



pynoddy Documentation

Release 1.0

Florian Wellmann, Sam Thiele

Aug 26, 2017

1	pynoddy	3
1.1	What is pynoddy	3
1.2	What is Noddy?	3
1.3	Installation	3
1.4	Installation of the pynoddy package	3
1.5	Installation of Noddy	4
1.6	Using a pre-compiled version of Noddy	4
1.7	Compiling Noddy from source files (recommended installation)	4
1.8	Placing the executable noddy in the Path	5
1.9	Noddy executable and GUI for Windows	5
1.10	Testing the installation	5
1.11	Testing noddy	5
1.12	Testing pynoddy	6
1.13	How to get started	6
1.14	Tutorial Jupyter notebooks	6
1.15	The Atlas of Strutural Geophysics	6
1.16	Documentation	6
1.17	Technical Notes	7
1.18	Dependencies	7
1.19	3-D Visualisation	7
1.20	References	7
2	pynoddy.noddy module	9
3	Simulation of a Noddy history and visualisation of output	11
3.1	Compute the model	11
3.2	Loading Noddy output files	12
3.3	Plotting sections through the model	12
3.4	Export model to VTK	13
4	Change Noddy input file and recompute model	15
4.1	Get basic information on the model	16
4.2	Change model cube size and recompute model	17
4.3	Estimating computation time for a high-resolution model	18
4.4	Simple convergence study	21
5	Geological events in pynoddy: organisation and adpatiation	23
5.1	Loading events from a Noddy history	23
5.2	Changing aspects of geological events	25
5.3	Changing the order of geological events	25
5.4	Determining the stratigraphic difference between two models	27

6	Creating a model from scratch	29
6.1	Defining a stratigraphy	29
6.2	Add a fault event	30
6.3	Complete Model Set-up	32
7	Read and Visualise Geophysical Potential-Fields	35
7.1	Read history file from Virtual Explorer	35
7.2	Visualise calculated geophysical fields	37
7.3	Change history and compare gravity	38
7.4	Figure with all results	42
8	Reproducible Experiments with pynoddy	45
8.1	Defining an experiment	45
8.2	Loading an example model from the Atlas of Structural Geophysics	46
9	Gippsland Basin Uncertainty Study	51
9.1	The Gippsland Basin Model	51
9.2	Generate randomised model realisations	52
9.3	Exporting results to VTK for visualisation	53
10	Sensitivity Analysis	55
10.1	Theory: local sensitivity analysis	55
10.2	Defining the responses	55
10.3	Setting up the base model	56
10.4	Define parameter uncertainties	57
10.5	Calculate total stratigraphic distance	58
10.6	Function to modify parameters	58
10.7	Full sensitivity analysis	59
11	Simulation of a Noddy history and analysis of its voxel topology	63
11.1	Compute the model	63
11.2	Loading Topology output files	64
12	Fault shapes	67
13	Pynoddy modules, classes and functions	69
13.1	Basic modules (low-level access)	69
13.2	Modules for Kinematic experiments	69

Contents:

Contents

- *pynoddy*
 - *What is pynoddy*
 - *What is Noddy?*
 - *Installation*
 - *Installation of the pynoddy package*
 - *Installation of Noddy*
 - *Using a pre-compiled version of Noddy*
 - *Compiling Noddy from source files (recommended installation)*
 - *Placing the executable noddy in the Path*
 - *Noddy executable and GUI for Windows*
 - *Testing the installation*
 - *Testing noddy*
 - *Testing pynoddy*
 - *How to get started*
 - *Tutorial Jupyter notebooks*
 - *The Atlas of Strutural Geophysics*
 - *Documentation*
 - *Technical Notes*
 - *Dependencies*
 - *3-D Visualisation*
 - *References*

What is pynoddy

`pynoddy` is a python package to write, change, and analyse kinematic geological modelling simulations. It provides methods to define, load, modify, and save 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.

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:

`Noddy` has been used to generate models for teaching and interpretation purposes, but also for scientific studies (e.g. [3]).

Installation

Installation of the pynoddy package

A successful installation of `pynoddy` requires two steps:

1. An installation of the python modules in the package `pynoddy`
2. The existence of an executable `Noddy (.exe)` program

Installation of the first part is straight-forward:

For the best (and most complete) installation, we suggest to clone the pynoddy repository on:

<https://github.com/flohorovicic/pynoddy>

To install pynoddy simply run:

```
python setup.py install
```

sufficient privileges are required (i.e. run in `sudo` with MacOSX/ Linux and set permissions on Windows)

The pynoddy packages themselves can also be installed directly from the Python Package Index (pypi.org) via `pip`:

```
pip install pynoddy
```

A Windows installer is also available on the Pypi page:

<https://pypi.python.org/pypi/pynoddy/>

Installation of Noddy

Noddy is a command line program, written in C, that performs the kinematic simulation itself. The program compilation is platform dependent, and therefore several ways for installation are possible (see below information for specific platforms).

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` or would like to add new one, see below for more information.

Compiling Noddy from source files (recommended installation)

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.

Placing the executable 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.

Noddy executable and GUI for Windows

The original graphical user interface for Noddy 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.

Testing the installation

Testing noddy

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

```
> 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. If this is not the case, please check if it is correctly placed in the path (see above).

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!**

How to get started

Tutorial Jupyter 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`.

The Atlas of Strutural Geophysics

The Atlas of Structural Geophysics contains a collection of structural models, together with their expression as geophysical potential fields (gravity and magnetics), with a focus on guiding the interpretation of observed features in potential-field maps.

The atlas is currently available on:

<http://tectonique.net/asg>

The structural models are created with Noddy and the history files can be downloaded from the atlas. Models from this Atlas can directly be loaded with `pynoddy`. See example notebooks and documentation for more details.

Documentation

An updated version of the documentation is available within the `pynoddy` repository (`pynoddy/docs`).

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

<http://pynoddy.readthedocs.org>

Technical Notes

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.

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/>

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!

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](http://dx.doi.org/10.1016/S1874-561X(96)80027-7).
- [3] Armit, R. J., Betts, P. G., Schaefer, B. F., & Ailleres, L. (2012). Constraints on long-lived Mesoproterozoic and Palaeozoic deformational events and crustal architecture in the northern Mount Painter Province, Australia. Gondwana Research, 22(1), 207–226. <http://doi.org/10.1016/j.gr.2011.11.003>

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:

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`.

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

```
%matplotlib inline
```

```
# 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 correctly below
repo_path = os.path.realpath('../..')
```

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:

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

# Path to example 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.

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 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:

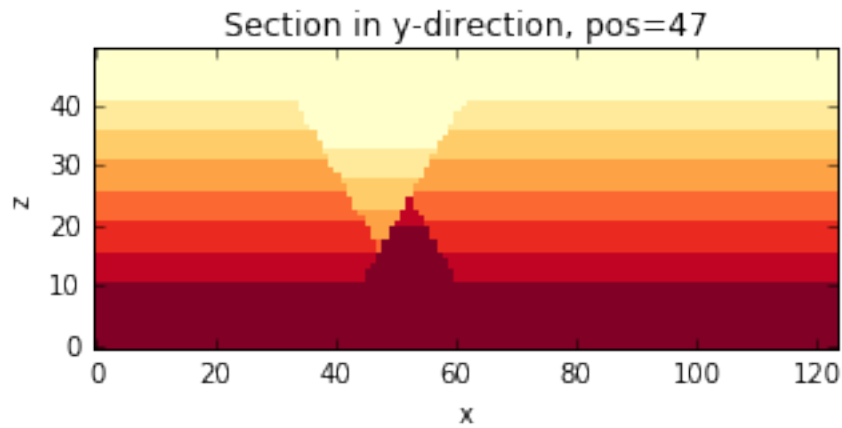
```
print("The model has an extent of %.0f m in x-direction, with %d cells of width %.
↪0f m" %
      (N1.extent_x, N1.nx, N1.delx))
```

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

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))
```

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.

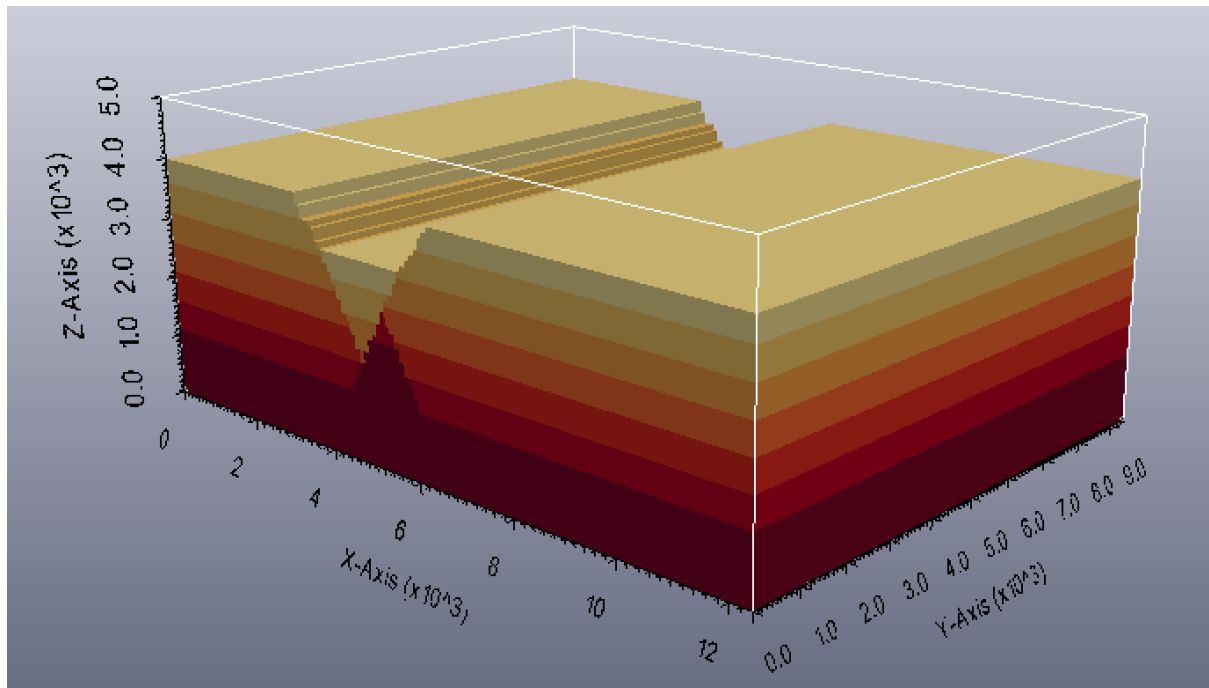


Fig. 3.1: 3-D Visualisation generated with Paraview (top layer transparent)

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.

```
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
```

```
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:

```
# 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!

