Sumatra: a toolkit for provenance capture and reuse

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Reproducibility in Computational and Experimental Mathematics
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“I thought I used the same parameters but I’m getting different results”

“I can’t remember which version of the code I used to generate figure 6”

“The new student wants to reuse that model I published three years ago but he can’t reproduce the figures”

“It worked yesterday”

“Why did I do that?”

Why isn’t it easy to reproduce a computational experiment exactly?

Why isn't it easy to reproduce a computational experiment exactly?

- complexity
  - dependence on small details, small changes have big effects
- entropy
  - computing environment, library versions change over time
- human memory limitations
  - forgetting, implicit knowledge not passed on

What can we do about it?

- complexity
  - use/teach good software-engineering practices (loose coupling, testing...)
- entropy
  - plan for reproducibility from the start: run in different environments, write tests, record dependencies
- human memory limitations
  - record everything

What can we do about it?

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- entropy
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  - record everything

- what code was run?
  - which executable?
    - name, location, version, compilation options
  - which script?
    - name, location, version
    - options, parameters
    - dependencies (name, location, version)
- what were the input data?
  - name, location, content
- what were the outputs?
  - data, logs, stdout/stderr
- who launched the computation?
- when was it launched/when did it run? (queueing systems)
- where did it run?
  - machine name(s), other identifiers (e.g. IP addresses)
  - processor architecture
  - available memory
  - operating system
- why was it run?
- what was the outcome?
- which project was it part of?

Recording all this by hand is tedious and error-prone

let's automate it

lab notebook by benjaminlansky http://www.flickr.com/photos/7274331@N08/3110638204/

Requirements

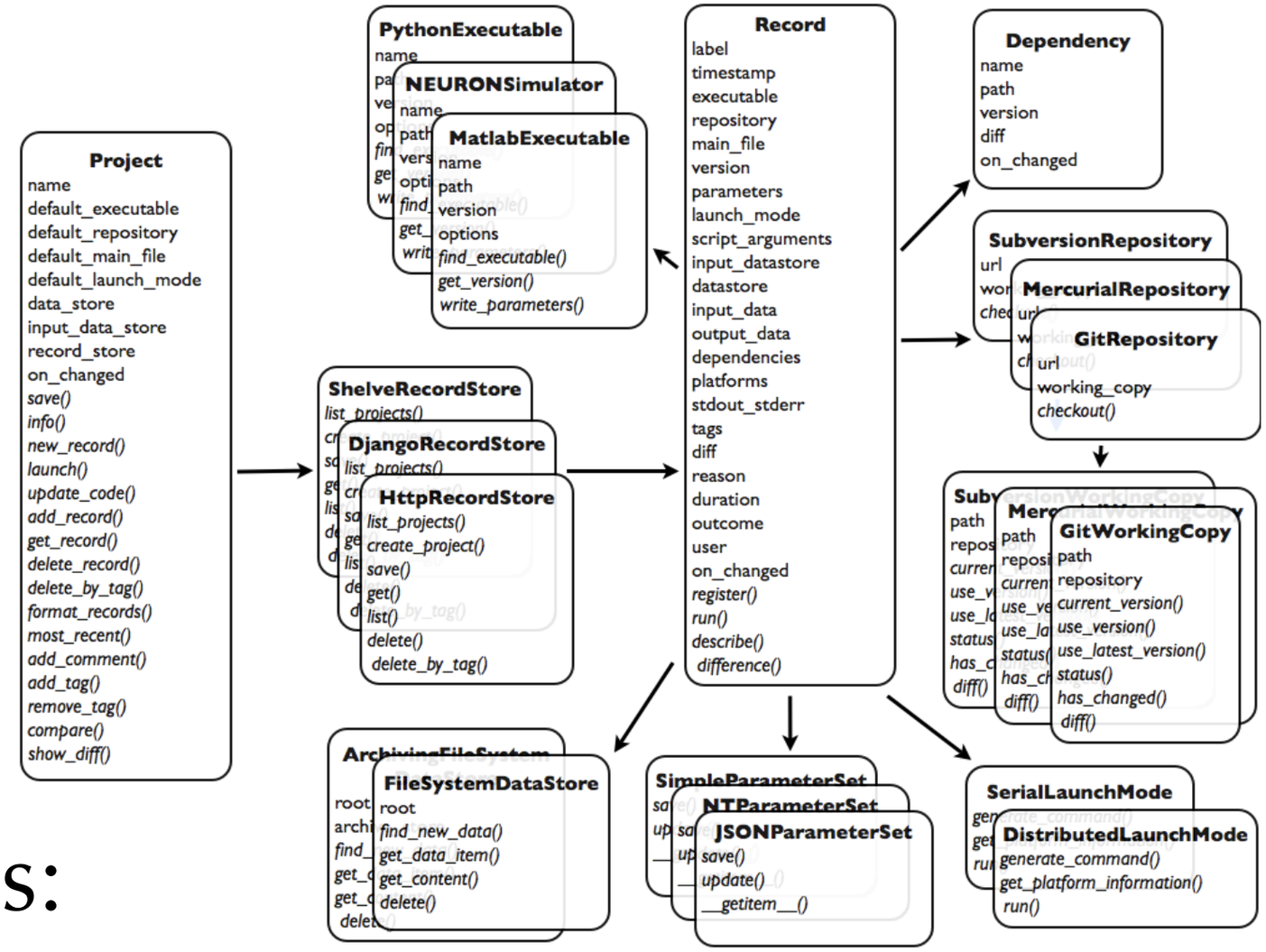
Different researchers, different workflows

