Geoscientific
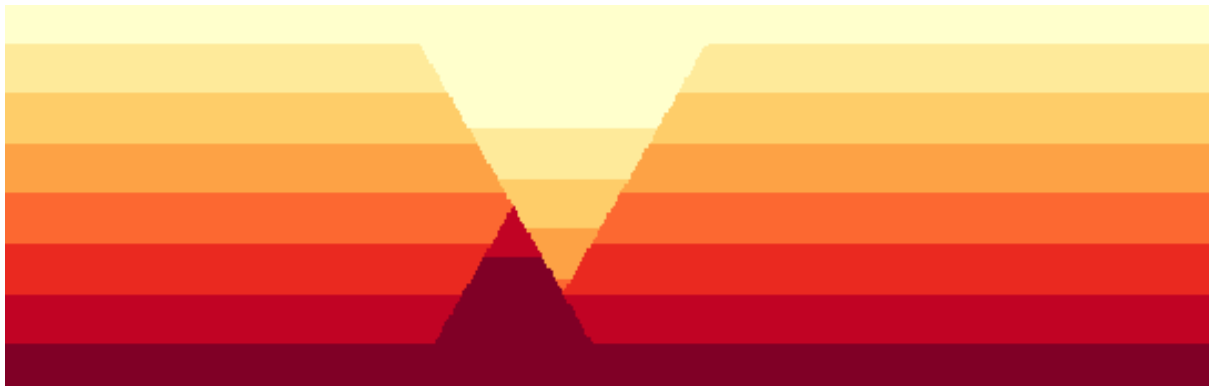Model Development
Discussions

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Supplement of

pynoddy 1.0: an experimental platform for automated 3-D kinematic and potential field modelling

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pynoddy Documentation

Release 1.0

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Contents:

PYNODDY

`pynoddy` is a python package to write, change, and analyse kinematic geological modelling simulations performed with Noddy (see below for more information on Noddy).

1.1 How does it work?

`pynoddy` provides methods to define, load, modify, and safe kinematic models for simulation with `Noddy`. In addition, the package contains an extensive range for postprocessing of results. One main aspect of `pynoddy` is that it enables the encapsulation of full scientific kinematic modelling experiments for full reproducibility of results.

A successful installation of `pynoddy` requires two steps:

1. An installation of the python modules in the package `pynoddy`

2. The existance of an executable `Noddy(.exe)` program

Currently, `pynoddy` and `Noddy` can be installed in two alternative ways: (a) directly from the source code with the full repository, or (b) with a direct installation from the Python Package Index and pre-compiled executables. We suggest to use option (a) for the most recent and most complete version of the code. Version (b) is suggested for less experienced users who would like to quickly test and apply kinematic modelling methods. We describe the installation the alternatives in the following.

Note: for clarity, we denote command line prompts with a > symbol below:

```
> command to be executed
```

1.2 Installation of `pynoddy`

1.2.1 Installing from the github repository

As a first step, we suggest to clone the current repository to your local machine. This step can be done with a github front-end, or simply with the usual `git` command in a terminal:

```
> git clone https://github.com/flohorovicic/pynoddy
```

Note: if you do not have a running version of installed, then you can also simply download the entire repository as a zip file from the github page. However, you then do not have the full flexibility of the entire repository, and therefore we recommend using `git`.

Once the repository is cloned (or downloaded), simply change to the main directory of `pynoddy` and install the Python package with the installation script:

```
> python setup.py install
```

Note that this command adds `pynoddy` to your global Python installation. If you plan to develop parts of further `pynoddy` yourself, then installation in development mode is suggested:

```
> python setup.py develop
```

In this mode, modifications in the cloned repository are directly considered when importing the modules in your Python scripts.

1.2.2 Installation from Python Package Index

`pynoddy` is hosted on the Python Package Index (https://pypi.python.org/pypi/pynoddy/) and the typical methods can be used to install the Python packages.

If `pip` is installed on your system, then the most straight-forward installation is directly though executing in a terminal:

```
> pip install pynoddy
```

Alternatively, the package source can be downloaded from the index page, as well as an installation program for Windows systems.

Please note that the Python package on the index is not always the newest version, but in a state that reflects the latest stable developments. For the most current state, we suggest an installation from the repository (Sec. [sec:inst-textsfpyn-from]).

1.3 Installation of the command line program `Noddy`

1.3.1 Using a pre-compiled version of `Noddy`

The easy way to obtain a executable version of `Noddy` is simply to download the appropriate version for your operating system. Currently, these executables versions are also stored on github (check the up-to-date online documentation if this should not anymore be the case) in the directory:

https://github.com/flohorovicic/pynoddy/tree/master/noddyapp

Furthermore, the executables for Windows are also available for download on the webpage:

http://www.tectonique.net/pynoddy

Download the appropriate app, rename it to *noddy*' or `noddy.exe` and place it into a folder that is in your local environment path variable. If you are not sure if a folder is in the path variable or would like to add new one, see below.

1.3.2 Compiling `Noddy` from source files (recommended)

The source code for the executable `Noddy` is located in the repository directory `noddy`. In order to perform the installation, a `gcc` compiler is required. This compiler should be available on Linux and MacOSX operating systems. On Windows, one possibility is to install MinGW. Otherwise, the code requires no specific libraries.

Note for MacOSX users: some header files have to be adapted to avoid conflicts with local libraries. The required adaptations are executed when running the script:

```
> adjust_for_MacOSX.sh
```

The compilation is then performed (in a Linux, MacOSX, or Windows MinGW terminal) with the command:

```
> compile.sh
```

Compilation usually produces multiple warnings, but should otherwise proceed successfully.

1.3.3 Placing `Noddy` in the Path

For the most general installation, the executable of `Noddy` should be placed in a folder that can be located from any terminal application in the system. This (usually) means that the folder with the executable has to be in the `PATH` environment variable. On Linux and MacOSX, a path can simply be added by:

```
> export PATH=path/to/executable/:$PATH
```

Note that this command should be placed into your `.bash_profile` file to ensure that the path is added whenever you start a new Python script.

On `Windows`, adding a folder to the local environment variable `Path`' is usually done through the System Control Panel (Start - Settings - Control Panel - System). in Advanced mode, open the Environment Variables sub-menu, and find the variable Path. Click to edit the variable, and add the location of your folder to this path.

1.3.4 Specifying path during `pynoddy` execution

Another option is to tell `pynoddy.compute_model()` the exact path to the `Noddy` executable:

```
pynoddy.compute_model(history, output_name,
                      noddy_path = 'path/to/program')
```

However, this method should only be used as the fall-back option if adding the executable to the path does not work. Also, in this case, the tests (see below) will most likely fail.

1.4 Testing the installation

1.4.1 Testing `Noddy`

Simply test the installation by running the generated (or downloaded) executable in a terminal window (on Windows:):

```
> noddy
```

or (depending on your compilation or naming convention):

```
> noddy.exe
```

Which should produce the general output:

```
Arguments <historyfile> <outputfile> <calc_mode>:
BLOCK
GEOPHYSICS
SURFACES
BLOCK_GEOPHYS
BLOCK_SURFACES
TOPOLOGY
ANOM_FROM_BLOCK
ALL
```

Note: if the executable is correctly placed in a folder which is recognised by the (Environment) path variable, then you should be able to run `Noddy` from any directory.

1.4.2 Testing `pynoddy`

The `pynoddy` package contains a set of tests which can be executed in the standard Python testing environment. If you cloned or downloaded the repository, then these tests can directly be performed through the setup script:

```
> python setup.py test
```

Of specific relevance is the test that determines if the `noddy(.exe)` executable is correctly accessible from `pynoddy`. If this is the case, then the `compute_model` test should return:

```
test_compute_model (test.TestHistory) ...  ok
```

If this test is not ok, then please check carefully the installation of the `noddy(.exe)` executable.

If all tests are successful, you are ready to go!

1.5 Noddy executable and GUI

The original graphical user interface for and the compiled executable program for Windows can be obtained from http://tinyurl.com/noddy-site. This site also contains the source code, as well as extensive documentation and tutorial material concerning the original implementation of the software, as well as more technical details on the modelling method itself.

1.6 Documentation

Documentation is available within the `pynoddy` repository (pynoddy/docs).

In addition, an up-to-date online html version of the documentation is also hosted on readthedocs:

http://pynoddy.readthedocs.org

1.7 How to get started: tutorial notebooks

The best way to get started with `pynoddy` is to have a look at the IPython notebooks in pynoddy/docs/notebooks. The numbered notebooks are those that are part of the documentation, and a good point to get started.

The notebooks require an installed Jupyter notebook. More information here:

https://jupyter.org

The notebook can be installed via `pip` or `conda`.

1.8 Dependencies

`pynoddy` depends on several standard Python packages that should be shipped with any standard distribution (and are easy to install, otherwise):

- numpy
- matplotlib
- pickle

The uncertainty analysis, quantification, and visualisation methods based on information theory are implemented in the python package pygeoinfo. This package is available on github and part of the python package index. It is automatically installed with the setup script provided with this package.

In addition, to export model results for full 3-D visualisation with VTK, the pyevtk package is used, available on bitbucket:

https://bitbucket.org/pauloh/pyevtk/src/9c19e3a54d1e?at=v0.1.0

The package is automatically downloaded and installed when running python setup.py install.

1.9 3-D Visualisation

At this stage, we do not supply methods for 3-D visualisation in python (although this may change in the future). However, we provide methods to export results into a VTK format. Exported files can then be viewed with the highly functional VTK viewers, and several free options are available, for example:

- Paraview: http://www.paraview.org
- Visit: https://wci.llnl.gov/simulation/computer-codes/visit/

- Mayavi: http://docs.enthought.com/mayavi/mayavi/

1.10 License

pynoddy is free software (see license file included in the repository). Please attribute the work when you use it and cite the publication if you use it in a scientific context - feel free to change and adapt it otherwise!

1.11 What is Noddy?

Noddy itself is a kinematic modelling program written by Mark Jessell [1][2] to simulate the effect of subsequent geological events (folding, unconformities, faulting, etc.) on a primary sedimentary pile. A typical example would be:

1. Create a sedimentary pile with defined thicknesses for multiple formations

2. Add a folding event (for example simple sinoidal folding, but complex methods are possible!)

3. Add an unconformity and, above it, a new stratigraphy

4. Finally, add a sequence of late faults affecting the entire system.

The result could look something like this:
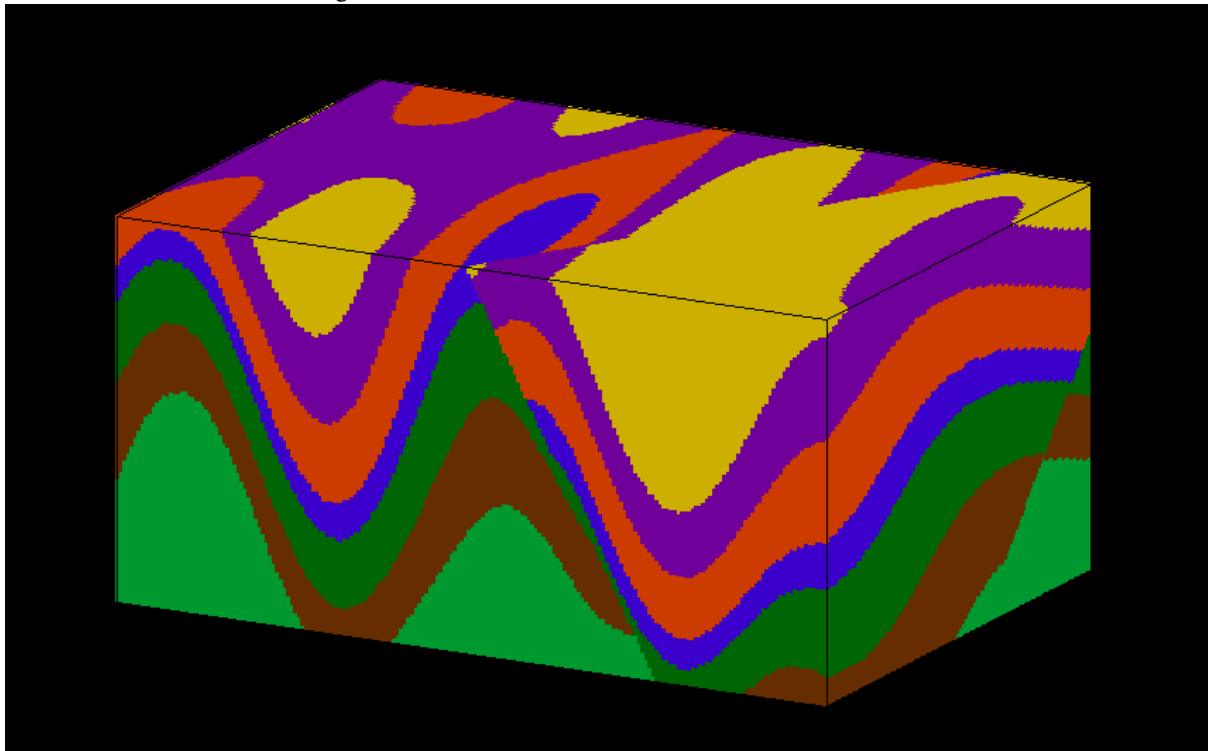
The software runs on Windows only, but the source files (written in C) are available for download to generate a command line version of the modelling step alone:

https://github.com/flohorovicic/pynoddy

It has been tested and compiled on MacOSX, Windows and Linux.

1.12 References

[1] Mark W. Jessell. Noddy, an interactive map creation package. Unpublished MSc Thesis, University of London. 1981. [2] Mark W. Jessell, Rick K. Valenta, Structural geophysics: Integrated structural and geophysical modelling, In: Declan G. De Paor, Editor(s), Computer Methods in the Geosciences, Pergamon, 1996, Volume 15, Pages 303-324, ISSN 1874-561X, ISBN 9780080424309, http://dx.doi.org/10.1016/S1874-561X(96)80027-7.

PYNODDY.NODDY MODULE

This module contains the Noddy code that is actually used to compute the kinematic models defined in .his files.

Note that this code *must be compiled* before `pynoddy.compute_model` will function correctly. It should compile easily (plus or minus a few thousand warnings) using the `compile.sh` script. Windows users will first need to install the GCC library (e.g. through MinGW), but otherwise the code requires no non-standard libraries.

Usage

The compiled noddy code can be run directly from the command line to a realisation of a model defined in a .his file, or called through `pynoddy.compute_model`.

If the binary is called from the command line it takes the following arguments:

```
noddy [history_file] [output_name] [calculation_mode]
```

Where:

- `history_file` is the filepath (including the extension) of the .his file defining the model
- `output_name` is the name that will be assigned to the noddy output files

The `mode` argument determines the type of output that noddy generates, and can be any one of:

- BLOCK - calculates the lithology block model
- GEOPHYSICS - calculates the geophysical expression (magnetics and gravity) of the model
- SURFACES - calculates surfaces representing the lithological contacts
- BLOCK_GEOPHYS - calculates the lithology block model and its geophysical expression
- BLOCK_SURFACES - calculates the lithology block model and lithological surfaces
- TOPOLOGY - calculates the lithology block model and associated topology information
- ANOM_FROM_BLOCK - calculates the geophysical expression of an existing lithology block (output_name.g12)
- ALL - calculates the block, geophysics, topology and surfaces

Python Wrapper

As mentioned earlier, the executable can also be accessed from python via pynoddy. This is performed by calling the `pynoddy.compute_model` function, as defined below:

pynoddy.**compute_model**(*history*, *output_name*, ***kwds*)
    Call Noddy and compute the history file

   Arguments:

- *history* = string : filename of history file
- *output_name* = string : basename for output files

   Optional Keywords:

- *sim_type* = 'BLOCK', 'GEOPHYSICS', 'SURFACES', 'BLOCK_GEOPHYS',

'TOPOLOGY', 'BLOCK_SURFACES', 'ALL': type of Noddy simulation (default: 'BLOCK')

- *program_name* **= string** [name of program] (default: noddy.exe or noddy, both checked)

- *verbose* = bool: verbose mode, print out information for debugging (default = False)

- *noddy_path* = path: location of Noddy executable (default: checks environment variable)

Returns: -Returns any text outputted by the noddy executable.

It is worth noting here that by default pynoddy looks for the compiled Noddy executable in the pynoddy.noddy directory. However this can be changed by updating the `pynoddy.noddyPath` variable to point to a new executable file (without any extension, .exe is added automatically to the path on windows machines).

SIMULATION OF A NODDY HISTORY AND VISUALISATION OF OUTPUT

This example shows how the module pynoddy.history can be used to compute the model, and how simple visualisations can be generated with pynoddy.output.

```python
from IPython.core.display import HTML
css_file = 'pynoddy.css'
HTML(open(css_file, "r").read())
```

```python
%matplotlib inline
```

```python
# Basic settings
import sys, os
import subprocess

# Now import pynoddy
import pynoddy
reload(pynoddy)
import pynoddy.output
import pynoddy.history

# determine path of repository to set paths corretly below
repo_path = os.path.realpath('../..')
```

3.1 Compute the model

The simplest way to perform the Noddy simulation through Python is simply to call the executable. One way that should be fairly platform independent is to use Python's own subprocess module:

```python
# Change to sandbox directory to store results
os.chdir(os.path.join(repo_path, 'sandbox'))

# Path to exmaple directory in this repository
example_directory = os.path.join(repo_path,'examples')
# Compute noddy model for history file
history_file = 'simple_two_faults.his'
history = os.path.join(example_directory, history_file)
output_name = 'noddy_out'
# call Noddy

# NOTE: Make sure that the noddy executable is accessible in the system!!
print subprocess.Popen(['noddy.exe', history, output_name, 'BLOCK'],
                       shell=False, stderr=subprocess.PIPE,
                       stdout=subprocess.PIPE).stdout.read()
#
```

For convenience, the model computation is wrapped into a Python function in pynoddy:

```
pynoddy.compute_model(history, output_name)
```

```
''
```

Note: The Noddy call from Python is, to date, calling Noddy through the subprocess function. In a future implementation, this call could be substituted with a full wrapper for the C-functions written in Python. Therefore, using the member function compute_model is not only easier, but also the more "future-proof" way to compute the Noddy model.

3.2 Loading Noddy output files

Noddy simulations produce a variety of different output files, depending on the type of simulation. The basic output is the geological model. Additional output files can contain geophysical responses, etc.

Loading the output files is simplified with a class class container that reads all relevant information and provides simple methods for plotting, model analysis, and export. To load the output information into a Python object:

```
N1 = pynoddy.output.NoddyOutput(output_name)
```

The object contains the calculated geology blocks and some additional information on grid spacing, model extent, etc. For example:

```
print("The model has an extent of %.0f m in x-direction, with %d cells of width %.0f m" %
       (N1.extent_x, N1.nx, N1.delx))
```

```
The model has an extent of 12400 m in x-direction, with 124 cells of width 100 m
```

3.3 Plotting sections through the model

The NoddyOutput class has some basic methods for the visualisation of the generated models. To plot sections through the model:

```
N1.plot_section('y', figsize = (5,3))
```
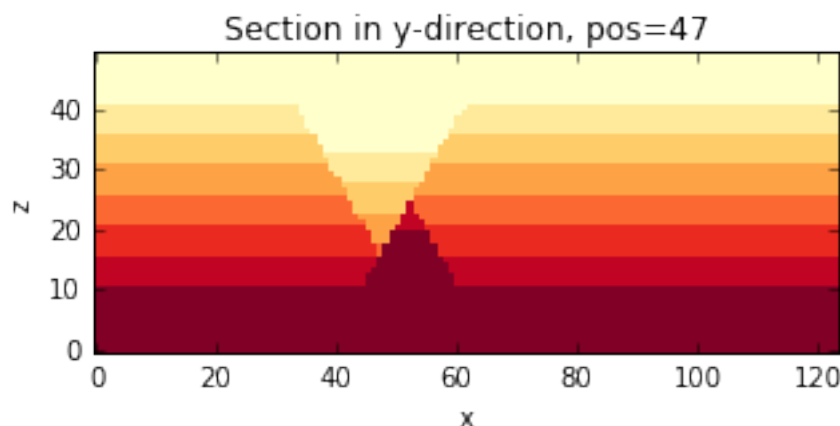

Fig. 3.1: png

3.4 Export model to VTK

A simple possibility to visualise the modeled results in 3-D is to export the model to a VTK file and then to visualise it with a VTK viewer, for example Paraview. To export the model, simply use:

```
N1.export_to_vtk()
```

The exported VTK file can be visualised in any VTK viewer, for example in the (free) viewer Paraview (www.paraview.org). An example visualisation of the model in 3-D is presented in the figure below.

Fig. 3.2: 3-D Visualisation generated with Paraview (top layer transparent)

CHANGE NODDY INPUT FILE AND RECOMPUTE MODEL

In this section, we will briefly present possibilities to access the properties defined in the Noddy history input file and show how simple adjustments can be performed, for example changing the cube size to obtain a model with a higher resolution.