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:

```
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:

```
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:

```
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}
```

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:

```
# 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_cubsize.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:

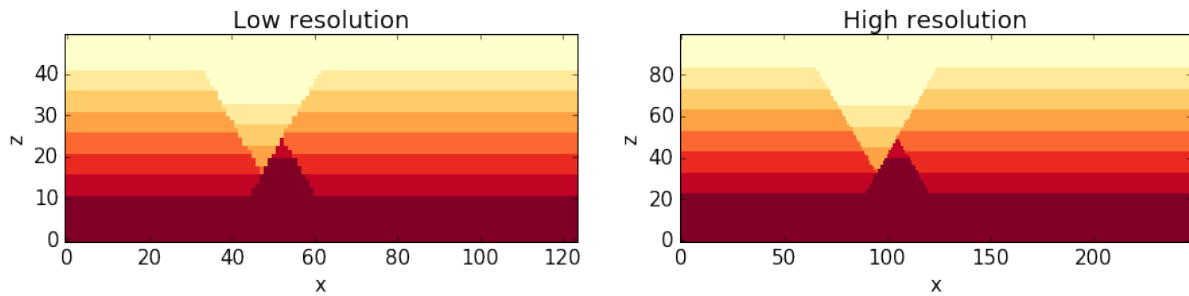
```
print("Model 1 contains a total of %7d cells with a blocksize %.0f m" %
      (NO1.n_total, NO1.delx))
print("Model 2 contains a total of %7d cells with a blocksize %.0f m" %
      (NO2.n_total, NO2.delx))
```

```
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()
```



Note: the following two subsections contain some slightly advanced examples on how to use the possibility to adjust cell sizes through scripts directly to automate 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.

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 significantly longer than the low-resolution model. In a practical case, this can be very important.

```
# We use here simply the time() function to evaluate the simulation 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 evaluate 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)
```

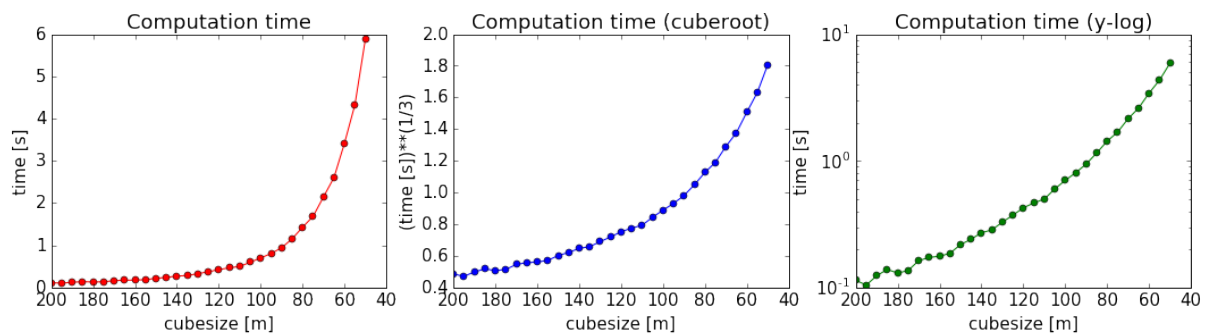
```
# create plot
fig = plt.figure(figsize=(18,4))
ax1 = fig.add_subplot(131)
ax2 = fig.add_subplot(132)
ax3 = fig.add_subplot(133)

ax1.plot(cube_sizes, np.array(times), 'ro-')
ax1.set_xlabel('cubeseize [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('cubeseize [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('cubeseize [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 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`:

```
# 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])
```

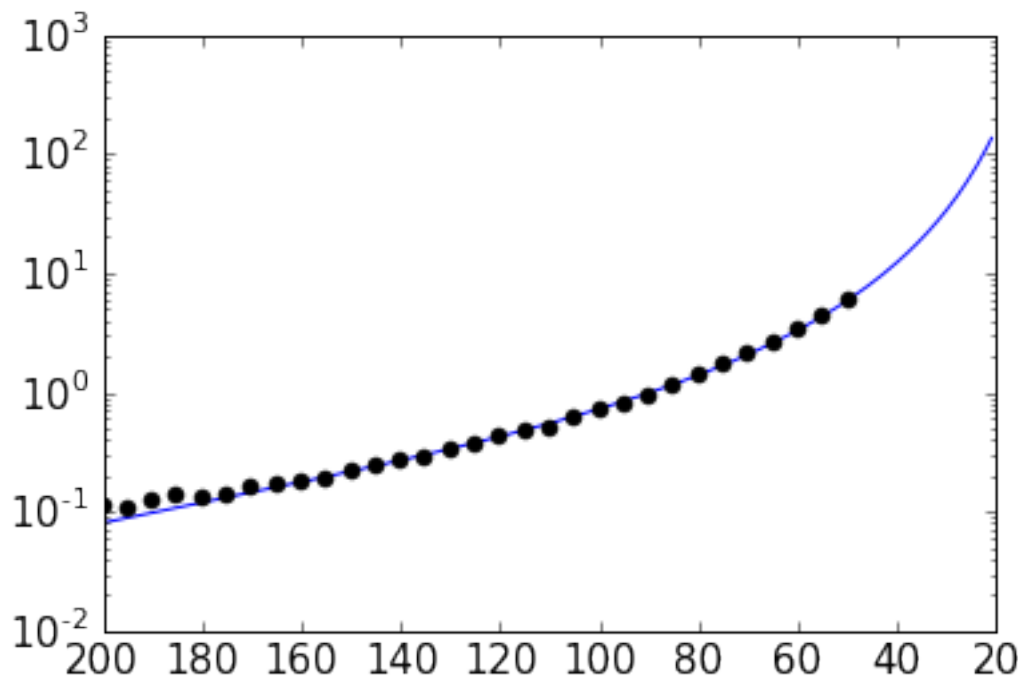
Interesting, it looks like Noody scales with something like:

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

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...

```
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:

```
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:

```
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()
time_comp = end_time - start_time

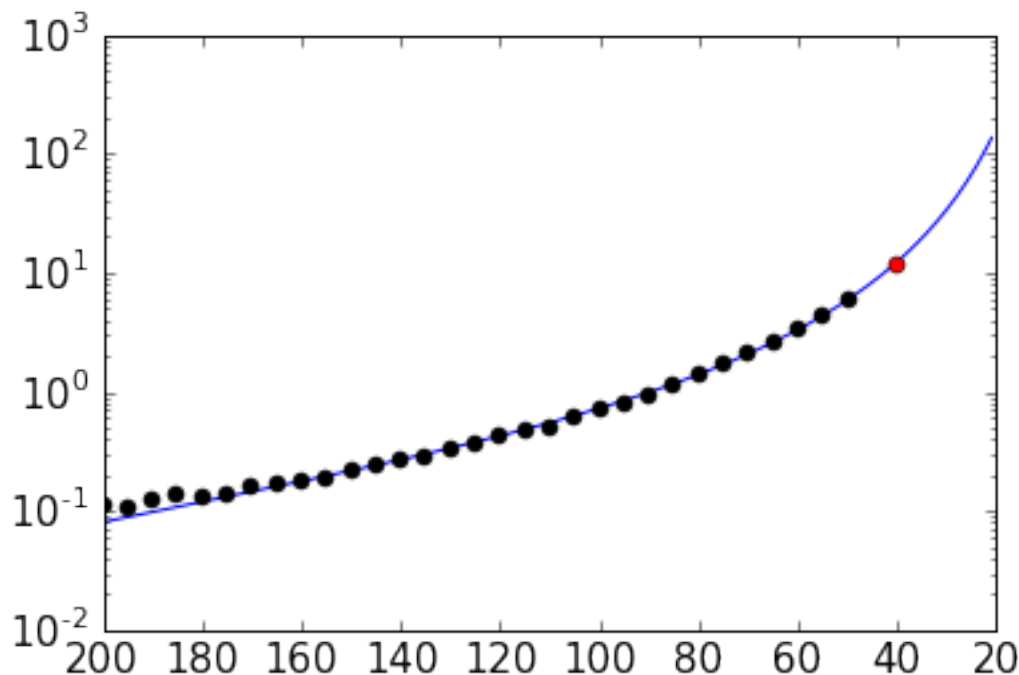
print("Actual computation time for a cube size of %d m: %.1f seconds" % (cube_size,
    ↪time_comp))
```


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 exercise 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)!

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 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 include 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:

```
# 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)
```

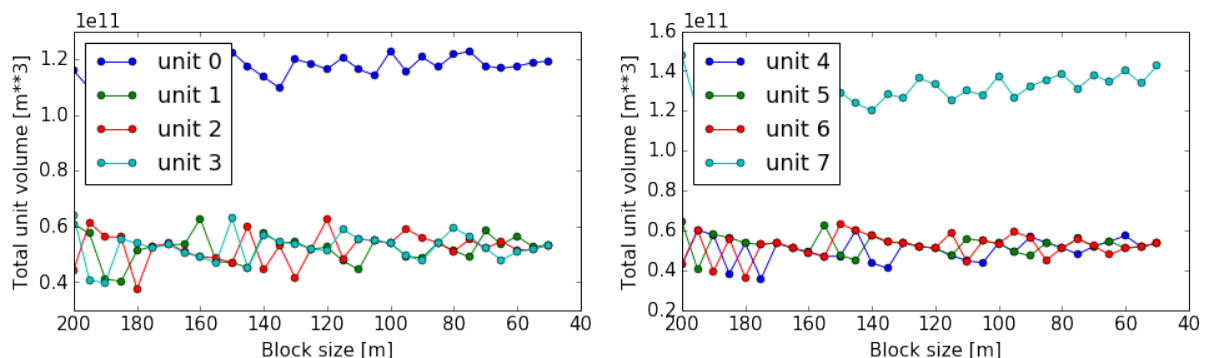
```
all_volumes = np.array(all_volumes)
fig = plt.figure(figsize=(16,4))
ax1 = fig.add_subplot(121)
ax2 = fig.add_subplot(122)

# 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>
```



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.