- command-line
- GUI
- batch jobs
- solo or collaborative
- any combination of these for different components and phases of the project

Requirements

- Integrate into the day-to-day workflow
- Be very easy to use, or only the very conscientious will use it

A core library of loosely-coupled components



Used to build interfaces:

- command-line interface for launching and capturing computations
- graphical interface for browsing/searching results
- remote server for sharing/communicating with others
- documentation-system interface for including results-with-provenance in publications
- integration with existing tools...

Installation

- Install Python bindings for your preferred version control system (`pysvn`, `mercurial`, `GitPython, bzrlib`)

- `pip install sumatra`

Command-line interface

```
$ cd myproject

$ smt init MyProject
```

```
$ python main.py default.param
```

```
$ python main.py default.param

$ smt run --executable=python --main=main.py default.param
```

```
$ python main.py default.param

$ smt run --executable=python --main=main.py default.param

$ smt configure --executable=python --main=main.py
```

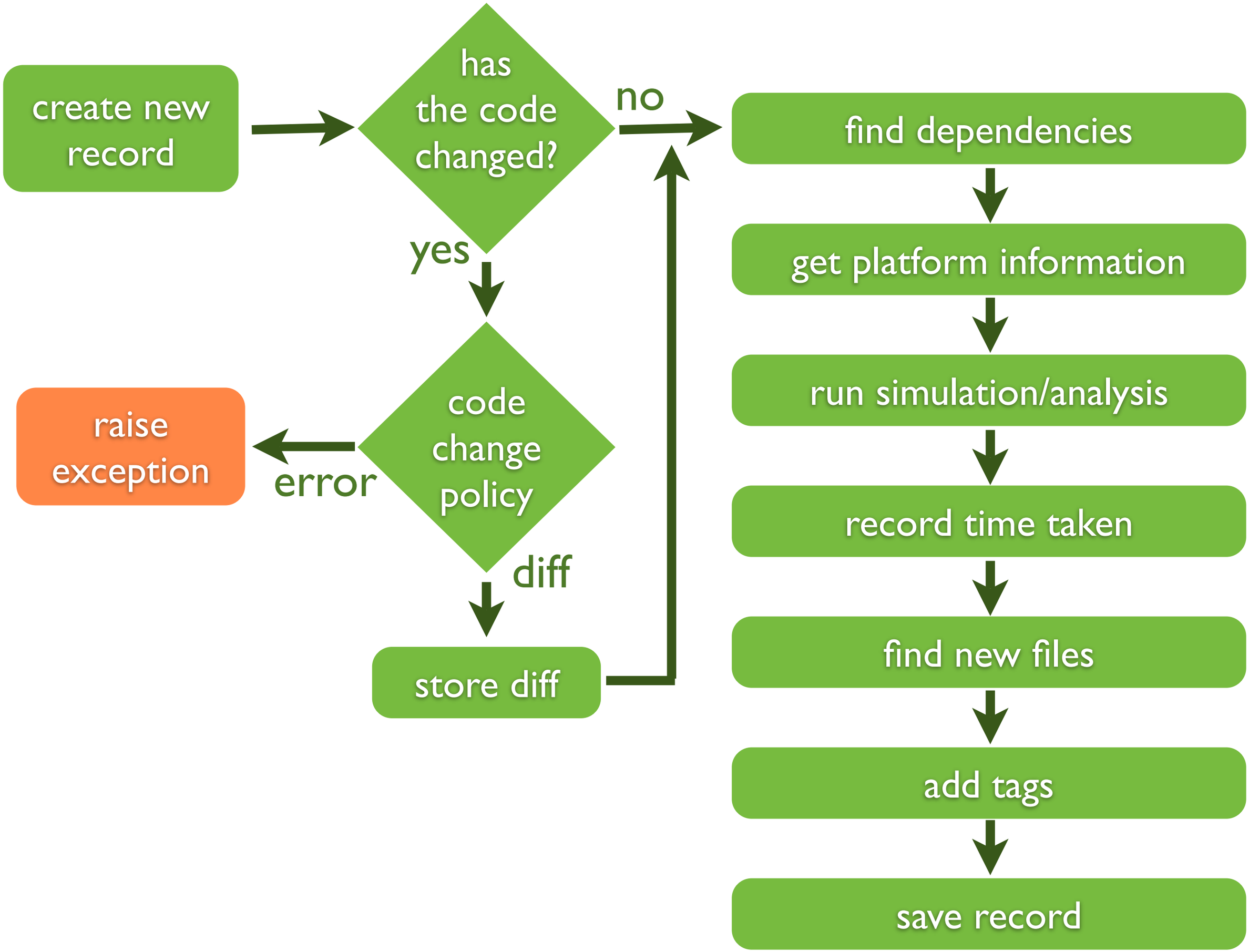
```
$ python main.py default.param

$ smt run --executable=python --main=main.py default.param

$ smt configure --executable=python --main=main.py

$ smt run default.param
```

```
$ smt run default.param
```

```
$ smt run default.param
Code has changed, please commit your changes.
```

```
$ smt run default.param
Code has changed, please commit your changes.

$ smt configure --on-changed=store-diff
```

```
$ smt run default.param
Code has changed, please commit your changes.

$ smt configure --on-changed=store-diff

$ smt run default.param
```


create new record
has the code changed?
no
yes
find dependencies
get platform information
run simulation/analysis
record time taken
find new files
add tags
save record
code change policy
error
raise exception
diff
store diff

```
$ smt list