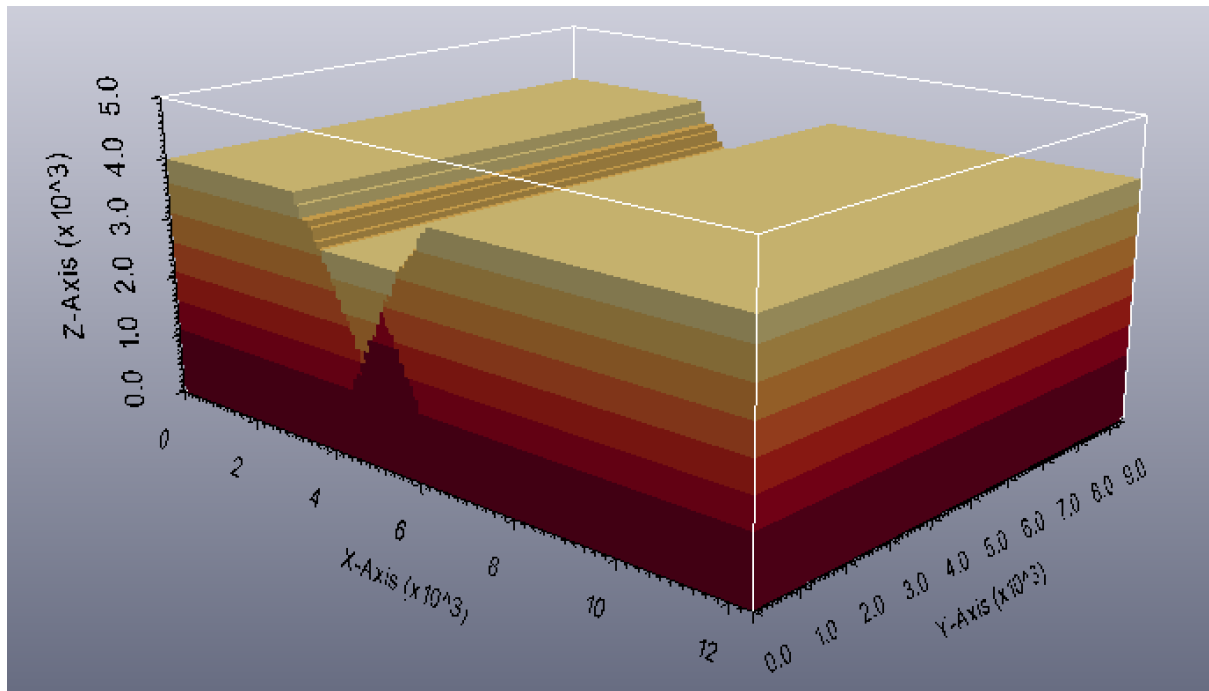Also outlined here is the way that events are stored in the history file as single objects. For more information on accessing and changing the events themselves, please be patient until we get to the next section.

```python
from IPython.core.display import HTML
css_file = 'pynoddy.css'
HTML(open(css_file, "r").read())
```

```
cd ../docs/notebooks/
```

```
/Users/flow/git/pynoddy/docs/notebooks
```

```
%matplotlib inline
```

```python
import sys, os
import matplotlib.pyplot as plt
import numpy as np
# adjust some settings for matplotlib
from matplotlib import rcParams
# print rcParams
rcParams['font.size'] = 15
# determine path of repository to set paths corretly below
repo_path = os.path.realpath('../..')
import pynoddy
import pynoddy.history
import pynoddy.output
```

First step: load the history file into a Python object:

```python
# Change to sandbox directory to store results
os.chdir(os.path.join(repo_path, 'sandbox'))
# Path to exmaple directory in this repository
example_directory = os.path.join(repo_path,'examples')
# Compute noddy model for history file
history_file = 'simple_two_faults.his'
history = os.path.join(example_directory, history_file)
output_name = 'noddy_out'
H1 = pynoddy.history.NoddyHistory(history)
```

Technical note: the `NoddyHistory` class can be accessed on the level of pynoddy (as it is imported in the `__init__.py` module) with the shortcut:

```
H1 = pynoddy.NoddyHistory(history)
```

I am using the long version `pynoddy.history.NoddyHistory` here to ensure that the correct package is loaded with the `reload()` function. If you don't make changes to any of the pynoddy files, this is not required. So for any practical cases, the shortcuts are absolutely fine!

4.1 Get basic information on the model

The history file contains the entire information on the Noddy model. Some information can be accessed through the NoddyHistory object (and more will be added soon!), for example the total number of events:

```python
print("The history contains %d events" % H1.n_events)
```

```
The history contains 3 events
```

Events are implemented as objects, the classes are defined in `H1.events`. All events are accessible in a list on the level of the history object:

```python
H1.events
```

```
{1: <pynoddy.events.Stratigraphy at 0x103ac2a50>,
 2: <pynoddy.events.Fault at 0x103ac2a90>,
 3: <pynoddy.events.Fault at 0x103ac2ad0>}
```

The properties of an event are stored in the event objects themselves. To date, only a subset of the properties (deemed as relevant for the purpose of pynoddy so far) are parsed. The .his file contains a lot more information! If access to this information is required, adjustments in pynoddy.events have to be made.

For example, the properties of a fault object are:

```python
H1.events[2].properties
# print H1.events[5].properties.keys()
```

```
{'Amplitude': 2000.0,
 'Blue': 254.0,
 'Color Name': 'Custom Colour 8',
 'Cyl Index': 0.0,
 'Dip': 60.0,
 'Dip Direction': 90.0,
 'Geometry': 'Translation',
 'Green': 0.0,
 'Movement': 'Hanging Wall',
 'Pitch': 90.0,
 'Profile Pitch': 90.0,
 'Radius': 1000.0,
 'Red': 0.0,
 'Rotation': 30.0,
 'Slip': 1000.0,
 'X': 5500.0,
 'XAxis': 2000.0,
 'Y': 3968.0,
 'YAxis': 2000.0,
 'Z': 0.0,
 'ZAxis': 2000.0}
```

4.2 Change model cube size and recompute model

The Noddy model itself is, once computed, a continuous model in 3-D space. However, for most visualisations and further calculations (e.g. geophysics), a discretised version is suitable. The discretisation (or block size) can be adapted in the history file. The according pynoddy function is change_cube_size.

A simple example to change the cube size and write a new history file:

```python
# We will first recompute the model and store results in an output file for comparison
NH1 = pynoddy.history.NoddyHistory(history)
pynoddy.compute_model(history, output_name)
NO1 = pynoddy.output.NoddyOutput(output_name)
```

```
# Now: change cubsize, write to new file and recompute
NH1.change_cube_size(50)
# Save model to a new history file and recompute (Note: may take a while to compute now)
new_history = "fault_model_changed_cubesize.his"
new_output_name = "noddy_out_changed_cube"
NH1.write_history(new_history)
pynoddy.compute_model(new_history, new_output_name)
NO2 = pynoddy.output.NoddyOutput(new_output_name)
```

The different cell sizes are also represented in the output files:

```
print("Model 1 contains a total of %7d cells with a blocksize %.0f m" %
      (NO1.n_total, NO1.delx))
print("Model 2 contains a total of %7d cells with a blocksize %.0f m" %
      (NO2.n_total, NO2.delx))
```

```
Model 1 contains a total of  582800 cells with a blocksize 100 m
Model 2 contains a total of 4662400 cells with a blocksize 50 m
```

We can compare the effect of the different model discretisations in section plots, created with the plot_section method described before. Let's get a bit more fancy here and use the functionality to pass axes to the plot_section method, and to create one figure as direct comparison:

```
# create basic figure layout
fig = plt.figure(figsize = (15,5))
ax1 = fig.add_subplot(121)
ax2 = fig.add_subplot(122)
NO1.plot_section('y', position=0, ax = ax1, colorbar=False, title="Low resolution")
NO2.plot_section('y', position=1, ax = ax2, colorbar=False, title="High resolution")

plt.show()
```
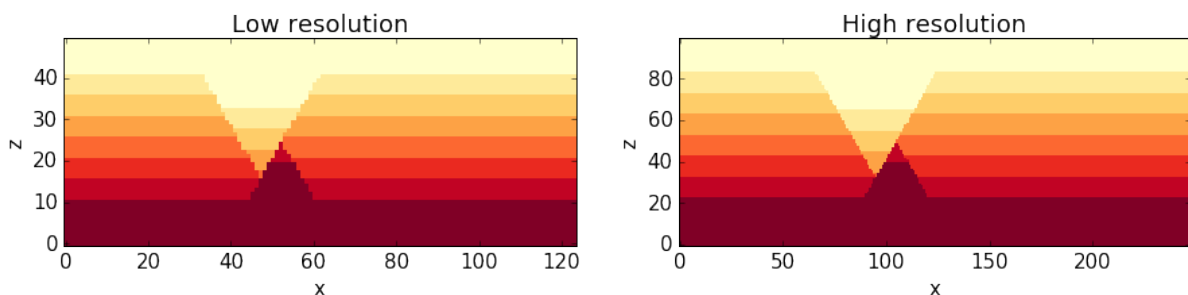

Fig. 4.1: png

Note: the following two subsections contain some slighly advanced examples on how to use the possibility to adjust cell sizes through scripts directly to autmote processes that are infeasible using the GUI version of Noddy - as a 'peek preview' of the automation for uncertainty estimation that follows in a later section. Feel free to skip those two sections if you are only interested in the basic features so far.

4.3 Estimating computation time for a high-resolution model

You surely realised (if you ran these examples in an actual interactive ipython notebook) that the computation of the high-resolution model takes siginficantly longer than the low-resolution model. In a practical case, this can be very important.

```
# We use here simply the time() function to evaulate the simualtion time.
# This is not the best possible way to do it, but probably the simplest.
import time
start_time = time.time()
```

```
pynoddy.compute_model(history, output_name)
end_time = time.time()

print("Simulation time for low-resolution model: %5.2f seconds" % (end_time - start_time))

start_time = time.time()
pynoddy.compute_model(new_history, new_output_name)
end_time = time.time()

print("Simulation time for high-resolution model: %5.2f seconds" % (end_time - start_time))
```

```
Simulation time for low-resolution model:  0.73 seconds
Simulation time for high-resolution model:  5.78 seconds
```

For an estimation of required computing time for a given discretisation, let's evaulate the time for a couple of steps, plot, and extrapolate:

```
# perform computation for a range of cube sizes
cube_sizes = np.arange(200,49,-5)
times = []
NH1 = pynoddy.history.NoddyHistory(history)
tmp_history = "tmp_history"
tmp_output = "tmp_output"
for cube_size in cube_sizes:
    NH1.change_cube_size(cube_size)
    NH1.write_history(tmp_history)
    start_time = time.time()
    pynoddy.compute_model(tmp_history, tmp_output)
    end_time = time.time()
    times.append(end_time - start_time)
times = np.array(times)
```

```
# create plot
fig = plt.figure(figsize=(18,4))
ax1 = fig.add_subplot(131)
ax2 = fig.add_subplot(132)
ax3 = fig.add_subplot(133)

ax1.plot(cube_sizes, np.array(times), 'ro-')
ax1.set_xlabel('cubesize [m]')
ax1.set_ylabel('time [s]')
ax1.set_title('Computation time')
ax1.set_xlim(ax1.get_xlim()[::-1])

ax2.plot(cube_sizes, times**(1/3.), 'bo-')
ax2.set_xlabel('cubesize [m]')
ax2.set_ylabel('(time [s])**(1/3)')
ax2.set_title('Computation time (cuberoot)')
ax2.set_xlim(ax2.get_xlim()[::-1])

ax3.semilogy(cube_sizes, times, 'go-')
ax3.set_xlabel('cubesize [m]')
ax3.set_ylabel('time [s]')
ax3.set_title('Computation time (y-log)')
ax3.set_xlim(ax3.get_xlim()[::-1])
```

```
(200.0, 40.0)
```

It is actually quite interesting that the computation time does not scale with cubesize to the power of three (as could be expected, given that we have a mesh in three dimensions). Or am I missing something?

Anyway, just because we can: let's assume that the scaling is somehow exponential and try to fit a model for a time prediction. Given the last plot, it looks like we could fit a logarithmic model with probably an additional
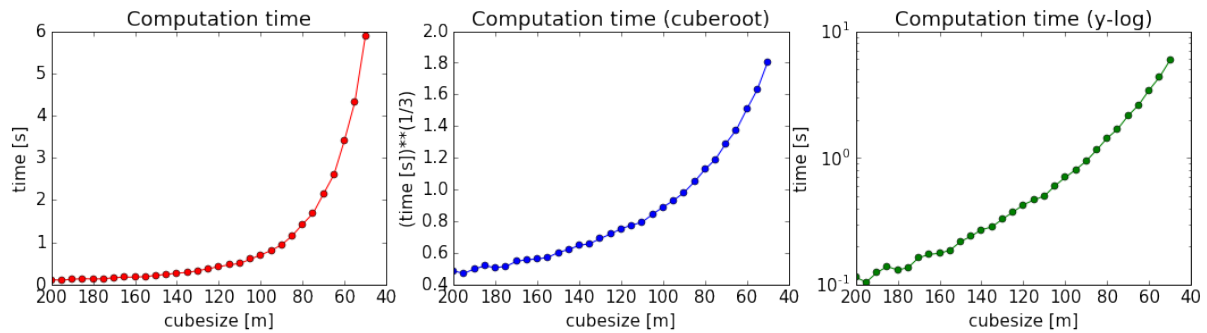
Fig. 4.2: png

exponent (as the line is obviously not straight), so something like:

$$f(x) = a + (b \log_{10}(x))^{-c}$$

Let's try to fit the curve with `scipy.optimize.curve_fit`:

```python
# perform curve fitting with scipy.optimize
import scipy.optimize
# define function to be fit
def func(x,a,b,c):
    return a + (b*np.log10(x))**(-c)

popt, pcov = scipy.optimize.curve_fit(func, cube_sizes, np.array(times), p0 = [-1, 0.5, 2])
popt
```

```
array([ -0.05618538,   0.50990774,  12.45183398])
```

Interesting, it looks like Noody scales with something like:

$$f(x) = (0.5 \log_{10}(x))^{-12}$$

Note: if you understand more about computational complexity than me, it might not be that interesting to you at all - if this is the case, please contact me and tell me why this result could be expected...

```python
a,b,c = popt
cube_range = np.arange(200,20,-1)
times_eval = func(cube_range, a, b, c)
fig = plt.figure()
ax = fig.add_subplot(111)
ax.semilogy(cube_range, times_eval, '-')
ax.semilogy(cube_sizes, times, 'ko')
# reverse x-axis
ax.set_xlim(ax.get_xlim()[::-1])
```

```
(200.0, 20.0)
```

Not too bad... let's evaluate the time for a cube size of 40 m:

```python
cube_size = 40 # m
time_est = func(cube_size, a, b, c)
print("Estimated time for a cube size of %d m: %.1f seconds" % (cube_size, time_est))
```

```
Estimated time for a cube size of 40 m: 12.4 seconds
```

Now let's check the actual simulation time:

```python
NH1.change_cube_size(cube_size)
NH1.write_history(tmp_history)
start_time = time.time()
```
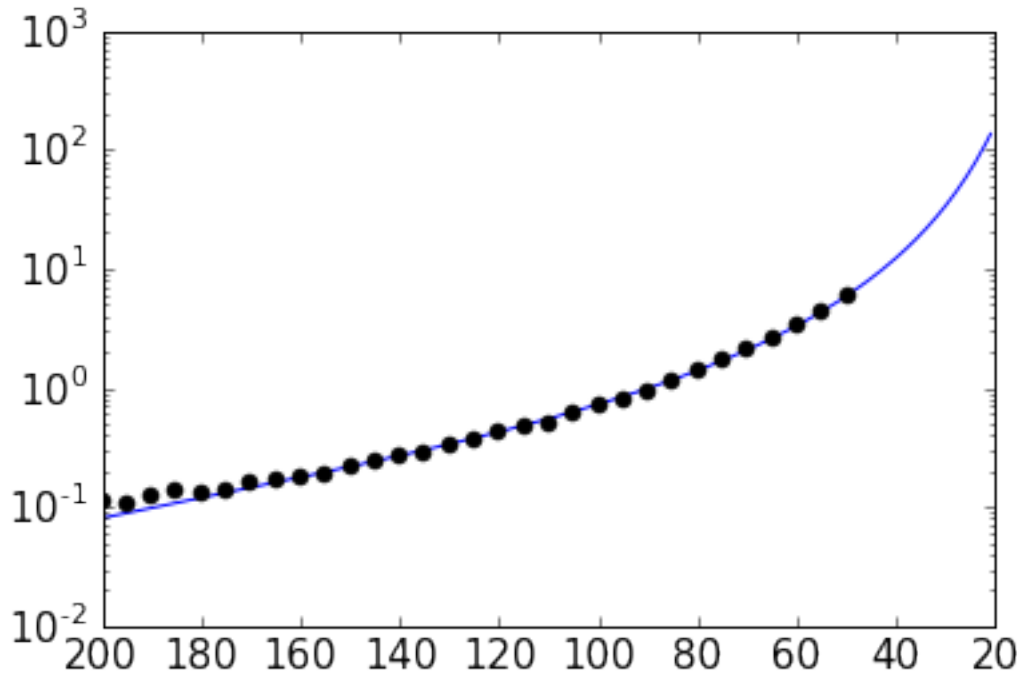
Fig. 4.3: png

```
pynoddy.compute_model(tmp_history, tmp_output)
end_time = time.time()
time_comp = end_time - start_time

print("Actual computation time for a cube size of %d m: %.1f seconds" % (cube_size, time_comp))
```

```
Actual computation time for a cube size of 40 m: 11.6 seconds
```

Not too bad, probably in the range of the inherent variability... and if we check it in the plot:

```
fig = plt.figure()
ax = fig.add_subplot(111)
ax.semilogy(cube_range, times_eval, '-')
ax.semilogy(cube_sizes, times, 'ko')
ax.semilogy(cube_size, time_comp, 'ro')
# reverse x-axis
ax.set_xlim(ax.get_xlim()[::-1])
```

```
(200.0, 20.0)
```

Anyway, the point of this excercise was not a precise evaluation of Noddy's computational complexity, but to provide a simple means of evaluating computation time for a high resolution model, using the flexibility of writing simple scripts using pynoddy, and a couple of additional python modules.

For a realistic case, it should, of course, be sufficient to determine the time based on a lot less computed points. If you like, test it with your favourite model and tell me if it proved useful (or not)!

4.4 Simple convergence study

So: why would we want to run a high-resolution model, anyway? Well, of course, it produces nicer pictures - but on a scientific level, that's completely irrelevant (haha, not true - so nice if it would be...).

Anyway, if we want to use the model in a scientific study, for example to evaluate volume of specific units, or to
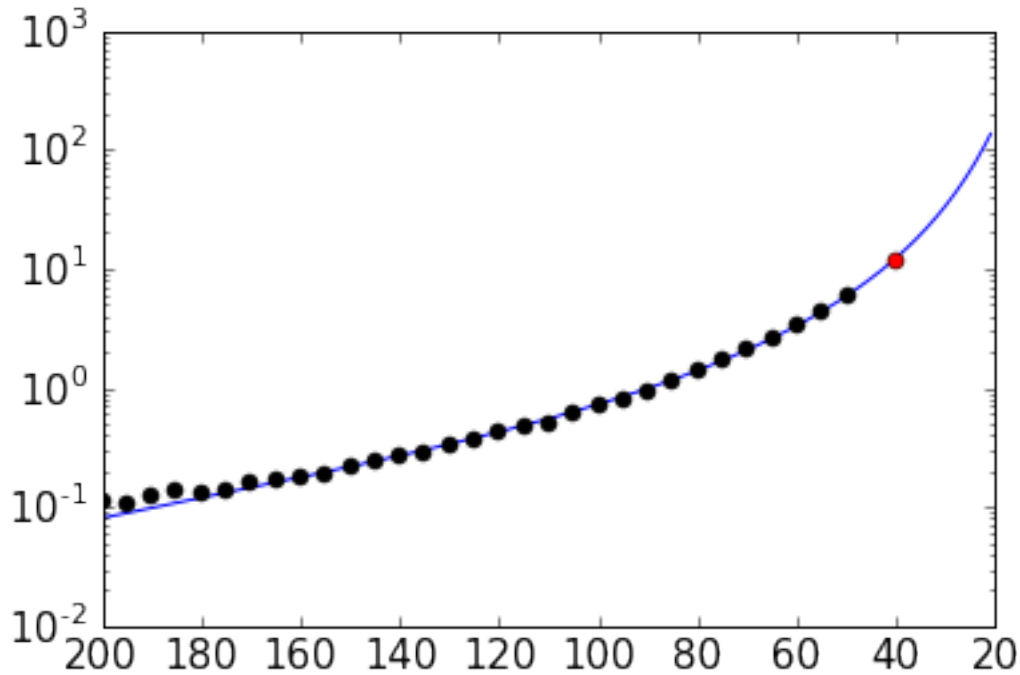
Fig. 4.4: png

estimate the geological topology (Mark is working on this topic with some cool ideas - example to be implemented here, "soon"), we want to know if the resolution of the model is actually high enough to produce meaningful results.

As a simple example of the evaluation of model resolution, we will here inlcude a volume convergence study, i.e. we will estimate at which level of increasing model resolution the estimated block volumes do not change anymore.