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

```
%matplotlib inline
```

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:

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

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

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

```
# Path to example 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}
```

Changing aspects of geological events

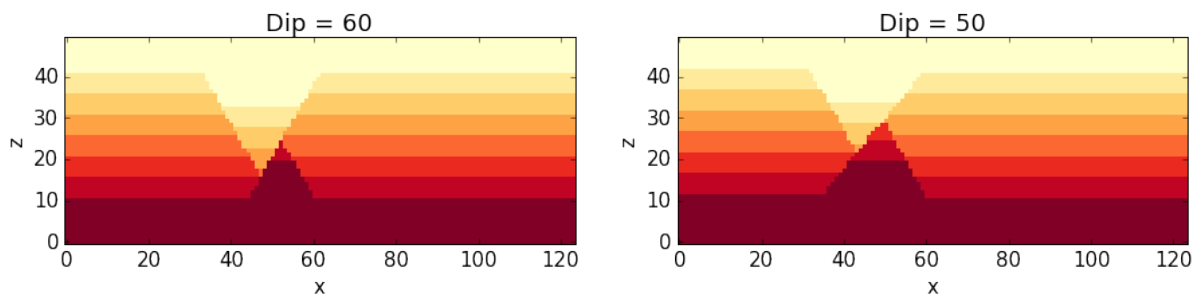
So what we now want to do, of course, is to change aspects of these events and to evaluate the effect on the resulting geological model. Parameters can directly be updated in the properties dictionary:

```
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=True, fig_filename="tmp.eps")
NO2.plot_section('y', position=1, ax = ax2, colorbar=False, title="Dip = %.0f" %
↳dip_new)
plt.show()
```



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 reflected in the events order now:
print H1.events[2].name
print H1.events[3].name
```

```
Fault1
Fault2
```

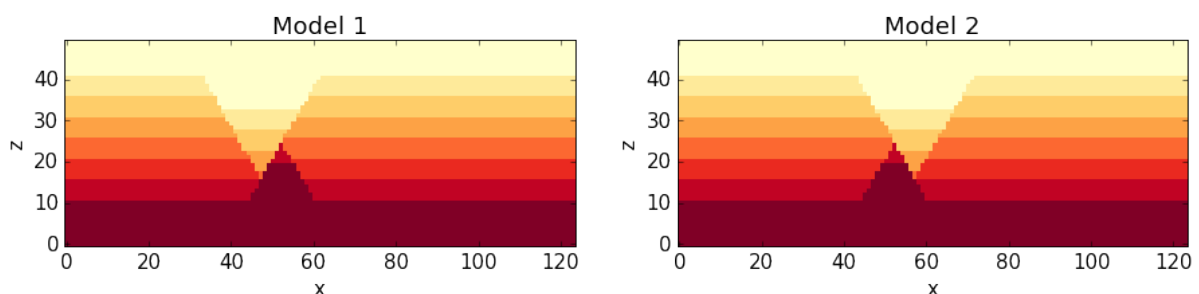
Now let's create a new history file and evaluate the effect of the changed order in a cross section view:

```
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()
```



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.

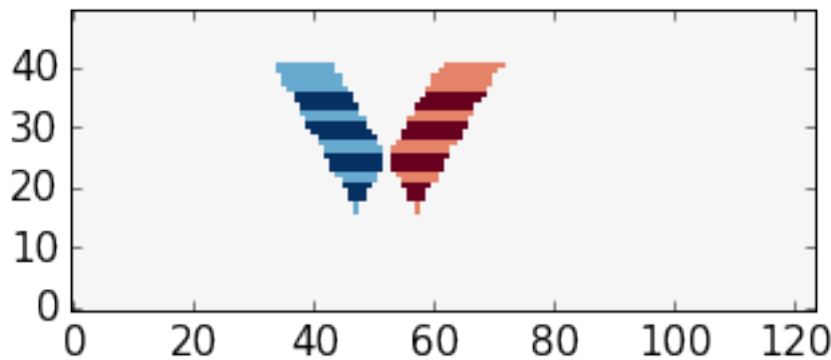
The geology data is stored in the `NoddyOutput.block` attribute. To evaluate the difference between two models, we can therefore simply compute:

```
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 exercise :-). Future versions of pynoddy might provide an automatic implementation for this step...)

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 calulated difference field:

```
NO1.export_to_vtk(vtk_filename = "model_diff", data = diff)
```

A 3-D view of the difference plot is presented below.

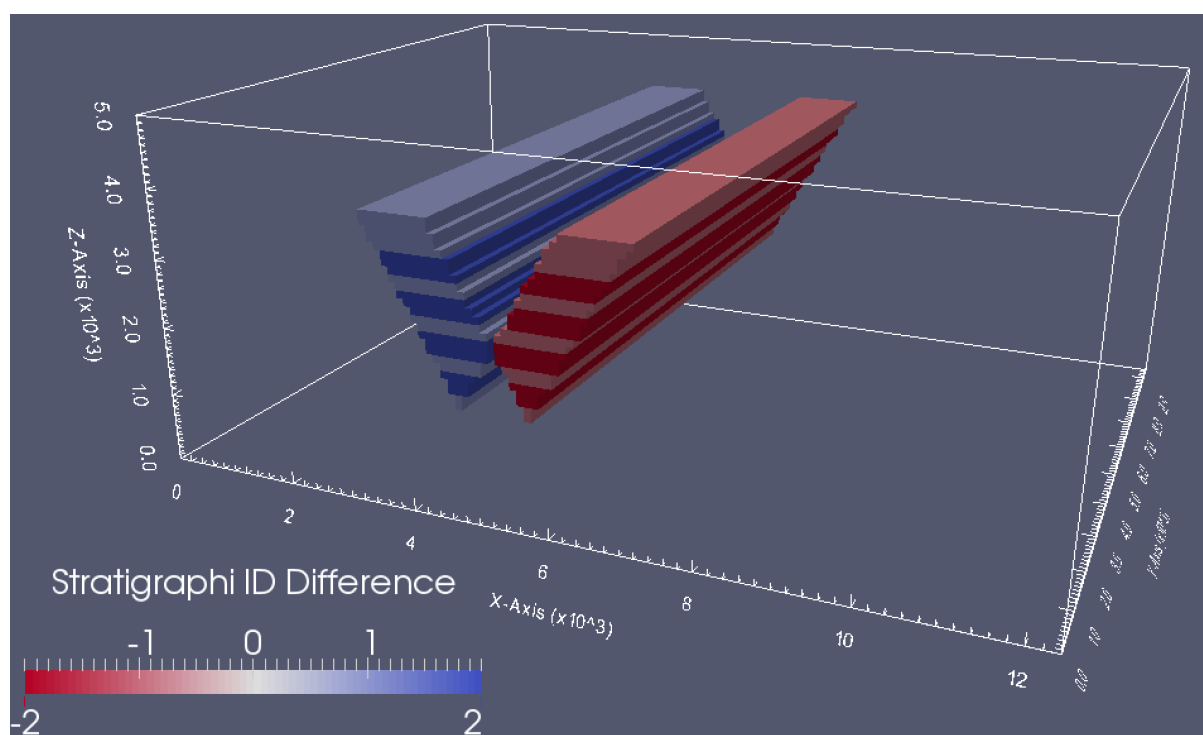


Fig. 5.1: 3-D visualisation of stratigraphic id difference

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 examples are shown in the following.

```
from matplotlib import rc_params
```

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

```
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 correctly below
repo_path = os.path.realpath('../..')
import pynoddy.history
```

```
%matplotlib inline
```

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

Defining a stratigraphy

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

```
# Combined: model generation and output vis to test:
history = "simple_model.his"
output_name = "simple_out"
```

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

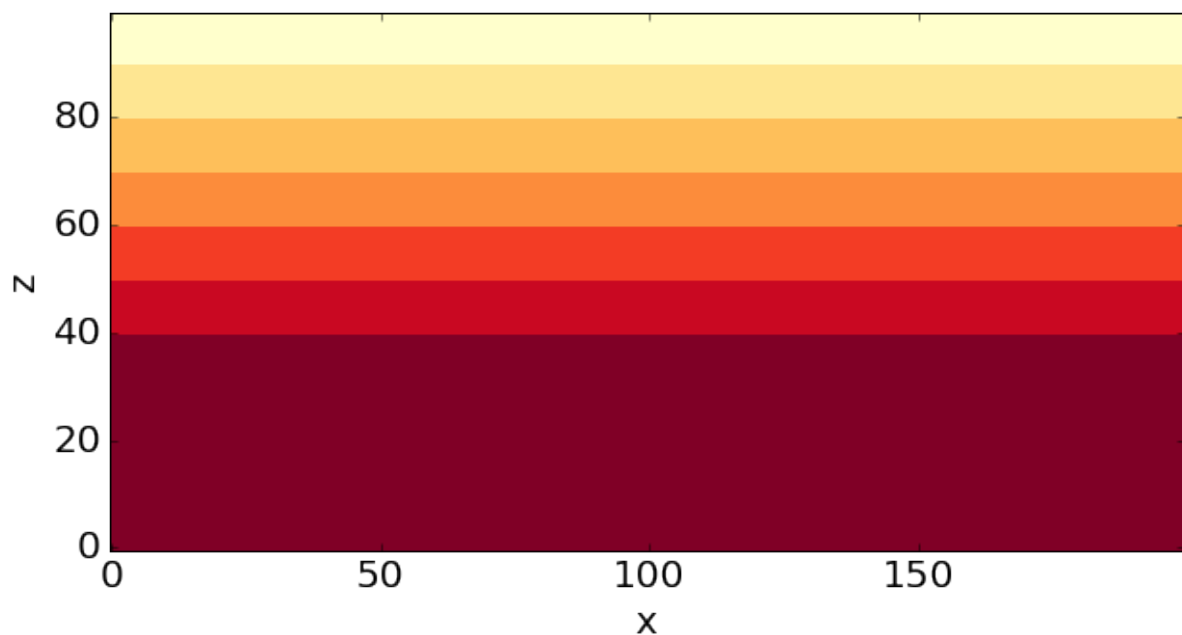
# create pynoddy object
nm = pynoddy.history.NoddyHistory()
# add stratigraphy
strati_options = {'num_layers' : 8,
                  'layer_names' : ['layer 1', 'layer 2', 'layer 3',
                                   'layer 4', 'layer 5', 'layer 6',
                                   'layer 7', 'layer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