20110713-174949
20110713-175111

$ smt list -l
-----------------------------------------------
Label             : 20110713-174949
Timestamp         : 2011-07-13 17:49:49.235772
Reason            :
Outcome           :
Duration          : 0.0548920631409
Repository        : MercurialRepository at /path/to/myproject
Main file         : main.py
Version           : rf9ab74313efe
Script arguments  : <parameters>
Executable        : Python (version: 2.6.2) at /usr/bin/python
Parameters        : seed = 65785
                  : distr = "uniform"
                  : n = 100
Input_Data        : []
Launch_Mode       : serial
Output_Data       :[example2.dat(43a47cb379df2a7008fdeb38c6172278d000f
Tags              :
.
.
.
```

```
$ smt run --label=haggling --reason="determine whether the
gourd is worth 3 or 4 shekels" romans.param
```

```
$ smt comment "apparently, it is worth NaN shekels."
```

```
$ smt comment 20110713-174949 "Eureka! Fields Medal
here we come."
```

```
$ smt tag “Figure 6”
```

```
$ smt run --reason="test effect of a smaller time
constant" default.param tau_m=10.0
```

```
$ smt repeat haggling
The new record exactly matches the original.
```

```
$ smt repeat haggling
The new record does not match the original. It
differs as follows.
Record 1                    : haggling
Record 2                    : haggling_repeat
Executable differs          : no
Code differs                : yes
  Repository differs        : no
  Main file differs         : no
  Version differs           : no
  Non checked-in code       : no
  Dependencies differ       : yes
Launch mode differs         : no
Input data differ           : no
Script arguments differ     : no
Parameters differ           : no
Data differ                 : no
```

```
$ smt
Usage: smt <subcommand> [options] [args]

Simulation/analysis management tool, version 0.4

Available subcommands:
  init
  configure
  info
  run
  list
  delete
  comment
  tag
  repeat
  diff
  help
  upgrade
  export
  sync
```