The entire procedure is very similar to the computational time evaluation above, only that we now also analyse the output and determine the rock volumes of each defined geological unit:

```python
# perform computation for a range of cube sizes
reload(pynoddy.output)
cube_sizes = np.arange(200,49,-5)
all_volumes = []
N_tmp = pynoddy.history.NoddyHistory(history)
tmp_history = "tmp_history"
tmp_output = "tmp_output"
for cube_size in cube_sizes:
    # adjust cube size
    N_tmp.change_cube_size(cube_size)
    N_tmp.write_history(tmp_history)
    pynoddy.compute_model(tmp_history, tmp_output)
    # open simulated model and determine volumes
    O_tmp = pynoddy.output.NoddyOutput(tmp_output)
    O_tmp.determine_unit_volumes()
    all_volumes.append(O_tmp.unit_volumes)
```

```python
all_volumes = np.array(all_volumes)
fig = plt.figure(figsize=(16,4))
ax1 = fig.add_subplot(121)
ax2 = fig.add_subplot(122)

# separate into two plots for better visibility:
for i in range(np.shape(all_volumes)[1]):
```

```
    if i < 4:
        ax1.plot(cube_sizes, all_volumes[:,i], 'o-', label='unit %d' %i)
    else:
        ax2.plot(cube_sizes, all_volumes[:,i], 'o-', label='unit %d' %i)

ax1.legend(loc=2)
ax2.legend(loc=2)
# reverse axes
ax1.set_xlim(ax1.get_xlim()[::-1])
ax2.set_xlim(ax2.get_xlim()[::-1])

ax1.set_xlabel("Block size [m]")
ax1.set_ylabel("Total unit volume [m**3]")
ax2.set_xlabel("Block size [m]")
ax2.set_ylabel("Total unit volume [m**3]")
```

```
<matplotlib.text.Text at 0x107eb7250>
```
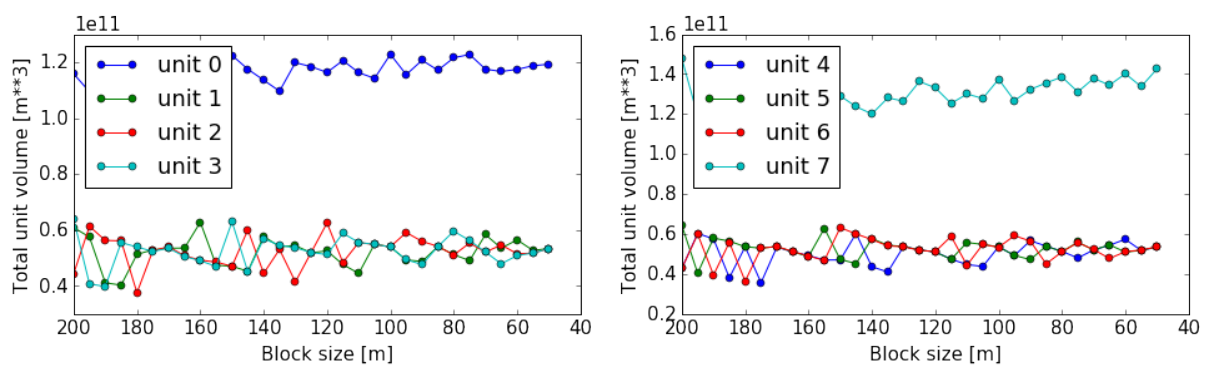

Fig. 4.5: png

It looks like the volumes would start to converge from about a block size of 100 m. The example model is pretty small and simple, probably not the best example for this study. Try it out with your own, highly complex, favourite pet model :-)

GEOLOGICAL EVENTS IN PYNODDY: ORGANISATION AND ADPATIATION

We will here describe how the single geological events of a Noddy history are organised within pynoddy. We will then evaluate in some more detail how aspects of events can be adapted and their effect evaluated.

```python
from IPython.core.display import HTML
css_file = 'pynoddy.css'
HTML(open(css_file, "r").read())
```

```python
%matplotlib inline
```

5.1 Loading events from a Noddy history

In the current set-up of pynoddy, we always start with a pre-defined Noddy history loaded from a file, and then change aspects of the history and the single events. The first step is therefore to load the history file and to extract the single geological events. This is done automatically as default when loading the history file into the History object:

```python
import sys, os
import matplotlib.pyplot as plt
# adjust some settings for matplotlib
from matplotlib import rcParams
# print rcParams
rcParams['font.size'] = 15
# determine path of repository to set paths correty below
repo_path = os.path.realpath('../..')

import pynoddy
import pynoddy.history
import pynoddy.events
import pynoddy.output
reload(pynoddy)
```

```
<module 'pynoddy' from '/Users/flow/git/pynoddy/pynoddy/__init__.pyc'>
```

```python
# Change to sandbox directory to store results
os.chdir(os.path.join(repo_path, 'sandbox'))

# Path to exmaple directory in this repository
example_directory = os.path.join(repo_path,'examples')
# Compute noddy model for history file
history = 'simple_two_faults.his'
history_ori = os.path.join(example_directory, history)
output_name = 'noddy_out'
reload(pynoddy.history)
reload(pynoddy.events)
H1 = pynoddy.history.NoddyHistory(history_ori)
```

```
# Before we do anything else, let's actually define the cube size here to
# adjust the resolution for all subsequent examples
H1.change_cube_size(100)
# compute model - note: not strictly required, here just to ensure changed cube size
H1.write_history(history)
pynoddy.compute_model(history, output_name)
```

```
''
```

Events are stored in the object dictionary "events" (who would have thought), where the key corresponds to the position in the timeline:

```
H1.events
```

```
{1: <pynoddy.events.Stratigraphy at 0x10cf2b410>,
 2: <pynoddy.events.Fault at 0x10cf2b450>,
 3: <pynoddy.events.Fault at 0x10cf2b490>}
```

We can see here that three events are defined in the history. Events are organised as objects themselves, containing all the relevant properties and information about the events. For example, the second fault event is defined as:

```
H1.events[3].properties
```

```
{'Amplitude': 2000.0,
 'Blue': 0.0,
 'Color Name': 'Custom Colour 5',
 'Cyl Index': 0.0,
 'Dip': 60.0,
 'Dip Direction': 270.0,
 'Geometry': 'Translation',
 'Green': 0.0,
 'Movement': 'Hanging Wall',
 'Pitch': 90.0,
 'Profile Pitch': 90.0,
 'Radius': 1000.0,
 'Red': 254.0,
 'Rotation': 30.0,
 'Slip': 1000.0,
 'X': 5500.0,
 'XAxis': 2000.0,
 'Y': 7000.0,
 'YAxis': 2000.0,
 'Z': 5000.0,
 'ZAxis': 2000.0}
```

5.2 Changing aspects of geological events

So what we now want to do, of course, is to change aspects of these events and to evaluate the effect on the resulting geological model. Parameters can directly be updated in the properties dictionary:

```
H1 = pynoddy.history.NoddyHistory(history_ori)
# get the original dip of the fault
dip_ori = H1.events[3].properties['Dip']

# add 10 degrees to dip
add_dip = -10
dip_new = dip_ori + add_dip

# and assign back to properties dictionary:
H1.events[3].properties['Dip'] = dip_new
# H1.events[2].properties['Dip'] = dip_new1
```

```
new_history = "dip_changed"
new_output = "dip_changed_out"
H1.write_history(new_history)
pynoddy.compute_model(new_history, new_output)
# load output from both models
NO1 = pynoddy.output.NoddyOutput(output_name)
NO2 = pynoddy.output.NoddyOutput(new_output)
# create basic figure layout
fig = plt.figure(figsize = (15,5))
ax1 = fig.add_subplot(121)
ax2 = fig.add_subplot(122)
NO1.plot_section('y', position=0, ax = ax1, colorbar=False, title="Dip = %.0f" % dip_ori, savefig
NO2.plot_section('y', position=1, ax = ax2, colorbar=False, title="Dip = %.0f" % dip_new)
plt.show()
```
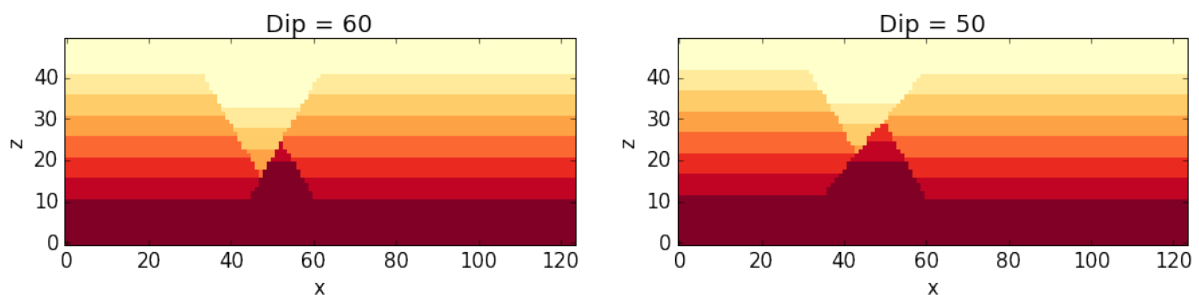

Fig. 5.1: png

5.3 Changing the order of geological events

The geological history is parameterised as single events in a timeline. Changing the order of events can be performed with two basic methods:

1. Swapping two events with a simple command

2. Adjusting the entire timeline with a complete remapping of events

The first method is probably the most useful to test how a simple change in the order of events will effect the final geological model. We will use it here with our example to test how the model would change if the timing of the faults is swapped.

The method to swap two geological events is defined on the level of the history object:

```
H1 = pynoddy.history.NoddyHistory(history_ori)
```

```
# The names of the two fault events defined in the history file are:
print H1.events[2].name
print H1.events[3].name
```

```
Fault2
Fault1
```

We now swap the position of two events in the kinematic history. For this purpose, a high-level function can directly be used:

```
# Now: swap the events:
H1.swap_events(2,3)
```

```
# And let's check if this is correctly relfected in the events order now:
print H1.events[2].name
print H1.events[3].name
```

```
Fault1
Fault2
```

Now let's create a new history file and evaluate the effect of the changed order in a cross section view:

```
new_history = "faults_changed_order.his"
new_output = "faults_out"
H1.write_history(new_history)
pynoddy.compute_model(new_history, new_output)
```

```
''
```

```
reload(pynoddy.output)
# Load and compare both models
NO1 = pynoddy.output.NoddyOutput(output_name)
NO2 = pynoddy.output.NoddyOutput(new_output)
# create basic figure layout
fig = plt.figure(figsize = (15,5))
ax1 = fig.add_subplot(121)
ax2 = fig.add_subplot(122)
NO1.plot_section('y', ax = ax1, colorbar=False, title="Model 1")
NO2.plot_section('y', ax = ax2, colorbar=False, title="Model 2")

plt.show()
```
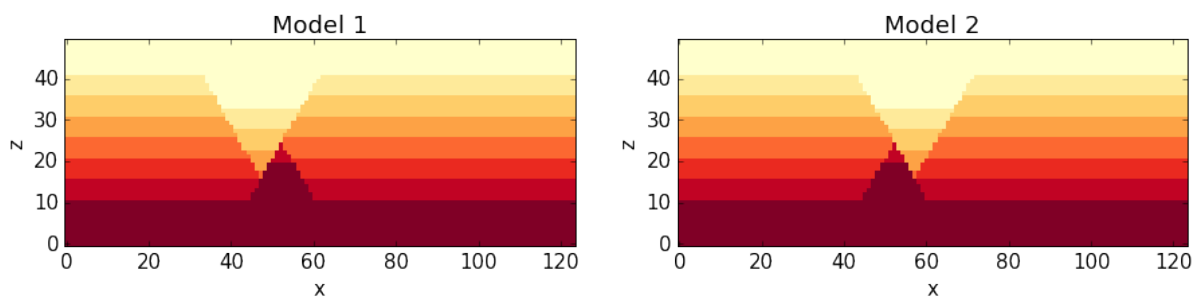

Fig. 5.2: png

5.4 Determining the stratigraphic difference between two models

Just as another quick example of a possible application of pynoddy to evaluate aspects that are not simply possible with, for example, the GUI version of Noddy itself. In the last example with the changed order of the faults, we might be interested to determine where in space this change had an effect. We can test this quite simply using the NoddyOutput objects.

The geology data is stored in the NoddyOutput.block attribute. To evaluate the difference between two models, we can therefore simply compute:

```
diff = (NO2.block - NO1.block)
```

And create a simple visualisation of the difference in a slice plot with:

```
fig = plt.figure(figsize = (5,3))
ax = fig.add_subplot(111)
ax.imshow(diff[:,10,:].transpose(), interpolation='nearest',
          cmap = "RdBu", origin = 'lower left')
```

```
<matplotlib.image.AxesImage at 0x10cf3be10>
```

(Adding a meaningful title and axis labels to the plot is left to the reader as simple excercise :-) Future versions of pynoddy might provide an automatic implementation for this step...)
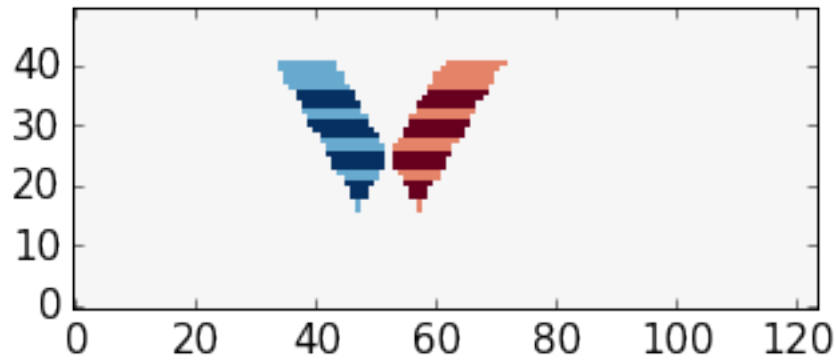
Fig. 5.3: png

Again, we may want to visualise results in 3-D. We can use the export_to_vtk-function as before, but now assing the data array to be exported as the calulcated differnce field:

```
NO1.export_to_vtk(vtk_filename = "model_diff", data = diff)
```
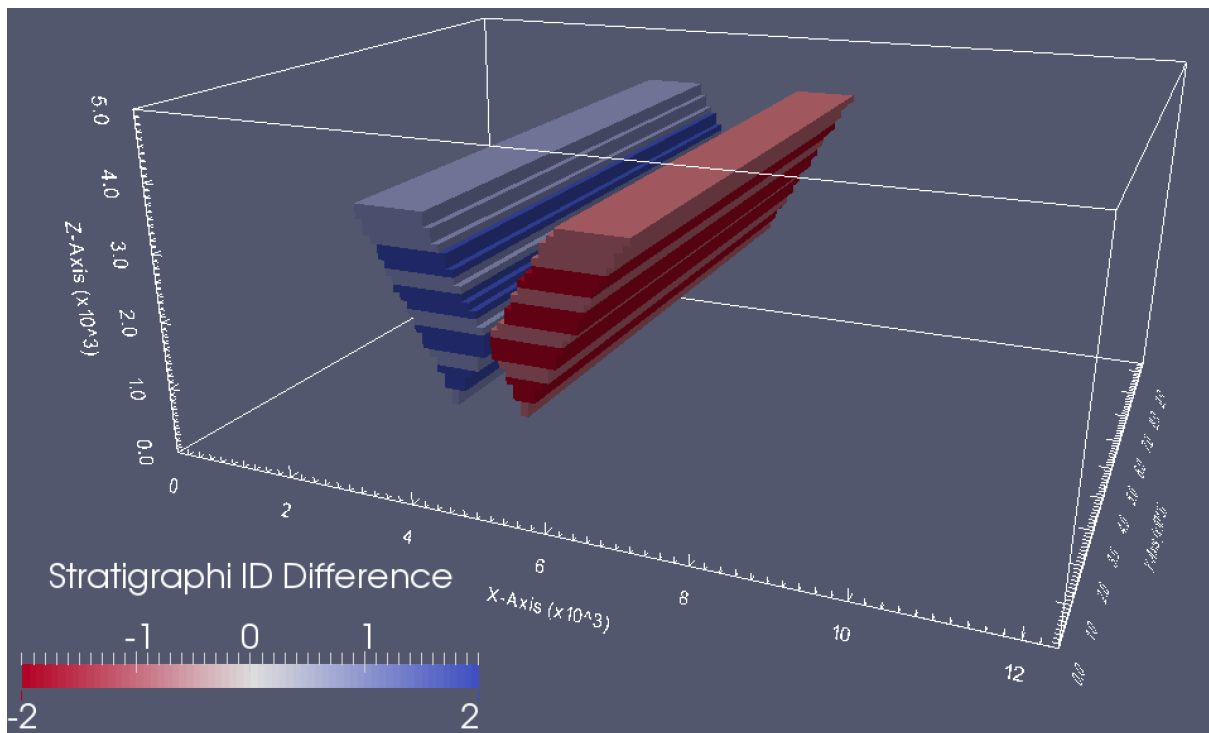
A 3-D view of the difference plot is presented below.

Fig. 5.4: 3-D visualisation of stratigraphic id difference

CREATING A MODEL FROM SCRATCH

We describe here how to generate a simple history file for computation with Noddy using the functionality of pynoddy. If possible, it is advisable to generate the history files with the Windows GUI for Noddy as this method provides, to date, a simpler and more complete interface to the entire functionality.

For completeness, pynoddy contains the functionality to generate simple models, for example to automate the model construction process, or to enable the model construction for users who are not running Windows. Some simple examlpes are shown in the following.

```python
from matplotlib import rc_params
```

```python
from IPython.core.display import HTML
css_file = 'pynoddy.css'
HTML(open(css_file, "r").read())
```

```python
import sys, os
import matplotlib.pyplot as plt
# adjust some settings for matplotlib
from matplotlib import rcParams
# print rcParams
rcParams['font.size'] = 15
# determine path of repository to set paths correltly below
repo_path = os.path.realpath('../..')
import pynoddy.history
```

```python
%matplotlib inline
```

```python
rcParams.update({'font.size': 20})
```

6.1 Defining a stratigraphy

We start with the definition of a (base) stratigraphy for the model.

```python
# Combined: model generation and output vis to test:
history = "simple_model.his"
output_name = "simple_out"
reload(pynoddy.history)
reload(pynoddy.events)

# create pynoddy object
nm = pynoddy.history.NoddyHistory()
# add stratigraphy
strati_options = {'num_layers' : 8,
                  'layer_names' : ['layer 1', 'layer 2', 'layer 3',
                                   'layer 4', 'layer 5', 'layer 6',
                                   'layer 7', 'layer 8'],
                  'layer_thickness' : [1500, 500, 500, 500, 500, 500, 500, 500]}
nm.add_event('stratigraphy', strati_options )
```

```
nm.write_history(history)
```

```
# Compute the model
reload(pynoddy)
pynoddy.compute_model(history, output_name)
```

```
''
```

```
# Plot output
import pynoddy.output
reload(pynoddy.output)
nout = pynoddy.output.NoddyOutput(output_name)
nout.plot_section('y', layer_labels = strati_options['layer_names'][::-1],
                  colorbar = True, title="",
                  savefig = False, fig_filename = "ex01_strati.eps")
```
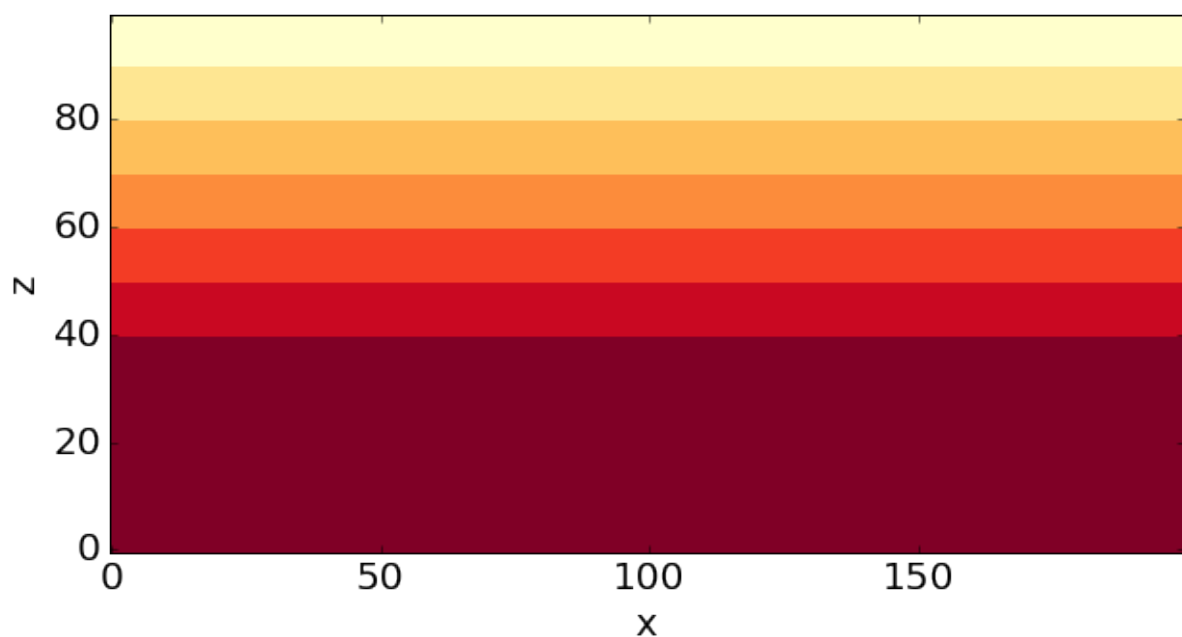

Fig. 6.1: png

6.2 Add a fault event

As a next step, let's now add the faults to the model.

```
reload(pynoddy.history)
reload(pynoddy.events)
nm = pynoddy.history.NoddyHistory()
# add stratigraphy
strati_options = {'num_layers' : 8,
                  'layer_names' : ['layer 1', 'layer 2', 'layer 3', 'layer 4', 'layer 5', 'layer
                  'layer_thickness' : [1500, 500, 500, 500, 500, 500, 500, 500]}
nm.add_event('stratigraphy', strati_options )




# The following options define the fault geometry:
fault_options = {'name' : 'Fault_E',
```

```
                      'pos' : (6000, 0, 5000),
                      'dip_dir' : 270,
                      'dip' : 60,
                      'slip' : 1000}

nm.add_event('fault', fault_options)
```

```
nm.events
```

```
{1: <pynoddy.events.Stratigraphy at 0x1073fc590>,
 2: <pynoddy.events.Fault at 0x107565fd0>}
```

```
nm.write_history(history)
```

```
# Compute the model
pynoddy.compute_model(history, output_name)
```

```
''
```

```
# Plot output
reload(pynoddy.output)
nout = pynoddy.output.NoddyOutput(output_name)
nout.plot_section('y', layer_labels = strati_options['layer_names'][::-1],
                  colorbar = True, title = "",
                  savefig = False, fig_filename = "ex01_fault_E.eps")
```
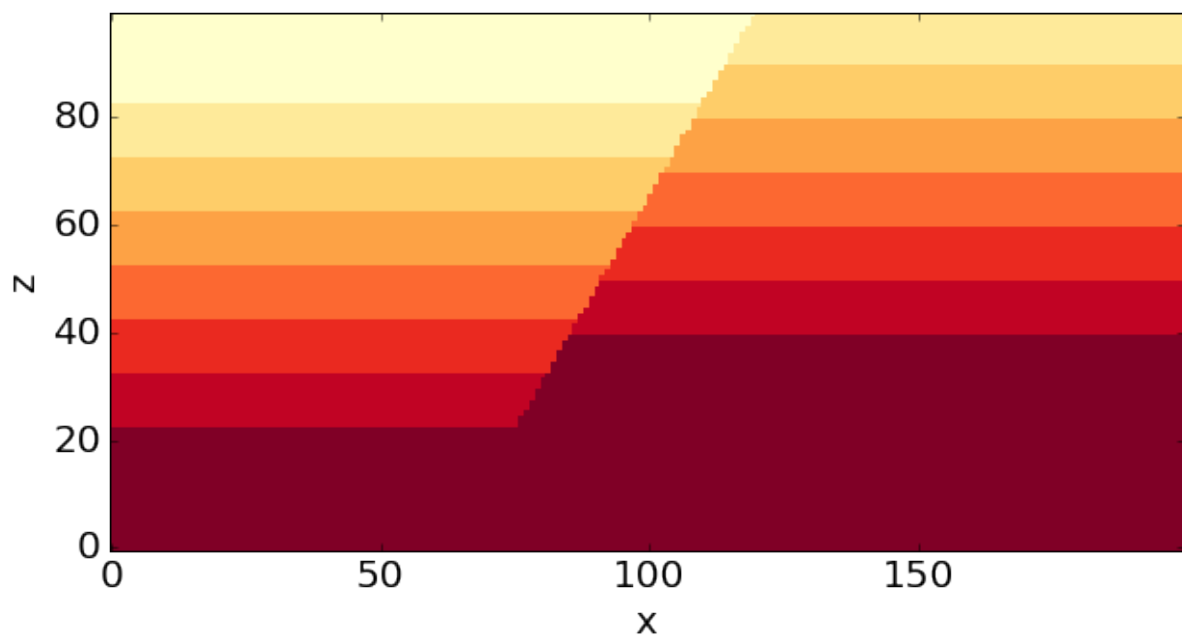