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 6', 'layer 7', 'layer 8'],
                  '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
```

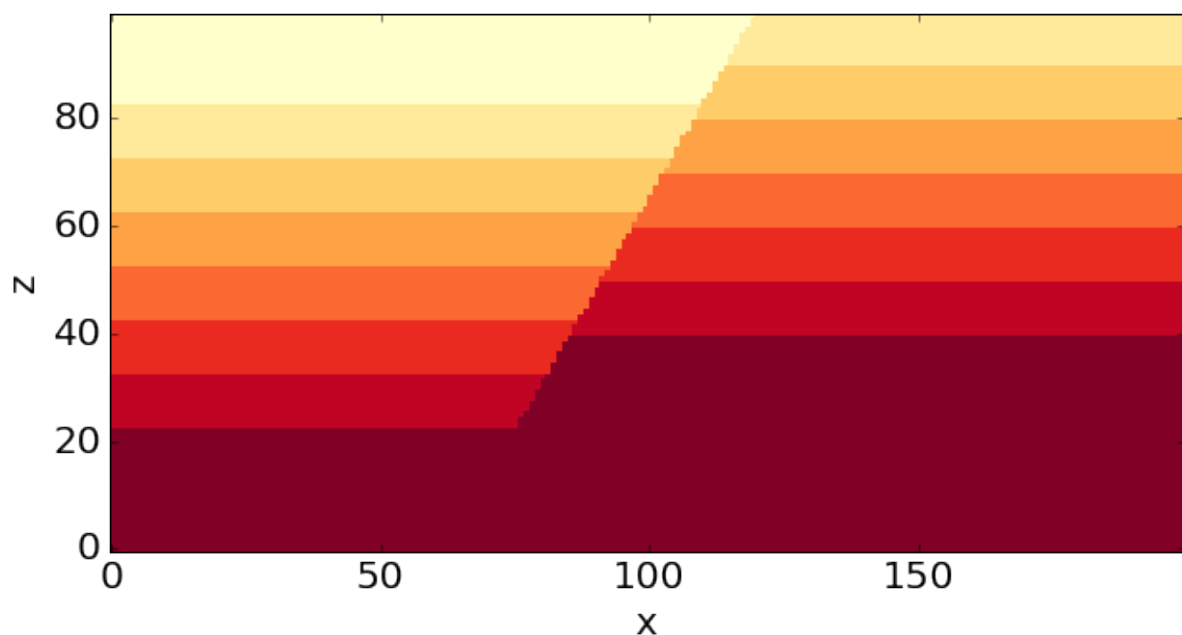
```
{1: <pynoddy.events.Stratigraphy at 0x1073fc590>,
 2: <pynoddy.events.Fault at 0x107565fd0>}
```

```
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")
```



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

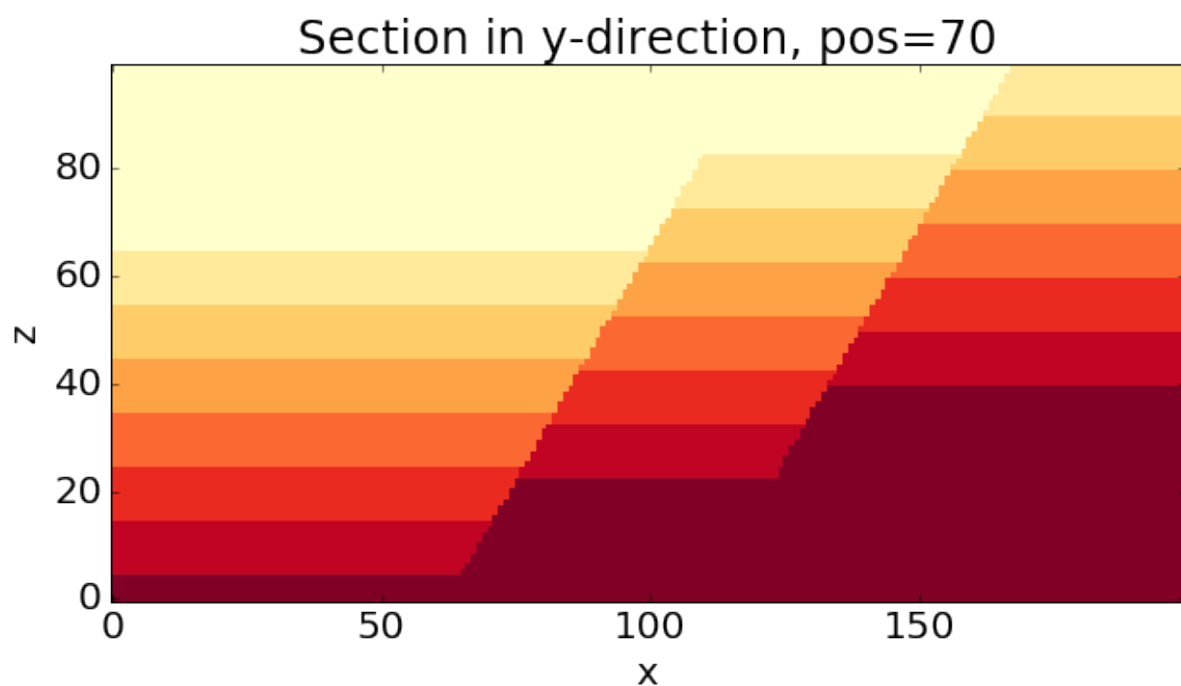
nm.add_event('fault', fault_options)
```

```
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)
```



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

```
nm1.get_extent()
```

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

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 )

# 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)

```

```

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

```

```

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

```

```

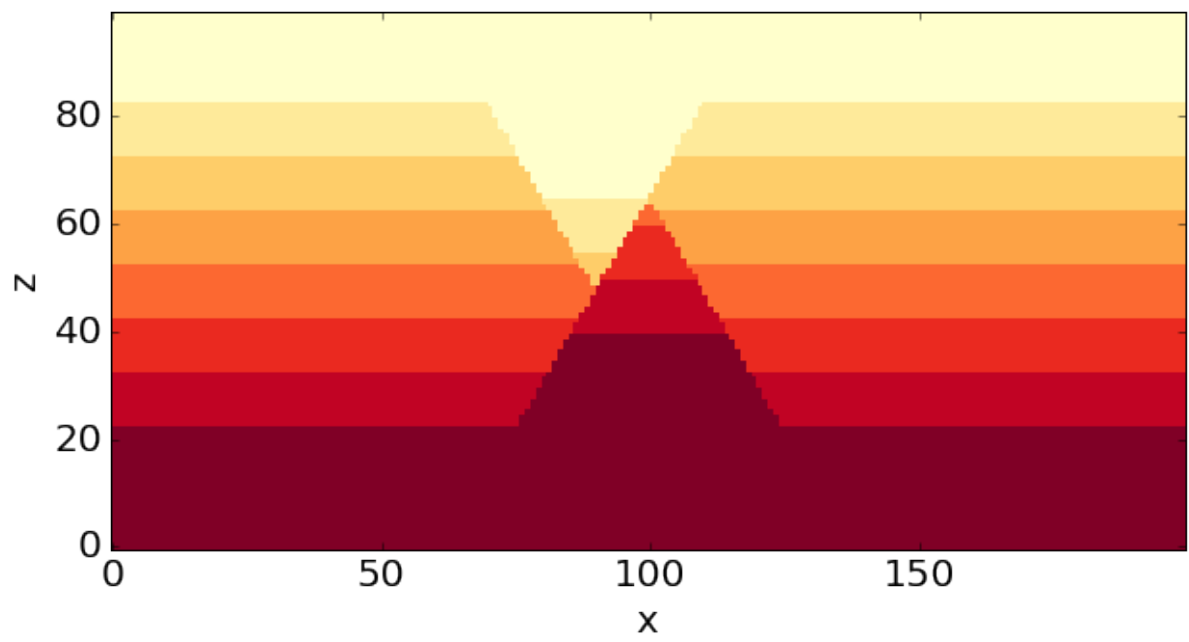
''

```

```

# 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 = True, fig_filename = "ex01_faults_combined.eps",
                  cmap = 'YlOrRd') # note: YlOrRd colourmap should be suitable for
↪ colorblindness!

```



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
```

```
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
```

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

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

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:

```
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()
```

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

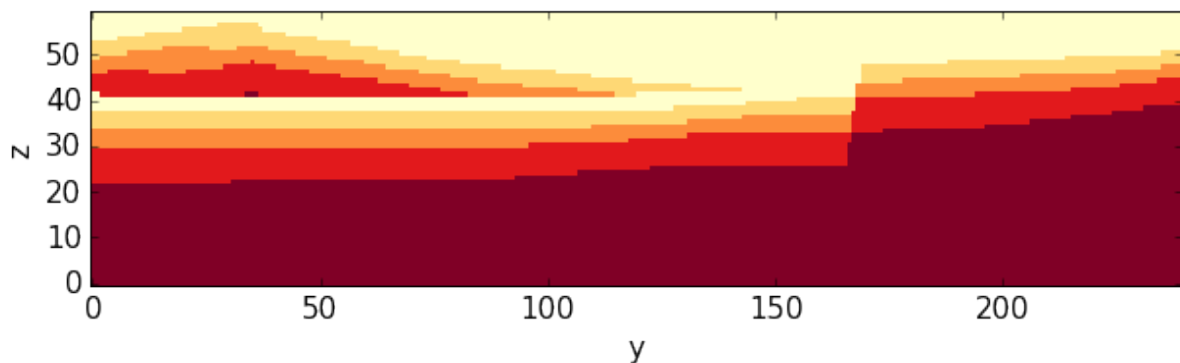
```
# Save to (local) file to compute and visualise model
history_name = "fold_thrust.his"
his.write_history(history_name)
# his = pynoddy.history.NoddyHistory(history_name)
```

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

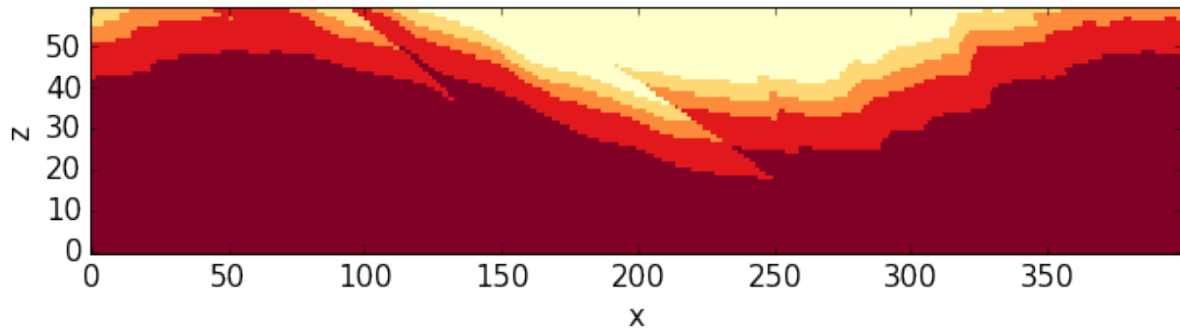
```
''
```

```
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')
```



```
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)
```

