radial	t2grid	constructs a radial TOUGH2 grid
rectgeo	(mulgrid, dict)	constructs a mulgrid object from a rectangular TOUGH2 grid
rename_blocks	–	renames blocks the grid
rename_rocktype	–	renames a rock type in the grid
reorder	–	reorders blocks and connections in the grid
rocktype_frequency	integer	frequency of use of a particular rock type
sort_rocktypes	–	sorts rock type list into alphabetical order by name
write_vtk	–	writes grid to VTK file

Table 3.2: Methods of a t2grid object

`add_rocktype(rock)`

Adds a rock type to the grid. If another rock type with the same name already exists, it is replaced.

Parameters:

- **rock**: rocktype
  Rock type to be added to the grid.

`block_index(blockname)`

Returns the block index (in the `blocklist` list) of a specified block name.

Parameters:

- **blockname**: string
  Name of the block.

`blockmap(geo, index = None)`

Returns a mapping from the block name list of the specified geometry object to the block names in the grid.

Parameters:

- **geo**: mulgrid
  Geometry object.

- **index**: list (or `None`)
  Specifies a list of integer indices defining which blocks in the grid to map to. If `None`, all blocks are mapped to.

`calculate_block_centres(geo)`

Calculates geometrical centres of all blocks in the grid, based on the specified geometry object `geo`.

Parameters:

- **geo**: mulgrid
  Geometry object associated with the grid.

`check(fix=False,silent=False)`

Checks a grid for errors and optionally fixes them. Errors checked for are: blocks not connected to any other blocks, and blocks with isolated rocktypes (not shared with any neighbouring blocks). Returns `True` if no errors were found, and `False` otherwise. If `fix` is `True`, any identified problems will be fixed. If `silent` is `True`, there is no printout (only really useful if `fix` is `True`).

Blocks not connected to any others are fixed by deleting them. Isolated-rocktype blocks are fixed by assigning them the most popular rocktype of their neighbours. Blocks with large volumes ($> 10^{20}$ m^3) are never considered isolated (because they often have a special rocktype, such as an atmosphere one, that their neighbours will never share).

Parameters:

- **fix**: Boolean
  Whether to fix any problems identified.

- **silent**: Boolean
  Whether to print out feedback or not.

`clean_rocktypes()`

Deletes any rock types from the grid which are not assigned to any block.

`connection_index(blocknames)`

Returns the connection index (in the `connectionlist` list) of the connection between a specified pair of block names.

Parameters:

- **blocknames**: tuple
  A pair of block names, each of type string.

`copy_connection_directions(geo,grid)`

Copies the connection permeability directions for horizontal connections from another grid. It is assumed that both grids have the same column structure, but may have different layer structures.

Parameters:

- **geo**: `mulgrid`
  Geometry object associated with the source grid.

- **grid**: `t2grid`
  The source grid from which the connection permeability directions are to be copied.

`delete_block(blockname)`

Deletes a block from the grid. This also deletes any connections involving the specified block.

Parameters:

- **blockname**: string
  Name of the block to be deleted from the grid.

`delete_connection(connectionname)`

Deletes a connection from the grid.

Parameters:

- **connectionname**: tuple (of string)
  Pair of block names identifying the connection to be deleted from the grid.

`delete_rocktype(rocktypename)`

Deletes a rock type from the grid.

Parameters:

- **rocktypename**: string
  Name of the rock type to be deleted from the grid.

`demote_block(blockname)`

Shifts a block (or blocks) to the end of the blocklist. This can be useful for making blocks inactive - by setting their volumes to zero or negative, and then shifting them to the end of the list (to avoid all blocks below them also being treated as inactive).

Parameters:

- **blockname**: string or list of strings
  Name(s) of the block(s) to be shifted to the end of the blocklist.

`embed(subgrid, connection)`

Returns a grid with a subgrid embedded inside one of its blocks. The connection specifies how the two grids are to be connected: the blocks to be connected and the connection distances, area etc. between them.

Parameters:

- **subgrid**: `t2grid`
  Subgrid to be embedded.

- **connection**: `t2connection`
  Connection specifying how the subgrid is to be embedded, including the connection distances and area. The first block should be the host block, the second the connecting block in the subgrid.

`empty()`

Empties the grid of all its blocks, rock types and connections.

`flux_matrix(geo, blockmap = {})`

Takes the grid and a corresponding `mulgrid` object, and constructs a sparse matrix (of type `scipy.sparse.lil_matrix`) which can be used to convert connection flow values on the grid to block-average fluxes (flows per unit area). Specifically, if an array of connection flow values (one for each connection in the grid) is multiplied by this sparse matrix, the result is a partitioned array containing the 3-component block-average flux for each of the (non-atmosphere) blocks.

The method for constructing the matrix is as follows. For each block, a distribution of flux is fitted to agree as closely as possible with the connection flow values. This distribution is either constant or linear, depending on how many connections the block has (linear for blocks with at least 6 connections). Fitting the connection values results in a small linear system to solve, which may be under- or over-determined, depending on the number of connections and the type of flux distribution. A pseudo-inverse matrix is calculated which will find the least-squares solution of this system. The total matrix is formed by assembling these matrices for each of the blocks into a global matrix.

Parameters:

- **geo**: `mulgrid`
  The `mulgrid` geometry object (see chapter 2).

- **blockmap**: dictionary
  Dictionary mapping the block names in the geometry to the block naming system used in the grid.

```
fromgeo(geo)
```

Returns a grid constructed from a `mulgrid` geometry object. (Any previous contents of the grid are first emptied.)

Parameters:

- **geo**: `mulgrid`
  The `mulgrid` geometry object (see chapter 2).

```
incons(values=(101.3e3,20.))
```

Returns a `t2incon` set of initial conditions for the grid, using the supplied values. Initial conditions can be specified for only one block, in which case they will be applied to all blocks, or for each block, in an array.

Parameters:

- **values**: `tuple` or `np.array`
  Initial conditions values, either a `tuple` of values for one block, or an `np.array` with each row containing a set of values for one block.

```
minc(volume_fractions, spacing=50., num_fracture_planes=1,
blocks=None, matrix_blockname=None, minc_rockname=None,
proximity=None, atmos_volume=1.e25, incon=None,
fracture_connection_distance=0.)
```

Creates "Multiple Interacting Continua" (MINC) blocks and connections in the grid, for simulating fracture flow with matrix blocks attached to each fracture block. This has capability similar to that of the GMINC program (Pruess, 1983), or of the MINC part of TOUGH2's MESHMAKER section (except that matrix-matrix flow is not supported).

This function returns a rank-2 integer `np.array` with one row for each MINC level, containing the indices of the blocks for that level. For example, the first row is a list of all fracture block indices, the second is a list of all MINC level 1 block indices, etc. This can be useful for identifying all blocks in a given MINC level, for plotting or other post-processing.

For example, if the output index array from this method is `minc_level`, and `T` is an array of temperatures computed over the entire MINC grid (e.g. extracted from the element table of a listing file), then the temperatures in MINC level `m` are given by:

```
T[minc_level[m]]
```

Note that plotting MINC results over a `mulgrid` geometry can be made easier (particularly for grids that have MINC applied over only part of the domain) by using the `minc_array()` method to create the solution vector to plot.

If the `incon` parameter is specified as a `t2incon` object (from the original grid), then this method will also return a new `t2incon` object for the MINC grid, with values copied from the original.

Fracture blocks retain the same block name as their original porous medium blocks. The naming of matrix blocks can be controlled using the `matrix_blockname` parameter.

Parameters:

- **volume_fractions**: list (or `np.array`)
  List or array of volume fractions. The first entry corresponds to the fractures, with subsequent entries specifying the volume fractions for each MINC level. The length of this list or array is therefore equal to one plus the number of matrix blocks to be used.

Entries for all MINC levels must be present, but they need not sum to 1- if they do not, they will be scaled so that the sum is 1. (This means, for example, that entries may be specified as percentage values.)

- **spacing**: float or list (or `np.array`)
  Fracture spacing parameters. If a float value is specified, this is applied to all sets of fracture planes (see below). If a list or array is specified, each entry is applied to its corresponding set of fracture planes.

- **num_fracture_planes**: integer
  Number of sets of fracture planes (1, 2 or 3).

- **blocks**: list (or `None`)
  List of blocks or block names, specifying which blocks are to have MINC applied. If this parameter is `None`, all blocks are processed (except inactive blocks).

- **matrix_blockname**: function (or `None`)
  Function returning the name of a MINC matrix block (string), given the original block name (string) and MINC level (integer > 0). If `None`, a default function will be used, which simply replaces the first character of the original block name with the MINC level.

- **minc_rockname**: function (or `None`)
  Function returning the MINC rocktype name, given the original rocktype name and MINC level (≥ 0). If `None`, a default function will be used, which leaves fracture blocks with their original rocktype (the properties of which can subsequently be edited), and for matrix blocks, simply replaces the first character of the original rocktype name with 'X'.

- **proximity**: function (or `None`)
  Proximity function, returning the total matrix volume within a given distance (float) from the fracture faces. If `None`, a default function will be used, corresponding to the `num_fracture_planes` parameter.

- **atmos_volume**: float
  Maximum block volume for blocks to be considered part of the geometrical grid. Blocks with volume greater than this will be assumed to be boundary condition blocks and no MINC processing will be applied to them.

- **incon**: `t2incon` (or `None`)
  Initial conditions object for the original grid, before MINC processing. If not `None`, then the method returns (as well as the block index array) a new `t2incon` object for the MINC grid, with values for each block copied from the original (for all MINC levels).

- **fracture_connection_distance**: float
  Connection distance between fracture and matrix blocks. Default is zero, as in MESHMAKER, but in some situations a finite value (e.g. 10^{-10} m) can work better.

```
radial(rblocks, zblocks, convention=0, atmos_type=2, origin=[0,0],
justify='r', case=None, dimension=2, blockmap={}, chars=ascii_lowercase, spaces=True)
```

Returns a radial TOUGH2 grid with the specified radial and vertical block sizes. Grid column and layer naming convention, atmosphere type and origin can be specified. The optional `justify` and `case` parameters control the formatting of the character part of the block names.

The `dimension` parameter sets the flow dimension for 'generalized radial flow', which can represent flow in fractured rocks and modifies the block volumes and areas (see Barker (1988)). The default `dimension` = 2 corresponds to standard radial flow.

Parameters:

- **rblocks**, **zblocks**: list (or `np.array`)
  Lists (or arrays) of block sizes in the r and z directions.

- **convention**: integer
  Naming convention for grid columns and layers - same as the naming convention for a `mulgrid` object.

- **atmos_type**: integer
  Type of atmosphere - also the same as the atmosphere type for a `mulgrid` object.

- **origin**: list (or `np.array`)
  Origin of the grid (of length 2 or 3). The first entry is the radial origin, i.e. the starting radius of the grid. The last entry is the vertical origin, i.e. the vertical position of the top of the grid. If of length 3, the middle entry is ignored.

- **justify**: string
  Specify 'r' for the character part of the block names (first three characters) to be right-justified, 'l' for left-justified.

- **case**: string
  Specify 'l' for the character part of the block names (first three characters) to be lower case, 'u' for upper case. Alternatively, use the more flexible `chars` parameter (see below).

- **dimension**: float
  Dimension for 'generalized radial flow', which can take any (possibly non-integer) value between 1 and 3. Dimension 1 corresponds to flow in a linear 'pipe', dimension 2 corresponds to standard radial flow in a disc-shaped reservoir and dimension 3 corresponds to flow in a spherically symmetric reservoir.

- **blockmap**: dictionary
  Dictionary mapping the block names in the geometry to the block naming system used in the grid.

- **chars**: string
  Specify a string of characters to be used to form the character part of block names. For example, to use both lowercase and uppercase characters, set `chars` to `ascii_lowercase + ascii_uppercase`, or to use uppercase letters only, specify `ascii_uppercase`.

- **spaces**: Boolean
  Specify `False` to disallow spaces in character part of block names. In this case, the first element of the `chars` parameter functions like a 'zero' and replaces spaces.

Visualization of radial $r-z$ model grids and results can be done in PyTOUGH by creating a 'dummy' vertical slice rectangular geometry, using the `mulgrid` `rectangular()` method, using its x direction for radius (and having only one block in the y direction - which is not used). The `slice_plot()` method can then be used to plot results.

```
rectgeo(origin_block=None, atmos_volume=1.e25, remove_inactive=False,
convention=0, atmos_type=2, justify='r', chars=ascii_lowercase,
spaces=True, layer_snap=0.1, block_order=None)
```

Creates a `mulgrid` geometry object from a rectangular TOUGH2 grid. It also returns a dictionary defining the mapping from the geometry block names to the grid block names. This block mapping can be used when the block naming convention used by the original TOUGH2 grid is not compatible with the layer/column based naming conventions assumed by a `mulgrid` geometry.

The method works within the following assumptions:

- the grid is in fact rectangular (results will not be predictable otherwise)
- block centre coordinates are present for all blocks in the grid
- the bottom layer of blocks is complete (no missing blocks)

The method should work on rectangular TOUGH2 grids that have been translated and/or horizontally rotated with respect to the coordinate axes. Grids with incomplete upper layers (e.g. representing topography) should also be OK.

Parameters:

- **origin_block**: string, `t2block` or `None`
  The block on the bottom layer of the geometry, at the origin of the axes defined by permeability directions 1 and 2. If `None`, it will be detected. Specify it manually if the algorithm does not detect it correctly.
- **atmos_volume**: float
  Block volume below which blocks are considered part of the geometrical grid. Blocks with volume greater than or equal to this value will be assumed to be boundary condition blocks and will not be represented geometrically.
- **remove_inactive**: Boolean
  Set `True` to remove inactive blocks from the geometry. TOUGH2 treats all blocks with zero or negative volume, and all subsequent blocks in the block list, to be inactive. If this option is used, the inactive blocks will be used to detect the surface elevations of the columns in the geometry. Otherwise, inactive blocks will be retained in the geometry.
- **convention**: integer
  Naming convention for grid columns and layers in the output geometry.
- **atmos_type**: integer
  Type of atmosphere for the output geometry.
- **justify**: string
  Specify 'r' for the character part of the block names (first three characters) to be right-justified, 'l' for left-justified.

- **chars**: string
  Specify a string of characters to be used to form the character part of block names. For example, to use both lowercase and uppercase characters, set `chars` to `ascii_lowercase + ascii_uppercase`, or to use uppercase letters only, specify `ascii_uppercase`.

- **spaces**: Boolean
  Specify `False` to disallow spaces in character part of block names. In this case, the first element of the `chars` parameter functions like a 'zero' and replaces spaces.

- **layer_snap**: float
  Smallest desired surface block thickness. Set to a positive value to eliminate surface blocks in the geometry with very small thicknesses (resulting from column surface elevations that are very close to the bottom of a layer). Default value is 0.1 m. Note that it is not recommended to use a value of zero, as spurious small-thickness surface blocks can arise from rounding errors in reading the data file. If this still occurs, try increasing the snap value until they disappear.

- **block_order**: string or `None`
  Specify `None` or 'layer_column' for default block ordering by layer and column, starting from the atmosphere. Specify 'dmplex' to order blocks by geometrical type (8-node hexahedrons first followed by 6-node wedges) as in PETSc DMPlex meshes.

`rename_blocks(`*`blockmap`* `= {}, `*`fix_blocknames`* `= True)`

Renames blocks in the grid according to the specified block mapping dictionary. Any block whose name is a key of the block mapping dictionary is renamed with the corresponding dictionary value. Related properties such as connections are also renamed.

Parameters:

- **blockmap**: dictionary
  Block mapping dictionary, mapping strings to strings.

- **fix_blocknames**: Boolean
  Set `True` (the default) to 'fix' block names in the dictionary, using the `fix_blockname()` function.