Fig. 6.2: png

```
# The following options define the fault geometry:
fault_options = {'name' : 'Fault_1',
                 'pos' : (5500, 3500, 0),
                 'dip_dir' : 270,
                 'dip' : 60,
                 'slip' : 1000}

nm.add_event('fault', fault_options)
```

```
nm.write_history(history)
```

```
# Compute the model
pynoddy.compute_model(history, output_name)
```

```
''
```

```
# Plot output
reload(pynoddy.output)
nout = pynoddy.output.NoddyOutput(output_name)
nout.plot_section('y', layer_labels = strati_options['layer_names'][::-1], colorbar = True)
```
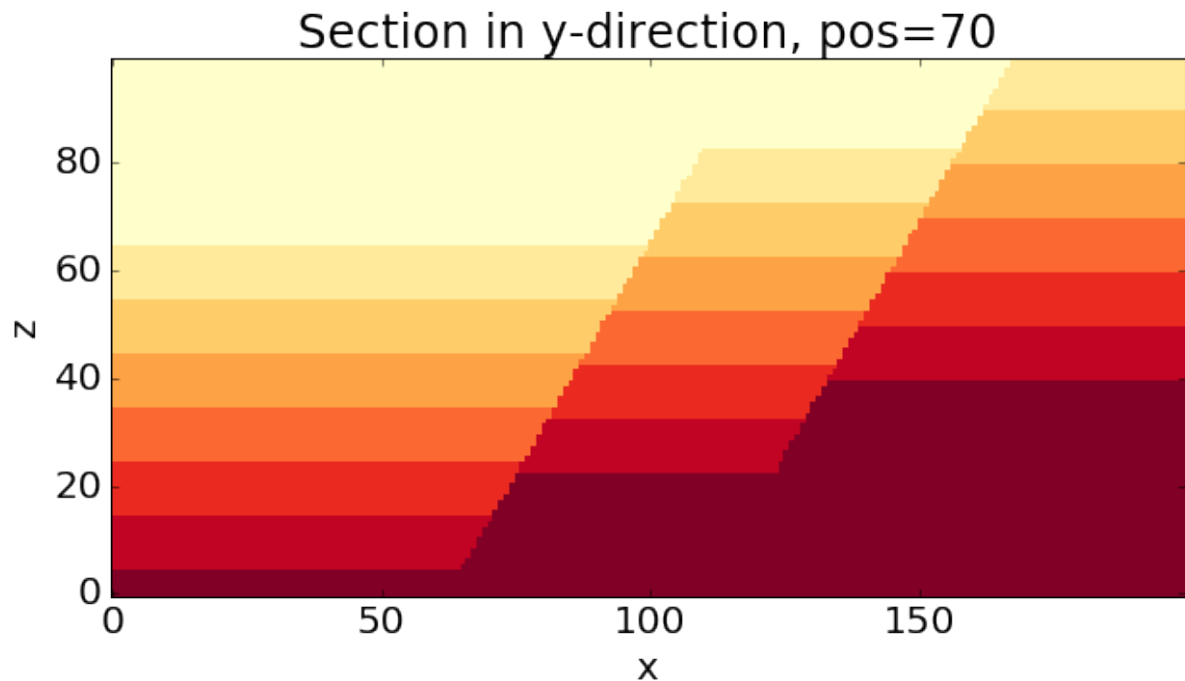

Fig. 6.3: png

```
nm1 = pynoddy.history.NoddyHistory(history)
```

```
nm1.get_extent()
```

```
(10000.0, 7000.0, 5000.0)
```

6.3 Complete Model Set-up

And here now, combining all the previous steps, the entire model set-up with base stratigraphy and two faults:

```
reload(pynoddy.history)
reload(pynoddy.events)
nm = pynoddy.history.NoddyHistory()
# add stratigraphy
strati_options = {'num_layers' : 8,
                  'layer_names' : ['layer 1', 'layer 2', 'layer 3',
                                   'layer 4', 'layer 5', 'layer 6',
                                   'layer 7', 'layer 8'],
                  'layer_thickness' : [1500, 500, 500, 500, 500,
                                       500, 500, 500]}
nm.add_event('stratigraphy', strati_options )
```

```python
# The following options define the fault geometry:
fault_options = {'name' : 'Fault_W',
                 'pos' : (4000, 3500, 5000),
                 'dip_dir' : 90,
                 'dip' : 60,
                 'slip' : 1000}

nm.add_event('fault', fault_options)
# The following options define the fault geometry:
fault_options = {'name' : 'Fault_E',
                 'pos' : (6000, 3500, 5000),
                 'dip_dir' : 270,
                 'dip' : 60,
                 'slip' : 1000}

nm.add_event('fault', fault_options)
nm.write_history(history)
```

```python
# Change cube size
nm1 = pynoddy.history.NoddyHistory(history)
nm1.change_cube_size(50)
nm1.write_history(history)
```

```python
# Compute the model
pynoddy.compute_model(history, output_name)
```

```python
''
```

```python
# Plot output
reload(pynoddy.output)
nout = pynoddy.output.NoddyOutput(output_name)
nout.plot_section('y', layer_labels = strati_options['layer_names'][::-1],
                  colorbar = True, title="",
                  savefig = True, fig_filename = "ex01_faults_combined.eps",
                  cmap = 'YlOrRd') # note: YlOrRd colourmap should be suitable for colorblindness
```
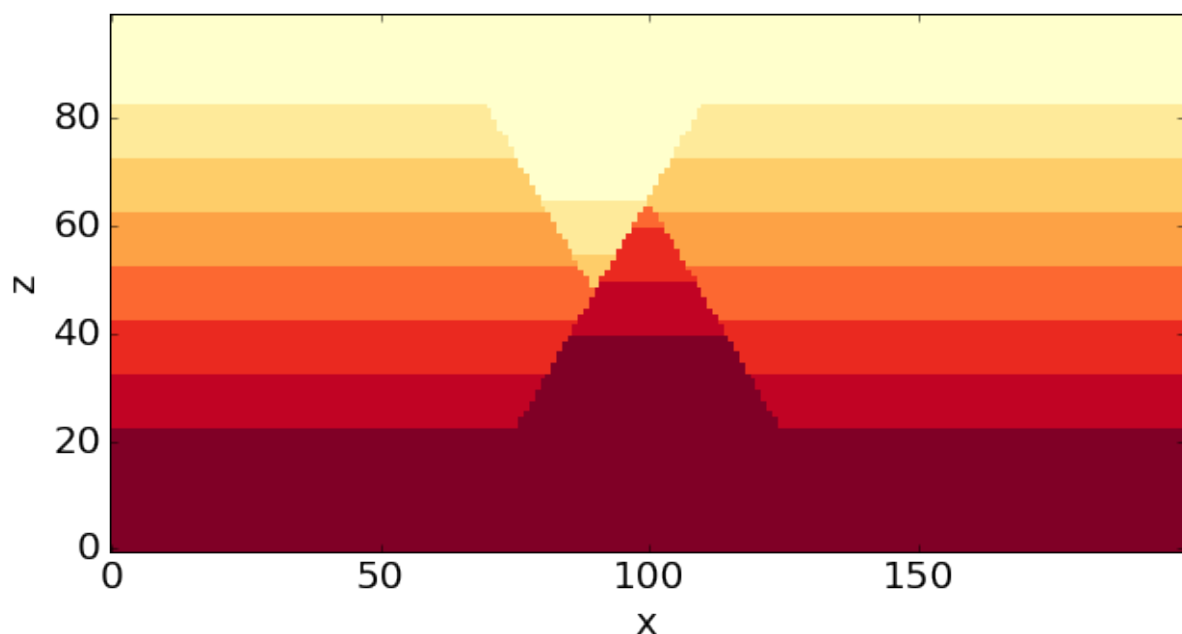

Fig. 6.4: png

READ AND VISUALISE GEOPHYSICAL POTENTIAL-FIELDS

Geophysical potential fields (gravity and magnetics) can be calculated directly from the generated kinematic model. A wide range of options also exists to consider effects of geological events on the relevant rock properties. We will here use pynoddy to simply and quickly test the effect of changing geological structures on the calculated geophysical response.

```
%matplotlib inline
```

```python
import sys, os
import matplotlib.pyplot as plt
# adjust some settings for matplotlib
from matplotlib import rcParams
# print rcParams
rcParams['font.size'] = 15
# determine path of repository to set paths corretly below
repo_path = os.path.realpath('../..')
import pynoddy
```

```python
import matplotlib.pyplot as plt
import numpy as np
```

```python
from IPython.core.display import HTML
css_file = 'pynoddy.css'
HTML(open(css_file, "r").read())
```

7.1 Read history file from Virtual Explorer

Many Noddy models are available on the site of the Virtual Explorer in the Structural Geophysics Atlas. We will download and use one of these models here as the base model.

We start with the history file of a "Fold and Thrust Belt" setting stored on:

```
http://tectonique.net/asg/ch3/ch3_5/his/fold_thrust.his
```

The file can directly be downloaded and opened with pynoddy:

```python
import pynoddy.history
reload(pynoddy.history)

his = pynoddy.history.NoddyHistory(url = \
            "http://tectonique.net/asg/ch3/ch3_5/his/fold_thrust.his")

his.determine_model_stratigraphy()
```

```python
his.change_cube_size(50)
```

```python
# Save to (local) file to compute and visualise model
history_name = "fold_thrust.his"
```

```
his.write_history(history_name)
# his = pynoddy.history.NoddyHistory(history_name)
```

```
output = "fold_thrust_out"
pynoddy.compute_model(history_name, output)
```

```
''
```

```
import pynoddy.output
# load and visualise model
h_out = pynoddy.output.NoddyOutput(output)
```

```
# his.determine_model_stratigraphy()
h_out.plot_section('x',
                   layer_labels = his.model_stratigraphy,
                   colorbar_orientation = 'horizontal',
                   colorbar=False,
                   title = '',
#                    savefig=True, fig_filename = 'fold_thrust_NS_section.eps',
                   cmap = 'YlOrRd')
```

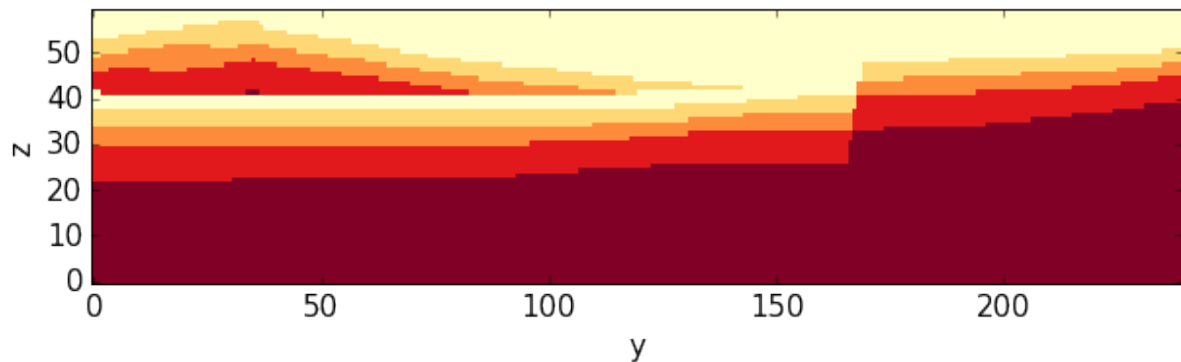

Fig. 7.1: png

```
h_out.plot_section('y', layer_labels = his.model_stratigraphy,
                   colorbar_orientation = 'horizontal', title = '', cmap = 'YlOrRd',
#                    savefig=True, fig_filename = 'fold_thrust_EW_section.eps',
                   ve=1.5)
```
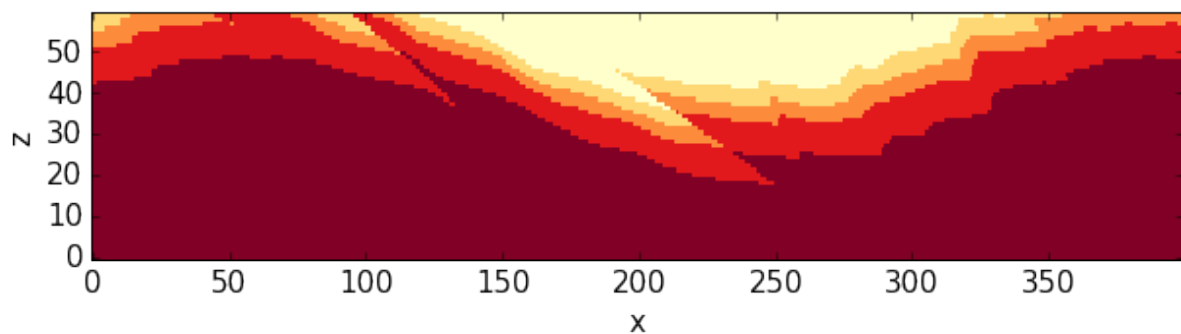

Fig. 7.2: png

```
h_out.export_to_vtk(vtk_filename = "fold_thrust")
```

7.2 Visualise calculated geophysical fields

The first step is to recompute the model with the generation of the geophysical responses

```
pynoddy.compute_model(history_name, output, sim_type = 'GEOPHYSICS')
```

```
''
```

We now get two files for the caluclated fields: '.grv' for gravity, and '.mag' for the magnetic field. We can extract the information of these files for visualisation and further processing in python:

```
reload(pynoddy.output)
geophys = pynoddy.output.NoddyGeophysics(output)
```

```
fig = plt.figure(figsize = (5,5))
ax = fig.add_subplot(111)
# imshow(geophys.grv_data, cmap = 'jet')
# define contour levels
levels = np.arange(322,344,1)
cf = ax.contourf(geophys.grv_data, levels, cmap = 'gray', vmin = 324, vmax = 342)
cbar = plt.colorbar(cf, orientation = 'horizontal')
# print levels
```
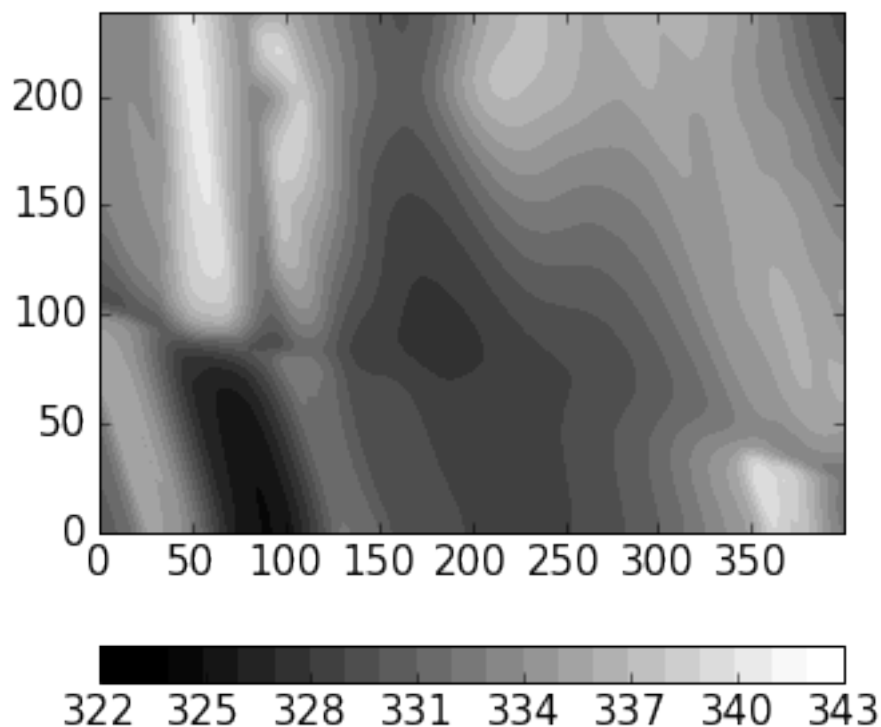

Fig. 7.3: png

7.3 Change history and compare gravity

As a next step, we will now change aspects of the geological history (paramtereised in as parameters of the kinematic events) and calculate the effect on the gravity. Then, we will compare the changed gravity field to the original field.

Let's have a look at the properties of the defined faults in the original model:

```python
for i in range(4):
    print("\nEvent %d" % (i+2))
    print "Event type:\t" + his.events[i+2].event_type
    print "Fault slip:\t%.1f" % his.events[i+2].properties['Slip']
    print "Fault dip:\t%.1f" % his.events[i+2].properties['Dip']
    print "Dip direction:\t%.1f" % his.events[i+2].properties['Dip Direction']
```

```
Event 2
Event type: FAULT
Fault slip: -5000.0
Fault dip:  0.0
Dip direction:  90.0

Event 3
Event type: FAULT
Fault slip: -3000.0
Fault dip:  0.0
Dip direction:  90.0

Event 4
Event type: FAULT
Fault slip: -3000.0
Fault dip:  0.0
Dip direction:  90.0

Event 5
Event type: FAULT
Fault slip: 12000.0
Fault dip:  80.0
Dip direction:  170.0
```

```python
reload(pynoddy.history)
reload(pynoddy.events)
his2 = pynoddy.history.NoddyHistory("fold_thrust.his")

print his2.events[6].properties
```

```
{'Dip': 130.0, 'Cylindricity': 0.0, 'Wavelength': 12000.0, 'Amplitude': 1000.0, 'Pitch': 0.0, 'Y'
```

As a simple test, we are changing the fault slip for all the faults and simply add 1000 m to all defined slips. In order to not mess up the original model, we are creating a copy of the history object first:

```python
import copy
his = pynoddy.history.NoddyHistory(history_name)
his.all_events_end += 1
his_changed = copy.deepcopy(his)

# change parameters of kinematic events
slip_change = 2000.
wavelength_change = 2000.
# his_changed.events[3].properties['Slip'] += slip_change
# his_changed.events[5].properties['Slip'] += slip_change
# change fold wavelength
his_changed.events[6].properties['Wavelength'] += wavelength_change
his_changed.events[6].properties['X'] += wavelength_change/2.
```

We now write the adjusted history back to a new history file and then calculate the updated gravity field:

```python
his_changed.write_history('fold_thrust_changed.his')
```

```python
# %%timeit
# recompute block model
pynoddy.compute_model('fold_thrust_changed.his', 'fold_thrust_changed_out')
```

```
''
```

```
# %%timeit
# recompute geophysical response
pynoddy.compute_model('fold_thrust_changed.his', 'fold_thrust_changed_out',
                      sim_type = 'GEOPHYSICS')
```

```
''
```

```
# load changed block model
geo_changed = pynoddy.output.NoddyOutput('fold_thrust_changed_out')
# load output and visualise geophysical field
geophys_changed = pynoddy.output.NoddyGeophysics('fold_thrust_changed_out')
```

```
fig = plt.figure(figsize = (5,5))
ax = fig.add_subplot(111)
# imshow(geophys_changed.grv_data, cmap = 'jet')
cf = ax.contourf(geophys_changed.grv_data, levels, cmap = 'gray', vmin = 324, vmax = 342)
cbar = plt.colorbar(cf, orientation = 'horizontal')
```
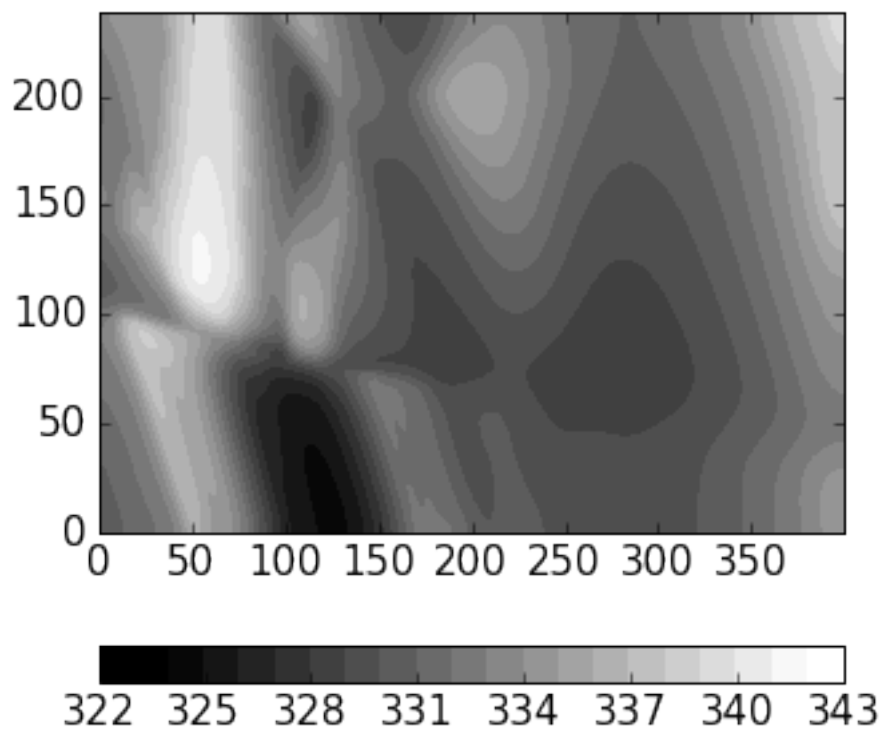