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

Visualise calculated geophysical fields

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

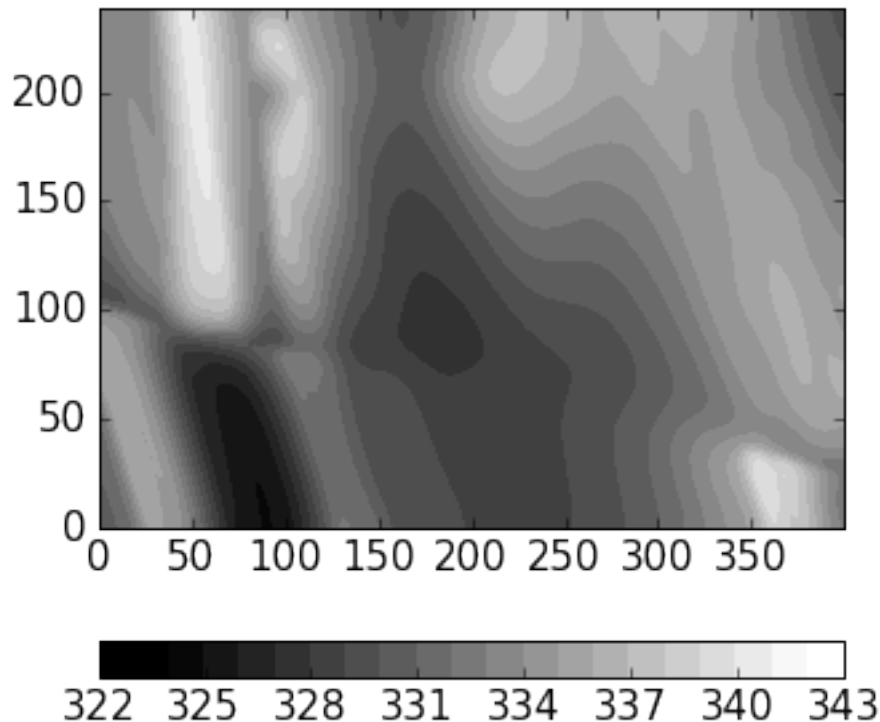
```
pynoddy.compute_model(history_name, output, sim_type = 'GEOPHYSICS')
```

```
''
```

We now get two files for the calculated 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
```



Change history and compare gravity

As a next step, we will now change aspects of the geological history (parameterised 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:

```
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
```

```
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': 0.0, 'X': 0.0, 'Single Fold': 'FALSE', 'Z': 0.0, 'Type':
↪ 'Fourier', 'Dip Direction': 110.0}
```

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:

```
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:

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

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

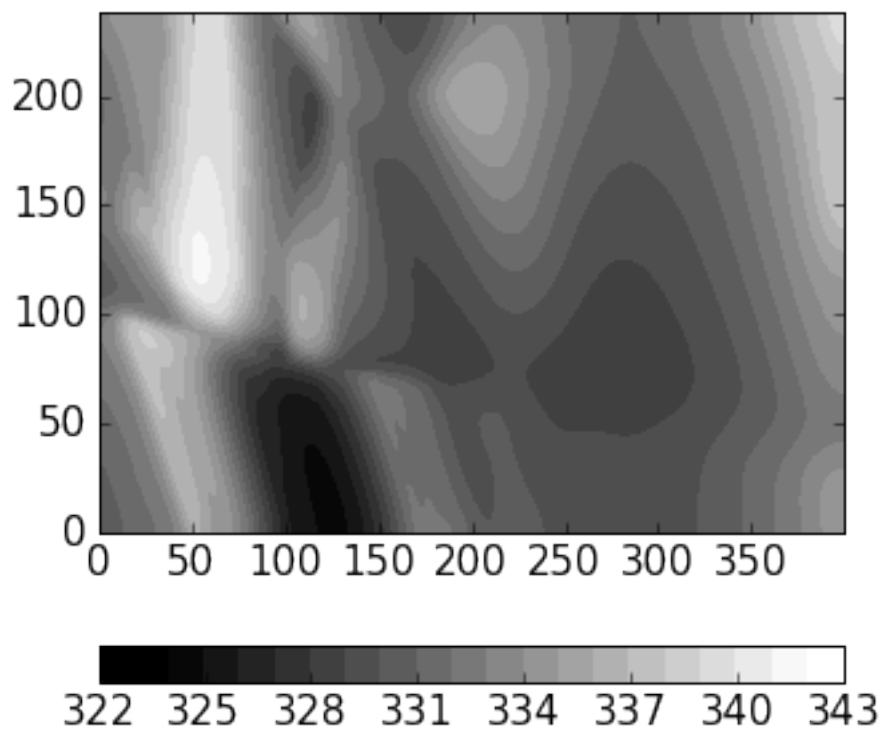
```
''
```

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

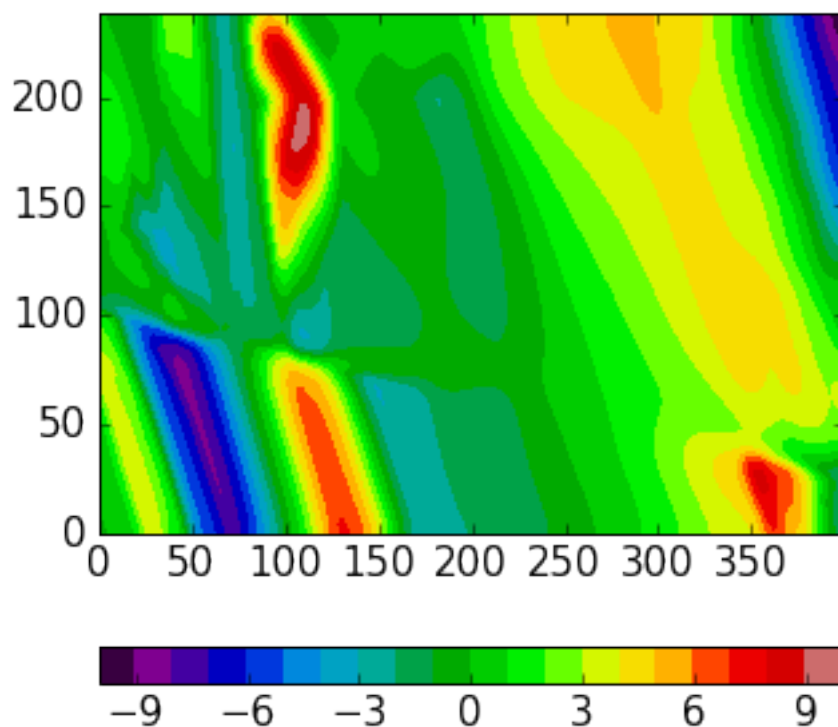
```
''
```

```
# 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')
```

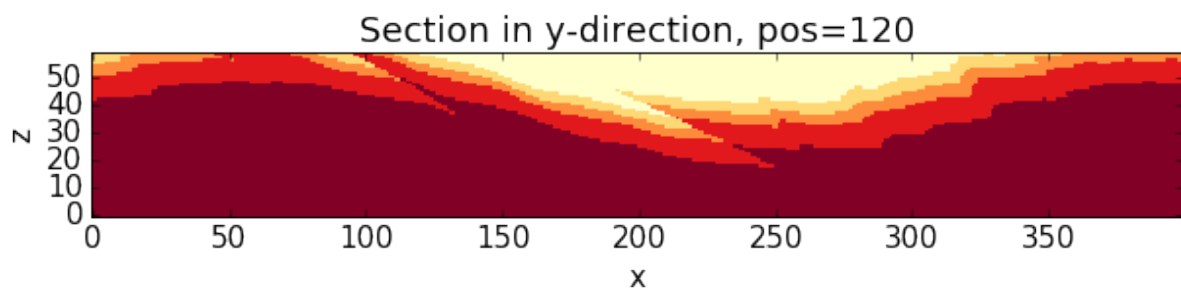
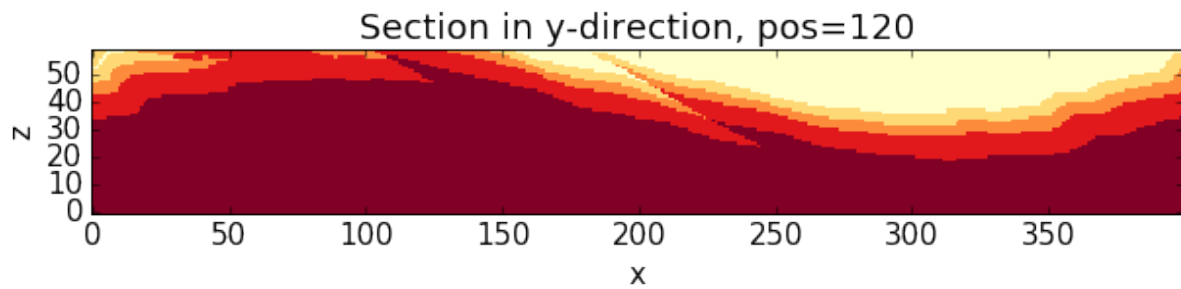
```
fig = plt.figure(figsize = (5,5))
ax = fig.add_subplot(111)
# imshow(geophys_changed.grv_data, cmap = 'jet')
cf = ax.contourf(geophys_changed.grv_data, levels, cmap = 'gray', vmin = 324, vmax_
↪ = 342)
cbar = plt.colorbar(cf, orientation = 'horizontal')
```



```
fig = 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)
```



```
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')
```

```
''
```