`rename_rocktype(`*`rockname`*`, `*`newrockname`*`)`

Renames a rock type in the grid. An exception is raised if the specified rocktype name does not exist, or if the new target rocktype name has already been used.

Parameters:

- **rockname**: string
  Name of the rock type to be renamed.

- **newrockname**: string
  New name for the rock type.

`reorder(`*`block_names`*`, `*`connection_names`*`=None, `*`geo`*`=None)`

Reorders the blocks (and optionally connections) in the grid.

Parameters:

- **block_names**: list of string (or `None`)
  List specifying the names of the blocks, in their desired order. Each block name must exist in the grid, otherwise an error will be raised. If this parameter is `None` (the default), blocks are not reordered (unless a geometry is specified instead).

- **connection_names**: list of string (or `None`)
  List specifying the names of the connections, in their desired order. Each item in the list should be a tuple of block names. The ordering of the block names in any tuple may be reversed with respect to the original connection naming. However an error will be raised if any tuple of block names in the list does not exist in the grid (in either its forward or reverse form). If this parameter is `None` (the default), connections are not reordered (unless a geometry is specified instead).

- **geo**: `mulgrid` geometry (or `None`)
  Geometry object to use for the reordering. If this is specified, the geometry's block and connection name lists are used (and the previous parameters are ignored). After reordering, the grid's blocks and connections will have the same ordering as if the grid had been created using the `fromgeo()` method.

`rocktype_frequency(`*`rockname`*`)`

Returns the frequency of use of the rock type with the specified name, i.e. how many blocks are assigned that rock type.

Parameters:

- **rockname**: string
  Name of the specified rock type.

`sort_rocktypes()`

Sorts the rocktype list into alphabetical order by name.

`write_vtk(`*`geo`*`, `*`filename`*`, `*`wells`*`=False, `*`blockmap`*` = {}, `*`surface_snap`*`=0.1)`

Writes a `t2grid` object to a VTK file on disk, for visualisation with VTK, Paraview, Mayavi etc. The grid is written as an 'unstructured grid' VTK object with data arrays defined on cells. The data arrays written, in addition to the defaults arrays for the associated `mulgrid` object, are: rock type index, porosity and permeability for each block. A separate VTK file for the wells in the grid can optionally be written.

Parameters:

- **geo**: `mulgrid`
  The `mulgrid` geometry object associated with the grid. This is required as the `t2grid` object does not contain any spatial information, e.g. locations of block vertices.

- **filename**: string
  Name of the VTK file to be written. This is also required.

- **wells**: Boolean
  Set to `True` if the wells from the `mulgrid` object are to be written to a separate VTK file.

- **blockmap**: dictionary
  Dictionary mapping the block names in the geometry to the block naming system used in the grid.

- **surface_snap**: float
  Tolerance for specifying how close column surface elevations need to be before being considered "equal" when constructing surface nodes.

3.3 Other objects (`rocktype`, `t2block` and `t2connection`)

A `t2grid` object contains lists of other types of objects: `rocktype`, `t2block` and `t2connection`. These classes are described below.

3.3.1 `rocktype` objects

A `rocktype` object represents a TOUGH2 rock type. The properties of a `rocktype` object, and their default values, are given in Table 3.3.

The main familiar properties of a rock type are referred to in a natural way, e.g. the porosity of a rock type `r` is given by `r.porosity`. The permeability property is a 3-element `np.array`, giving the permeability in each of the three principal axes of the grid, so e.g. the vertical permeability of a rock type `r` would normally be given by `r.permeability[2]` (recall that array indices in Python are zero-based, so that the third element has index 2).

Some rock type properties are optional, and only need be specified when the property `nad` is greater than zero. An example is the relative permeability and capillarity functions that can be specified for a rock type when `nad` ≥ 2. The way these functions are specified is described in chapter 4.

Example:

```
r = rocktype(name = 'ignim', permeability = [10.e-15, 10.e-15, 2.e-15],
    specific_heat = 850)
```

declares a rocktype object called `r` with name 'ignim', permeability of 10 mD in the first and second directions and 2 mD in the vertical direction, and specific heat 850 J.kg^{-1}.K^{-1}.

(Note that when declaring rock types, the permeability can for convenience be specified as a list, which will be converted internally to an `np.array`.)

3.3.2 `t2block` objects

A `t2block` object represents a block in a TOUGH2 grid. The properties of a `t2block` object are given in Table 3.4. These reflect the specifications of a TOUGH2 block as given in a TOUGH2 data file, with the exception of the `atmosphere`, `centre`, `connection_name`, `neighbour_name` and `num_connections` properties.

The `atmosphere` property determines whether the block is to be treated as an atmosphere block. The `centre` property can optionally be used to specify the coordinates of the centre of a block. Block centres are automatically calculated when a `t2grid` object is constructed from a `mulgrid` object using the `fromgeo` method). The `connection_name` property is a set containing the names (as tuples of strings) of all connections involving the block.

A `t2block` object has no methods.

Property	Type	Description	Default
capillarity	dictionary	capillarity function	–
compressibility	float	compressibility	0 $m^2.N^{-1}$
conductivity	float	heat conductivity	1.5 $W.m^{-1}.K^{-1}$
density	float	rock grain density	2600 $kg.m^{-3}$
dry_conductivity	float	dry heat conductivity	wet heat conductivity
expansivity	float	expansivity	0 K^{-1}
klinkenberg	float	Klinkenberg parameter	0 Pa^{-1}
nad	integer	number of extra data lines	0
name	string	rock type name	'dfalt'
permeability	np.array	permeability	np.array([10^{-15}]*3) m^2
porosity	float	porosity	0.1
relative_permeability	dictionary	relative permeability function	–
specific_heat	float	rock grain specific heat	900 $J.kg^{-1}.K^{-1}$
tortuosity	float	tortuosity factor	0
xkd3	float	used by EOS7R	0 $m^3.kg^{-1}$
xkd4	float	used by EOS7R	0 $m^3.kg^{-1}$

Table 3.3: Properties of a rocktype object

Property	Type	Description
ahtx	float	interface area for heat exchange (TOUGH2 only)
atmosphere	Boolean	whether block is an atmosphere block or not
centre	np.array	block centre (optional)
connection_name	set	names of connections involving the block
nadd	integer	increment between block numbers in sequence
name	string	block name
neighbour_name	set	names of neighbouring (connected) blocks
nseq	integer	number of additional blocks in sequence
num_connections	integer	number of connections containing the block
pmx	float	permeability modifier (TOUGH2 only)
rocktype	rocktype	rock type
volume	float	block volume

Table 3.4: Properties of a t2block object

Property	Type	Description
area	float	connection area
block	list	two-element list of blocks
dircos	float	gravity direction cosine
direction	integer	permeability direction (1, 2, or 3)
distance	list	two-element list of connection distances
nad1,nad2	integer	increments in sequence numbering
nseq	integer	number of additional connections in sequence
sigma	float	radiant emittance factor (TOUGH2 only)

Table 3.5: Properties of a t2connection object

3.3.3 t2connection objects

A t2connection object represents a connections between two TOUGH2 blocks. The properties of a t2connnection object are given in Table 3.5. These correspond to the properties of a connection specified in a TOUGH2 data file. Note that the block property returns t2block objects, not just the names of the blocks in the connection. Hence, for example, the volume of the first block in a connection object con is given simply by con.block[0].volume.

A t2connection object has no methods.

3.4 Example

The following piece of Python script creates a rectangular 2-D slice TOUGH2 grid with two rock types, and assigns these rock types to blocks in the grid according to their position along the slice.

```
from t2grids import *

geo = mulgrid().rectangular([500]*20, [1000], [100]*20, atmos_type = 0,
    convention = 2)
geo.write('2Dgrd.dat')
grid = t2grid().fromgeo(geo)

grid.add_rocktype(rocktype('greyw', permeability = [1.e-15]*2 + [0.1e-15]))
grid.add_rocktype(rocktype('fill ', permeability = [15.e-15]*2 + [5.e-15]))

for blk in grid.blocklist[1:]:
    if 200 <= blk.centre[0] <= 400: blk.rocktype = grid.rocktype['fill ']
    else: blk.rocktype = grid.rocktype['greyw']
```

The first line just imports the required PyTOUGH library. (It is not necessary to import the mulgrids library explicitly, because it is used and therefore imported by the t2grids library.)

The second block of code creates a rectangular MULgraph geometry object with 20 columns (each 500 m wide) along the slice and 20 layers (each 100 m thick), writes this to a geometry file on disk, and creates a TOUGH2 grid from it.

Then the two rock types are created, 'greyw' and 'fill '. (Note that rock types are

expected by TOUGH2 to have names 5 characters long, so it is necessary to add spaces to shorter names.)

The final part assigns the rock types to the blocks in the grid. The loop starts from 1 instead of 0, so that the atmosphere block is skipped. In this example, the blocks in the grid are assigned the `'fill '` rock type if they are between 200 m and 400 m along the slice. Blocks outside this region are assigned the `'greyw'` rock type.

Chapter 4

TOUGH2 data files

4.1 Introduction

The `t2data` library in PyTOUGH contains classes and routines for creating, editing and saving TOUGH2 or AUTOUGH2 data files. It can be imported using the command:

```
from t2data import *
```

4.2 `t2data` objects

The `t2data` library defines a `t2data` class, used for representing TOUGH2 data files.

Example:

```
dat = t2data()
```

creates an empty `t2data` object called `dat`.

```
dat = t2data(filename)
```

creates a `t2data` object called `dat` and reads its contents from file `filename`. (It is also possible to read the mesh part of the `t2data` object from separate files - see below.)

Because a `t2data` object contains a large number of different parameters, it is usually easier to load one from an existing TOUGH2 data file and edit it, rather than creating a new one from scratch.

4.2.1 Properties

The main properties of a `t2data` object are listed in Table 4.1. In general, each of these properties corresponds to an input block in a TOUGH2 data file. Most of these input blocks contain a number of different parameters, so that the `t2data` property corresponding to each input block is usually in the form of a dictionary, containing a number of keys representing sub-properties.

For example, the maximum number of time steps for the simulation is controlled by `max_timesteps` key in the `parameter` property, which for a `t2data` object called `dat` would be accessed by `dat.parameter['max_timesteps']`.

The details of all the `t2data` properties are given below.

Property	Type	Description	Input block
capillarity	dictionary	capillarity function	RELP
diffusion	list	diffusion coefficients	DIFFU
echo_extra_precision	Boolean	echoing extra precision sections to main data file (AUTOUGH2 only)	–
end_keyword	string	keyword to end file	ENDCY or ENDFI
extra_precision	list	data sections read from extra precision auxiliary file (AUTOUGH2 only)	–
filename	string	file name on disk	–
generator	dictionary	generators (by block name and generator name)	GENER
generatorlist	list	generators (by index)	GENER
grid	t2grid	model grid	ELEME, CONNE
history_block	list	history blocks (TOUGH2 only)	FOFT
history_connection	list	history connections (TOUGH2 only)	COFT
history_generator	list	history generators (TOUGH2 only)	GOFT
incon	dictionary	initial conditions	INCON
indom	dictionary	rocktype-specific initial conditions	INDOM
lineq	dictionary	linear equation solver options (AUTOUGH2 only)	LINEQ
meshfilename	string or tuple	file name(s) on disk containing mesh data	–
meshmaker	list	mesh generation options	MESHM
more_option	array of integer	additional parameter options	MOMOP
multi	dictionary	EOS configuration	MULTI
noversion	Boolean	suppressing printing of version summary	NOVER
num_generators	integer	number of generators	–
output_times	dictionary	times to write output	TIMES
parameter	dictionary	run-time parameters	PARAM
relative_permeability	dictionary	relative permeability function	RELP
selection	dictionary	selection parameters	SELEC
short_output	dictionary	short output (AUTOUGH2 only)	SHORT
simulator	string	simulator name (AUTOUGH2 only)	SIMUL
solver	dictionary	linear equation solver options (TOUGH2 only)	SOLVR
start	Boolean	run initialisation option	START
title	string	simulation title	TITLE
type	string	simulator type (AUTOUGH2 or TOUGH2)	–

Table 4.1: Properties of a `t2data` object

Key	Type	Description	TOUGH2 parameter
`parameters`	array (7) of float	function parameters	CP
`type`	integer	type of capillarity function	ICP

Table 4.2: `capillarity` property keys

`capillarity` property

A dictionary property specifying the capillarity function used, corresponding to the second line of the **RPCAP** input block in the TOUGH2 data file. The individual keys of this property are given in Table 4.2.

`diffusion` property

A list property specifying diffusion coefficients for each mass component simulated, corresponding to the **DIFFU** input block in the TOUGH2 data file. The list has length `multi['num_components']` (i.e. NK in TOUGH2 terminology), and each element is a list of the diffusion coefficients for each component (with length `multi['num_phases']`, or NPH).

`echo_extra_precision` property

A Boolean property (AUTOUGH2 only) governing whether data written to an auxiliary extra-precision file is also echoed to the main data file. If `True`, all extra-precision data sections are echoed to the main file.

`end_keyword` property

A string property containing the keyword used in the data file to end the file. Normally this is 'ENDCY', but 'ENDFI' can also be used.

`extra_precision` property

A list property determining which data sections will be written to an auxiliary extra-precision file (AUTOUGH2 only). Recent versions of AUTOUGH2 support an additional data file containing some data written with extra precision. Possible extra-precision data sections are ROCKS, ELEME, CONNE, RPCAP and GENER. Typical usage of this extra-precision data is for automatic model calibration using PEST or similar software, where calculation of derivatives of model outputs with respect to model parameters requires higher precision than is possible with the standard TOUGH2 data file format.

The `extra_precision` parameter may be a list containing names of sections to be written in extra precision (e.g. ['RPCAP', 'GENER']), or set to `False` to disable extra precision (equivalent to []), or to `True` to specify that all possible sections should be written in extra precision.

The `read()` method of a `t2data` object determines whether extra precision data are available by searching for an additional file with the same base name as the data file itself, but with a '.pdat' or '.PDAT' extension (depending on the case of the main data file name). If no such file exists, then no extra precision data will be read.

filename property

A string property containing the name of the TOUGH2 data file on disk. (This does not correspond to any parameter in the TOUGH2 data file.)

generator property

A dictionary property containing the generators for the simulation, accessed by tuples of block name and generator name. Each generator is an object of type `t2generator`, which is described in section 4.3.

generatorlist property

A list property containing the generators for the simulation, accessed by index.

grid property

A `t2grid` object (see chapter 3) representing the simulation grid, corresponding to the **ELEME** and **CONNE** input blocks in a TOUGH2 data file.

history_block property

A list property containing blocks for which time history output is required, corresponding to the **FOFT** input block in a TOUGH2 data file. If the `t2data` object contains grid data, the items in this list are `t2block` objects; otherwise, they are block names (i.e. strings).

history_connection property

A list property containing connections for which time history output is required, corresponding to the **COFT** input block in a TOUGH2 data file. If the `t2data` object contains grid data, the items in this list are `t2connection` objects; otherwise, they are tuples of block names (i.e. tuples of strings).

history_generator property

A list property containing blocks in which generators are defined and for which time history output is required, corresponding to the **GOFT** input block in a TOUGH2 data file. If the `t2data` object contains grid data, the items in this list are `t2block` objects; otherwise, they are block names (i.e. strings).

incon property

A dictionary property representing the initial conditions for the simulation, accessed by block name, corresponding to the **INCON** input block in a TOUGH2 data file. The value of each element of the dictionary is a list consisting of the porosity of the block, followed by a list of the specified initial primary thermodynamic variables in the block. If the TOUGH2 NSEQ and NADD values are used, these are stored after the thermodynamic variables. If they are not used, they can either be set to `None` or simply omitted.