Fig. 7.4: png

```
fig = plt.figure(figsize = (5,5))
ax = fig.add_subplot(111)
# imshow(geophys.grv_data - geophys_changed.grv_data, cmap = 'jet')
maxval = np.ceil(np.max(np.abs(geophys.grv_data - geophys_changed.grv_data)))
# comp_levels = np.arange(-maxval,1.01 * maxval, 0.05 * maxval)
cf = ax.contourf(geophys.grv_data - geophys_changed.grv_data, 20,
                 cmap = 'spectral')
cbar = plt.colorbar(cf, orientation = 'horizontal')
```

```
# compare sections through model
geo_changed.plot_section('y', colorbar = False)
h_out.plot_section('y', colorbar = False)
```
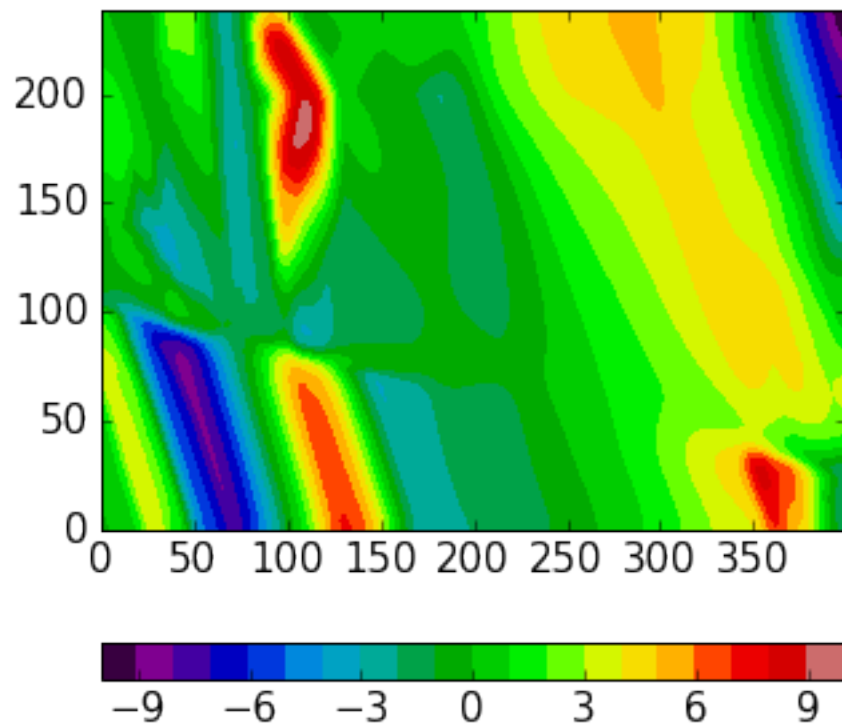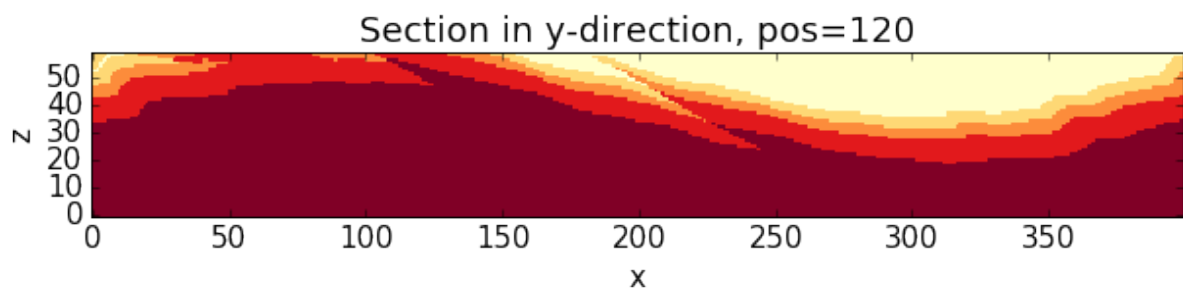
Fig. 7.5: png
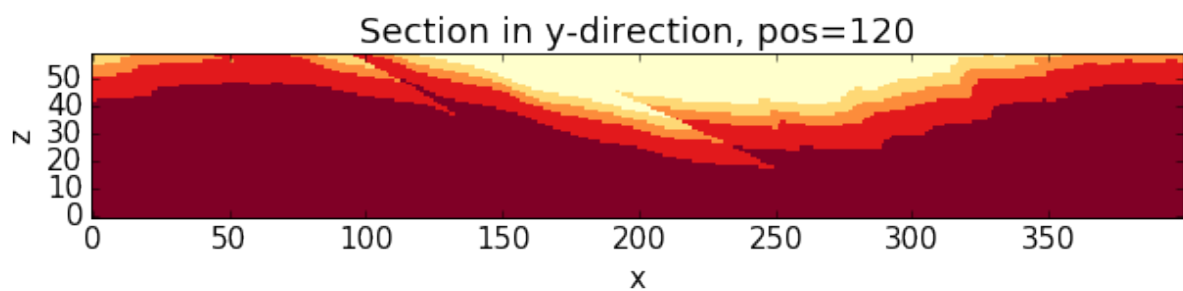

Fig. 7.6: png

Fig. 7.7: png

```
for i in range(4):
    print("Event %d" % (i+2))
    print his.events[i+2].properties['Slip']
    print his.events[i+2].properties['Dip']
    print his.events[i+2].properties['Dip Direction']
```

```
Event 2
-5000.0
0.0
90.0
Event 3
-3000.0
0.0
90.0
Event 4
-3000.0
0.0
90.0
Event 5
12000.0
80.0
170.0
```

```
# recompute the geology blocks for comparison:
pynoddy.compute_model('fold_thrust_changed.his', 'fold_thrust_changed_out')
```

```
''
```

```
geology_changed = pynoddy.output.NoddyOutput('fold_thrust_changed_out')
```

```
geology_changed.plot_section('x',
#                   layer_labels = his.model_stratigraphy,
                    colorbar_orientation = 'horizontal',
                    colorbar=False,
                    title = '',
#                    savefig=True, fig_filename = 'fold_thrust_NS_section.eps',
                    cmap = 'YlOrRd')
```
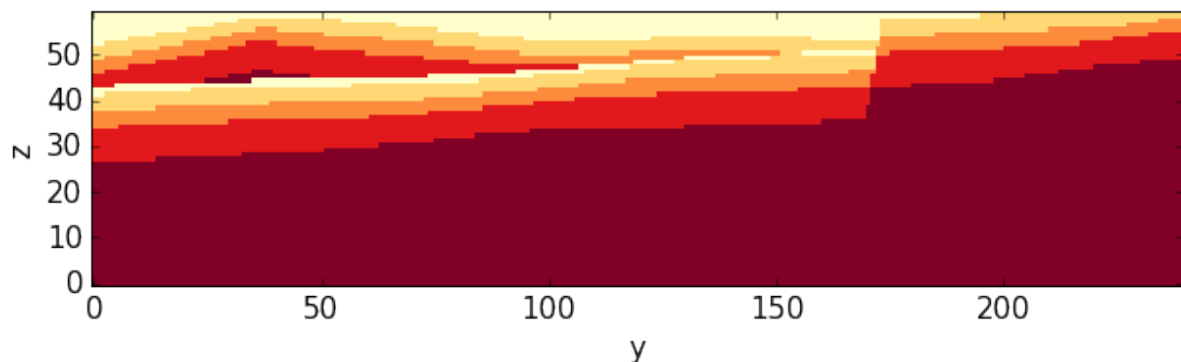

Fig. 7.8: png

```
geology_changed.plot_section('y',
#                     layer_labels = his.model_stratigraphy,
                    colorbar_orientation = 'horizontal', title = '', cmap = 'YlOrRd',
#                     savefig=True, fig_filename = 'fold_thrust_EW_section.eps',
                    ve=1.5)
```

```
# Calculate block difference and export as VTK for 3-D visualisation:
import copy
```
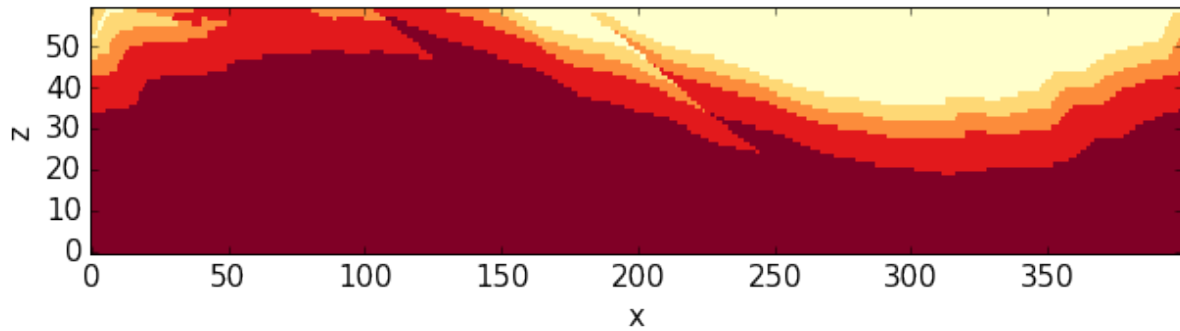
Fig. 7.9: png

```
diff_model = copy.deepcopy(geology_changed)
diff_model.block -= h_out.block
```

```
diff_model.export_to_vtk(vtk_filename = "diff_model_fold_thrust_belt")
```

7.4 Figure with all results

We now create a figure with the gravity field of the original and the changed model, as well as a difference plot to highlight areas with significant changes. This example also shows how additional equations can easily be combined with pynoddy classes.

```
fig = plt.figure(figsize=(20,8))
ax1 = fig.add_subplot(131)
# original plot
levels = np.arange(322,344,1)
cf1 = ax1.contourf(geophys.grv_data, levels, cmap = 'gray', vmin = 324, vmax = 342)
# cbar1 = ax1.colorbar(cf1, orientation = 'horizontal')
fig.colorbar(cf1, orientation='horizontal')
ax1.set_title('Gravity of original model')

ax2 = fig.add_subplot(132)




cf2 = ax2.contourf(geophys_changed.grv_data, levels, cmap = 'gray', vmin = 324, vmax = 342)
ax2.set_title('Gravity of changed model')
fig.colorbar(cf2, orientation='horizontal')

ax3 = fig.add_subplot(133)


comp_levels = np.arange(-10.,10.1,0.25)
cf3 = ax3.contourf(geophys.grv_data - geophys_changed.grv_data, comp_levels, cmap = 'RdBu_r')
ax3.set_title('Gravity difference')

fig.colorbar(cf3, orientation='horizontal')

plt.savefig("grav_ori_changed_compared.eps")
```
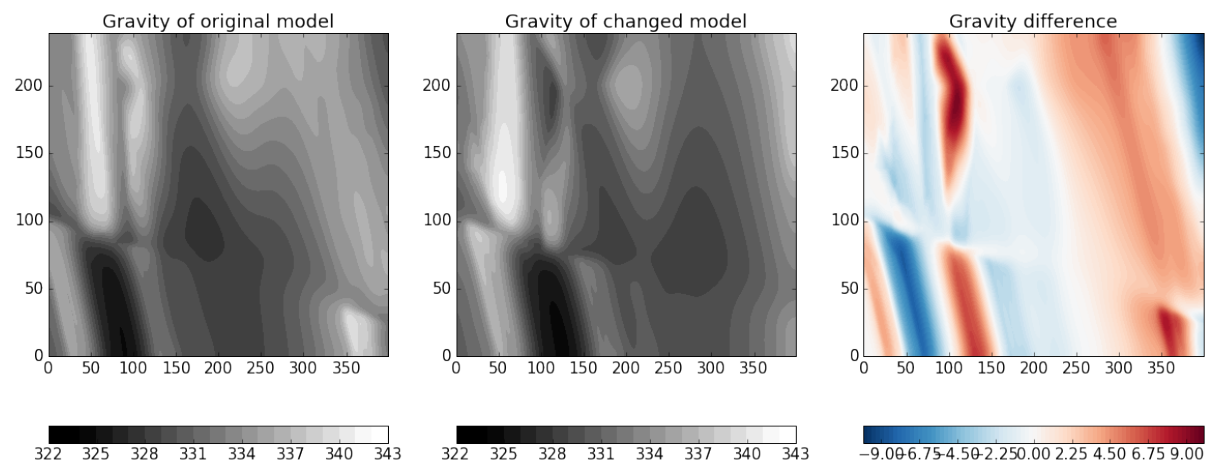
Fig. 7.10: png

REPRODUCIBLE EXPERIMENTS WITH PYNODDY

All `pynoddy` experiments can be defined in a Python script, and if all settings are appropriate, then this script can be re-run to obtain a reproduction of the results. However, it is often more convenient to encapsulate all elements of an experiment within one class. We show here how this is done in the `pynoddy.experiment.Experiment` class and how this class can be used to define simple reproducible experiments with kinematic models.

```python
from IPython.core.display import HTML
css_file = 'pynoddy.css'
HTML(open(css_file, "r").read())
```

```python
%matplotlib inline
```

```python
# here the usual imports. If any of the imports fails,
# make sure that pynoddy is installed
# properly, ideally with 'python setup.py develop'
# or 'python setup.py install'
import sys, os
import matplotlib.pyplot as plt
import numpy as np
# adjust some settings for matplotlib
from matplotlib import rcParams
# print rcParams
rcParams['font.size'] = 15
# determine path of repository to set paths corretly below
repo_path = os.path.realpath('../..')
import pynoddy.history
import pynoddy.experiment
reload(pynoddy.experiment)
rcParams.update({'font.size': 15})
```

8.1 Defining an experiment

We are considering the following scenario: we defined a kinematic model of a prospective geological unit at depth. As we know that the estimates of the (kinematic) model parameters contain a high degree of uncertainty, we would like to represent this uncertainty with the model.

Our approach is here to perform a randomised uncertainty propagation analysis with a Monte Carlo sampling method. Results should be presented in several figures (2-D slice plots and a VTK representation in 3-D).

To perform this analysis, we need to perform the following steps (see main paper for more details):

1. Define kinematic model parameters and construct the initial (base) model;

2. Assign probability distributions (and possible parameter correlations) to relevant uncertain input parameters;

3. Generate a set of n random realisations, repeating the following steps:

    (a) Draw a randomised input parameter set from the parameter distribu- tion;

    (b) Generate a model with this parameter set;

     (c) Analyse the generated model and store results;

4. Finally: perform postprocessing, generate figures of results

It would be possible to write a Python script to perform all of these steps in one go. However, we will here take another path and use the implementation in a Pynoddy Experiment class. Initially, this requires more work and a careful definition of the experiment - but, finally, it will enable a higher level of flexibility, extensibility, and reproducibility.

8.2 Loading an example model from the Atlas of Structural Geophysics

As in the example for geophysical potential-field simulation, we will use a model from the Atlas of Structural Geophysics as an examlpe model for this simulation. We use a model for a fold interference structure. A discretised 3-D version of this model is presented in the figure below. The model represents a fold interference pattern of "Type 1" according to the definition of Ramsey (1967).
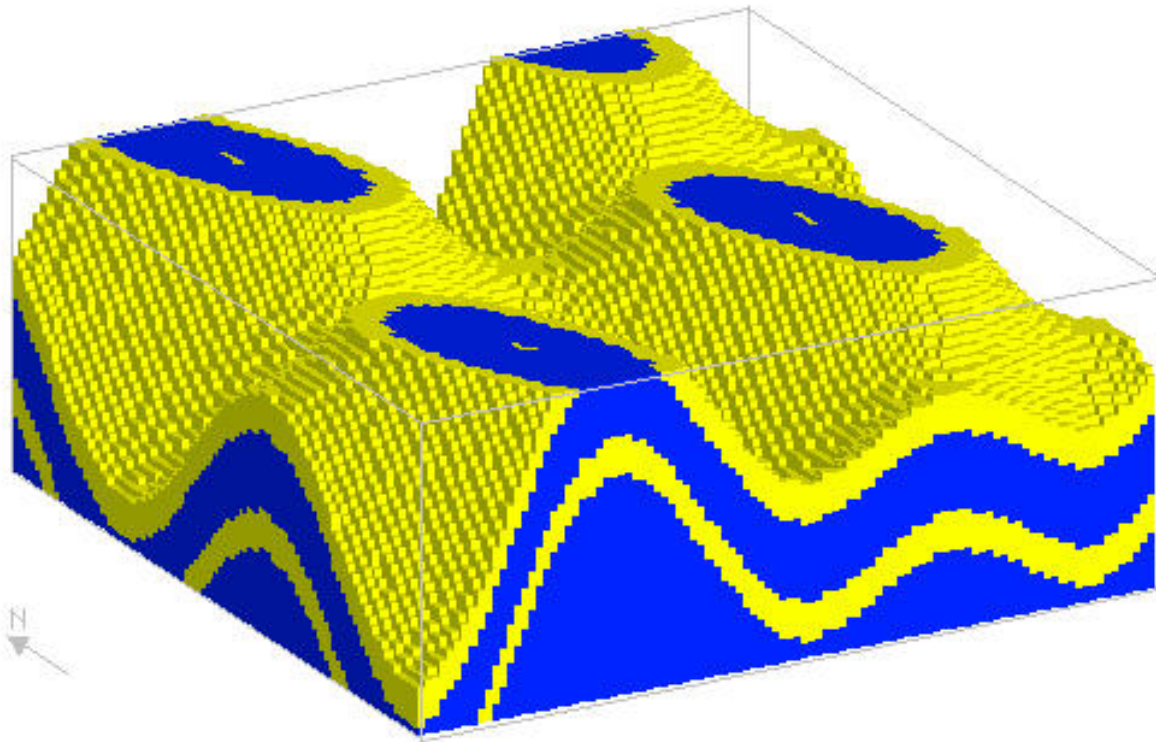

Fig. 8.1: Fold interference pattern

Instead of loading the model into a history object, we are now directly creating an experiment object:

```
reload(pynoddy.history)
reload(pynoddy.experiment)

from pynoddy.experiment import monte_carlo
model_url = 'http://tectonique.net/asg/ch3/ch3_7/his/typeb.his'
ue = pynoddy.experiment.Experiment(url = model_url)
```

For simpler visualisation in this notebook, we will analyse the following steps in a section view of the model.