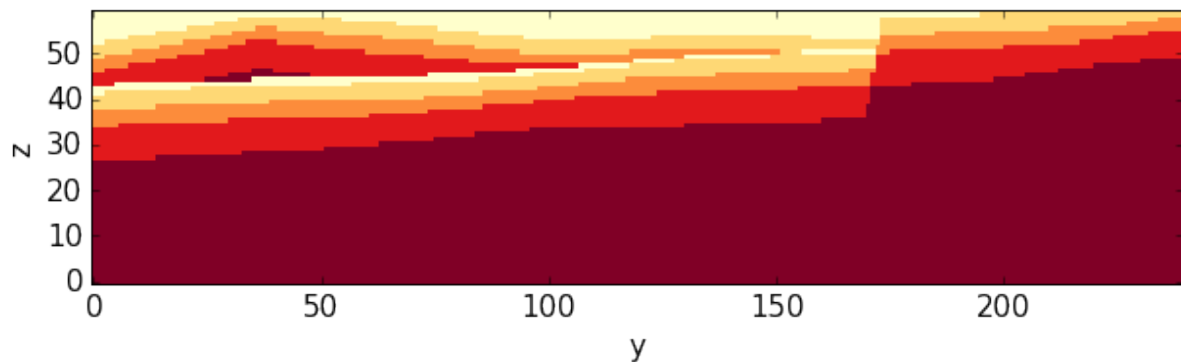
```
geology_changed = pynoddy.output.NoddyOutput('fold_thrust_changed_out')
```

```
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')

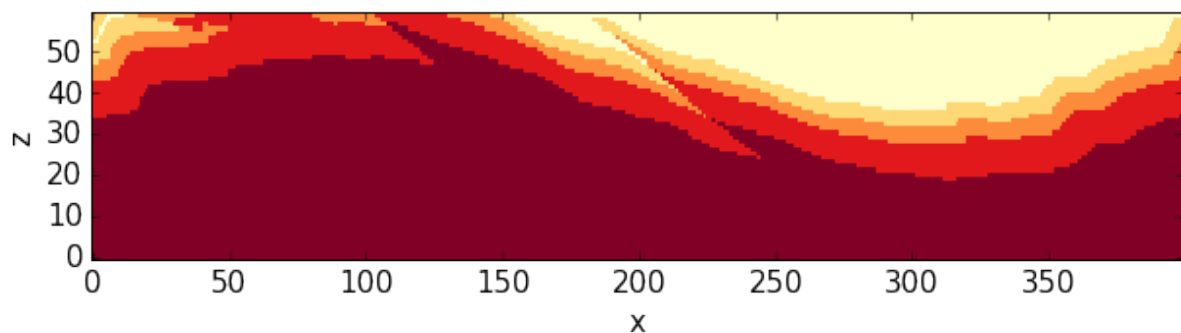
```



```

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

```

```

diff_model.export_to_vtk(vtk_filename = "diff_model_fold_thrust_belt")

```

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')

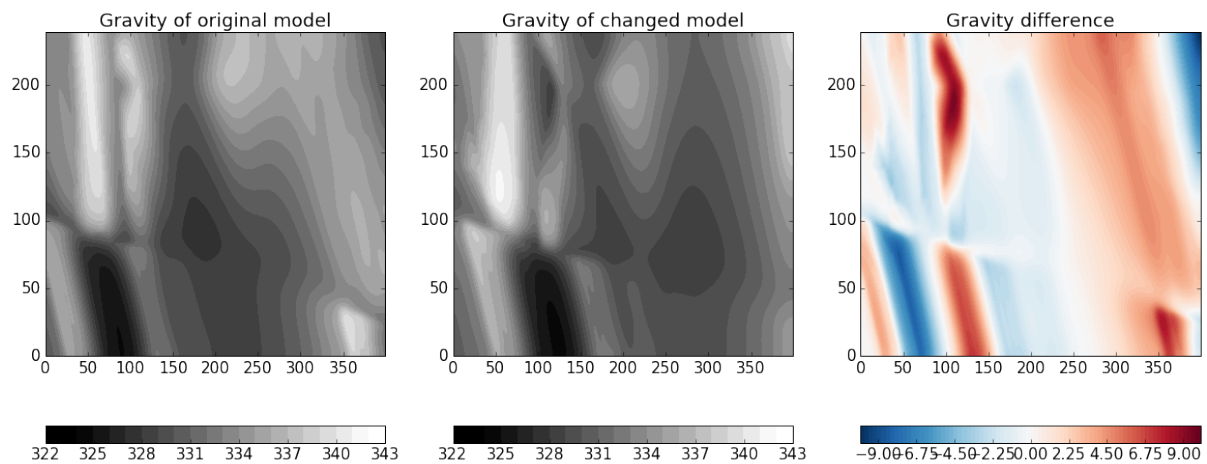
ax3 = fig.add_subplot(133)

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")

```



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.

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

```
%matplotlib inline
```

```
# 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})
```

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 distribution;
 - (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.

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 example 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).

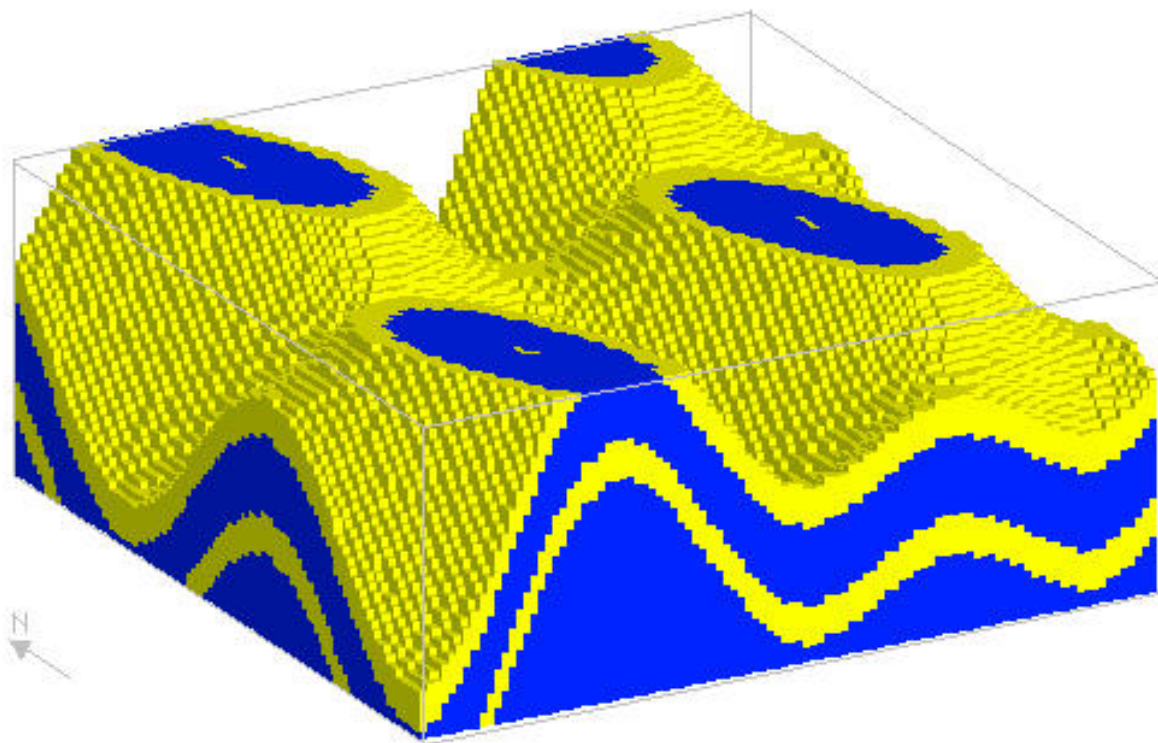


Fig. 8.1: Fold interference pattern

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)

```

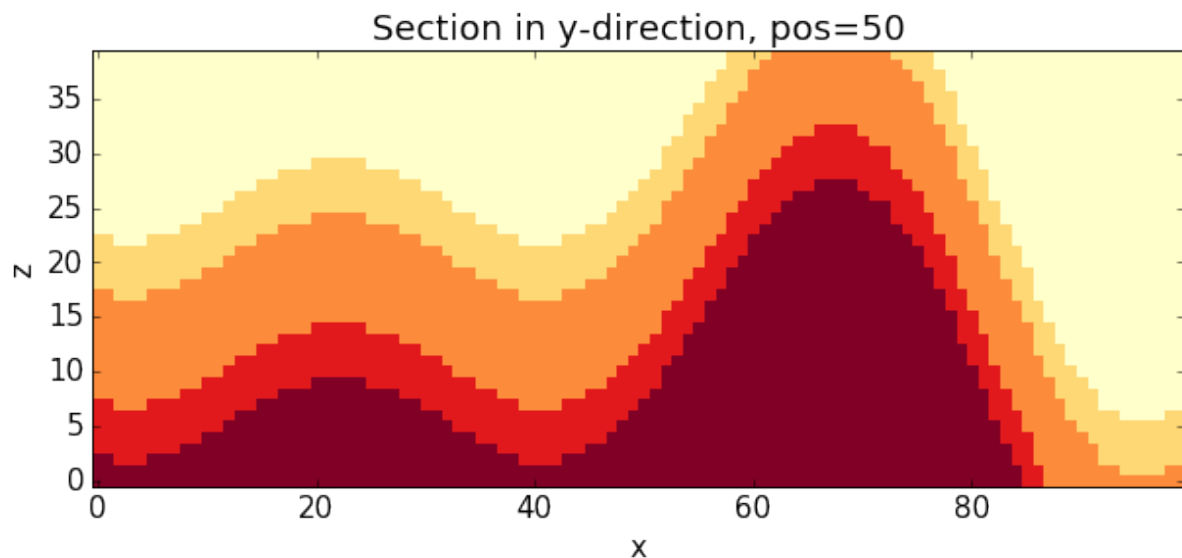
For simpler visualisation in this notebook, we will analyse the following steps in a section view of the model.