Key	Type	Description	AUTOUGH2 parameter
`epsilon`	float	solver tolerance	EPN
`gauss`	integer	Gauss elimination parameter	IGAUSS
`max_iterations`	integer	max. number of iterations	MAXIT
`num_orthog`	integer	number of orthogonalisations	NORTH
`type`	integer	type of solver (1 or 2)	ISOLVR

Table 4.3: `lineq` property keys

For example, to specify porosity 0.1 and initial conditions (101.3E3, 20.0) in block `'AB105'` of a `t2data` object called `dat`, set `dat.incon['AB105'] = [0.1, [101.3e3, 20.0]]`.

To specify these same conditions but with NSEQ = 10 and NADD = 2, set `dat.incon['AB105'] = [0.1, [101.3e3, 20.0], 10, 2]`.

Porosity can be specified as `None` if default porosity (from the rocktype) is to be used.

`indom` property

A dictionary property representing the initial conditions for the simulation, accessed by rocktype name, corresponding to the **INDOM** input block in a TOUGH2 data file. The value of each element of the dictionary is a list consisting of the specified initial primary thermodynamic variables for the rocktype.

`lineq` property

A dictionary property representing linear equation solver options, corresponding to the **LINEQ** input block in an AUTOUGH2 data file. The individual keys of this property are given in Table 4.3.

`meshfilename` property

A string property (or tuple of strings) containing the name(s) of files on disk containing the mesh data. (This does not correspond to any parameter in the TOUGH2 data file.) Its default value is an empty string which means mesh data will be read from the main data file.

If `meshfilename` is a single (non-empty) string, this is interpreted as the name of a formatted text file containing 'ELEME' and 'CONNE' sections specifying the mesh (e.g. the 'MESH' file created by TOUGH2 or TOUGH2_MP).

If `meshfilename` is a tuple of two strings, these are interpreted as the names of two binary files containing the mesh data, e.g. the 'MESHA' and 'MESHB' files created by TOUGH2_MP.

`meshmaker` property

A list property representing mesh generation options, corresponding to the **MESHM** input block in a TOUGH2 data file. For more detail on the use of **MESHM** data, consult the TOUGH2 users' guide (Pruess et al., 1999).

The **MESHM** data may contain multiple sections (e.g. creation of a rectilinear XYZ grid followed by MINC processing), so the `meshmaker` property is structured as a list of

Key	Type	Description	TOUGH2 parameter
radii sub-section keys			
`radii`	list	specified mesh radii	RC
equid sub-section keys			
`dr`	float	radial increment	DR
`nequ`	integer	number of equidistant radii	NEQU
logar sub-section keys			
`dr`	float	reference radial increment	DR
`nlog`	integer	number of logarithmic radii	NLOG
`rlog`	float	largest radius	RLOG
layer sub-section keys			
`layer`	list	layer thicknesses	H

Table 4.4: `rz2d` data keys

two-element tuples, each containing the type of section (`rz2d`, `xyz` or `minc`) followed by the section data itself.

The form of the section data varies depending on the section type. For the `rz2d` type it is also structured as a list, as these types may contain variable numbers of sub-sections. (For example, data for the `rz2d` type may contain multiple `logar` sub-sections for different logarithmic radial parts of the mesh.) Each sub-section is again a two-element tuple, consisting of the sub-section type (a string) followed by a dictionary containing the data for the sub-section.

Data for the `xyz` type are also structured as a list, with the first element containing the stand-alone `deg` parameter (a float), followed by the other sub-sections, corresponding to the **NX**, **NY** and **NZ** sub-sections in the TOUGH2 data file. The `minc` type does not have sub-sections so MINC data are not structured as a list but simply a dictionary.

Possible sub-section types for `rz2d` data are `radii`, `equid`, `logar` and `layer`, corresponding to their (uppercase) keyword counterparts in the TOUGH2 data file. Data keys for these types are given in Table 4.4. Data keys for the `xyz` and `minc` data are given in Tables 4.5 and 4.6.

Example: The easiest way to understand how the `meshmaker` property works is to read some example input data into a `t2data` object and examine the result. The **MESHM** data for the standard TOUGH2 test problem 'rhbc' ('Production from a geothermal reservoir with hypersaline brine') is represented as a `t2data meshmaker` property as follows:

```
[('rz2d',[
 ('radii', {'radii': [5.0]}),
 ('equid', {'dr': 2.0, 'nequ': 1}),
 ('logar', {'rlog': 100.0, 'nlog': 50}),
 ('logar', {'rlog': 1000.0, 'nlog': 20}),
 ('equid', {'dr': 0.0, 'nequ': 1}),
 ('layer', {'layer': [500.0]})
 ])
]
```

Key	Type	Description	TOUGH2 parameter
deg parameter			
deg	float	angle between y-axis and horizontal	DEG
NX, NY and NZ keys			
del	float	constant grid increment	DEL
deli	list	variable grid increments	DEL
no	integer	number of grid increments	DR
ntype	string	axis direction ('NX', 'NY' or 'NZ')	NTYPE

Table 4.5: xyz data keys

Key	Type	Description	TOUGH2 parameter
dual	string	treatment of global matrix-matrix flow	DUAL
num_continua	integer	number of interacting continua	J
spacing	list	fracture spacings	PAR
type	string	proximity function type	TYPE
vol	list	volume fractions	VOL
where	string	direction of volume fraction specification	WHERE

Table 4.6: minc data keys

more_option property

An array property containing additional integer parameter options, corresponding to the **MOMOP** input block in a TOUGH2 data file (it is not recognised by AUTOUGH2). Introduced by iTOUGH2, this is an extension of the parameter.option property. It is of length 21 and is populated with zeros by default. Like the parameter.option property, values are accessed using 1-based (not zero-based) indices.

multi property

A dictionary property selecting the equation of state (EOS) module used and setting associated parameters, corresponding to the **MULTI** input block in a TOUGH2 or AUTOUGH2 data file. The individual keys of this property are given in Table 4.7.

noversion property

A Boolean property specifying whether to suppress printing of version and date information, corresponding to the **NOVER** input block in a TOUGH2 data file.

num_generators property

A read-only integer property returning the number of generators.

output_times property

Key	Type	Description	TOUGH2 parameter
eos	string	EOS name (AUTOUGH2 only)	NAMEOS
num_components	integer	number of components	NK
num_equations	integer	number of equations	NEQ
num_inc	integer	number of mass components in INCON data (TOUGH2 only)	NKIN
num_phases	integer	number of phases	NPH
num_secondary_parameters	integer	number of secondary parameters	NB

Table 4.7: multi property keys

Key	Type	Description	TOUGH2 parameter
max_timestep	float	maximum time step	DELAF
num_times_specified	integer	number of times specified	ITI
num_times	integer	total number of times	ITE
time	list of float	times at which output is required	TIS
time_increment	float	time increment after specified times	TINTER

Table 4.8: output_times property keys

A dictionary property specifying the times at which model output is required, corresponding to the **TIMES** input block in a TOUGH2 data file. The individual keys of this property are given in Table 4.8.

`parameter` property

A dictionary property specifying run-time parameters, corresponding to the **PARAM** input block in a TOUGH2 data file. The individual keys of this property are given in Table 4.9.

The `option` parameter (MOP array in TOUGH2) is an array of 24 integers, and has a 1-based index so that its indices are the same as those in the TOUGH2 documentation. (In fact it is really zero-based, like all other Python arrays, but has an extra unused zeroth element).

`relative_permeability` property

A dictionary property specifying the relative permeability function used, corresponding to the first line of the **RPCAP** input block in the TOUGH2 data file. The individual keys of this property are given in Table 4.10.

`selection` property

A dictionary property representing selection parameters for the simulation (only used by some EOS modules, e.g. EOS7, EOS7R, EWASG), corresponding to the **SELEC** block in the TOUGH2 data file.

The dictionary contains two keys: 'integer' and 'float', the first of which accesses a list of the integer selection parameters (the first line of the **SELEC** block), while the second accesses a list of the float selection parameters (the remaining lines of the **SELEC** block).

`short_output` property

A dictionary property representing blocks, connections and generators for which short output is required, corresponding to the **SHORT** input block in an AUTOUGH2 data file.

The dictionary contains four keys: 'frequency', 'block', 'connection' and 'generator'. The last three of these access lists of blocks, connections and generators respectively for short output. (Note that each of these lists contains `t2block`, `t2connection` or `t2generator` objects, rather than names.) The 'frequency' key accesses the time step frequency (an integer) for which short output is required.

`simulator` property

A string property specifying the type of simulator, corresponding to the **SIMUL** input block in an AUTOUGH2 data file.

`solver` property

A dictionary property representing linear equation solver options, corresponding to the **SOLVR** input block in a TOUGH2 data file. The individual keys of this property are given in Table 4.11.

Key	Type	Description	TOUGH2 parameter
absolute_error	float	absolute convergence tolerance	RE2
be	float	enhanced vapour diffusion	BE
const_timestep	float	time step length	DELTEN
default_incons	list of float	default initial conditions	DEP
derivative_increment	float	numerical derivate increment factor	DFAC
diff0	float	diffusive vapour flux (AUTOUGH2 only)	DIFF0
gravity	float	gravitational acceleration	GF
max_duration	integer	maximum simulation duration (machine seconds)	MSEC
max_iterations	integer	maximum number of iterations per time step	NOITE
max_timesteps	integer	maximum number of time steps	MCYC
max_timestep	float	maximum time step size	DELTMX
newton_weight	float	Newton-Raphson weighting factor	WNR
option	array(24) of integer	simulation options	MOP
pivot	float	pivoting parameter for linear solver	U
print_block	string	block name for short printout	ELST
print_interval	integer	time step interval for printing	MCYPR
print_level	integer	amount of printout	KDATA
relative_error	float	relative convergence tolerance	RE1
scale	float	grid scale factor	SCALE
texp	float	binary diffusion temperature parameter	TEXP
timestep_reduction	float	time step reduction factor	REDLT
timestep	list of float	specified time step sizes	DLT
tstart	float	start time (seconds)	TSTART
tstop	float	stop time	TIMAX
upstream_weight	float	upstream weighting factor	WUP

Table 4.9: `parameter` property keys

Key	Type	Description	TOUGH2 parameter
parameters	array (7) of float	function parameters	RP
type	integer	type of relative permeability function	IRP

Table 4.10: relative_permeability property keys

Key	Type	Description	TOUGH2 parameter
closure	float	convergence criterion	CLOSUR
relative_max_iterations	float	relative max. number of iterations	RITMAX
type	integer	solver type	MATSLV
o_precond	string	O-preconditioning type	OPROCS
z_precond	string	Z-preconditioning type	ZPROCS

Table 4.11: solver property keys

start property

A Boolean property specifying whether the flexible start option is used, corresponding to the **START** input block in a TOUGH2 data file.

title property

A string property containing the simulation title, corresponding to the **TITLE** input block in a TOUGH2 data file.

type property

A string property specifying the simulator type ('AUTOUGH2' or 'TOUGH2'). Changing the value of this property will cause one of the convert_to_TOUGH2() or convert_to_AUTOUGH2() methods to be executed, with default method parameters. Hence, changing the type property to 'AUTOUGH2' causes the EOS to be set to the default 'EW'. It is also not possible to specify TOUGH2_MP options when setting type. For more control over how the conversion is carried out, use the conversion methods directly instead of setting type.

4.2.2 Functions for reading data from file

It is possible to specify customized functions to control how data are read from a TOUGH2 data file. This is done using the optional read_function parameter when a t2data object is created- in exactly the same way it is done for a mulgrid object. For more details, see the corresponding documentation for mulgrid objects in section 2.2.1. By default, the read functions for t2data objects are given by the default_read_function dictionary.

4.2.3 Methods

The main methods of a t2data object are listed in Table 4.12. Details of these methods are given below.

Method	Type	Description
add_generator	–	adds a generator
clear_generators	–	deletes all generators
convert_to_AUTOUGH2	–	converts from TOUGH2 input to AUTOUGH2
convert_to_TOUGH2	–	converts from AUTOUGH2 input to TOUGH2
delete_generator	–	deletes a generator
delete_orphan_generators	–	deletes orphaned generators
effective_incons	list or t2incon	effective initial conditions
generator_index	integer	returns index of generator with specified name and block name
json	dictionary	Waiwera JSON input
read	t2data	reads data file from disk
rename_blocks	–	renames blocks
run	–	runs a TOUGH2 simulation
specific_generation	np.array	generation per unit volume in each block
total_generation	np.array	total generation in each block
transfer_from	–	transfers data from another t2data object
write	–	writes to data file on disk

Table 4.12: Methods of a t2data object

`add_generator(generator)`

Adds a generator to the data file object.

Parameters:

- **generator**: t2generator
  Generator to be added to the data file object.

`convert_to_AUTOUGH2(warn=True, MP=False, simulator='AUTOUGH2.2', eos='EW')`

Converts a TOUGH2 (or TOUGH2_MP) data file for use with AUTOUGH2. Various parameter options are altered to try to make the AUTOUGH2 simulation give similar results to the original TOUGH2 simulation. If necessary, the `filename` property is changed to end in '.dat' (or '.DAT', depending on the case of the base file name), as required by AUTOUGH2.

The simulator and EOS name can also be specified, as AUTOUGH2 data files contain this information in the SIMUL and MULTI sections.

Parameters:

- **warn**: Boolean
  If `True`, warnings will be printed regarding TOUGH2 options used in the original data file which are not supported in AUTOUGH2.

- **MP**: Boolean
  if `True`, treats the original `t2data` object as a TOUGH2_MP data file, which uses some of the parameters differently (e.g. MOP(20)).

- **simulator**: string
  Simulator name, used for the leading part of the AUTOUGH2 SIMUL data section. Possible values are 'MULKOM', 'TOUGH2', 'TOUGH2.2', 'AUTOUGH2' and 'AUTOUGH2.2'.

- **eos**: string
  EOS name, used for the trailing part of the AUTOUGH2 SIMUL data section (e.g. 'EW', 'EWC', 'EWA', 'EWAV' etc.)

`convert_to_TOUGH2(warn=True, MP=False)`

Converts an AUTOUGH2 data file for use with TOUGH2 (or compatible simulators such as TOUGH2_MP). Various parameter options are altered to try to make the TOUGH2 simulation give similar results to the original AUTOUGH2 simulation. This particularly affects AUTOUGH2 options related to backward compatibility with MULKOM. In particular, if these are used then the heat conductivities in the ROCKS block have to be altered to give the same results. Data blocks specific to AUTOUGH2 (e.g. SIMULATOR, LINEQ, and SHORT) are removed, and AUTOUGH2-specific generator types are converted to their TOUGH2 equivalents if possible, or otherwise deleted.

Parameters:

- **warn**: Boolean
  If `True`, warnings will be printed regarding AUTOUGH2 options used in the original data file which are not supported in TOUGH2.

- **MP**: Boolean
  if `True`, converts to a TOUGH2_MP data file, which treats some of the parameters differently (e.g. MOP(20)). The `filename` property is also changed to INFILE, as required by TOUGH2_MP.

`clear_generators()`

Deletes all generators from the data file object.

`delete_generator(blocksourcenames)`

Deletes the generator with the specified block and generator (source) name, if it exists.

Parameters:

- **blocksourcenames**: tuple
  Tuple of block name and generator name (both strings) of the generator to be deleted.

`delete_orphan_generators()`

Deletes all generators with block names that are not in the grid.

`effective_incons(incons = None)`

Returns effective initial conditions, based on on the specified initial conditions in combination with any initial conditions specified in the `t2data` object itself – whether as default initial conditions specified via the `parameter` property, or via the `incon` property, or the `indom` property (or any combination of these).

Any `indom` specifications override the defaults in the `parameter` property. Values in the `incon` property override both the defaults and values in `indom`. Finally, values passed into this method via the `incons` parameter override any other specifications. Note that any of these may contain incomplete specifications (i.e. values are not specified for all blocks in the grid).