We consider a section in y-direction through the model:

```
ue.write_history("typeb_tmp3.his")
```

```
ue.write_history("typeb_tmp2.his")
```

```
ue.change_cube_size(100)
ue.plot_section('y')
```
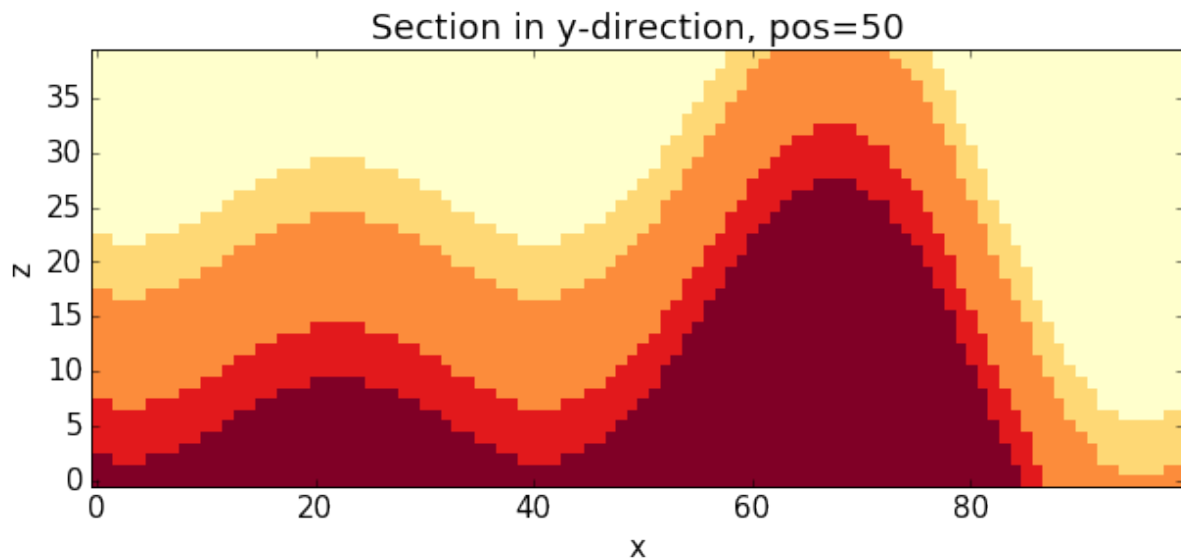

Fig. 8.2: png

Before we start to draw random realisations of the model, we should first store the base state of the model for later reference. This is simply possibel with the freeze() method which stores the current state of the model as the "base-state":

```
ue.freeze()
```

We now intialise the random generator. We can directly assign a random seed to simplify reproducibility (note that this is not *essential*, as it would be for the definition in a script function: the random state is preserved within the model and could be retrieved at a later stage, as well!):

```
ue.set_random_seed(12345)
```

The next step is to define probability distributions to the relevant event parameters. Let's first look at the different events:

```
ue.info(events_only = True)
```

```
This model consists of 3 events:
    (1) - STRATIGRAPHY
    (2) - FOLD
    (3) - FOLD
```

```
ev2 = ue.events[2]
```

```
ev2.properties
```

```
{'Amplitude': 1250.0,
 'Cylindricity': 0.0,
 'Dip': 90.0,
 'Dip Direction': 90.0,
 'Pitch': 0.0,
 'Single Fold': 'FALSE',
```

```
'Type': 'Sine',
'Wavelength': 5000.0,
'X': 1000.0,
'Y': 0.0,
'Z': 0.0}
```

Next, we define the probability distributions for the uncertain input parameters:

```
param_stats = [{'event' : 2,
                'parameter': 'Amplitude',
                'stdev': 100.0,
                'type': 'normal'},
               {'event' : 2,
                'parameter': 'Wavelength',
                'stdev': 500.0,
                'type': 'normal'},
               {'event' : 2,
                'parameter': 'X',
                'stdev': 500.0,
                'type': 'normal'}]

ue.set_parameter_statistics(param_stats)
```

```
resolution = 100
ue.change_cube_size(resolution)
tmp = ue.get_section('y')
prob_4 = np.zeros_like(tmp.block[:,:,:])
n_draws = 100


for i in range(n_draws):
    ue.random_draw()
    tmp = ue.get_section('y', resolution = resolution)
    prob_4 += (tmp.block[:,:,:] == 4)

# Normalise
prob_4 = prob_4 / float(n_draws)
```

```
fig = plt.figure(figsize = (12,8))
ax = fig.add_subplot(111)
ax.imshow(prob_4.transpose()[:,0,:],
          origin = 'lower left',
          interpolation = 'none')
plt.title("Estimated probability of unit 4")
plt.xlabel("x (E-W)")
plt.ylabel("z")
```

```
<matplotlib.text.Text at 0x10ba80250>
```

This example shows how the base module for reproducible experiments with kinematics can be used. For further specification, child classes of `Experiment` can be defined, and we show examples of this type of extension in the next sections.
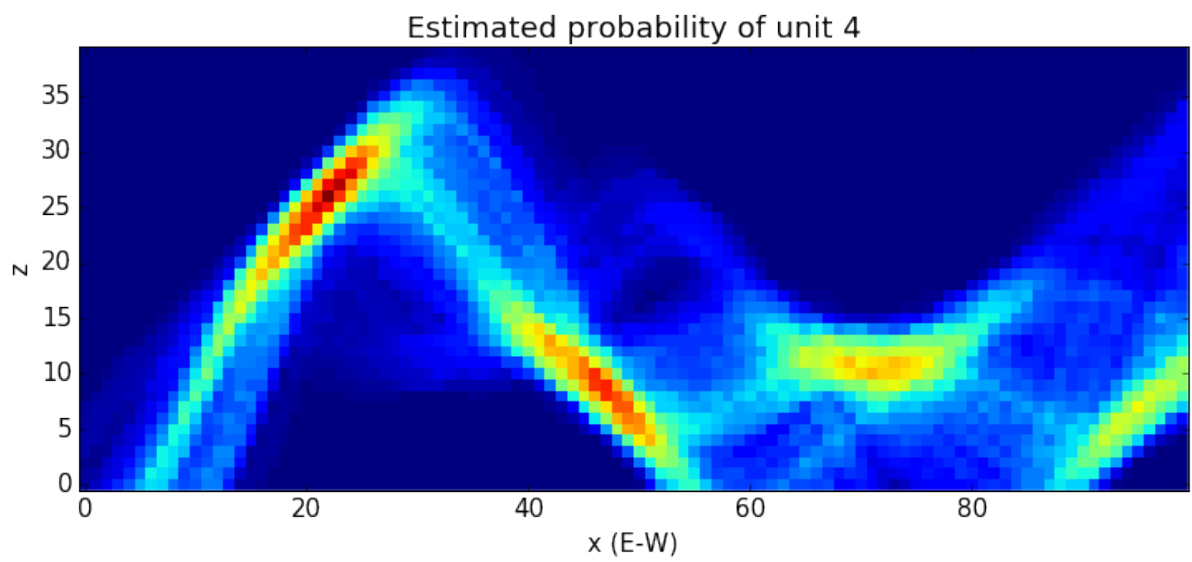
Fig. 8.3: png

GIPPSLAND BASIN UNCERTAINTY STUDY

```python
from IPython.core.display import HTML
css_file = 'pynoddy.css'
HTML(open(css_file, "r").read())
```

```python
%matplotlib inline
```

```python
#import the ususal libraries + the pynoddy UncertaintyAnalysis class

import sys, os, pynoddy
# from pynoddy.experiment.UncertaintyAnalysis import UncertaintyAnalysis

# adjust some settings for matplotlib
from matplotlib import rcParams
# print rcParams
rcParams['font.size'] = 15

# determine path of repository to set paths corretly below
repo_path = os.path.realpath('../..')
import pynoddy.history
import pynoddy.experiment.uncertainty_analysis
rcParams.update({'font.size': 20})
```

9.1 The Gippsland Basin Model

In this example we will apply the UncertaintyAnalysis class we have been playing with in the previous example to a 'realistic' (though highly simplified) geological model of the Gippsland Basin, a petroleum field south of Victoria, Australia. The model has been included as part of the PyNoddy directory, and can be found at `pynoddy/examples/GBasin_Ve1_V4.his`

```python
reload(pynoddy.history)
reload(pynoddy.output)
reload(pynoddy.experiment.uncertainty_analysis)
reload(pynoddy)

# the model itself is now part of the repository, in the examples directory:
history_file = os.path.join(repo_path, "examples/GBasin_Ve1_V4.his")
```

While we could hard-code parameter variations here, it is much easier to store our statistical information in a csv file, so we load that instead. This file accompanies the `GBasin_Ve1_V4` model in the pynoddy directory.

```python
params = os.path.join(repo_path,"examples/gipps_params.csv")
```

9.2 Generate randomised model realisations

Now we have all the information required to perform a Monte-Carlo based uncertainty analysis. In this example we will generate 100 model realisations and use them to estimate the information entropy of each voxel in the model, and hence visualise uncertainty. It is worth noting that in reality we would need to produce several thousand model realisations in order to adequately sample the model space, however for convinience we only generate a small number of models here.

```
# %%timeit    # Uncomment to test execution time
ua = pynoddy.experiment.uncertainty_analysis.UncertaintyAnalysis(history_file, params)
ua.estimate_uncertainty(100,verbose=False)
```

A few utility functions for visualising uncertainty have been included in the UncertaintyAnalysis class, and can be used to gain an understanding of the most uncertain parts of the Gippsland Basin. The probabability voxels for each lithology can also be accessed using `ua.p_block[lithology_id]`, and the information entropy voxset accessed using `ua.e_block`.

Note that the Gippsland Basin model has been computed with a vertical exaggeration of 3, in order to highlight vertical structure.

```
ua.plot_section(direction='x',data=ua.block)
ua.plot_entropy(direction='x')
```
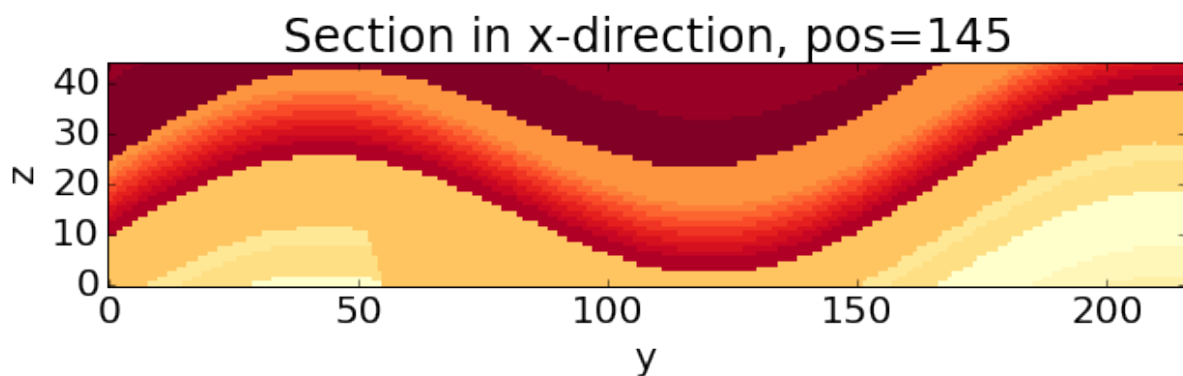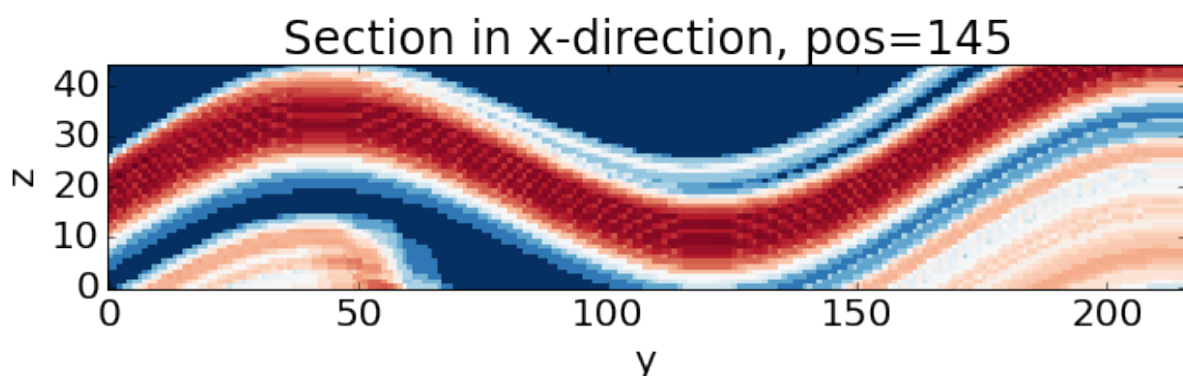

Fig. 9.1: png

Fig. 9.2: png

It is immediately apparent (and not particularly surprising) that uncertainty in the Gippsland Basin model is concentrated around the thin (but economically interesting) formations comprising the La Trobe and Strzelecki Groups. The faults in the model also contribute to this uncertainty, though not by a huge amount.

9.3 Exporting results to VTK for visualisation

It is also possible (and useful!) to export the uncertainty information to .vtk format for 3D analysis in software such as ParaView. This can be done as follows:

```
ua.extent_x = 29000
ua.extent_y = 21600
ua.extent_z = 4500

output_path = os.path.join(repo_path,"sandbox/GBasin_Uncertainty")
ua.export_to_vtk(vtk_filename=output_path,data=ua.e_block)
```

The resulting vtr file can (in the sandbox directory) can now be loaded and properly analysed in a 3D visualisation package such as ParaView.
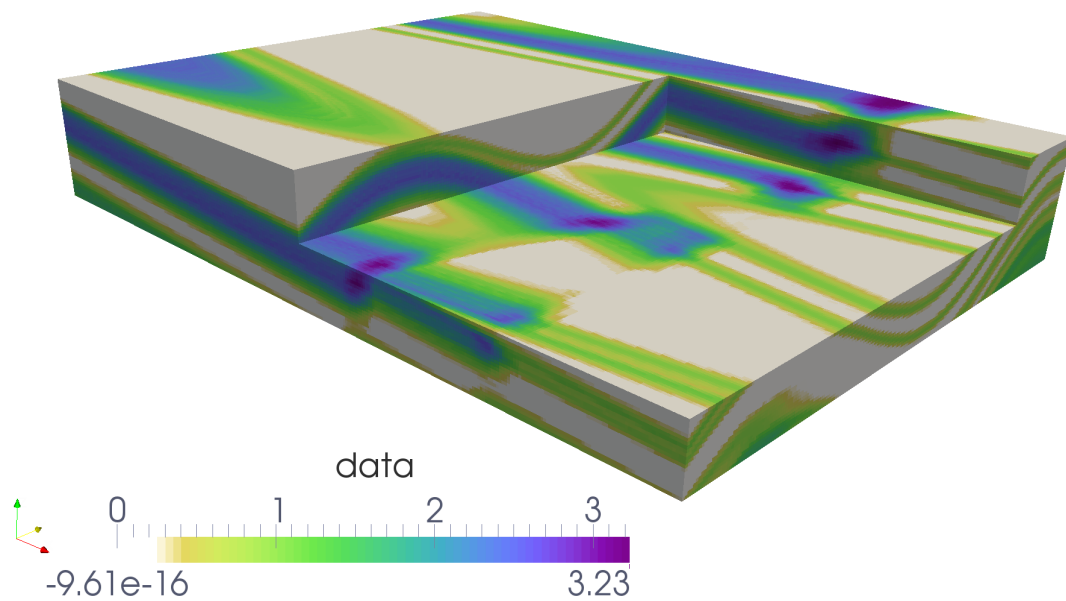

Fig. 9.3: 3-D visualisation of cell information entropy

SENSITIVITY ANALYSIS

Test here: (local) sensitivity analysis of kinematic parameters with respect to a defined objective function. Aim: test how sensitivity the resulting model is to uncertainties in kinematic parameters to:

1. Evaluate which the most important parameters are, and to

2. Determine which parameters could, in principle, be inverted with suitable information.

10.1 Theory: local sensitivity analysis

Basic considerations:

- parameter vector $\vec{p}$

- residual vector $\vec{r}$

- calculated values at observation points $\vec{z}$

- Jacobian matrix $J_{ij} = \frac{\partial \vec{z}}{\partial \vec{p}}$

Numerical estimation of Jacobian matrix with central difference scheme (see Finsterle):

$$J_{ij} = \frac{\partial z_i}{\partial p_j} \approx \frac{z_i(\vec{p}; p_j + \delta p_j) - z_i(\vec{p}; p_j - \delta p_j)}{2\delta p_j}$$

where δp_j is a small perturbation of parameter j, often as a fraction of the value.

10.2 Defining the responses

A meaningful sensitivity analysis obviously depends on the definition of a suitable response vector $\vec{z}$. Ideally, these responses are related to actual observations. In our case, we first want to determine how sensitive a kinematic structural geological model is with respect to uncertainties in the kinematic parameters. We therefore need calculatable measures that describe variations of the model.

As a first-order assumption, we will use a notation of a stratigraphic distance for discrete subsections of the model, for example in single voxels for the calculated model. We define distance d of a subset ω as the (discrete) difference between the (discrete) stratigraphic value of an ideal model, $\hat{s}$, to the value of a model realisation s_i:

$$d(\omega) = \hat{s} - s_i$$

In the first example, we will consider only one response: the overall sum of stratigraphic distances for a model realisation r of all subsets (= voxels, in the practical sense), scaled by the number of subsets (for a subsequent comparison of model discretisations):

$$D_r = \frac{1}{n} \sum_{i=1}^{n} d(\omega_i)$$

Note: mistake before: not considering distances at single nodes but only the sum - this lead to "zero-difference" for simple translation! Now: consider more realistic objective function, squared distance:

$$r = \sqrt{\sum_i (z_{icalc} - z_{iref})^2}$$

```python
from IPython.core.display import HTML
css_file = 'pynoddy.css'
HTML(open(css_file, "r").read())
```

```python
%matplotlib inline
```

10.3 Setting up the base model

For a first test: use simple two-fault model from paper

```python
import sys, os
import matplotlib.pyplot as plt
import numpy as np
# adjust some settings for matplotlib
from matplotlib import rcParams
# print rcParams
rcParams['font.size'] = 15
# determine path of repository to set paths corretly below
repo_path = os.path.realpath('../..')
import pynoddy.history
import pynoddy.events
import pynoddy.output
```

```python
reload(pynoddy.history)
reload(pynoddy.events)
nm = pynoddy.history.NoddyHistory()
# add stratigraphy
strati_options = {'num_layers' : 8,
                  'layer_names' : ['layer 1', 'layer 2', 'layer 3', 'layer 4', 'layer 5', 'layer
                  'layer_thickness' : [1500, 500, 500, 500, 500, 500, 500, 500]}
nm.add_event('stratigraphy', strati_options )

# The following options define the fault geometry:
fault_options = {'name' : 'Fault_W',
                 'pos' : (4000, 3500, 5000),
                 'dip_dir' : 90,
                 'dip' : 60,
                 'slip' : 1000}

nm.add_event('fault', fault_options)
# The following options define the fault geometry:
fault_options = {'name' : 'Fault_E',
                 'pos' : (6000, 3500, 5000),
                 'dip_dir' : 270,
                 'dip' : 60,
                 'slip' : 1000}

nm.add_event('fault', fault_options)
history = "two_faults_sensi.his"
nm.write_history(history)
```

```python
output_name = "two_faults_sensi_out"
# Compute the model
pynoddy.compute_model(history, output_name)
```

```
''
```

```
# Plot output
nout = pynoddy.output.NoddyOutput(output_name)
nout.plot_section('y', layer_labels = strati_options['layer_names'][::-1],
                  colorbar = True, title="",
                  savefig = False)
```
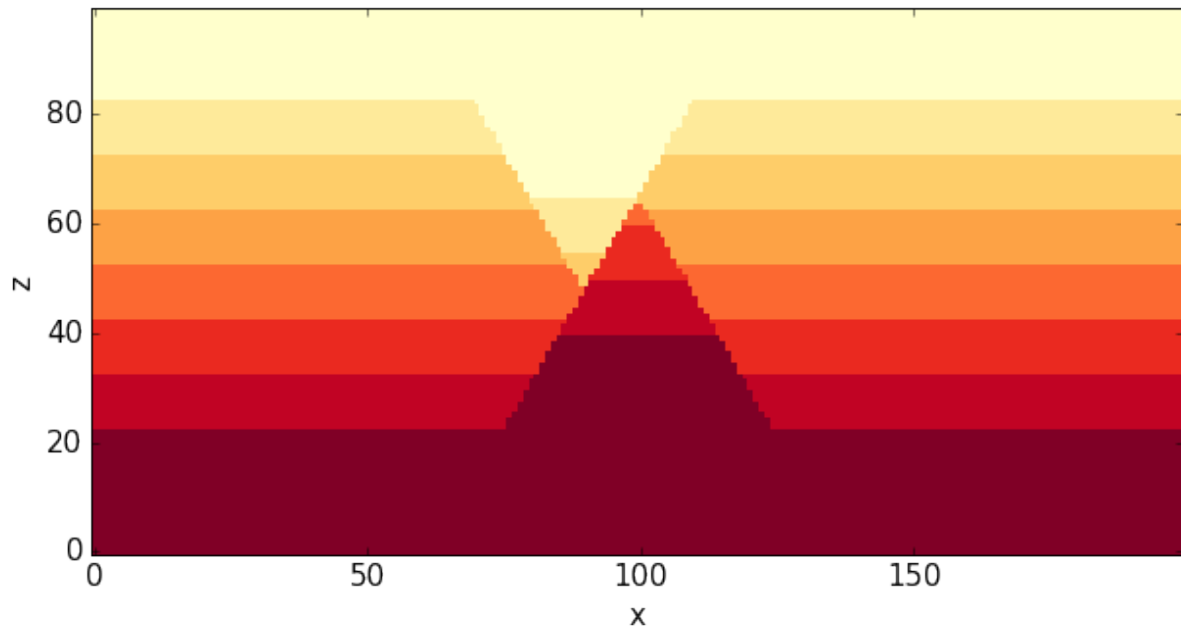

Fig. 10.1: png

10.4 Define parameter uncertainties

We will start with a sensitivity analysis for the parameters of the fault events.

```
H1 = pynoddy.history.NoddyHistory(history)
# get the original dip of the fault
dip_ori = H1.events[3].properties['Dip']
# dip_ori1 = H1.events[2].properties['Dip']
# add 10 degrees to dip
add_dip = -20
dip_new = dip_ori + add_dip
# dip_new1 = dip_ori1 + add_dip

# and assign back to properties dictionary:
H1.events[3].properties['Dip'] = dip_new
```

```
reload(pynoddy.output)
new_history = "sensi_test_dip_changed.his"
new_output = "sensi_test_dip_changed_out"
H1.write_history(new_history)
pynoddy.compute_model(new_history, new_output)
# load output from both models
NO1 = pynoddy.output.NoddyOutput(output_name)
NO2 = pynoddy.output.NoddyOutput(new_output)

# create basic figure layout
fig = plt.figure(figsize = (15,5))
```

```
ax1 = fig.add_subplot(121)
ax2 = fig.add_subplot(122)
NO1.plot_section('y', position=0, ax = ax1, colorbar=False, title="Dip = %.0f" % dip_ori)
NO2.plot_section('y', position=0, ax = ax2, colorbar=False, title="Dip = %.0f" % dip_new)

plt.show()
```
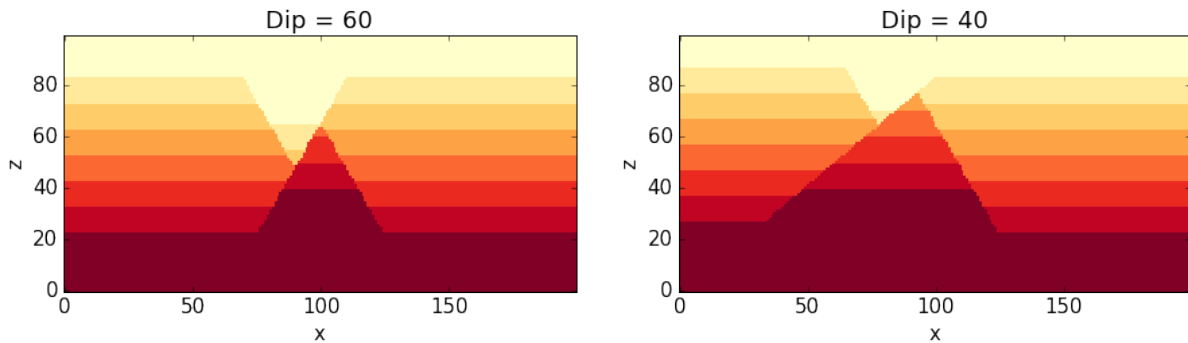