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')
```



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 possible with the `freeze()` method which stores the current state of the model as the “base-state”:

```
ue.freeze()
```

We now initialise 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)
```

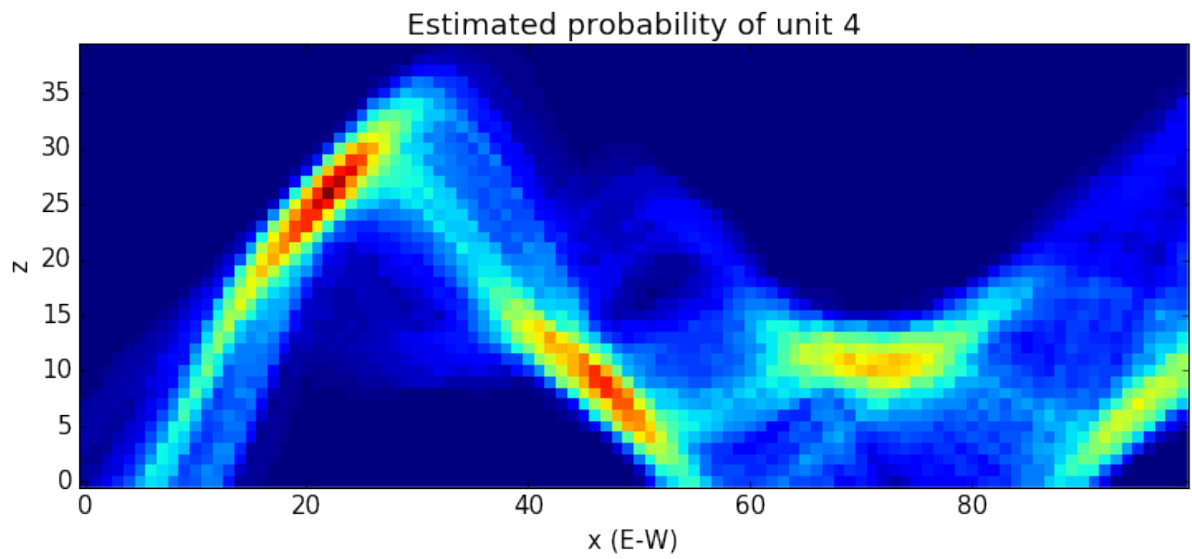
```
resolution = 100
ue.change_cube_size(resolution)
tmp = ue.get_section('y')
prob_4 = np.zeros_like(tmp.block[:, :, :])
n_draws = 100

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.

Gippsland Basin Uncertainty Study

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

```
%matplotlib inline
```

```
#import the usual 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})
```

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_Vel_V4.his`

```
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_Vel_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_Vel_V4 model in the pynoddy directory.

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

Generate randomised model realisations

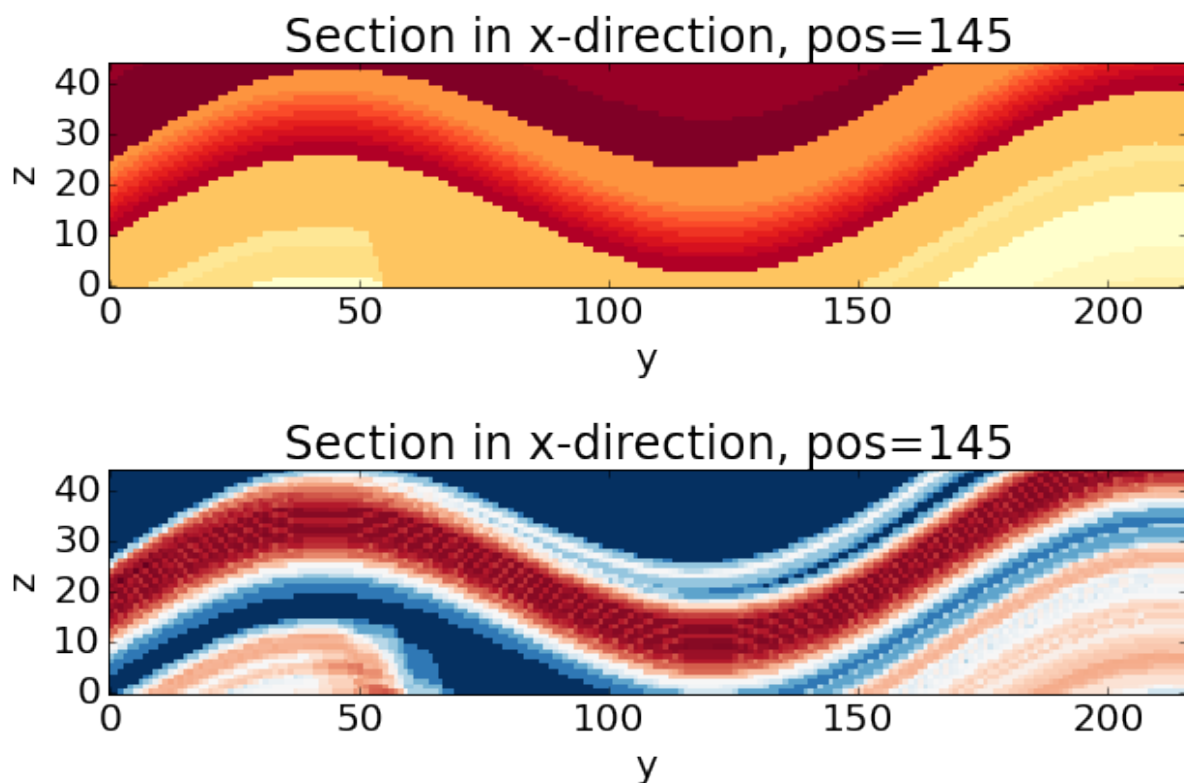
Now we have all the information required to perform a Monte-Carlo based uncertainty analysis. In this example we will generate 100 model realisations and use them to estimate the information entropy of each voxel in the model, and hence visualise uncertainty. It is worth noting that in reality we would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



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.

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.

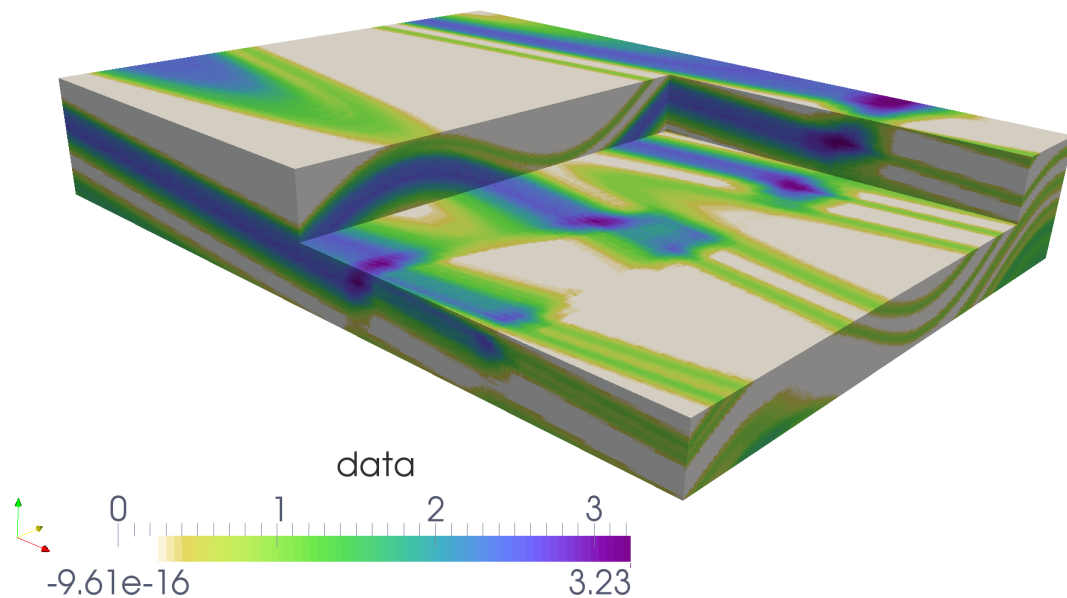


Fig. 9.1: 3-D visualisation of cell information entropy

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.

Theory: local sensitivity analysis

Basic considerations:

- parameter vector \vec{p}
- residual vector \vec{r}
- calculated values at observation points \vec{z}
- Jacobian matrix $J_{ij} = \frac{\partial z_i}{\partial p_j}$

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.

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 (= voxets, 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:

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

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

```
%matplotlib inline
```

Setting up the base model

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

```
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
```

```
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)

# 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)

```

```

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

```

```

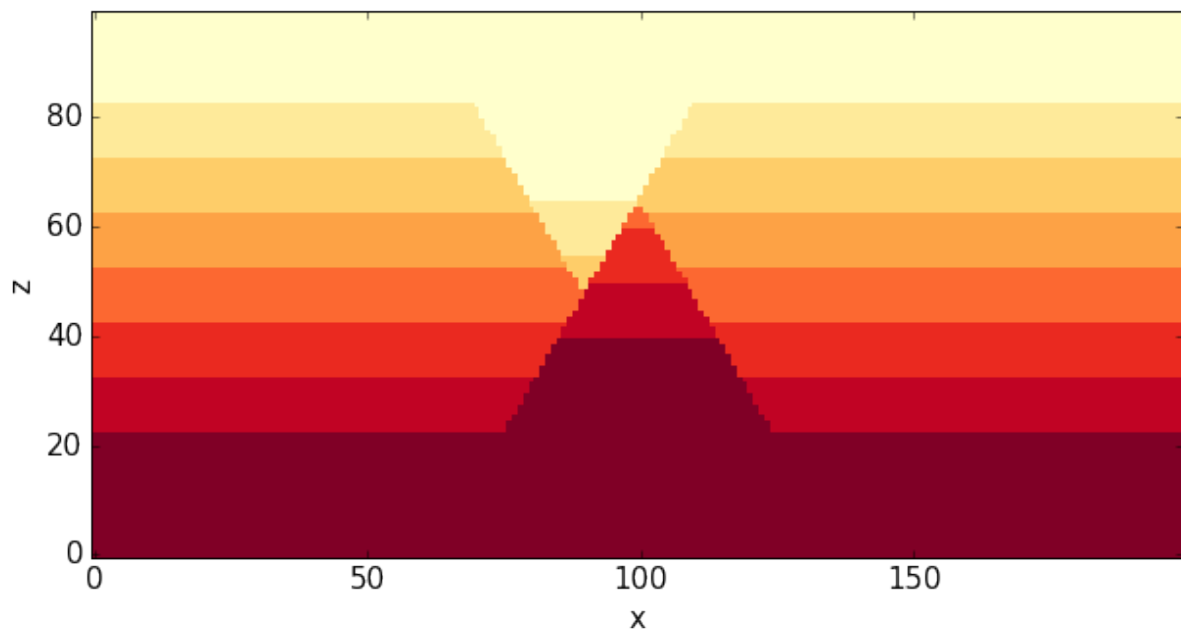
''