If only default homogeneous initial conditions are in effect, then a list of the primary variables is returned. Otherwise, a `t2incon` object is returned with initial conditions values for every block.

Parameters:

- **incons**: `t2incon` or `None`
  Initial conditions object, usually representing the contents of a separate initial conditions file.

```
generator_index(blocksourcenames)
```

Returns the index (in the `generatorlist` list) of the generator with the specified block and generator name.

Parameters:

- **blocksourcenames**: tuple
  Tuple of block name and generator name (both strings) of the generator.

```
json(geo, mesh_filename, atmos_volume = 1.e25, incons = None, eos = None,
bdy_incons = None, mesh_coords = 'xyz')
```

Returns a JSON dictionary representing the contents of the `t2data` object (and associated mesh geometry), suitable for input to the Waiwera simulator (`http://waiwera.github.io`).

Parameters:

- **geo**: `mulgrid`
  Geometry object. Note that geometric meshes with column surface elevations that do not correspond to layer elevations are not supported in Waiwera. For meshes of this type, the column surface elevations can be "snapped" to layer elevations using the `snap_columns_to_nearest_layers()` method. In that case the `t2grid` in the `t2data` object must be updated so it corresponds to the snapped mesh geometry, and other parts of the data file updated to reference the new mesh (e.g. using the `transfer_from()` method). The geometry's `block_order` property should be set to 'dmplex', particularly if it contains mixtures of 3- and 4-sided columns.

- **mesh_filename**: string
  The filename of the mesh file (e.g. ExodusII or GMSH mesh) for the Waiwera simulation.

- **atmos_volume**: float
  Maximum block volume for blocks to be considered part of the geometric grid. Blocks with volume greater than this value (or zero) will be treated as boundary condition (e.g. atmosphere) blocks rather than part of the simulation mesh.

- **incons**: `t2incon`, string, or `None`
  Initial conditions for the Waiwera model. If specified as a string, this should be the filename of the Waiwera HDF5 output file for restarting the simulation from the output of a previous run. If `None` is specified, then default initial conditions will be applied from the `parameter` property (see 4.2.1).

- **eos**: string, integer or `None`
  Equation of state used for the simulation. For AUTOUGH2 simulations, this can generally be set to `None`, and the EOS will be read from the `t2data simulator` or `multi` properties. Otherwise, it can be specified as an integer corresponding to the EOS number (1 being pure water, 2 being water / CO_2 etc.) or as a string corresponding to the AUTOUGH2 EOS names (EOS1 being 'EW', EOS2 being 'EWC' etc.). Note that only EOS modules 1, 2 and 4 (i.e. 'W', 'EW', 'EWC' and 'EWAV' in terms of AUTOUGH2 EOS names) are supported.

- **bdy_incons**: `t2incon`, or `None`
  TOUGH2 initial conditions from which boundary conditions are to be derived. In many cases this parameter is not needed, because boundary conditions are taken from the `incons` parameter: if the `incons` parameter is specified as a `t2incon` object, then the `bdy_incons` parameter can be set to `None`. If, however, `incons` is a string or `None`, then it will not contain boundary condition data, in which case boundary conditions can be specified by passing a `t2incon` object as the `bdy_incons` parameter; otherwise, if this is set to `None` then default boundary conditions will be applied from the default initial conditions in the `t2data parameter` property. Faces on which to apply boundary conditions are identified by the presence of connections to blocks with either zero or large volume (above the volume specified by the `atmos_volume` parameter). Note that for side boundary conditions (with horizontal connections), the boundary blocks must have centres defined, otherwise it is not possible to calculate the appropriate normal vector for the boundary condition.

- **mesh_coords**: string
  String representing the coordinate system to be used in the Waiwera model. 3-D Cartesian meshes are identified as 'xyz'. 2-D Cartesian meshes may be identified as either 'xy', 'xz', or 'yz' (depending on orientation), while 2-D radial meshes are identified as 'rz'.

`read(filename, meshfilename='')`

Reads a `t2data` object from a TOUGH2 data file on disk. The mesh data may optionally be read from auxiliary files, if it is not present in the main data file. (Note that if the main data file does contain mesh information (the 'ELEME' and 'CONNE' sections), any auxiliary mesh files will not be read.)

Parameters:

- **filename**: string
  Name of the TOUGH2 data file to be read.

- **meshfilename**: string or tuple
  Name of separate mesh file(s) to read, containing element and connection data. If empty, then mesh data will be read from the main data file. If a non-empty string is given, this is interpreted as the name of a formatted text file containing 'ELEME' and 'CONNE' data sections (as in the 'MESH' files created by TOUGH2 and TOUGH2_MP). If a tuple of two filenames is given, these are interpreted as the names of the two binary MESHA and MESHB files used by TOUGH2_MP.

Note that it is possible to create a `t2data` object and read its contents in from disk files in one step, e.g.: `dat = t2data(filename,meshfilename)`.

```
rename_blocks(blockmap={}, invert=False, fix_blocknames = True)
```

Renames blocks in the model according to the specified block mapping dictionary. Any block whose name is a key of the block mapping dictionary is renamed with the corresponding dictionary value. The blocks in the `t2grid` object are renamed using its own `rename_blocks()` method. Other `t2data` properties such as generators, initial conditions and history specifications are similarly renamed.

Parameters:

- **blockmap**: dictionary
  Block mapping dictionary, mapping strings to strings.

- **invert**: Boolean
  Set `True` to invert the block mapping dictionary, i.e. to map its values to its keys. This can be used, for example, to rename the blocks to correspond to a geometry created using the `t2grid rectgeo()` method, via the block mapping dictionary also created by that method.

- **fix_blocknames**: Boolean
  Set `True` (the default) to 'fix' block names in the dictionary, using the `fix_blockname()` function.

```
run(save_filename='', incon_filename='', simulator='AUTOUGH2_2',
silent=False, output_filename='')
```

Runs an AUTOUGH2 or TOUGH2 (but not TOUGH2_MP) simulation using the data file corresponding to a `t2data` object. The contents of the `t2data` object must first have been written to disk using the `write` function. If the file names for the save file or initial conditions file are not specified, they are constructed by changing the file extension of the data file name. The name of the TOUGH2 executable can be specified.

For running TOUGH2 (rather than AUTOUGH2), the name of the TOUGH2 executable must be specified via the `simulator` parameter. However, the `save_filename` and `incon_filename` parameters do not need to be specified. Initial conditions will be read from the file INCON and final results written to SAVE. The listing file name will be the same as the data file name, but with the extension changed to *.listing, unless the `output_filename` is specified.

Running TOUGH2_MP is generally done via MPI rather than directly, and the exact syntax for doing so may vary with different implementations of MPI (OpenMPI, MPICH2 etc.) It is also necessary to specify the number of processors to use. However it is still possible to run TOUGH2_MP from a Python script using a system call, e.g.:

```
from os import system
system("mpirun -np 16 t2eos1_mp")
```

Parameters:

- **save_filename**: string
  Name of the save file to be written to disk during the simulation (AUTOUGH2 only). Default is 'base.save' where the AUTOUGH2 data file name is 'base.dat'.

- **incon_filename**: string
  Name of the initial conditions file for the simulation (AUTOUGH2 only). Default is 'base.incon' where the AUTOUGH2 data file name is 'base.dat'.

- **simulator**: string
  Name of the AUTOUGH2 or TOUGH2 executable. Default is 'AUTOUGH2_2'.

- **silent**: Boolean
  Set to `True` to suppress output to the display while running (default is `False`).

- **output_filename**: string
  Name of the output listing file for the simulation (TOUGH2 only). Default is 'base.listing' where the base name of the TOUGH2 data file (without file extension) is 'base'.

```
specific_generation(type='MASS', name='')
```

Returns an `np.array` containing the total specific generation rate in each block (i.e. generation rate per unit volume) for the specified generator type and name.

Parameters:

- **type**: string
  Generation type ('HEAT', 'MASS' etc.) – default is 'MASS'.

- **name**: string
  Regular expression to match generator names (e.g. 'SP...' (or '^SP') will match all generators with names beginning with 'SP'.)

```
transfer_from(source, sourcegeo, geo, top_generator=[], bottom_generator=[],
sourceinconfilename='', inconfilename='', rename_generators=False,
preserve_generation_totals=False)
```

Transfers data from another `t2data` object, and its associated `mulgrid` object. Parameters, rock types and rock type assignments, and optionally initial conditions files are transferred. In general the data for a given block in the geometry is found by identifying the nearest block in the source geometry and transferring data from that block. There are, however, exceptions, such as for generators that need to remain on the surface or bottom of the model. The `top_generator` and `bottom_generator` lists specify the 'layer' part of the generator name for generators that should remain on the top or bottom of the model, respectively.

For generator types in which the `gx` and `rate` properties represent generation rates (as opposed to other types for which these properties are used to represent other things, e.g. productivity index for wells on deliverability), the values of `gx` and `rate` are scaled to account for the different volume of the block the generator has been mapped into. If `preserve_generation_totals` is `True`, and a generator with generation rate G is mapped into n blocks with volumes $V_1, V_2, \ldots, V_n$, then the generation rate for the new generator in block i will be $GV_i / \sum_{k=1}^{n} V_k$. This should preserve the total generation rate over the model. (For generator types matching the `bottom_generator` or `top_generator` specifications, the column area instead of the block volume is used to determine the appropriate scaling.) Note that of the columns a top or bottom generator is mapped into, only those with centres inside the source geometry are included in the scaling calculations. The generator types for which this scaling is carried out are: ' AIR', 'COM1', 'COM2', 'COM3', 'COM4', 'COM5', 'HEAT', 'MASS', 'NACL', 'TRAC' and ' VOL'.

If both `sourceinconfilename` and `inconfilename` are specified, a new initial conditions file with filename `inconfilename` is written to disk, with initial conditions transferred from the file `sourceinconfilename`.

Parameters:

- **source**: t2data
  The `t2data` object to transfer data from.
- **sourcegeo**: mulgrid
  The `mulgrid` object corresponding to `source`.
- **geo**: mulgrid
  The `mulgrid` object corresponding to the destination `t2data` object.
- **top_generator**: list
  A list of generator 'layer' identifier strings for generators that need to be kept at the top of the model (e.g. rain generators).
- **bottom_generator**: list
  A list of generator 'layer' identifier strings for generators that need to be kept at the bottom of the model (e.g. basement heat and mass inputs).
- **sourceinconfilename**: string
  Name of the (optional) initial conditions file to transfer initial conditions data from (corresponding to `source`).
- **inconfilename**: string
  Name of the (optional) initial conditions file to write, corresponding to the destination `t2data` object.
- **rename_generators**: Boolean
  If `False`, generators other than those at the top and bottom of the model retain their original names. Otherwise, they will be renamed according to their column names in the new grid.
- **preserve_generation_totals**: Boolean
  If `False` (the default), the transfer of generators will attempt to preserve the distribution of specific generation of the original model; otherwise, it will attempt to preserve the total generation over the model.

```
total_generation(type='MASS', name='')
```

Returns an `np.array` containing the total generation rate in each block for the specified generator type and name.

Parameters:

- **type**: string
  Generation type ('HEAT', 'MASS' etc.) – default is 'MASS'.
- **name**: string
  Regular expression to match generator names (e.g. 'SP...' (or '^SP') will match all generators with names beginning with 'SP'.)

```
write(filename='', meshfilename='', extra_precision=None,
echo_extra_precision=None)
```

Writes a `t2data` object to a TOUGH2 data file on disk. If the `meshfilename` parameter is used, mesh information can be written to auxiliary mesh files.

Parameters:

- **filename**: string
  Name of the TOUGH2 data file to be written. If no file name is specified, the object's own `filename` property is used.

- **meshfilename**: string or tuple
  Name of auxiliary mesh file(s) to be written. If this is empty (the default), the object's own `meshfilename` property is used. Otherwise, if a single (non-empty) string is given, this in interpreted as the name of a file to write formatted mesh information to (as in the 'MESH' files produced by TOUGH2 and TOUGH2_MP). If a tuple of two strings is given, this in interpreted as the names of two binary files (as in the 'MESHA' and 'MESHB' files produced by TOUGH2_MP).

- **extra_precision**: list or Boolean
  Controls whether to write extra precision data to auxiliary file (AUTOUGH2 only). If set to `True`, then all possible sections will be written to the extra precision file. Currently the possible extra-precision sections are the ROCKS, ELEME, CONNE, RPCAP and GENER sections. If set to `False` or [], then no extra-precision data will be written. If set to a list of section names (e.g. ['RPCAP', 'GENER']), then only those sections will be written in extra precision. If set to `None` (the default), then the value of the data object's `extra_precision` property is used. Otherwise, the value of this property is overwritten by the value specified here.

- **echo_extra_precision**: Boolean or None
  Controls whether to echo all extra-precision data sections to the main data file (AUTOUGH2 only). If `None`, the value of the data object's `echo_extra_precision` property is used. Otherwise, the value of this property is overwritten by the value specified here.

4.3 `t2generator` objects

A `t2generator` object represents a generator in a TOUGH2 simulation (i.e. an item in the generation table). The properties of a `t2generator` object are given in Table 4.13. These correspond closely to the parameters specified in the TOUGH2 **GENER** input block. A `t2generator` object has no methods.

4.4 Example

The following piece of Python script opens a MULgraph geometry file and TOUGH2 data file, changes some TOUGH2 run-time parameters and assigns heat generators to the blocks in the bottom layer inside a defined area, with the specified total heat divided uniformly amongst the generators.

```
geo = mulgrid('gmodel.dat')
dat = t2data('model.dat')

dat.parameter['max_timesteps'] = 300
dat.parameter['print_interval'] = dat.parameter['max_timesteps']/10
```

Property	Type	Description	TOUGH2 parameter
block	string	name of block containing the generator	EL, NE
enthalpy	list of float	generation enthalpies (|ltab| >1, itab<>‘’)	F3
ex	float	enthalpy for injection	EX
gx	float	generation rate (or productivity index for deliverability)	GX
hg	float	layer thickness for deliverability	HG
fg	float	separator pressure/ injectivity etc.	FG
itab	string	blank unless table of specific enthalpies specified	ITAB
ltab	integer	number of generation times (or open layers for deliverability)	LTAB
nadd	integer	successive block increment	NADD
nads	integer	successive generator increment	NADS
name	string	generator name	SL, NS
nseq	integer	number of additional generators	NSEQ
rate	list of float	generation rates (|ltab| >1)	F2
time	list of float	generation times (|ltab| >1)	F1
type	string	generator type (default ‘MASS’)	TYPE

Table 4.13: Properties of a `t2generator` object

```
dat.parameter['option'][16] = 5 # time step control

dat.clear_generators()
totalheat = 10.e6
layer = geo.layerlist[-1]  # bottom layer
cols = [col for col in geo.columnlist if 10.e3 <= col.centre[0] <= 20.e3]
totalarea = sum([col.area for col in cols])
q = totalheat / totalarea

for col in cols:
    blockname = geo.block_name(layer.name, col.name)
    gen = t2generator(name = ' q'+col.name, block = blockname, type =
        'HEAT', gx = q*col.area)
    dat.add_generator(gen)

dat.write()
```

Chapter 5

TOUGH2 initial conditions

5.1 Introduction

The `t2incons` library in PyTOUGH contains classes and routines for reading, editing and writing TOUGH2 initial conditions and files. It can be imported using the command:

```
from t2incons import *
```

The initial conditions files used by TOUGH2 and AUTOUGH2 have the same format. PyTOUGH also supports TOUGHREACT initial conditions files, which have a slightly different format – permeabilities are included for each block, and timing information at the bottom of the file is formatted differently.