Fig. 10.2: png

10.5 Calculate total stratigraphic distance

```python
# def determine_strati_diff(NO1, NO2):
#     """calculate total stratigraphic distance between two models"""
#     return np.sum(NO1.block - NO2.block) / float(len(NO1.block))

def determine_strati_diff(NO1, NO2):
    """calculate total stratigraphic distance between two models"""
    return np.sqrt(np.sum((NO1.block - NO2.block)**2)) / float(len(NO1.block))



diff = determine_strati_diff(NO1, NO2)
print(diff)
```

```
5.56205897128
```

10.6 Function to modify parameters

Multiple event parameters can be changed directly with the function `change_event_params`, which takes a dictionary of events and parameters with according changes relative to the defined parameters. Here a brief example:

```python
# set parameter changes in dictionary

changes_fault_1 = {'Dip' : -20}
changes_fault_2 = {'Dip' : -20}
param_changes = {2 : changes_fault_1,
                 3 : changes_fault_2}
```

```python
reload(pynoddy.history)
H2 = pynoddy.history.NoddyHistory(history)
H2.change_event_params(param_changes)
```

```
new_history = "param_dict_changes.his"
new_output = "param_dict_changes_out"
H2.write_history(new_history)
pynoddy.compute_model(new_history, new_output)
# load output from both models
NO1 = pynoddy.output.NoddyOutput(output_name)
NO2 = pynoddy.output.NoddyOutput(new_output)

# create basic figure layout
fig = plt.figure(figsize = (15,5))
ax1 = fig.add_subplot(121)
ax2 = fig.add_subplot(122)
NO1.plot_section('y', position=0, ax = ax1, colorbar=False, title="Original Model")
NO2.plot_section('y', position=0, ax = ax2, colorbar=False, title="Changed Model")

plt.show()
```
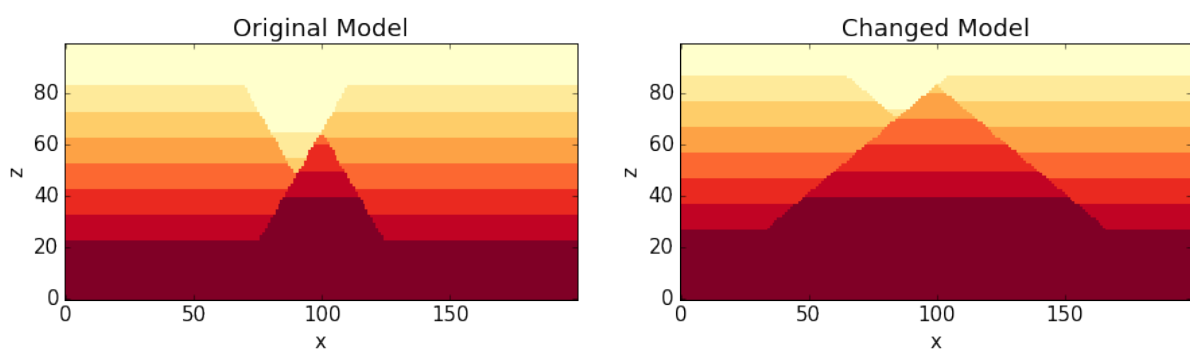

Fig. 10.3: png

10.7 Full sensitivity analysis

Perform now a full sensitivity analysis for all defined parameters and analyse the output matrix. For a better overview, we first create a function to perform the sensitivity analysis:

```
import copy
new_history = "sensi_tmp.his"
new_output = "sensi_out"
def noddy_sensitivity(history_filename, param_change_vals):
    """Perform noddy sensitivity analysis for a model"""
    param_list = [] # list to store parameters for later analysis
    distances = [] # list to store calcualted distances
    # Step 1:
    # create new parameter list to change model
    for event_id, event_dict in param_change_vals.items(): # iterate over events
        for key, val in event_dict.items(): # iterate over all properties separately
            changes_list = dict()
            changes_list[event_id] = dict()
            param_list.append("event_%d_property_%s" % (event_id, key))
            for i in range(2):
                # calculate positive and negative values
                his = pynoddy.history.NoddyHistory(history_filename)
                if i == 0:
                    changes_list[event_id][key] = val
                    # set changes
                    his.change_event_params(changes_list)
                    # save and calculate model
                    his.write_history(new_history)
```

```python
                    pynoddy.compute_model(new_history, new_output)
                    # open output and calculate distance
                    NO_tmp = pynoddy.output.NoddyOutput(new_output)
                    dist_pos = determine_strati_diff(NO1, NO_tmp)
                    NO_tmp.plot_section('y', position = 0, colorbar = False,
                                        title = "Dist: %.2f" % dist_pos,
                                        savefig = True,
                                        fig_filename = "event_%d_property_%s_val_%d.png" \
                                        % (event_id, key,val))
                if i == 1:
                    changes_list[event_id][key] = -val
                    his.change_event_params(changes_list)
                    # save and calculate model
                    his.write_history(new_history)
                    pynoddy.compute_model(new_history, new_output)
                    # open output and calculate distance
                    NO_tmp = pynoddy.output.NoddyOutput(new_output)
                    dist_neg = determine_strati_diff(NO1, NO_tmp)
                    NO_tmp.plot_section('y', position=0, colorbar=False,
                                        title="Dist: %.2f" % dist_neg,
                                        savefig=True,
                                        fig_filename="event_%d_property_%s_val_%d.png" \
                                        % (event_id, key,val))
            # calculate central difference
            central_diff = (dist_pos + dist_neg) / (2.)
            distances.append(central_diff)
    return param_list, distances
```

As a next step, we define the parameter ranges for the local sensitivity analysis (i.e. the δp_j from the theoretical description above):

```python
changes_fault_1 = {'Dip' : 1.5,
                   'Dip Direction' : 10,
                   'Slip': 100.0,
                   'X': 500.0}
changes_fault_2 = {'Dip' : 1.5,
                   'Dip Direction' : 10,
                   'Slip': 100.0,
                   'X': 500.0}
param_changes = {2 : changes_fault_1,
                 3 : changes_fault_2}
```

And now, we perform the local sensitivity analysis:

```python
param_list_1, distances = noddy_sensitivity(history, param_changes)
```

The function passes back a list of the changed parameters and the calculated distances according to this change. Let's have a look at the results:

```python
for p,d in zip(param_list_1, distances):
    print "%s \t\t %f" % (p, d)
```

```
event_2_property_X          2.716228
event_2_property_Dip           1.410039
event_2_property_Dip Direction        2.133553
event_2_property_Slip         1.824993
event_3_property_X          3.323528
event_3_property_Dip           1.644589
event_3_property_Dip Direction        2.606573
event_3_property_Slip         1.930455
```

Results of this local sensitivity analysis suggest that the model is most sensitive to the X-position of the fault, when we evaluate distances as simple stratigraphic id differences. Here just a bar plot for better visualisation (feel free to add proper labels):

```
d = np.array([distances])
fig = plt.figure(figsize=(5,3))
ax = fig.add_subplot(111)
ax.bar(np.arange(0.6,len(distances),1.), np.array(distances[:]))
```
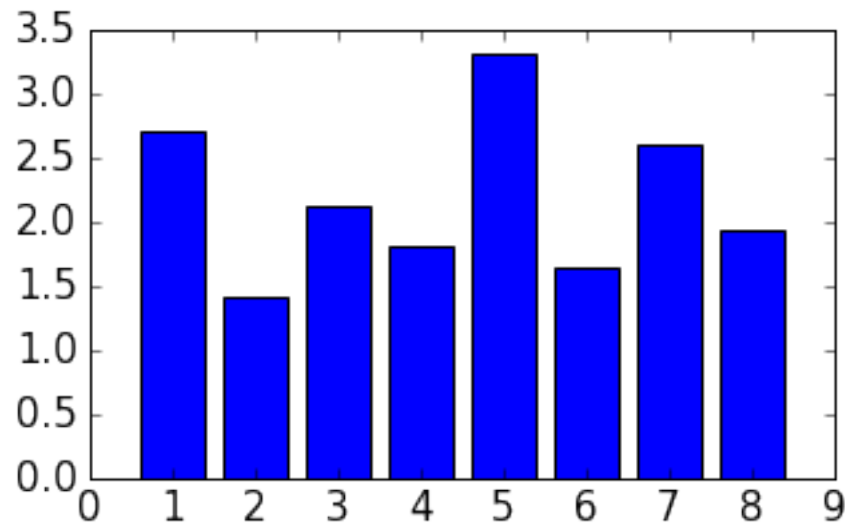
```
<Container object of 8 artists>
```


Fig. 10.4: png

The previous experiment showed how `pynoddy` can be used for simple scientific experiments. The sensitivity analysis itself is purely local. A better way would be to use (more) global sensitivity analysis, for example using the Morris or Sobol methods. These methods are implemented in the Python package `SALib`, and an experimental implementation of this method into `pynoddy` exists, as well (see further notebooks on repository, note: no guaranteed working, so far!).

SIMULATION OF A NODDY HISTORY AND ANALYSIS OF ITS VOXEL TOPOLOGY

Example of how the module can be used to run Noddy simulations and analyse the output.

```python
from IPython.core.display import HTML
css_file = 'pynoddy.css'
HTML(open(css_file, "r").read())
```

```python
# Basic settings
import sys, os
import subprocess

# Now import pynoddy
import pynoddy
%matplotlib inline

# determine path of repository to set paths corretly below

repo_path = os.path.realpath('../..')
```

11.1 Compute the model

The simplest way to perform the Noddy simulation through Python is simply to call the executable. One way that should be fairly platform independent is to use Python's own subprocess module:

```python
# Change to sandbox directory to store results
os.chdir(os.path.join(repo_path, 'sandbox'))

# Path to exmaple directory in this repository
example_directory = os.path.join(repo_path,'examples')
# Compute noddy model for history file
history_file = 'strike_slip.his'
history = os.path.join(example_directory, history_file)
nfiles = 1
files = '_'+str(nfiles).zfill(4)
print "files", files
root_name = 'noddy_out'
output_name = root_name + files
print root_name
print output_name
# call Noddy

# NOTE: Make sure that the noddy executable is accessible in the system!!
sys
print subprocess.Popen(['noddy.exe', history, output_name, 'TOPOLOGY'],
                       shell=False, stderr=subprocess.PIPE,
                       stdout=subprocess.PIPE).stdout.read()
```

```
#
sys
print subprocess.Popen(['topology.exe', root_name, files],
                        shell=False, stderr=subprocess.PIPE,
                        stdout=subprocess.PIPE).stdout.read()
```

```
files _0001
noddy_out
noddy_out_0001
```

For convenience, the model computations are wrapped into a Python function in pynoddy:

```
pynoddy.compute_model(history, output_name)
pynoddy.compute_topology(root_name, files)
```

Note: The Noddy call from Python is, to date, calling Noddy through the subprocess function. In a future implementation, this call could be subsituted with a full wrapper for the C-functions written in Python. Therefore, using the member function compute_model is not only easier, but also the more "future-proof" way to compute the Noddy model.

11.2 Loading Topology output files

Here we load the binary adjacency matrix for one topology calculation and display it as an image

```
from matplotlib import pyplot as plt
import matplotlib.image as mpimg
import numpy as np

N1 = pynoddy.NoddyOutput(output_name)
AM= pynoddy.NoddyTopology(output_name)

am_name=root_name +'_uam.bin'
print am_name
print AM.maxlitho

image = np.empty((int(AM.maxlitho),int(AM.maxlitho)), np.uint8)

image.data[:] = open(am_name).read()
cmap=plt.get_cmap('Paired')
cmap.set_under('white')  # Color for values less than vmin

plt.imshow(image, interpolation="nearest", vmin=1, cmap=cmap)
plt.show()
```

```
maxlitho = 7

noddy_out_uam.bin
7
```
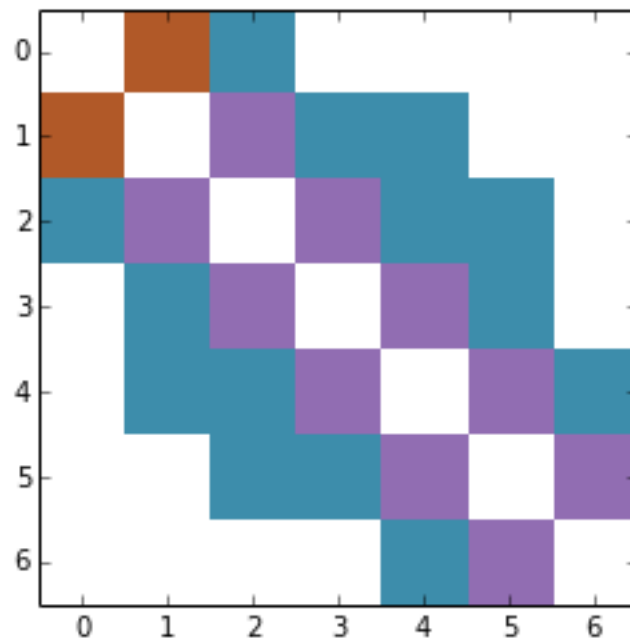
Fig. 11.1: png

PYNODDY MODULES, CLASSES AND FUNCTIONS

12.1 Basic modules (low-level access)

The modules in this section provide low-level access to the functionality in Noddy. Basically, these modules provide parsers for Noddy input and output files and class definitions for suitable Noddy elements.

12.1.1 Main module

Package initialization file for pynoddy

pynoddy.**compute_model**(*history*, *output_name*, ***kwds*)

Call Noddy and compute the history file

Arguments:

- *history* = string : filename of history file

- *output_name* = string : basename for output files

Optional Keywords:

- *sim_type* = 'BLOCK', 'GEOPHYSICS', 'SURFACES', 'BLOCK_GEOPHYS',

'TOPOLOGY', 'BLOCK_SURFACES', 'ALL': type of Noddy simulation (default: 'BLOCK')

- ***program_name* = string** [name of program] (default: noddy.exe or noddy, both checked)

- *verbose* = bool: verbose mode, print out information for debugging (default = False)

- *noddy_path* = path: location of Noddy executable (default: checks environment variable)

Returns: -Returns any text outputted by the noddy executable.

pynoddy.**compute_topology**(*rootname*, ***kwds*)

Call the topology executable to compute a models topology.

Arguments:

- *rootname* = string : rootname of the noddy model to calculate topology for

Optional Keywords:

- *ensure_discrete_volumes* = True if topological units are broken down into separate, spatially continuous volumes. Otherwise some topological units may represent two separate rock volumes (eg. if a folded unit has been truncated by an unconformity). Default is True, though this is a global variable (pynoddy.ensure_discrete_volumes) so it can be changed during runtime.

- *null_volume_threshold* = The smallest non-null volume. volumes smaller than this are ignored by the topology algorithm (as they represent pixelation artefacts). The default is 20 voxels, though this is a global variable and can be changed with pynoddy.null_volume_threshold.

- *topology_path* = path: location of executable for topology calculation

Returns -Returns any text outputted by the topology executable, including errors.

pynoddy.**which**(*program*)

12.1.2 History file parser: pynoddy.history

Noddy history file wrapper Created on 24/03/2014

@author: Florian Wellmann

class pynoddy.history.**NoddyHistory**(*history=None*, ***kwds*)
    Bases: object

    Class container for Noddy history files

    add_event(*event_type*, *event_options*, ***kwds*)
        Add an event type to history

        Arguments:

            • *event_type* = string : type of event, legal options to date are:

            'stratigraphy', 'fault', 'fold', 'unconformity' - *event_options* = list : required options to create event (event dependent)

        Optional keywords:

            • *event_num* = int : event number (default: implicitly defined with increasing counter)

    change_cube_size(*cube_size*, ***kwds*)
        Change the model cube size (isotropic)

        Arguments:

            • *cube_size* = float : new model cube size

    change_event_params(*changes_dict*)
        Change multiple event parameters according to settings in changes_dict

        Arguments:

            • *changes_dict* = dictionary : entries define relative changes for (multiple) parameters

        Per default, the values in the dictionary are added to the event parameters.

    copy_events()
        Create a copy of the current event state

    create_footer_from_template()
        Create model footer (with all settings) from template

    create_new_history()
        Methods to create a Noddy model

    determine_events(***kwds*)
        Determine events and save line numbers

        Note:

        Parsing of the history file is based on a fixed Noddy output order. If this is, for some reason (e.g. in a changed version of Noddy) not the case, then this parsing might fail!

        Optional Keywords:

            • verbose = True if this function is should write to the print bufffer, otherwise False. Default is False.

    determine_model_stratigraphy()
        Determine stratigraphy of entire model from all events

get_cube_size(***kwds*)
>   Determine cube size for model export **Optional Args**

>> -type: choose geology or geophysics cube size to return. Should be either 'Geology' (default) or 'Geophysics'

get_date_saved()
>   Determine the last savepoint of the file

get_drillhole_data(*x*, *y*, ***kwds*)
>   Get geology values along 1-D profile at position x,y with a 1 m resolution

>   The following steps are performed: 1. creates a copy of the entire object, 2. sets values of origin, extent and geology cube size, 3. saves model to a temporary file, 4. runs Noddy on that file 5. opens and analyses output 6. deletes temporary files

>   Note: this method only works if write access to current directory is enabled and noddy can be executed!

>   **Arguments:**

>> - *x* = float: x-position of drillhole

>> - *y* = float: y-position of drillhole

>   **Optional Arguments:**

>> - *z_min* = float : minimum depth of drillhole (default: model range)

>> - *z_max* = float : maximum depth of drillhole (default: model range)

>> - *resolution* = float : resolution along profile (default: 1 m)

get_ev_counter()
>   Event counter for implicit and continuous definition of events

get_event_param(*event_number*, *name*)
>   Returns the value of a given parameter for a given event.

>   **Arguments:**

>> - *event_number* = the event to get a parameter for (integer)

>> - *name* = the name of the parameter to retreive (string)

>>> **Returns**

>>> - Returns the value of the request parameter, or None if it does not exists.

get_event_params(*event_number*)
>   Returns the parameter dictionary for a given event.

>   **Arguments:**

>> - *event_number* = the event to get a parameter for (integer)

>>> **Returns**

>>> - Returns the parameter dictionary for the requested event

get_extent()
>   Get model extent and return and store in local variables

>   **Returns**: (extent_x, extent_y, extent_z)

get_filename()
>   Determine model filename from history file/ header

get_footer_lines()
>   Get the footer lines from self.history_lines

>   The footer contains everything below events (all settings, etc.)

---

get_info_string(***kwds*)
> Get model information as string

>> **Optional keywords:**

>>> • *events_only* = bool : only information on events

get_origin()
> Get coordinates of model origin and return and store in local variables

>> **Returns**: (origin_x, origin_y, origin_z)

info(***kwds*)
> Print out model information

>> **Optional keywords:**

>>> • *events_only* = bool : only information on events

load_history(*history*)
> Load Noddy history

>> **Arguments:**

>>> • *history* = string : Name of Noddy history file

load_history_from_url(*url*)
> Directly load a Noddy history from a URL

> This method is useful to load a model from the Structural Geophysics Atlas on the pages of the Virtual Explorer. See: http://tectonique.net/asg

>> **Arguments:**

>>> • *url* : url of history file

reorder_events(*reorder_dict*)
> Reorder events accoring to assignment in reorder_dict

>> **Arguments:**

>>> • *reorder_dict* = dict : for example {1 : 2, 2 : 3, 3 : 1}

set_event_params(*params_dict*)
> set multiple event parameters according to settings in params_dict

>> **Arguments:**

>>> • *params_dict* = dictionary : entries to set (multiple) parameters

set_extent(*extent_x*, *extent_y*, *extent_z*)
> Set model extent and update local variables

>> **Arguments:**

>>> • *extent_x* = float : extent in x-direction

>>> • *extent_y* = float : extent in y-direction

>>> • *extent_z* = float : extent in z-direction

set_origin(*origin_x*, *origin_y*, *origin_z*)
> Set coordinates of model origin and update local variables

>> **Arguments:**

>>> • *origin_x* = float : x-location of model origin

>>> • *origin_y* = float : y-location of model origin

>>> • *origin_z* = float : z-location of model origin

swap_events(*event_num_1*, *event_num_2*)
> Swap two geological events in the timeline

Arguments:

- *event_num_1/2* = int : number of events to be swapped ("order")

update_all_event_properties()
> Update properties of all events - in case changes were made

update_event_numbers()
> Update event numbers in 'Event #' line in noddy history file

write_history(*filename*)
> Write history to new file

Arguments:

- *filename* = string : filename of new history file

Hint: Just love it how easy it is to 'write history' with Noddy ;-)

12.1.3 Output file parser: pynoddy.output

Noddy output file analysis Created on 24/03/2014

@author: Florian Wellmann, Sam Thiele

class pynoddy.output.**NoddyGeophysics**(*output_name*)
> Bases: object

> Definition to read, analyse, and visualise calculated geophysical responses

> **read_gravity**()
> > Read calculated gravity response

> **read_magnetics**()
> > Read caluclated magnetic field response

class pynoddy.output.**NoddyOutput**(*output_name*)
> Bases: object

> Class definition for Noddy output analysis

> **compare_dimensions_to**(*other*)
> > Compare model dimensions to another model

> **determine_unit_volumes**()
> > Determine volumes of geological units in the discretized block model

> **export_to_vtk**(***kwds*)
> > Export model to VTK

> > Export the geology blocks to VTK for visualisation of the entire 3-D model in an external VTK viewer, e.g. Paraview.