```

```

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

```



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

```

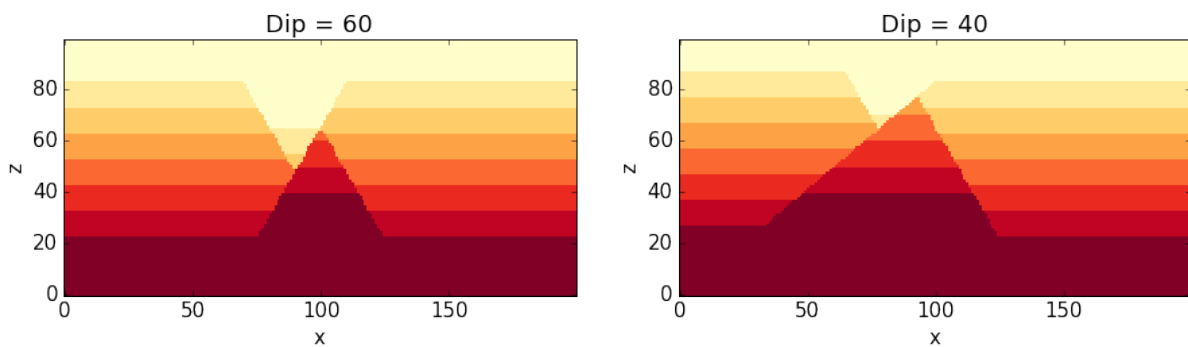
```

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()

```



Calculate total stratigraphic distance

```

# 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
```

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:

```
# set parameter changes in dictionary
```

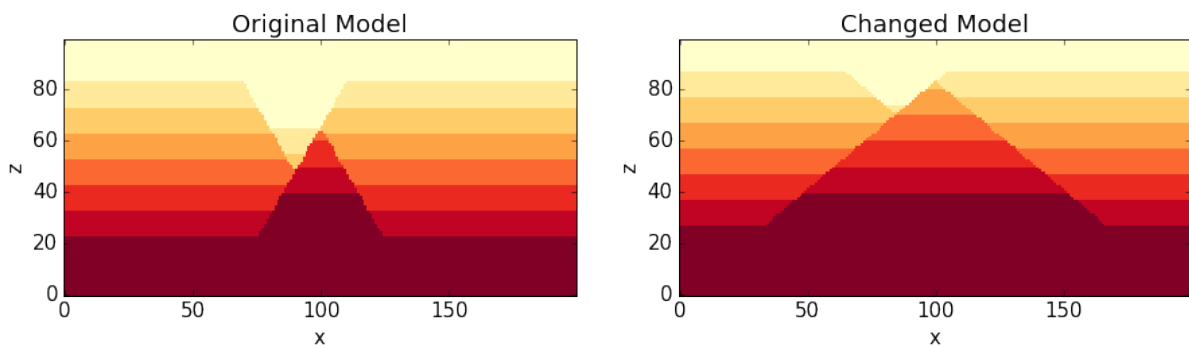
```
changes_fault_1 = {'Dip' : -20}
changes_fault_2 = {'Dip' : -20}
param_changes = {2 : changes_fault_1,
                  3 : changes_fault_2}
```

```
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()
```



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 calculated 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)
        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):

```

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:

```
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:

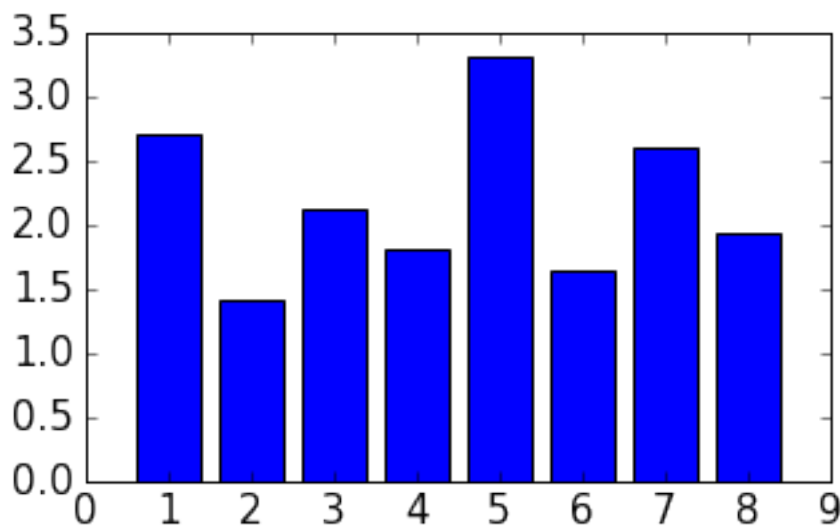

```
for p,d in zip(param_list_1, distances):
    print "%s \t\t %f" % (p, d)
```

```
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>
```



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.

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

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

# Now import pynoddy
import pynoddy
%matplotlib inline

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

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:

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

# Path to example 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 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.

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

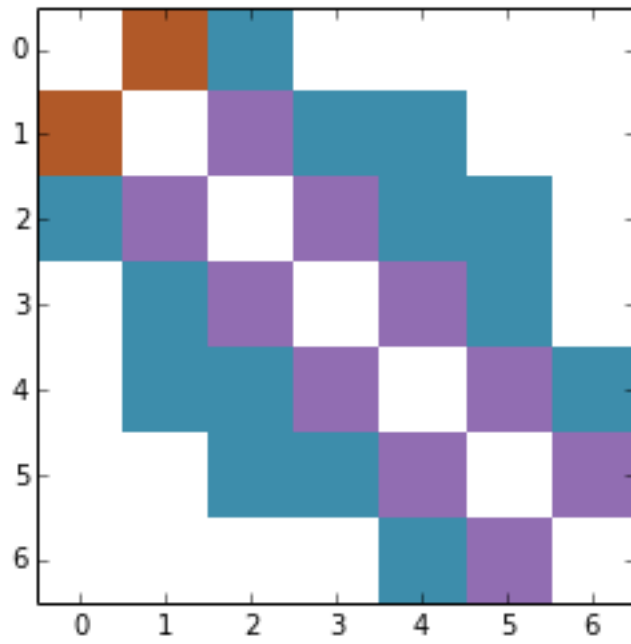
image = np.empty((int(AM.maxlitho),int(AM.maxlitho)), np.uint8)

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
```



CHAPTER 12

Fault shapes

We are here briefly showing the possibility of Noddy to model more complex fault shapes than simple planar faults.

```
from matplotlib import rc_params
```

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

```
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 correctly below
repo_path = os.path.realpath('../..')
import pynoddy.history
import pynoddy.experiment
import pynoddy.events
```

```
<module 'pynoddy.experiment' from '/Users/flow/git/pynoddy/pynoddy/experiment/___
↳init__.pyc'>
```

```
%matplotlib inline
```

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

We will create a model with a listric fault from scratch. In addition to the previous parameters for creating a fault (see notebook 4-Create-model), we now change the fault “geometry” to “Curved” and add parameters defining the amplitude and radius of influence:

```
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' : [1000, 500, 500, 500, 500, 500, 1000, 2000]}
nm.add_event('stratigraphy', strati_options )

# The following options define the fault geometry:
fault_options = {'name' : 'Fault_E',
                 'pos' : (3000, 0, 4000),
                 'dip_dir' : 90,
                 'dip' : 30,
                 'slip' : 1000,
                 'amplitude' : 1000.,
                 'radius' : 2000,
                 'geometry' : 'Curved',
                 'xaxis': 5000.,
                 'yaxis': 5000.0,
                 'zaxis' : 39999.0}
nm.add_event('fault', fault_options)
nm.change_cube_size(50)

```

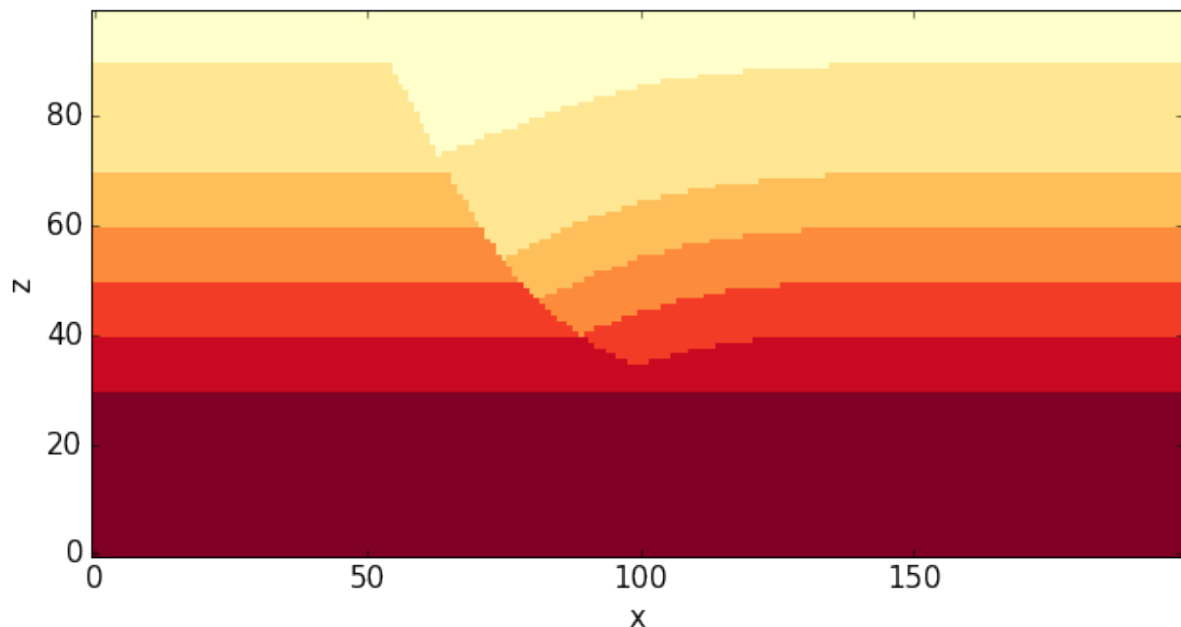
With these settings, we obtain an example of a listric fault in Noddy:

```

history = "listric_example.his"
outout_name = "listric_out"

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_listric.eps")

```



Pynoddy modules, classes and functions

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.

Main module

History file parser: `pynoddy.history`

Output file parser: `pynoddy.output`

Additional useful classes

`pynoddy.events`

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.

Base classes for pynoddy experiments

The base class for any type of experiments is defined in the `pynoddy.experiment` module.

MonteCarlo class

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

SensitivityAnalysis class