5.2 `t2incon` objects

The `t2incons` library defines a `t2incon` class, used for representing TOUGH2 initial conditions.

Example:

```
inc = t2incon()
```

creates an empty `t2incon` object called `inc`.

```
inc = t2incon(filename)
```

creates a `t2incon` object called `inc` and reads its contents from file `filename`.

5.2.1 Properties

The main properties of a `t2incon` object are listed in Table 5.1. Once a set of initial conditions is loaded into a `t2incon` object, conditions for individual blocks can be accessed by block name or index. For example, for a `t2incon` object `inc`, the initial conditions in block 'blockname' are given simply by `inc[blockname]`. This returns a `t2blockincon` object (see section 5.3). Similarly, `inc[i]` returns the initial conditions at the block with (zero-based) index `i`.

Each column in the initial conditions file can be accessed by adding an integer (zero-based) index after the `t2blockincon` object, so for example:

```
t = inc['aa 20'][1]
```

assigns the variable `t` the value of the second primary thermodynamic variable (index 1) in block `'AA 20'`. Initial conditions can be edited in a similar way, for example:

```
inc['aa 20'][0] = p
```

assigns the value of `p` to the first primary variable (usually pressure) in block `'AA 20'`. For convenience, initial conditions for a given block can also be specified as a simple list or tuple of values, for example:

```
inc['ab 25'] = (101.3e5,25.0)
```

sets the initial conditions at block `'ab 25'` to the specified values. This will work even if no initial conditions have been previously specified for the given block.

An `np.array` of the values of the variables at all blocks can be found from the `variable` property. For example:

```
inc.variable[:,2]
```

returns an `np.array` of the third variable (index 2) in each block. The `variable` property can also be set to a given array. Note, however, that the whole array must be set, not just part of it. For example, adding an offset `P0` to all pressures (variable 0) in the initial conditions could be done by:

```
v = inc.variable
v[:,0] += P0
inc.variable = v
```

The `porosity` property may be set to assign values of porosity to all blocks. The assigned value may be an `np.array` with a value for each block, or a scalar float (in which case the same value is assigned to all blocks), or `None` which assigns the value in each block to `None`.

Similarly, for TOUGHREACT initial conditions files, the `permeability` property can be used to read or assign permeabilities for all blocks. When assigning this property, the value can be an `np.array` of shape (`num_blocks`, 3), (i.e. a row for each block), or a single `np.array` with 3 elements, to be applied to all blocks, a single scalar float (to assign isotropic permeabilities to all blocks) or `None` which assigns `None` to all block permeabilities.

The `timing` property of a `t2incon` object contains the optional timing information at the end of the file. This is a dictionary property with keys `'kcyc'`, `'iter'`, `'nm'`, `'tstart'` and `'sumtim'`, corresponding to the values stored on this line.

The `simulator` string property is 'TOUGH2' by default, and is set to 'TOUGHREACT' if permeabilities are detected while reading from file. Setting this property back to 'TOUGH2' will cause the file to be written out in TOUGH2 format (no permeabilities, and different format for timing information) if the `write()` method is executed.

Functions for reading data from file

It is possible to specify customized functions to control how data are read from a TOUGH2 initial conditions file. This is done using the optional `read_function` parameter when a `t2incon` object is created- in exactly the same way it is done for a `mulgrid` object. For more details, see the corresponding documentation for `mulgrid` objects in section 2.2.1. By default, the read functions for `t2incon` objects are given by the `fortran_read_function` dictionary.

Property	Type	Description
`blocklist`	list	ordered list of block names in the initial conditions file
`num_blocks`	integer	number of blocks at which conditions are specified
`num_variables`	integer	number of thermodynamic variables specified at each block
`permeability`	`np.array`	array of permeability values specified at each block (TOUGHREACT only)
`porosity`	`np.array`	array of porosity values specified at each block
`simulator`	string	simulator type ('TOUGH2' or 'TOUGHREACT')
`timing`	dictionary	additional timing information for restarting
`variable`	`np.array`	two-dimensional array of thermodynamic variable values at each block

Table 5.1: Properties of a `t2incon` object

Specifying the number of primary variables

Most common TOUGH2 EOS modules have no more than four primary variables, in which case the variables for a given block all fit on one line in the initial conditions file. However, some EOS modules (e.g. EOS7c and EOS7r) have more than four primary variables. For these, the variables for a given block are specified over multiple lines in the initial conditions file.

In this case, it is not possible for PyTOUGH to reliably detect the number of primary variables, as it does when there are no more than four variables. Instead, the number of primary variables must be specified when the `t2incon` object is created (or its `read()` method is executed). This can be done by setting the optional integer `num_variables` parameter, which defaults to `None` (meaning PyTOUGH will detect the number of variables). For example:

```
from t2incons import *
inc = t2incon('model.incon', num_variables = 6)
```

opens initial conditions for an EOS using six primary variables.

For writing initial conditions files with more than four primary variables, no extra parameters need be set, as the data stored in the `t2incon` object determines the number of primary variables, and they will be written out over multiple lines as required.

5.2.2 Methods

The main methods of a `t2incon` object are listed in Table 5.2. Details of these methods are given below.

`add_incon(`*`incon`*`)`

Adds a set of initial conditions for a single block.

Parameters:

- **incon**: `t2blockincon`
  Initial conditions for the block.

Method	Type	Description
add_incon	–	adds a set of initial conditions for one block
delete_incon	–	deletes the initial conditions for one block
empty	–	deletes all initial conditions from the object
insert_incon	–	inserts initial conditions for one block at a specified index
read	–	reads initial conditions from file
transfer_from	–	transfers initial conditions from one grid to another
write	–	writes initial conditions to file

Table 5.2: Methods of a `t2incon` object

`delete_incon(`*`blockname`*`)`

Deletes a set of initial conditions for a single block.
Parameters:
- **blockname**: string
  Name of the block at which initial conditions are to be deleted.

`empty()`

Deletes initial conditions for all blocks.

`insert_incon(`*`index`*`,`*`incon`*`)`

Inserts a set of initial conditions for a single block at the specified index.
Parameters:
- **index**: integer
  Index (zero-based) at which to insert the initial conditions.
- **incon**: `t2blockincon`
  Initial conditions for the block.

`read(`*`filename`*`, `*`num_variables`*` = None)`

Reads initial conditions from file.
Parameters:
- **filename**: string
  Name of the initial conditions file to be read.
- **num_variables**: integer or `None`
  If reading initial conditions files with more than four primary variables, set to the number of primary variables. Otherwise, the default `None` value can be used, in which case the number of primary variables will be detected automatically.

`transfer_from(`*`sourceinc`*`, `*`sourcegeo`*`, `*`geo`*`, `*`mapping={}`*`, `*`colmapping={}`*`)`

Transfers initial conditions from another `t2incon` object `sourceinc`, using the two corresponding `mulgrid` geometry objects `sourcegeo` and `geo`, and optionally the block and column mappings between the two grids (which are created if not specified).

Parameters:

- **sourceinc**: t2incon
  Source initial conditions object.
- **sourcegeo**: mulgrid
  Geometry object corresponding to the source initial conditions.
- **geo**: mulgrid
  Geometry object for the grid to be transferred to.
- **mapping**: dictionary
  Dictionary mapping block names from `geo` to `sourcegeo`.
- **colmapping**: dictionary
  Dictionary mapping column names from `geo` to `sourcegeo`.

`write(filename, reset=True)`

Writes initial conditions to file.

Parameters:

- **filename**: string
  Name of the initial conditions file to be written.
- **reset**: Boolean
  Set to `False` if timing information is not to be reset - e.g. if restarting a transient simulation.

5.3 t2blockincon objects

A `t2blockincon` object represents the initial conditions for a particular block. The properties of a `t2blockincon` object are given in Table 5.3. The `permeability` property is used only by TOUGHREACT. If no values are specified for `porosity`, `permeability`, `nseq` or `nadd`, their values are `None`. A `t2blockincon` object has no methods.

The `variable` property of a `t2blockincon` can be more easily accessed simply by adding the required (zero-based) variable index after the object. For example, for a `t2blockincon` object `b`, the value of the second variable is given simply by `b[1]`.

To create a new `t2blockincon` object, simply invoke the class name with values of the desired properties, e.g.:

```
binc = t2blockincon(block = 'abc10', porosity = 0.1, variable =
    [101.3e3, 28.])
```

5.4 Reading save files and converting to initial conditions

TOUGH2 writes a save file (SAVE, or *.save for AUTOUGH2) at the end of the simulation, which has a format almost the same as that of an initial conditions file and can be used to

Property	Type	Description
`block`	string	block name
`nadd`	integer or `None`	optional block index increment between additional blocks with the same initial conditions
`nseq`	integer or `None`	optional number of additional blocks with the same initial conditions
`permeability`	`np.array` or `None`	optional permeability for the block (TOUGHREACT only)
`porosity`	float or `None`	optional porosity for the block
`variable`	list	list of thermodynamic variable values for the block

Table 5.3: Properties of a `t2blockincon` object

start a subsequent run. A save file generally has some extra timing information at the end which can be used to restart a simulation at a particular time. However, in many cases, e.g when running natural state simulations, we want to restart at the original start time and this timing information must be discarded.

PyTOUGH will read a save file into a `t2incon` object. This can then be written to file, providing a simple way to convert save files into incon files. By default, the timing information is discarded when writing (it can be retained by setting the `reset` parameter of the `write` method to `False`). For example:

```
t2incon('model1.save').write('model2.incon')
```

will read the save file `'model1.save'`, convert it to initial conditions, and write it to the initial conditions file `'model2.incon'`.

5.5 Example

The following piece of Python script reads in a save file and prints out a table of block names and temperatures for the first 10 blocks. It then adds an extra variable to each initial condition and gives it a constant value (giving a new column in the initial conditions file), and finally writes out the edited initial conditions to a new file.

Adding a new variable to each initial condition can be useful when e.g. changing from one TOUGH2 equation of state (EOS) module to another, as different EOS modules may have different numbers of primary thermodynamic variables.

```
from t2incons import *
inc = t2incon('model1.save')
for blk in inc[0:10]:
    print 'Block %5s: temperature = %5.1f' % (blk.block,blk[1])
patm = 101.3e3
for blk in inc: blk.variable.append(patm)
inc.write('model2.incon')
```

Chapter 6

TOUGH2 listing files

6.1 Introduction

The `t2listing` library in PyTOUGH contains classes and routines for reading TOUGH2 listing files. It can be imported using the command:

```
from t2listing import *
```

Listing files produced by AUTOUGH2, TOUGH2, TOUGH2_MP, TOUGH+ and TOUGH3 have different formats but are all supported. The main listing files produced by TOUGHREACT are also supported. (There is also a separate `toughreact_tecplot` class for handling the additional Tecplot output files produced by TOUGHREACT.)

6.2 `t2listing` objects

The `t2listing` library defines a `t2listing` class, used for representing TOUGH2 listing files.

Example:

```
lst = t2listing()
```

creates an empty `t2listing` object called `lst`.

```
lst = t2listing(filename)
```

creates a `t2listing` object called `lst` and reads its contents from file `filename`.

6.2.1 Properties

The main properties of a `t2listing` object are listed in Table 6.1.

Element, connection and generation tables

There are three main 'table' properties, corresponding to the **element**, **connection** and **generation** tables in the listing file. These are all of type `listingtable` (see section 6.3) and provide access to the simulation results. Not all of these tables will necessarily be present - this depends on the settings in the data file which produced the results. For TOUGH2

results, a fourth **primary** table may also be present, containing primary variables and their changes, if the KDATA parameter is set to 3. TOUGH+ results can also contain additional element tables containing other calculated quantities; these are named **element1**, **element2** etc. A list of names of all available tables is given by the `table_names` property.

For example, for a `t2listing` object `lst`, `lst.element['AR210']['Temperature']` gives the temperature at block 'AR210', at the current time. Blocks can also be identified by index rather than name, so that `lst.element[120]['Pressure']` gives the pressure at the block with (zero-based) index 120.

These tables can also be accessed to give all results for a given block, or for a given column in the table. For example, `lst.element['AR210']` returns a dictionary containing all results at block 'AR210', referred to by the name of each table column. `lst.element['Temperature']` returns an `np.array` containing the temperatures at all blocks in the model. (Hence, `lst.element['Pressure'][120]` gives the same result as `lst.element[120]['Pressure']`.)

The connection and generation tables work very similarly to the element table, except that connections are referred to by tuples of block names (rather than single block names), and generators are referred to by tuples of block names and generator names. So for example, the mass flow rate between blocks 'AB300' and 'AC300' might be given by `lst.connection['AB300', 'AC300']['Mass flow']`.

The names of the columns for each table are read directly from the listing file, and will depend on the TOUGH2 equation of state (EOS) being used.

Skipping tables

The default behaviour is for a `t2listing` object to read all tables present in the listing file. However, it is possible to skip the reading of specified tables if required. This can be useful for speeding up reading of large listing files where not all tables are required. For example, sometimes the connection data are not required, but for large models the connection table is often much bigger than the others, so skipping it can make reading significantly faster. Data in skipped tables are not available either via their corresponding properties or via the `history()` method.

To skip tables, specify their table names (`element`, `connection` etc.) in the optional `skip_tables` parameter when creating the `t2listing` object. (By default, this parameter is an empty list.) For example, to read a listing file with name 'output.listing' into the object `lst` and skip reading the connection and generation tables:

```
lst = t2listing('output.listing', skip_tables = ['connection',
    'generation'])
```

File encoding

It is possible to specify the file encoding for the listing file using the optional `encoding` parameter when creating the `t2listing` object. The default for this parameter is "latin-1" encoding which should be fine for reading in most listing files. If you encounter exotic characters in your listing files which are not read correctly using the default encoding you may want to try other encodings.

Full and short output

AUTOUGH2 allows the use of 'short' output, in which a specified selection of block, connection or generator properties are printed at time steps between normal full output. A

t2listing object will read short output results, if they are present, when producing time histories using the history() method. However it is not possible to navigate to short output results or access them via the t2listing table properties above.

TOUGH2, TOUGH2_MP, TOUGHREACT, TOUGH+ and TOUGH3 do not support short output.

Navigating in time using time, index and step

The time property returns the time (in seconds) corresponding to the current set of results. It is also possible to set the time property to navigate to a specific set of full results. For example, lst.time=1.e9 navigates to the set of full results with time closest to 10^9s.

The index property gives the index of the current set of results, and can take any value between 0 and num_fulltimes-1. The value of index can also be set to change to a different set of results in the listing file (e.g. lst.index=12). It can be incremented and decremented like any other Python integer variable, e.g. lst.index+=1 or lst.index-=2 to go to the next set of results, or the second to last set respectively.

The step property gives the time step number for the current set of results. This is the number of time steps carried out in the simulation up to the current set of results (recall that results are not necessarily written to the listing file at every time step). Again, its value can be set to navigate through the results, e.g. lst.step=100 navigates to the set of full results with time step number nearest to 100.

The times property returns an np.array of all times at which results (including short output) are given in the listing file. It has length equal to num_times. The fulltimes property returns an np.array of times at which full results are given (not including short output), and has length equal to num_fulltimes.

A t2listing object also has methods (as well as properties) for navigating through time (see section 6.2.2).

Listing diagnostics

t2listing objects have two properties that provide diagnostics on the results of the TOUGH2 run.

The convergence property is a dictionary of the maximum absolute differences in the element table between the second to last and last sets of results in the listing file. This can be used to check convergence of steady-state simulations. For example:

```
lst.convergence['Temperature']
```

gives the largest absolute temperature change between the second to last and last sets of results.

The reductions property is a list of tuples of time step indices at which the time step size was reduced during the simulation, and the block name at which the maximum residual occurred prior to each reduction. This gives an indication of problematic times and blocks which caused time step reductions.