> > ..Note:: Requires pyevtk, available for free on: https://github.com/firedrakeproject/firedrake/tree/master/python/evtk

> > **Optional keywords:**

> > - *vtk_filename* = string : filename of VTK file (default: output_name)

> > - *data* = np.array : data array to export to VKT (default: entire block model)

> **get_section_lines**(*direction='y'*, *position='center'*, ***kwds*)
> > Create and returns a list of lines representing a section block through the model

> > **Arguments:**

> > - *direction* = 'x', 'y', 'z' : coordinate direction of section plot (default: 'y')

- *position* = **int or 'center'** [cell position of section as integer value] or identifier (default: 'center')

Returns: A tuple of lists of dictionaries.... ie: ([dictionary of x coordinates, with lithology pairs as keys, separated by an underscore],

[dictionary of y coordinates, with lithology pairs as keys, separated by an underscore], [dictionary of z coordinates, with lithology pairs as keys, separated by an underscore], [dictionary of colours, with lithologies as keys])

For example: get_section_lines()[0]["1_2"] returns a list of all the x coordinates from the contact between lithology 1 and lithology 2. Note that the smaller lithology index always comes first in the code.

get_section_voxels (*direction='y'*, *position='center'*, ***kwds*)
Create and returns section block through the model

Arguments:

- *direction* = 'x', 'y', 'z' : coordinate direction of section plot (default: 'y')

- *position* = **int or 'center'** [cell position of section as integer value] or identifier (default: 'center')

Optional Keywords:

- *data* = np.array : data to plot, if different to block data itself

- *litho_filter* = a list of lithologies to draw. All others will be ignored.

get_surface_grid (*lithoID*, ***kwds*)
Returns a grid of lines that define a grid on the specified surface. Note that this cannot handle layers that are repeated in the z direction...

Arguments:

- *lithoID* **- the top surface of this lithology will be calculated. If a list is passed,** the top surface of each lithology in the list is calculated.

Keywords:

- *res* - the resolution to sample at. Default is 2 (ie. every second voxel is sampled).

Returns: a tuple containing lists of tuples of x, y and z coordinate dictionaries and colour dictionaries, one containing the east-west lines and one the north-south lines: ((x,y,z,c),(x,y,z,c)). THe dictionary keys are the lithoID's passed in the lithoID parameter.

load_geology ()
Load block geology ids from .g12 output file

load_model_info ()
Load information about model discretisation from .g00 file

plot_section (*direction='y'*, *position='center'*, ***kwds*)
Create a section block through the model

Arguments:

- *direction* = 'x', 'y', 'z' : coordinate direction of section plot (default: 'y')

- *position* = **int or 'center'** [cell position of section as integer value] or identifier (default: 'center')

Optional Keywords:

- *ax* = matplotlib.axis : append plot to axis (default: create new plot)

- *figsize* = (x,y) : matplotlib figsize

- *colorbar* = bool : plot colorbar (default: True)

- *colorbar_orientation* = **'horizontal' or 'vertical'** [orientation of colorbar] (default: 'vertical')

- *title* = string : plot title

- *savefig* = bool : save figure to file (default: show directly on screen)

- *cmap* = matplotlib.cmap : colormap (default: YlOrRd)

- *fig_filename* = string : figure filename

- *ve* = float : vertical exaggeration

- *layer_labels* = list of strings: labels for each unit in plot

- *layers_from* = noddy history file : get labels automatically from history file

- *data* = np.array : data to plot, if different to block data itself

- *litho_filter* = a list of lithologies to draw. All others will be ignored.

set_basename(*name*)
> Set model basename

class pynoddy.output.**NoddyTopology**(*noddy_model*, ***kwds*)
> Bases: object

> Definition to read, analyse, and visualise calculated voxel topology

> **calculate_difference**(*G2*, *data=False*)
> > Calculates the difference between this NoddyTopology and another NoddyTopology or networkX graph

> > **Arguments**

> > - *G2* = a valid NoddyTopology object or NetworkX graph that this topology is to be compared with

> > **Returns** A tuple containing: - The number of different edges - a list of these edges

> **calculate_overlap**(*G2*)
> > Calculates the overlap between this NoddyTopology and another NoddyTopology or networkX graph

> > **Arguments**

> > - *G2* = a valid NoddyTopology object or NetworkX graph that this topology is to be compared with

> > **Returns**

> > - The number of overlapping edges

> > - A list of these edges

> **static calculate_unique_topologies**(*topology_list*, ***kwds*)
> > Calculates the number of unique topologies in a list of NoddyTopologies

> > **Arguments:**

> > - *topology_list* = The list of NoddyTopologies to search through.

> > **Optional Keywords:**

> > - *output* = A File or list to write cumulative observed topologies distribution. Default is None (nothing written).

> > - *ids* = A list to write the unique topology id's for each topology in the provided topology_list (in that order). Default is None.

> > - *frequency* = A list to write frequency counts to.

> > **Returns:**

> > - Returns a list of unique topologies.

collapse_stratigraphy()
> Collapses all stratigraphic edges in this network to produce a network that only contains structurally bound rock volumes. Essentially this is a network built only with Topology codes and ignoring lithology

> **Returns**

>> • a new NoddyTopology object containing the collapsed graph. The original object is not modified.

collapse_structure(*verbose=False*)
> Collapses all topology codes down to the last (most recent) difference. Information regarding specific model topology is generalised, eg. lithology A has a fault and stratigrappic contact with B (regardless of how many different faults are involved).

> **Optional Arguments:**

>> • *verbose* = True if this function should write to the print buffer. Default is False.

> **Returns**

>> • a new NoddyTopology object containing the collapsed graph. The original object is not modified.

static combine_topologies(*topology_list*)
> Combines a list of topology networks into a weighted 'super-network'. This is designed for estimating the likelyhood of a given edge occuring using a series of networks generated in a Monte-Carlo type analysis.

> **Arguments**

>> • *topology_list* = A list of networkX graphs or NoddyTopology objects to build supernetwork from.

> **Returns**

>> • A NetworkX graph object containing all edges from the input graphs and weighted ('weight' parameter) according to their observed frequency.

draw_3d_network(***kwds*)
> Draws a 3D network using matplotlib.

> **Optional Keywords:**

>> • *show* = If True, the 3D network is displayed immediatly on-screen in an interactive matplotlib viewer. Default is True.

>> • *output* = If defined an image of the network is saved to this location.

>> • *node_size* = The size of the nodes. Default is 40.

>> • *geology* = a NoddyOutput object to draw with the network

>> • *res* = resolution to draw geology at. Default is 4 (ie 1/4 of all voxels are drawn)

>> • *horizons* = a list of geology surfaces to draw. Default is nothing (none drawn). Slow! See NoddyOutput.get_surface_grid for details.

>> • *sections* = draw geology sections. Default is True.

draw_adjacency_matrix(***kwds*)
> Draws an adjacency matrix representing this topology object.

> **Keywords:**

>> • *path* = The path to save this image to. If not provided, the image is drawn to the screen

>> • *dpi* = The resolution to save this image. Default is 300

>> • *size* = The size of the image to save (in inches). This value will be used as the width and the height

draw_difference_matrix(*G2*, ***kwds*)
>   Draws an adjacency matrix containing the difference between this topology and the provided topology

>   **Arguments:**

>   >   • *G2* = A different NoddyTopology or NetworkX Graph to compare to

>   **Optional Keywords:**

>   >   • *strat* = A dictionary linking node names to stratigraphic heights and names. Should be as follows { node_name : (height,name) }.

>   >   • *path* = The path to save this image to. If not provided, the image is drawn to the screen

>   >   • *dpi* = The resolution to save this image. Default is 300

>   >   • *size* = The size of the image to save (in inches). This value will be used as the width and the height

static **draw_graph_matrix**(*G*, ***kwds*)
>   Draws an adjacency matrix representing the specified graph object. Equivalent to NoddyTopology.draw_matrix_image() but for a networkX graph object.

>   **Keywords:**

>   >   • *strat* = A dictionary linking node names to stratigraphic heights and names. Should be as follows { node_name : (height,name) }.

>   >   • *path* = The path to save this image to. If not provided, the image is drawn to the screen

>   >   • *dpi* = The resolution to save this image. Default is 300

>   >   • *size* = The size of the image to save (in inches). This value will be used as the width and the height

draw_mayavi(***kwds*)
>   Draws this network with mayavi. This requires the Mayavi python library (mayavi.mlab)

>   **Optional Keywords:**

>   >   • *node_size* = The size of the nodes. Default is 40.

>   >   • *edge_thickness* = The thickness of the edges. Default is 4

>   >   • *show* = If true, the model is displayed in the mayavi viewer after exporting. Default is True

>   >   • *path* = A path to save the mayavi vtk file to after generating it.

static **draw_mayavi_graph**(*G*, ***kwds*)
>   Draws the provided network with mayavi. This requires the Mayavi python library (mayavi.mlab)

>   **Optional Keywords:**

>   >   • *node_size* = The size of the nodes. Default is 40.

>   >   • *edge_thickness* = The thickness of the edges. Default is 4

>   >   • *show* = If true, the model is displayed in the mayavi viewer after exporting. Default is True

>   >   • *path* = A path to save the mayavi vtk file to after generating it.

draw_network_hive(***kwds*)
>   Draws a network hive plot (see https://github.com/ericmjl/hiveplot). The axes of the hive are: node lithology, edge age & edge area.

>   ie. the top axis lists the nodes in stratigraphic order. The second axis lists edges in structural age & thrid axis lists edges by surface area.

>   Nodes are joined to edge-nodes by lines on the graph if they are topologically linked (ie. if an edge has that node as an end point).

>   **Optional Keywords:**

- *path* = the path to save this figure

- *dpi* = the resolution of the figure

- *bg* = the background color. Default is black.

- *axes* = The color of the axes and labels.

draw_network_image (*outputname=''*, ***kwds*)
Draws a network diagram of this NoddyTopology to the specified image

Arguments:

- *outputname* = the path of the image being written. If left as '' the image is written to the same directory as the basename.

Optional Keywords:

- *dimension* = '2D' for a 2D network diagram or '3D' for a 3D network diagram. Default is '2D'.

- *axis* = the axis to view on for 3D network diagrams

- *perspective* = True to use perspective projection, or False for orthographic projection. Default is False.

- *node_size* = The size that nodes are drawn. Default is 1500.

- *layout* = The layout algorithm used in 2D. Options are 'spring_layout' (default), 'shell_layout', 'circular_layout' and 'spectral_layout'.

- *verbose* = True if this function is allowed to write to the print buffer, otherwise false. Default is False.

filter_node_volumes (*min_volume=50*)
Removes all nodes with volumes less than the specified size

Arguments:

- *min_volume* = the threshold volume. Nodes with smaller volumes are deleted.

Returns

- returns the number of deleted nodes

find_first_match (*known*)
Identical to is_unique, except that the index of the first match is returned if this matches, otherwise -1 is returned.

Arguments: *-known* = a list of valid NoddyTopology objects or NetworkX graphs to compare with.

Returns:

- Returns the index of the first matching topology object, or -1

find_matching (*known*)
Finds the first matching NoddyTopology (or NetworkX graph) in the specified list

Arguments: *-known* = a list of valid NoddyTopology objects or NetworkX graphs to compare with.

Returns:

- Returns the first matching object (jaccard coefficient = 1), or otherwise None

is_unique (*known*)
Returns True if the topology of this model is different (ie. forms a different network) to a list of models.

Arguments: *-known* = a list of valid NoddyTopology objects or NetworkX graphs to compare with.

Returns:

- Returns true if this topology is unique, otherwise false

jaccard_coefficient(*G2*)
> Calculates the Jaccard Coefficient (ratio between the intersection & union) of the graph representing this NOddyTopology and G2.

> **Arguments**
>> • *G2* = a valid NoddyTopology object or NetworkX graph that this topology is to be compared with

> **Returns**
>> • The jaccard_coefficient

loadNetwork()
> Loads the topology network into a NetworkX datastructure

read_adjacency_matrix()
> *Depreciated* Reads max number of lithologies aross all models

read_properties()

write_summary_file(*path*, *append=True*)
> Writes summary information about this network to a file

> **Optional Arguments**
>> • *append* = True if summary information should be appended to the file. If so the file is written as a csv spreadsheet. Default is true. If False is passed, a single, detailed summary is written for this network.

12.1.4 Additional useful classes

pynoddy.events

Module for reading and manipulating geological events Created on Mar 26, 2014

@author: Florian Wellmann

class pynoddy.events.**Dyke**(***kwds*)
> Bases: *pynoddy.events.Event*

> Dyke event

> **parse_event_lines**(*lines*)
>> Read specific event lines from history file **Arguments**:

>>> •*lines* = list of lines : lines with event information (as stored in .his file)

class pynoddy.events.**Event**(***kwds*)
> Bases: object

> Main class container for geological events

> Include here all elements that events have in common (position, etc. - possibly even things like color and other aspects that are defined in the history... Parse for equal settings and include here!)

> **set_event_lines**(*lines*)
>> Explicitly define event lines

> **set_event_number**(*num*)
>> Set number in 'Event #' line to num

> **update_properties**(***kwds*)
>> Update properties (required if self.properties assignment changed!)

class pynoddy.events.**Fault**(***kwds*)
> Bases: *pynoddy.events.Event*

> Fault event

---

parse_event_lines(*lines*)
    Read specific event lines from history file

    Arguments:

    • *lines* = list of lines : lines with event information (as stored in .his file)

class pynoddy.events.**Fold**(***kwds*)
    Bases: *pynoddy.events.Event*

    Folding event

    parse_event_lines(*lines*)
        Read specific event lines from history file

        Arguments:

        • *lines* = list of lines : lines with event information (as stored in .his file)

class pynoddy.events.**Plug**(***kwds*)
    Bases: *pynoddy.events.Event*

    Plug event

    parse_event_lines(*lines*)
        Read specific event lines from history file **Arguments**:

        •*lines* = list of lines : lines with event information (as stored in .his file)

class pynoddy.events.**Shear**(***kwds*)
    Bases: *pynoddy.events.Event*

    Shear zone event

    parse_event_lines(*lines*)
        Read specific event lines from history file

        Arguments:

        • *lines* = list of lines : lines with event information (as stored in .his file)

class pynoddy.events.**Strain**(***kwds*)
    Bases: *pynoddy.events.Event*

    Strain event

    parse_event_lines(*lines*)
        Read specific event lines from history file **Arguments**:

        •*lines* = list of lines : lines with event information (as stored in .his file)

class pynoddy.events.**Stratigraphy**(***kwds*)
    Bases: *pynoddy.events.Event*

    Sedimentary pile with defined stratigraphy

    parse_event_lines(*lines*)
        Read specific event lines from history file

        Arguments:

        • *lines* = list of lines : lines with event information (as stored in .his file)

class pynoddy.events.**Tilt**(***kwds*)
    Bases: *pynoddy.events.Event*

    Tilt event

    parse_event_lines(*lines*)
        Read specific event lines from history file

        Arguments:

- *lines* = list of lines : lines with event information (as stored in .his file)

class pynoddy.events.**Unconformity**(***kwds*)
Bases: *pynoddy.events.Event*

Unconformity event

change_height(*val*)
Change the vertical position (i.e. height) of the entire stratigraphic pile above the unconformity

---

Note: This is not identical to changing only the 'Z' property as the height of all layers has to be adjusted for (geological) consistency

---

Arguments:

- *val* = float : value added to current z-values

parse_event_lines(*lines*)
Read specific event lines from history file

Arguments:

- *lines* = list of lines : lines with event information (as stored in .his file)

12.2 Modules for Kinematic experiments

The modules described in this section are designed to provide a high-level access to the kinematic modelling functionality in Noddy. The modules encapsulate the required aspects of complete experiments, including input file generation, adaptation of parameters, random number generation, model computation, and postprocessing.

12.2.1 Base classes for pynoddy experiments

The base class for any type of experiments is defined in the pynoddy.experiment module. Base class from which PyNoddy experiments should inherit.

Much basic functionality (random perturbation, plotting etc. is defined here).

Thought: perhaps drawing functions etc. should be moved into NoddyOutput class?

@author: flohorovicic, samthiele

class pynoddy.experiment.**Experiment**(*history=None*, ***kwds*)
Bases: *pynoddy.history.NoddyHistory*, *pynoddy.output.NoddyOutput*

Noddy experiment container, inheriting from both noddy history and output methods

export_to_vtk(***kwds*)
Export model to VTK

Export the geology blocks to VTK for visualisation of the entire 3-D model in an external VTK viewer, e.g. Paraview.

..Note:: Requires pyevtk, available for free on: https://github.com/firedrakeproject/firedrake/tree/master/python/evtk

Optional keywords:

- *vtk_filename* = string : filename of VTK file (default: output_name)

- *data* = np.array : data array to export to VKT (default: entire block model)

- *recompute* = bool : recompute the block model (default: True)

- *model_type* = 'current', 'base' : model type (base "freezed" model can be plotted for comparison)

..Note:: If data is defined, the model is not recomputed and the data from this array is plotted

freeze (***kwds*)
> Freeze the current model state: store the event settings for later comparison

get_sampling_line_data (*xyz_from*, *xyz_to*)
> Get computed model along a line, for example as a drillhole position

> **Arguments:**

>> • *xyz_from* = [x, y, z] : list of float values for starting position

>> • *xyz_to* = [x, y, z] : list of float values for starting position

get_section (*direction='y'*, *position='center'*, ***kwds*)
> Get geological section of the model (re-computed at required resolution) as noddy object

> **Arguments:**

>> • *direction* = 'x', 'y', 'z' : coordinate direction of section plot (default: 'y')

>> • **position = int or 'center'** [cell position of section as integer value] or identifier (default: 'center')

> **Optional arguments:**

>> • *resolution* = float : set resolution for section (default: self.cube_size)

>> • *model_type* = 'current', 'base' : model type (base "freezed" model can be plotted for comparison)

>> • *compute_output* = bool : provide output from command line call (default: True)

get_up_to_date ()
> Get model state

is_up_to_date
> Model state

load_parameter_file (*filename*, ***kwds*)
> Load parameter statistics from external csv file

> The csv file should contain a header row with the relevant keywords identifying columns. In order to be read in correctly, the header should contain the labels:

>> •'event' : event id

>> •'parameter' : Noddy parameter ('Dip', 'Dip Direction', etc.)

>> •'mean' : mean parameter value

>> •'type' = 'normal', 'vonmises' or 'uniform'.

> In addition, it is necessary to define PDF type and parameters. For now, the following settings are supported: - '+-' = Defines the 2.5th and 97.5th percentiles of the distribution,

>> similar to a 95% confidence interval.

>> •'stdev' = standard deviation. Only works if type='normal'.

>> •'min' = The minimum value of a uniform distribution (if type='uniform')

>> •'max' = The maximum value of a uniform distribution (if type='uniform')

> **Arguments:**

>> • *filename* = string : filename

> **Optional arguments:**

>> • *delim* = string : delimiter (default: ',' or ';', both checked)

plot_section(*direction='y'*, *position='center'*, ***kwds*)

    Extended version of plot_section method from pynoddy.output class

    Arguments:

- *direction* = 'x', 'y', 'z' : coordinate direction of section plot (default: 'y')

- *position* **= int or 'center'** [cell position of section as integer value] or identifier (default: 'center')

    Optional Keywords:

- *ax* = matplotlib.axis : append plot to axis (default: create new plot)

- *figsize* = (x,y) : matplotlib figsize

- *colorbar* = bool : plot colorbar (default: True)

- *colorbar_orientation* **= 'horizontal' or 'vertical'** [orientation of colorbar] (default: 'vertical')

- *title* = string : plot title

- *savefig* = bool : save figure to file (default: show directly on screen)

- *cmap* = matplotlib.cmap : colormap (default: YlOrRd)

- *fig_filename* = string : figure filename

- *ve* = float : vertical exaggeration

- *layer_labels* = list of strings: labels for each unit in plot

- *layers_from* = noddy history file : get labels automatically from history file

- *resolution* = float : set resolution for section (default: self.cube_size)

- *model_type* = 'current', 'base' : model type (base "freezed" model can be plotted for comparison)

- *data* = np.array : data to plot, if different to block data itself

random_draw(***kwds*)

    Perform a random draw for parameter distributions as defined, and calculate model

    This method is based on the model "base-state", and not the current state (as opposed to the self.random_perturbation() method).

    Optional Keywords:

- *verbose* = bool: print out parameter changes as they happen (default: False)

- *store_params* = bool : store random parameter set (default: True)

random_perturbation(***kwds*)

    Perform a random perturbation of the model according to parameter statistics defined in self.param_stats.

    Note that by default, this function is identical to random_draw. If model_type is set to 'current', then parameters are varied according using the *current values* as distribution means - this allows 'random walk' away from the initial model state, which is usually not desired.

    Optional arguments:

- *store_params* = bool : store random parameter set (default: True)

- *verbose* = bool: print out parameter changes as they happen (default: False)

- *model_type* **= 'base', 'current'** [perturb on basis of current model,] or use base model (default: 'base' model)

reset_base()

    Set events back to base model (stored in self.base_events)

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reset_random_seed ()
> Reset random seed to defined value (stored in self.seed, set with self.set_random_seed)

set_parameter_statistics (*param_stats*)
> Define parameter statistics for uncertainty simulation and sensitivity analysis

> param_stats = list : list with relevant statistics defined for event parameters list is organised as: param_stats[event_id][parameter_name][stats_type] = value

> Example: param_stats[2]["Dip"]["min"] = 200.

> **Possible statistics are:**
>> • min = float : minimum bound
>>
>> • max = float : maximum bound
>>
>> • type = 'normal', 'uniform' : distribution type
>>
>> • stdev = float : standard deviation (if normal distribution)

set_random_seed (*random_seed*)
> Set random seed for reproducible experiments

> **Arguments:**
>> • *random_seed* = int (or array-like) : define seed

set_up_to_date ()
> Set boolean variable for valid object

shuffle_event_order (*event_ids*)
> Randomly shuffle order of events

> **Arguments:**
>> • *event_ids* = [list of event ids] : event ids to be randomly shuffeled

update ()
> Update model computation

write_parameter_changes (*filepath*)

12.2.2 MonteCarlo class

This class provides the basic functionality to perform MonteCarlo error propagation experiments with Noddy.

12.2.3 SensitivityAnalysis class

p