6.2.2 Methods

The main methods of a t2listing object are listed in Table 6.2. Details of these methods are given below.

Property	Type	Description
`connection`	`listingtable`	connection table for current set of results
`convergence`	dictionary	maximum differences in element table between second to last and last sets of results
`element`	`listingtable`	element table for current set of results
`element1` etc.	`listingtable`	additional element table for current set of results (TOUGH+ only)
`filename`	string	name of listing file on disk
`fullsteps`	`np.array`	array of time step numbers (integer) for full results
`fulltimes`	`np.array`	array of times (float) for full results
`generation`	`listingtable`	generation table for current set of results
`index`	integer	index of current set of results
`num_fulltimes`	integer	number of sets of full results
`num_times`	integer	number of sets of all results (full and short)
`primary`	`listingtable`	primary variable table for current set of results (TOUGH2 only)
`reductions`	list	time step indices at which time step was reduced during the simulation
`short_types`	list of string	types of short output present
`simulator`	string	detected simulator ('AUTOUGH2', 'TOUGH2' etc.)
`step`	integer	time step number of current set of results
`steps`	`np.array`	array of time step numbers (integer) for all results (full and short)
`table_names`	list	names of available tables
`time`	float	time of current set of results
`times`	`np.array`	array of times (float) for all results (full and short)
`title`	string	simulation title

Table 6.1: Properties of a `t2listing` object

Method	Type	Description
`add_side_recharge`	–	adds side recharge generators to a `t2data` object
`close`	–	closes listing file
`first`	–	navigates to the first set of full results
`get_difference`	dictionary	maximum differences in element table between two sets of results
`history`	list or tuple	time history for a selection of locations and table columns
`last`	–	navigates to the last set of full results
`next`	Boolean	navigates to the next set of full results
`prev`	Boolean	navigates to the previous set of full results
`write_vtk`	–	writes results to VTK file

Table 6.2: Methods of a `t2listing` object

`add_side_recharge(geo, dat)`

Adds side recharge generators to a `t2data` object `dat` for a production run, calculated according to the final results in the listing. These generators represent side inflows due to pressure changes in the blocks on the model's horizontal boundaries. Recharge generators are given the names of their blocks- any existing generators with the same names will be overwritten.

Parameters:

- **geo**: `mulgrid`
  Geometry object associated with the listing.
- **dat**: `t2data`
  TOUGH2 data object for the side recharge generators to be added to.

`close()`

Closes the listing file after use.

`first()`

Navigates to the first set of full results in the listing file.

`get_difference(indexa=None, indexb=None)`

Returns dictionary of maximum differences, and locations of difference, of all element table properties between two sets of results.

Parameters:

- **indexa**, **indexb**: integer or `None`
  Indices of results between which the maximum differences are to be calculated. If both indexa and indexb are provided, the result is the difference between these two result indices. If only one index is given, the result is the difference between the given index and the one before that. If neither are given, the result is the difference between the last and penultimate sets of results.

`history(selection, short=True, start_datetime=None)`

Returns a list of time histories (as `np.arrays`) for specified locations and table columns in the element, connection or generation tables. For each selection, a tuple of two `np.arrays` is returned, one each for times and values. Short output (AUTOUGH2 only) can be omitted from the history results by setting the `short` parameter to `False`. If the `start_datetime` parameter is given, times in the output are given as datetimes rather than seconds from the start.

Parameters:

- **selection**: list of tuples
  Selection of listing tables, locations (or indices) and table columns to produce histories for. Each tuple contains three elements: the listing **table type** ('e', 'c', 'p' or 'g' for element, connection, primary or generation table respectively), the **block/ connection/ generator name** (or index) and the **table column name**. (If only a single tuple is given instead of a list of tuples, just the single tuple of times and values

for that selection is returned.) For history of additional element tables in TOUGH+ results, use 'e1', 'e2' etc. instead of 'e'. Note that, as for listing tables, connection and generator names (or 'keys') are specified as two-element tuples (see Table 6.3). If the second element of a selection tuple is an integer, it will be interpreted as the (zero-based) index of the block, connection or generator in the corresponding table.

- **short**: Boolean
  Whether short output (AUTOUGH2 only) is to be included in the history results - default is `True`.

- **start_datetime**: datetime or `None`
  Datetime of the start of the simulation. If `None` (the default), output times are given as seconds from the start of the simulation. If a Python datetime is given, then output times are given as datetimes.

Examples:

```
[(tt,temp), (tq,q), (tg,g)] = lst.history([('e', 'AR210', 'Temperature'),
('c', ('AB300','AC300'), 'Mass flow'), ('g', ('BR110','SO  1'),
    'Generation rate')])
```

returns a list of three tuples of `np.arrays`, `(tt,temp)`, `(tq,q)` and `(tg,g)`, giving the times and values of temperature at block 'AR210', mass flow at the connection between blocks 'AB300' and 'AC300', and generation rate in the generator 'SO 1' in block 'BR110' respectively.

```
from datetime import datetime
t0 = datetime(1955, 1, 1)
t,T = lst.history(('e', 'AR210', 'Temperature'), start_datetime = t0)
```

returns `T` as an `np.array` of temperature values, and `t` as an `np.array` of Python datetimes, starting at 1 January 1955.

`last()`

Navigates to the last set of full results in the listing file.

`next()`

Navigates to the next set of full results in the listing file. Returns `False` if already at the last set of results (and `True` otherwise).

`prev()`

Navigates to the previous set of full results in the listing file. Returns `False` if already at the first set of results (and `True` otherwise).

`write_vtk(`*`geo`*`, `*`filename`*`, `*`grid`*`=None, `*`indices`*`=None, `*`flows`*`=False, `*`wells`*`=False, `*`start_time`*`=0, `*`time_unit`*`='s', `*`flux_matrix`*`=None, `*`blockmap`*` = {}, `*`surface_snap`*`=0.1)`

Writes a `t2listing` object to a set of VTK files on disk, for visualisation with VTK, Paraview, Mayavi etc. The results in the listing object are written as an 'unstructured grid' VTK object with data arrays defined on cells. The data arrays written correspond to the variables given in the columns of the element table of the `t2listing` object. (For TOUGH+ results, variables from the additional element tables are also included.) In addition, data arrays from an associated `mulgrid` and (optionally) `t2grid` objects can be included.

If `flows` is `True` (and a `grid` is specified and the listing contains connection data), approximate block-average flux vectors at the centre of each block are also written, for all variables in the connection table with names ending in 'flow'.

One *.vtu file is produced for each time step in the `t2listing` object at which full results are present, and a *.pvd file is also written. This is usually the file that should actually be opened in Paraview or other software as it contains time information associated with each *.vtu file.

Optionally, only a subset of the time indices present in the `t2listing` can be written, according to the `indices` parameter. A start time and time unit for the output can optionally be specified.

Parameters:

- **geo**: `mulgrid`
  The `mulgrid` geometry object associated with the results. For flexibility, this geometry need not be fully compatible with the results – for example, it may contain only a subset of the blocks for which results are present, or the blocks may be in a different order. However, if it is not fully compatible, the writing process will be slower, and flux vectors will not be written (even if `flows` is set to `True`).

- **filename**: string
  Name of the *.pvd file to be written. Names of the individual *.vtu files for each time step are similar but with a time index appended and the file extension changed.

- **grid**: `t2grid`
  Name of optional `t2grid` object associated with the results.

- **indices**: list or tuple
  Optional specification of time indices to include in the output. If set to `None` (the default), all time indices will be included.

- **flows**: Boolean
  Set to `True` if approximate block-centred flux vectors are to be calculated and written, for visualising flows. Default is `False`. **Note**: flow vectors can only be calculated if a **grid** is specified.

- **wells**: Boolean
  Set to `True` if a separate VTK file for the wells in the `mulgrid` object is to be written. Default is `False`.

- **start_time**: float
  Optional start time of the simulation, i.e. time associated with the first set of results. Default is zero.

- **time_unit**: string
  Optional time unit for the output. TOUGH2 results are given at times in seconds, but this option allows them to be converted to other units. Options are: 's', 'h', 'd' and 'y', for seconds, hours, days and years respectively. Default is 's'.

- **flux_matrix**: `scipy.sparse.lil_matrix`
  Sparse matrix that multiplies a vector of connection values to produce a partition vector of 3-D block average flows at the (underground) block centres. One of these can be produced using the `t2grid.flux_matrix()` method, and a corresponding `mulgrid` object. A flux matrix will be calculated internally if not supplied.

- **blockmap**: dictionary
  Dictionary mapping the block names in the geometry to the block naming system used in the listing.

- **surface_snap**: float
  Tolerance for specifying how close column surface elevations need to be before being considered "equal" when constructing surface nodes.

6.3 `listingtable` objects

A `listingtable` object represents a table of results in a TOUGH2 listing file (whether it is an element, connection or generation table). The column headings of the table are taken directly from the corresponding table in the listing file. The rows of the table may be accessed either by (zero-based) index, or by the 'key' for the table row, which depends on the table type (see Table 6.3).

Table type	Key
`element`	block name
`connection`	(block name 1, block name 2)
`generation`	(block name, generator name)

Table 6.3: Keys for different listing table types

Hence, the value in the element table for a given block and column can be accessed by `lst.element[blockname][columnname]`, or by `lst.element[blockindex][columnname]` (for a `t2listing` object `lst`). Note that for connection and generation tables, the keys are tuples of two strings. For connection tables, the order of these two strings (the block names) is not important; if the listing file contains results for (block1, block2), then results for (block2, block1) can be accessed via the corresponding `listingtable` object (though the results will have the opposite sign to those in the file, as they will represent flows in the opposite direction).

The values for an entire row or column of the table can also be accessed, for example `lst.element[blockname]` gives the row in the table for a specified block, with the values arranged in a dictionary which can be accessed using the column names of the table (e.g. `lst.element['AR231']['Temperature']`). This dictionary for each row also contains an additional `'key'` item which returns the key for that row. Conversely, `lst.element[columnname]` gives the column in the table for a specified column name, with the values returned in an `np.array` (one value for each block in the grid, for an element table).

Property	Type	Description
column_name	list	column headings
DataFrame	pandas DataFrame	data in DataFrame format
num_columns	integer	number of columns
num_keys	integer	number of keys per row
num_rows	integer	number of rows
row_name	list	keys for each row

Table 6.4: Properties of a `listingtable` object

6.3.1 `listingtable` properties

The properties of a `listingtable` object are given in Table 6.4. The entire list of key values for a `listingtable` may be accessed via the `row_name` property, which contains the key value for each row. The column headings of the table can similarly be accessed via the `column_name` list property. The `num_rows` and `num_columns` properties of a `listingtable` object return the numbers of rows and columns respectively. The `num_keys` property just returns the number of keys used to identify each row - generally 1 for an element table and 2 for connection and generation tables.

6.3.2 Adding and subtracting

It is possible to perform addition and subtraction operations on `listingtable` objects. Subtraction can be useful, for example, when comparing results from different runs. These operations can only be carried out when the row and column names of the two tables are identical. The resulting table will have the same row and column names as the original tables, but will contain the element-wise sums or differences.

6.3.3 Converting to DataFrames

A `listingtable` object has a `DataFrame` property which returns the entire table in the form of a `pandas` (http://pandas.pydata.org/) DataFrame object. `pandas` is a Python library for data analysis, which you will need to have installed before you can use the `DataFrame` property. With `pandas` you can do advanced data analysis on your TOUGH2 results. See the `pandas` documentation for more details.

6.3.4 `listingtable` methods

`listingtable` objects have one method as described below.

```
rows_matching(pattern, index=0, match_any=False)
```

Returns a list of rows in the table with keys matching the specified regular expression string, `pattern`.

For tables with multiple keys, `pattern` can be a list or tuple of regular expressions. If a single string pattern is given for a multiple-key table, the pattern is matched on the indexth key (and any value of the other key - unless the `match_any` option is used; see below).

If `match_any` is set to `True`, rows are returned with keys matching any of the specified patterns (instead of all of them). If this option is used in conjunction with a single string pattern, the specified pattern is applied to all keys.

Parameters:

- **pattern**: string, list or tuple
  Regular expression string specifying the pattern to match. For multiple-key tables, this can be a list or tuple of regular expression strings.
- **index**: integer
  Index of the key to which the pattern is to be applied, for multiple-key tables and when `pattern` is specified as a single string.
- **match_any**: Boolean
  If `False`, return only rows with keys matching *all* of their corresponding patterns. If `True`, return rows with keys matching *any* of the specified patterns - and if a single string pattern is given, apply this to all keys.

6.4 `t2historyfile` objects

In addition to the main listing file, TOUGH2 can optionally produce extra files containing time history data from selected blocks, connections or generators, named `FOFT`, `COFT` and `GOFT` files respectively. TOUGH+ can optionally name these files `Elem_Time_Series`, `Conx_Time_Series` and `SS_Time_Series` instead. (AUTOUGH2 does not produce separate history files, but can instead produce 'short output' at selected blocks, connections or generators within the listing file itself.)

The `t2listing` module contains a `t2historyfile` class for reading and manipulating these history files. History files produced by TOUGH2, TOUGH2_MP and TOUGH+ are supported, although they all have different formats. The same class is used for FOFT, COFT and GOFT files. A history file of any of these types can be opened using a command such as:

```
hist = t2historyfile(filename)
```

where *`filename`* is the name of the file. It may contain wildcards (*) so that several files matching a pattern are read in to the same object. This is useful for reading output from TOUGH2_MP, which creates separate history files for each processor used in the calculation (e.g. `FOFT_P.000`, `FOFT_P.001`, etc.). It is assumed that all files opened are however of the same type (FOFT, COFT or GOFT).

Once a history file has been read in, history results for a particular key (i.e. block, connection or generator) can be extracted. For TOUGH2_MP, the keys are the block names for FOFT files, tuples of block names for COFT files, and tuples of block names and source names for GOFT files. For example:

```
foft = t2historyfile('FOFT_P.*')
blockname = 'fmq20'
results = foft[blockname]
```

This will return a dictionary containing an `np.array` for each column in the file, indexed by the column name. For example the temperature history at this block would be given by:

Property	Type	Description
column_name	list	column headings
key_name	list	names of keys
num_times	integer	number of times
num_columns	integer	number of data columns
num_rows	integer	total number of data (for all keys)
simulator	string	detected simulator ('TOUGH2' or 'TOUGH2_MP')
times	np.array	times at which results are given
type	string	history type ('FOFT', 'COFT' or 'GOFT')

Table 6.5: Properties of a t2historyfile object

```
temp = foft[blockname]['TEMPERATURE']
```

Results at a particular time can also be found:

```
time = 3.156e7
result = foft[blockname, time]
```

Again, this will return a dictionary with one item for each column, but in this case each item is just a single floating point number instead of an array.

For **TOUGH2** rather than TOUGH2_MP, the keys are integer indices of blocks, connections or generators, rather than names or tuples of names. Similarly, the column names are just integers. This is because the key names and column names are not given in TOUGH2 history files. Aside from these differences, they can be used in the same way as TOUGH2_MP history files, for example:

```
foft = t2historyfile('FOFT')
blkindex = 123
temp = foft[blkindex][1]
```

For **TOUGH+** connection and generator history files (COFT and GOFT, or Conx_Time_Series and SS_Time_Series), multiple connections and generators can be specified as usual in the TOUGH2 input data file, but individual results for them are not written to the history file. Instead, the results for them are summed. As a result, there are no 'keys' as such for accessing individual results, and the t2historyfile works a little differently. An array containing the data in each column can be accessed by specifying the column name, for example:

```
ct = t2historyfile('Conx_Time_Series')
qh = ct['HeatFlow']
```

The properties of a t2historyfile object are given in Table 6.5.

6.5 toughreact_tecplot objects

The t2listing library also defines a toughreact_tecplot class, used for representing the additional Tecplot output files produced by TOUGHREACT.

Example:

Property	Type	Description
element	listingtable	element table for current set of results
filename	string	name of listing file on disk
index	integer	index of current set of results
num_times	integer	number of sets of results
time	float	time of current set of results
times	np.array	array of times (float) for all results

Table 6.6: Properties of a toughreact_tecplot object

```
tp = toughreact_tecplot(filename, blocks)
```

creates a toughreact_tecplot object called tp and reads its contents from file filename. The blocks object passed in as a second parameter specifies the block names (see 6.5.2).

6.5.1 Differences from t2listing objects

A toughreact_tecplot object is similar to a t2listing object in many respects. Apart from the need to specify the block names on creation (see 6.5.2), the other main difference is that unlike a t2listing object, which usually contains several listingtable objects, a toughreact_tecplot object contains only one: the element table. Because of this, when using the history method, tables need not be specified.

These Tecplot files do not contain any information about time step numbers, so t2listing properties like step and steps are not present in a toughreact_tecplot object. There is also no title property, as this is not present in the Tecplot file.

There is also no 'short' output in a Tecplot file, so a toughreact_tecplot object does not have properties like fulltimes, as this would just be the same as the times property. There are also no diagnostic methods like convergence or reductions.

6.5.2 Specifying block names

In the Tecplot file, results are not associated with block names, though they appear in the same order as in the TOUGH2 data file used to generate the results. To make results accessible by block name, a second parameter containing the block names must be specified when a toughreact_tecplot object is created. This parameter is not optional. It can be either:

- a list of strings specifying the block names
- a mulgrid geometry object
- a t2grid object

6.5.3 Properties

The main properties of a toughreact_tecplot object are listed in Table 6.6. For more details, see the corresponding properties of the t2listing class.

Method	Type	Description
close	–	closes file
first	–	navigates to the first set of full results
history	list or tuple	time history for a selection of locations and table columns
last	–	navigates to the last set of full results
next	Boolean	navigates to the next set of full results
prev	Boolean	navigates to the previous set of full results
write_vtk	–	writes results to VTK file

Table 6.7: Methods of a `toughreact_tecplot` object

6.5.4 Methods

The methods of a `toughreact_tecplot` object are listed in Table 6.7. Details of these methods are given below.

`close()`

Closes the file after use.

`first()`

Navigates to the first set of results in the Tecplot file.

`history(selection)`

Returns a list of time histories (as `np.arrays`) for specified locations and table columns in the element table. For each selection, a tuple of two `np.arrays` is returned, one each for times and values.

Parameters:

- **selection**: list of tuples
  Selection of locations (or indices) and table columns to produce histories for. Each tuple contains two elements: **block name** and **table column name**. (If only a single tuple is given instead of a list of tuples, just the single tuple of times and values for that selection is returned.)

`last()`

Navigates to the last set of results in the Tecplot file.

`next()`

Navigates to the next set of results in the Tecplot file. Returns `False` if already at the last set of results (and `True` otherwise).

`prev()`

Navigates to the previous set of results in the Tecplot file. Returns `False` if already at the first set of results (and `True` otherwise).

```
write_vtk(geo, filename, grid=None, indices=None, start_time=0,
time_unit='s', blockmap = {}, surface_snap=0.1)
```

Writes a `toughreact_tecplot` object to a set of VTK files on disk, for visualisation with VTK, Paraview, Mayavi etc. The results in the element table of the Tecplot file object are written as an 'unstructured grid' VTK object with data arrays defined on cells. The data arrays written correspond to the variables given in the columns of the element table of the `toughreact_tecplot` object. In addition, data arrays from an associated `mulgrid` and (optionally) `t2grid` objects can be included.

One *.vtu file is produced for each time step in the `toughreact_tecplot` object, and a *.pvd file is also written. This is usually the file that should actually be opened in Paraview or other software as it contains time information associated with each *.vtu file.

Optionally, only a subset of the time indices present in the `toughreact_tecplot` can be written, according to the `indices` parameter. A start time and time unit for the output can optionally be specified.

Parameters:

- **geo**: `mulgrid`
  The `mulgrid` geometry object associated with the results. For flexibility, this geometry need not be fully compatible with the results – for example, it may contain only a subset of the blocks for which results are present, or the blocks may be in a different order. However, if it is not fully compatible, the writing process will be slower.

- **filename**: string
  Name of the *.pvd file to be written. Names of the individual *.vtu files for each time step are similar but with a time index appended and the file extension changed.

- **grid**: `t2grid`
  Name of optional `t2grid` object associated with the results.

- **indices**: list or tuple
  Optional specification of time indices to include in the output. If set to `None` (the default), all time indices will be included.

- **start_time**: float
  Optional start time of the simulation, i.e. time associated with the first set of results. Default is zero.

- **time_unit**: string
  Optional time unit for the output. TOUGHREACT Tecplot results are given at times in years, but this option allows them to be converted to other units. Options are: 's', 'h', 'd' and 'y', for seconds, hours, days and years respectively. Default is 's'.

- **blockmap**: dictionary
  Dictionary mapping the block names in the geometry to the block naming system used in the Tecplot output.

- **surface_snap**: float
  Tolerance for specifying how close column surface elevations need to be before being considered "equal" when constructing surface nodes.

6.6 Examples

6.6.1 Slice plot of drawdown

This script shows a vertical slice plot along the model's x-axis of the difference in pressure (i.e. drawdown) between the start and end of a simulation.

```
from mulgrids import *
from t2listing import *
from copy import copy

geo = mulgrid('gmodel.dat')
results = t2listing('model.listing')

results.first()
p0 = copy(results.element['Pressure'])
results.last()
p1 = results.element['Pressure']

geo.slice_plot('x', (p1-p0)/1.e5, 'Pressure\ difference', 'bar')
```

(Note: the `copy` command is needed, otherwise the arrays `p0` and `p1` would both contain the final values of pressure after the `results.last()` command.)

6.6.2 Pressure-temperature diagram

This script plots model results from a specified block on a pressure-temperature diagram.

```
from t2listing import *
import matplotlib.pyplot as plt

lst = t2listing('model.listing')
blk = ' n 60'
[(tp,p), (tt,t)] = lst.history([('e', blk, 'Pressure'), ('e', blk,
    'Temperature')])

plt.plot(t, p/1.e5, 'o-')
plt.xlabel('T ($\degree$C)')
plt.ylabel('P (bar)')
plt.show()
```

6.6.3 Comparing results of two models

This script reads grids and results for two different models, a coarse model and a fine one, and produces a comparison plot of the time history of temperature for both models at a given point.

```
from mulgrids import *
from t2listing import *
import matplotlib.pyplot as plt
```

```
geoc, geof = mulgrid('gcoarse.dat'), mulgrid('gfine.dat')
coarse, fine = t2listing('coarse.listing'), t2listing('fine.listing')

p = [47.e3, 0.0, -7000.0]
blkc = geoc.block_name_containing_point(p)
blkf = geof.block_name_containing_point(p)

tc, tempc = coarse.history(('e', blkc, 'Temperature'))
tf, temp = fine.history(('e', blkf, 'Temperature'))

plt.plot(tc, tempc, 'o-', label = 'coarse model')
plt.plot(tf, tempf, 's-', label = 'fine model')
plt.xlabel('time (s)')
plt.ylabel('Temperature ($\degree$C)')
plt.legend()

plt.show()
```

Chapter 7

TOUGH2 thermodynamics

7.1 Introduction

The `t2thermo` library in PyTOUGH contains a Python implementation of the thermodynamic routines used in TOUGH2. These can be used to calculate the thermodynamic properties of water and steam under a range of conditions. They are based on a subset of the IFC-67 thermodynamic formulation (IFC, 1967).

The `t2thermo` library can be imported using the command:

```
from t2thermo import *
```

The functions available through the `t2thermo` library are listed in Table 7.1 and described below.

7.2 Thermodynamic functions

The thermodynamic routines used in TOUGH2 provide functions for liquid water and dry steam. These functions calculate secondary parameters from the primary thermodynamic variables. Their names follow the subroutine names used in the TOUGH2 code.

Function	Type	Description
`cowat`	tuple	density and internal energy of liquid water
`sat`	float	saturation pressure as a function of temperature
`region`	integer	thermodynamic region
`separated_steam_fraction`	float	separated steam fraction for given enthalpy and separator pressure
`supst`	tuple	density and internal energy of dry steam
`tsat`	float	saturation temperature as a function of pressure
`visw`	float	dynamic viscosity of water
`viss`	float	dynamic viscosity of steam

Table 7.1: `t2thermo` functions

7.2.1 Liquid water: `cowat(t, p, bounds = False)`

The `cowat` function returns a two-element tuple (`d`,`u`) of density (kg/m^3) and internal energy (J/kg) of liquid water as a function of temperature `t` (°C) and pressure `p` (Pa).

Parameters:

- **t**: float
  Temperature (°C)
- **p**: float
  Pressure (Pa)
- **bounds**: Boolean
  If `True`, return `None` if the input temperature and pressure are outside the operating range of the routine (as defined by thermodynamic region 1 of the IFC-67 specification).

7.2.2 Dry steam: `supst(t, p, bounds = False)`

The `supst` function returns a two-element tuple (`d`,`u`) of density (kg/m^3) and internal energy (J/kg) of dry steam as a function of temperature `t` (°C) and pressure `p` (Pa).

Parameters:

- **t**: float
  Temperature (°C)
- **p**: float
  Pressure (Pa)
- **bounds**: Boolean
  If `True`, return `None` if the input temperature and pressure are outside the operating range of the routine (as defined by thermodynamic region 2 of the IFC-67 specification).

7.3 Viscosity

7.3.1 Liquid water: `visw(t,p,ps)`

The `visw` function returns the dynamic viscosity (Pa.s) of liquid water as a function of temperature `t` (°C), pressure (Pa) and saturation pressure (Pa).

Parameters:

- **t**: float
  Temperature (°C)
- **p**: float
  Pressure (Pa)
- **ps**: float
  Saturation pressure (Pa), calculated for example using the `sat` function.

7.3.2 Dry steam: `viss(t,d)`

The `viss` function returns the dynamic viscosity (Pa.s) of dry steam as a function of temperature `t` (°C) and density `d` (kg/m^3).

Parameters:

- **t**: float
  Temperature (°C)
- **d**: float
  Density (kg/m^3)

7.4 Saturation line: `sat(t)` and `tsat(p)`

7.4.1 `sat(t, bounds = False)`

The `sat` function returns the saturation pressure (Pa) at a given temperature `t` (°C), for temperatures below the critical temperature.

Parameters:

- **t**: float
  Temperature (°C)
- **bounds**: Boolean
  If `True`, return `None` if the input temperature is outside the operating range of the routine (i.e. less than 0.01°C or greater than the critical temperature, 374.15°C).

7.4.2 `tsat(p, bounds = False)`

The `tsat` function returns the saturation temperature (°C) at a given pressure `p` (Pa), for pressures below the critical pressure.

Note that the IFC-67 formulation did not include an explicit formula for calculating saturation temperature as a function of pressure, so here (as in TOUGH2) this is calculated using an iterative root-finding process on the `sat` function. The root-finding function is from the `scipy` library, so this library must be installed before the `tsat` function will work.

Parameters:

- **p**: float
  Pressure (Pa)
- **bounds**: Boolean
  If `True`, return `None` if the input pressure is outside the operating range of the routine (i.e. less than `sat(0.01)` or greater than the critical pressure, 22.12 MPa).

7.5 Other functions

7.5.1 Separated steam fraction

`separated_steam_fraction(h, separator_pressure, separator_pressure2 = None)`

Returns the separated steam fraction for a given enthalpy `h` and separator pressure. A second separator pressure may be specified in the case of two-stage flash.

Parameters:

- **h**: float
  Enthalpy (J/kg)
- **separator_pressure**: float
  Steam separator pressure (Pa)
- **separator_pressure2**: float (or `None`)
  Second separator pressure (Pa) for two-stage flash – set to `None` (the default) for single-stage.

7.5.2 Determining thermodynamic region

`region(t, p)`

Returns the thermodynamic region (integer, or `None`) corresponding to the given temperature (°C) and pressure (Pa), as defined by the IFC-67 specification. The regions are:

1. liquid water
2. dry steam
3. supercritical
4. near-critical

If the input temperature and/or pressure are outside the operating range of the IFC-67 formulation, the routine will return `None`.

Parameters:

- **t**: float
  Temperature (°C)
- **Pressure**: float
  Pressure (Pa)

7.6 Example

The following script reads in a geometry file and writes an initial conditions file with approximate hydrostatic conditions corresponding to a specified vertical temperature gradient. In this case, the model has a simple flat surface, so that each column has the same number of layers. The `cowat` function is used to calculate the fluid density at each layer, and hence the approximate vertical pressure distribution.

```
from mulgrids import *
from t2thermo import *

geo = mulgrid('gmodel.dat')

patm, tatm = 101.325e3, 15.0
ptblk = np.zeros((geo.num_blocks, 2))
ptblk[:,0] = patm; ptblk[:,1] = tatm
```

```
g = 9.8
p, t = patm, tatm
thick = 0.0
tgradient = 30 # deg C/km
for lay in geo.layerlist[1:]:
    d = cowat(t, p)[0]
    thisthick = lay.top - lay.bottom
    h = 0.5 * (thick + thisthick)
    p += d * g * h
    t += tgradient / 1.e3 * h
    thick = thisthick
    for col in geo.columnlist:
        blkname = geo.block_name(lay.name, col.name)
        iblk = geo.block_name_index[blkname]
        ptblk[iblk] = [p, t]
inc = dat.grid.incons(ptblk)
inc.write('model.incon')
```

Chapter 8

IAPWS-97 thermodynamics

8.1 Introduction

The `IAPWS97` library in PyTOUGH contains a Python implementation of the main functions of the International Association for the Properties of Water and Steam 1997 (IAPWS-97) thermodynamic formulation (Wagner et al., 2000). These can be used to calculate the thermodynamic properties of water, steam and supercritical water. The IAPWS-97 supersedes the IFC-67 formulation used in TOUGH2 (see section 7), being generally faster and more accurate, as well as having a simpler representation of the thermodynamic region around the critical point.

The operating range of the IAPWS-97 formulation is shown in the pressure-temperature plot below. It covers temperatures up to 800 °C and pressures up to 100 MPa, and is divided into four thermodynamic regions:

1. liquid water
2. dry steam
3. supercritical fluid
4. two-phase

The two-phase region (4) follows the saturation line on the pressure-temperature plot (the boundary between liquid water and dry steam), up to the critical point C ($T = 373.946$ °C, $P = 22.064$ MPa), where the distinction between liquid water and steam disappears. Region 3 covers supercritcal fluid (above the critical point) and also near-critical fluid, just below the critical point. The boundary between regions 1 and 3 (liquid water and supercritical) is aribitrarily set at $T = 350$ °C. The boundary between regions 2 and 3 (dry steam and supercritical) is described by the `b23p` and `b23t` functions, given in section 8.4.2.

The `IAPWS97` library can be imported using the command:

```
from IAPWS97 import *
```

The functions available through the `IAPWS97` library are listed in Table 8.1 and described below.

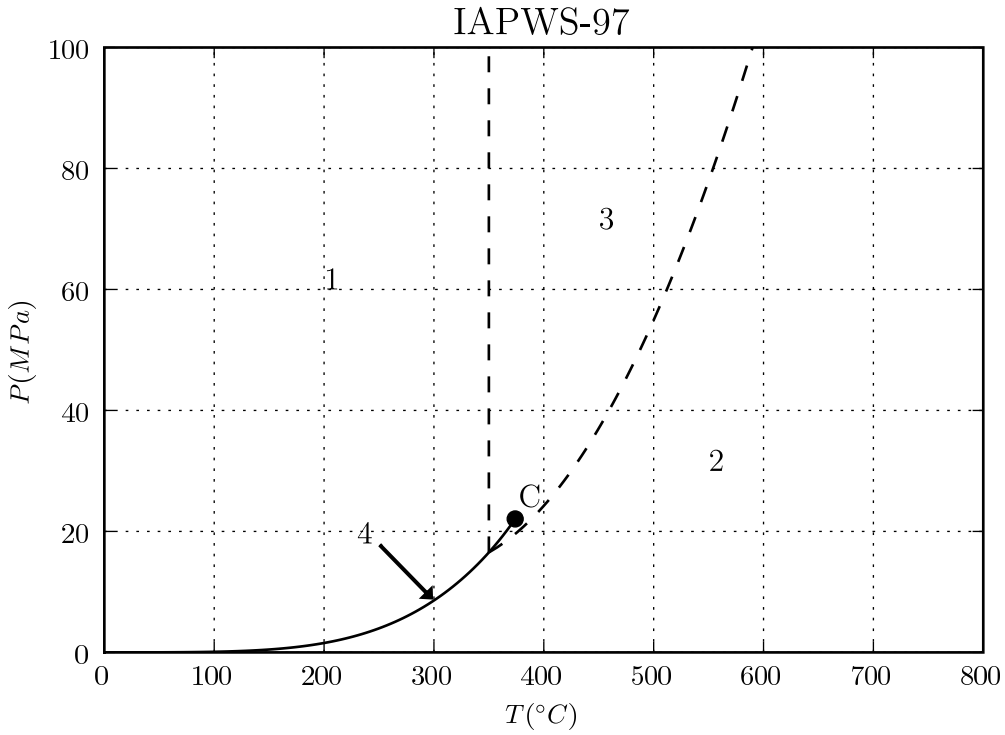

Figure 8.1: Operating range of the IAPWS-97 thermodynamic formulation

Function	Type	Description
b23p	float	pressure on boundary between steam and supercritical regions, as a function of temperature
b23t	float	temperature on boundary between steam and supercritical regions, as a function of pressure
cowat	tuple	density and internal energy of liquid water
density_temperature_plot	–	draws region boundaries on a density-temperature plot
pressure_temperature_plot	–	draws region boundaries on a pressure-temperature plot
region	integer	thermodynamic region
sat	float	saturation pressure as a function of temperature
super	tuple	pressure and internal energy of supercritical fluid
supst	tuple	density and internal energy of dry steam
tsat	float	saturation temperature as a function of pressure
visc	float	dynamic viscosity of water, steam or supercritical fluid

Table 8.1: `IAPWS97` functions

8.2 Thermodynamic functions

The IAPWS-97 formulation provides thermodynamic functions for liquid water, dry steam and supercritical fluid. These functions calculate secondary parameters from the primary thermodynamic variables.

8.2.1 Liquid water: `cowat(t,p)`

The `cowat` function returns a two-element tuple (`d`,`u`) of density (kg/m^3) and internal energy (J/kg) of liquid water as a function of temperature `t` (°C) and pressure `p` (Pa).

Parameters:

- **t**: float
  Temperature (°C)
- **p**: float
  Pressure (Pa)

8.2.2 Dry steam: `supst(t,p)`

The `supst` function returns a two-element tuple (`d`,`u`) of density (kg/m^3) and internal energy (J/kg) of dry steam as a function of temperature `t` (°C) and pressure `p` (Pa).

Parameters:

- **t**: float
  Temperature (°C)

- **p**: float
  Pressure (Pa)

8.2.3 Supercritical fluid: `super(d,t)`

The `super` function returns a two-element tuple (`p`,`u`) of pressure (Pa) and internal energy (J/kg) of supercritical fluid as a function of density `d` (kg/m^3) and temperature `t` (°C).

Parameters:

- **d**: float
  Density (kg/m^3)
- **t**: float
  Temperature (°C)

8.3 Viscosity: `visc(d,t)`

The `visc` function returns the dynamic viscosity (Pa.s) of liquid water, dry steam or supercritical fluid as a function of density `d` (kg/m^3) and temperature `t` (°C). This function is based on the supplementary "IAPWS Formulation 2008 for the Viscosity of Ordinary Water Substance", without the critical enhancement of viscosity near the critical point.

Parameters:

- **d**: float
  Density (kg/m^3)
- **t**: float
  Temperature (°C)

8.4 Region boundaries

These functions describe the boundaries between the four thermodynamic regions of the IAPWS-97 formulation (see Figure 8.1). There is no equation for the boundary between regions 1 and 3 as this is simply the line $T = 350$°C.

8.4.1 Saturation line: `sat(t)` and `tsat(p)`

`sat(t)`

The `sat` function returns the saturation pressure (Pa) at a given temperature `t` (°C), for temperatures below the critical temperature.

Parameters:

- **t**: float
  Temperature (°C)

`tsat(p)`

The `tsat` function returns the saturation temperature (°C) at a given pressure `p` (Pa), for pressures below the critical pressure.

Parameters:

- **p**: float
  Pressure (Pa)

8.4.2 Steam/supercritical boundary

`b23p(t)`

The `b23p` function returns the pressure (Pa) on the boundary of the dry steam and supercritical regions (regions 2 and 3) at a given temperature `t` (°C).

Parameters:

- **t**: float
  Temperature (°C)

`b23t(p)`

The `b23t` function returns the temperature (°C) on the boundary of the dry steam and supercritical regions (regions 2 and 3) at a given pressure `p` (Pa).

Parameters:

- **p**: float
  Pressure (Pa)

8.5 Determining thermodynamic region

`region(t, p)`

Returns the thermodynamic region (integer, or `None`) corresponding to the given temperature (°C) and pressure (Pa), as defined by the IAPWS-97 specification. The regions are:

1. liquid water
2. dry steam
3. supercritical

If the input temperature and/or pressure are outside the operating range of the IAPWS-97 formulation, the routine will return `None`.

Parameters:

- **t**: float
  Temperature (°C)
- **Pressure**: float
  Pressure (Pa)

8.6 Plotting functions

The `IAPWS97` library contains two functions used for including the IAPWS-97 thermodynamic region boundaries on plots.

8.6.1 `pressure_temperature_plot(plt)`

Draws the IAPWS-97 thermodynamic region boundaries on a pressure-temperature diagram.

Parameters:

- **plt**: `matplotlib.pyplot` instance
  An instance of the `matplotlib.pyplot` library, imported in the calling script using e.g. `import matplotlib.pyplot as plt`.

8.6.2 `density_temperature_plot(plt)`

Draws the IAPWS-97 thermodynamic region boundaries on a density-temperature diagram. (This function requires the Scientific Python (`scipy`) library to be installed.)

Parameters:

- **plt**: `matplotlib.pyplot` instance
  An instance of the `matplotlib.pyplot` library, imported in the calling script using e.g. `import matplotlib.pyplot as plt`.

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Appendix A

MULgraph geometry file format

A.1 Introduction

This appendix gives a format specification of the MULgraph geometry file. These files can be used to give a geometrical description of a TOUGH2 model grid, useful for creating grids and visualizing simulation results.

MULgraph geometry files were originally developed for use with MULgraph, a graphical post-processor for TOUGH2 and AUTOUGH2 (O'Sullivan and Bullivant, 1995) developed at the University of Auckland in the 1990s. However, MULgraph geometry files can be used independently of MULgraph. PyTOUGH is able to represent the contents of a MULgraph geometry file in a Python script via the `mulgrid` class.

A.2 Grid structure

A.2.1 Layers and columns

MULgraph geometry files implicitly assume a layered structure, with blocks arranged in layers and columns, and the same arrangement of columns in each layer. The only exception to this is at the top surface of the model, where layers are allowed to be incomplete (i.e. not contain all columns) in order to represent topography.

The layers are always of constant vertical thickness. However, the blocks in the top layer are allowed to vary in height, again to represent variations in ground surface elevation.

A.2.2 Atmosphere blocks

The blocks in the top layer may optionally be connected to the atmosphere- either a single atmosphere block connected to all columns, or a separate atmosphere block over each column (see section A.4).

A.2.3 Tilted geometries

It is possible to tilt the geometry coordinate axes with respect to the vertical, to represent non-horizontal geometries. When a TOUGH2 grid is created from such a tilted geometry, only the gravity cosines of the grid connections are affected.

A.2.4 Rotating permeability directions

It is also possible to rotate the permeability principal directions with respect to the coordinate axes- for example, to align permeabilities with a dominant fault direction. When a TOUGH2 grid is created, this can change the permeability index associated with each connection.

A.3 Geometry types

The original MULgraph file specification allowed for three types of geometry: 'general', 'rectangular' and 'radial'. Only the 'general' geometry type is supported by PyTOUGH. It is intended for representing general grids with arbitrary, possibly unstructured horizontal column arrangements.

The 'rectangular' type was a special type for grids with rectangular horizontal column structures. These can also be represented using the 'general' geometry type. Since PyTOUGH contains methods for constructing rectangular grids within the 'general' geometry type, there is usually no longer any significant benefit from using the 'rectangular' type.

The 'radial' type was intended for grids with radial horizontal column structure. PyTOUGH also contains methods for creating radial TOUGH2 grids. Simulation results from radial models can also be visualized using a simple one- or two-dimensional rectangular 'general' geometry to represent the grid structure in the radial direction.

A.4 Naming conventions and atmosphere types

The grid block naming convention and atmosphere type used in a MULgraph geometry file are both integers which can be given the value 0, 1 or 2. The meanings of these values are shown in Table A.1 and A.2.

Note that the grid nodes (vertices) are also named according to the column part of the block naming convention. If naming nodes, columns or layers manually, while the names can in principle be arbitrary (within the naming convention), it is safest to right-justify them.

The MULgraph block naming conventions all use part of the block name to indicate the layer, and part of it to indicate the column. In PyTOUGH, it is also possible to use MULgraph geometry files in conjunction with TOUGH2 grids that follow other naming conventions, by means of a block mapping dictionary.

0	3 characters for column followed by 2 digits for layer
1	3 characters for layer followed by 2 digits for column
2	2 characters for layer followed by 3 digits for column

Table A.1: MULgraph geometry file naming conventions

0	A single atmosphere block
1	One atmosphere block over each column
2	No atmosphere blocks

Table A.2: MULgraph geometry file atmosphere types

A.5 File format

MUlgraph geometry files are simple formatted ASCII text files with a header line at the top, followed by a number of sections. Each section begins with a keyword and ends with a blank line. Each line has **fixed** format, so the different values have to be specified in the right text columns.

If you use PyTOUGH scripts to create and manipulate your grid geometries, you don't need to know anything about the format of a MULgraph geometry file, because PyTOUGH will handle reading and writing them for you. If, however, for some reason you do need to know how these files are structured, the format specification for a 'general' type geometry file is given below.

A.5.1 Header

This is a single line containing a number of global parameters of the geometry. Its format is given in table A.3.

Note that the block ordering parameter is an extension to the original MULgraph file format.

A.5.2 Vertices

This section defines the horizontal locations of the grid vertices (nodes), at the corners of the columns. The first line just contains the keyword 'VERTI'. Each subsequent line defines the position of a vertex, and has the format given in table A.4. The vertices section is terminated by a blank line.

A.5.3 Grid

This section specifies the vertices making up each column. The first line just contains the keyword 'GRID'.

For each grid column, there is then a sub-header line with information about the column, followed by a line for each vertex making up the column. The sub-header line has the format given in table A.5, and the line for each vertex has the format given in table A.6. There are no blank lines between the definitions of the grid columns, but there is a blank line at the end of the section.

A.5.4 Connections

This section defines the horizontal connections between columns. The first line just contains the keyword 'CONNE'.

Each subsequent line defines a connection between two columns, and has the format given in table A.7. There is a blank line at the end of the section.

A.5.5 Layers

This section defines the grid layers. The first line just contains the keyword 'LAYER'.

Each subsequent line defines a layer, with format given by table A.8. There are no blank lines between layers, but there is a blank line at the end of the section.

Name	Type	Length	Columns	Description
Geometry type	character	5	1–5	'GENER' for general geometry type; 'RECTA' or 'RADIA' for other types (but these are not supported by PyTOUGH)
Naming convention	integer	1	6	Block naming convention: see table A.1
Atmosphere type	integer	1	7	Type of atmosphere: see table A.2
Atmosphere volume	float	10	8–17	Volume of each atmosphere block (default $10^{20}m^3$)
Atmosphere connection distance	float	10	18–27	Connection distance for each atmosphere block (default $10^{-6}m$)
Length unit	character	5	28–32	Default is metres (blank); for feet specify 'FEET'
x-direction cosine	float	10	33–42	Cosine of angle between x-axis and gravity vector (default zero); set positive for tilt in the x-direction
y-direction cosine	float	10	43–52	Cosine of angle between y-axis and gravity vector (default zero); set positive for tilt in the y-direction
Connection type	integer	1	53	Method of calculating connection parameters (default zero)-not supported by PyTOUGH
Permeability angle	float	10	54–63	Horizontal angle (degrees anticlockwise) between first permeability direction and x-axis
Block ordering	integer	2	64–65	Block ordering scheme: 0 for original MULgraph layer/column ordering; 1 for PETSc DMPlex ordering (sorted by block type)

Table A.3: MULgraph geometry file header line format

Name	Type	Length	Columns	Description
Vertex name	character	3	1–3	Name of the vertex (honouring the column naming convention)
x	float	10	4–13	x-coordinate of the vertex
y	float	10	14–23	y-coordinate of the vertex

Table A.4: MULgraph geometry file vertices format

Name	Type	Length	Columns	Description
Column name	character	3	1–3	Name of the column (honouring the column naming convention)
Centre specified	integer	1	4–5	Set non-zero to specify the column centre location, or zero (default) to calculate it as the centroid of the column
Number of vertices	integer	2	6–7	Number of vertices in the column
Column centre x	float	10	8–17	x-coordinate of column centre
Column centre y	float	10	18–27	y-coordinate of column centre

Table A.5: MULgraph geometry file column header format

Name	Type	Length	Columns	Description
Vertex name	character	3	1–3	Name of the vertex, as specified in the vertices section

Table A.6: MULgraph geometry file column vertex format

A.5.6 Surface elevation

This section is optional, and can be used to define the surface elevation at any or all columns in the grid, to represent topography. The first line just contains the keyword 'SURFA'.

Each subsequent line defines the surface elevation at a column, with format given by table A.9. There is a blank line at the end of the section.

A.5.7 Wells

This section is optional, and can be used to define the positions of wells (including their tracks) within the geometry. Deviated wells are supported. The first line of the section just contains the keyword 'WELLS'.

Each subsequent line defines the location of one point on a well track, with format given by table A.10. At least two points are required to define each well (one for the wellhead and one for the bottom), with more than two points needed to define a deviated well. There is a blank line at the end of the section.

Name	Type	Length	Columns	Description
First column name	character	3	1–3	Name of the first column
Second column name	character	3	4–6	Name of the second column

Table A.7: MULgraph geometry file connection format

Name	Type	Length	Columns	Description
Layer name	character	3	1–3	Name of the layer (honouring the layer naming convention)
Bottom elevation	float	10	4–13	Elevation of the bottom of the layer
Centre elevation	float	10	14–23	Elevation of the centre of the layer

Table A.8: MULgraph geometry file layer format

Name	Type	Length	Columns	Description
Column name	character	3	1–3	Name of the column
Surface elevation	float	10	4–13	Surface elevation of the column

Table A.9: MULgraph geometry file surface elevation format

Name	Type	Length	Columns	Description
Well name	character	5	1–5	Name of the well
x	float	10	6–15	x-coordinate of the well location
y	float	10	16–25	y-coordinate of the well location
z	float	10	26–35	z-coordinate of the well location

Table A.10: MULgraph geometry file well format

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