Browser interface

```
$ smtweb -p 8008 &
```

Browser interface

ProjectGlass | Search | Search | Settings

New record

ProjectGlass

1 – 8 of 8

Repository	Label	Tag	Reason	Outcome	Duration	Date	Time	Executable name	Executable version	Main file	Version	Arguments
Glass	20121026-174545	Precise, default,	Fixed to work with the new numpy.histogram() function		3.85s	26/10/2012	17:45:45	Python	2.6.5	glass_sem_analysis.py	924a3	<parameters> MV_HFV_012.jpg
Glass	20121026-172642	error,	Running on Ubuntu 12.04	TypeError: histogram() got an unexpected keyword argument 'new'	3.07s	26/10/2012	17:26:42	Python	2.6.5	glass_sem_analysis.py	432ff	<parameters> MV_HFV_012.jpg
Glass	20121025-173606	Lucid,	No filtering, but more cleaning		2.82s	25/10/2012	17:36:06	Python	2.6.5	glass_sem_analysis.py	432ff	<parameters> MV_HFV_012.jpg
Glass	20121025-173350	Lucid,	Trying a different colourmap ("hot")	"Copper" is nicer	4.08s	25/10/2012	17:33:50	Python	2.6.5	glass_sem_analysis.py	432ff	<parameters> MV_HFV_012.jpg
Glass	20121025-173036	Lucid,	No filtering		2.83s	25/10/2012	17:30:36	Python	2.6.5	glass_sem_analysis.py	432ff	<parameters> MV_HFV_012.jpg
Glass	20121025-172833	Lucid, default,	Parameters are now in a separate file		3.85s	25/10/2012	17:28:33	Python	2.6.5	glass_sem_analysis.py	432ff	<parameters> MV_HFV_012.jpg
Glass	20121025-170718	Lucid, default,	Image file now specified on command line		3.73s	25/10/2012	17:07:18	Python	2.6.5	glass_sem_analysis.py	9d24b	MV_HFV_012.jpg
Glass	20121025-163949	Lucid, default,	First run with Sumatra		3.76s	25/10/2012	16:39:49	Python	2.6.5	glass_sem_analysis.py	89af3	

General info

Label: 20121025-170718

Reason:

Outcome:

Timestamp: 25/10/2012 17:07:18

Duration: 3.73s

Executable: Python version 2.6.5 (/usr/bin/python)

Launch mode: serial

Repository: /home/bob/Projects/Glass

Main file: glass_sem_analysis.py

Version: 9d24b099b5f3

Arguments: MV_HFV_012.jpg

Tags:

Save changes Delete record

Input files

/
MV_HFV_012.jpg 5d789282b10a0da7a91560f33f8baf7272f7543d 0 bytes

Output files

./Data

20121025/MV_HFV_012_170722_phases.png	c9955f84ca3c19123d24ccc4c87d197514d9e01e	image/png	82.2 KB
20121025/MV_HFV_012_170722_sand.png	20bd5420d37ee589f3c2542a12438cb78663974b	image/png	34.3 KB
20121025/MV_HFV_012_170722_histogram.png	e7884dc5f3e9ce2c0d713cb3e9ddffb07bf2010c	image/png	27.7 KB

Parameters

no parameters

Output files

./Data

20121025/MV_HFV_012_170722_phases.png	c9955f84ca3c19123d24ccc4c87d197514d9e01e	image/png	82.2 KB
20121025/MV_HFV_012_170722_sand.png	20bd5420d37ee589f3c2542a12438cb78663974b	image/png	34.3 KB
20121025/MV_HFV_012_170722_histogram.png	e7884dc5f3e9ce2c0d713cb3e9ddffb07bf2010c	image/png	27.7 KB

Parameters

no parameters

Dependencies

Name	Path	Version
dateutil	/usr/lib/pymodules/python2.6/dateutil	1.4.1
glib	/usr/lib/pymodules/python2.6/gtk-2.0/glib	unknown
gobject	/usr/lib/pymodules/python2.6/gtk-2.0/gobject	unknown
matplotlib	/usr/lib/pymodules/python2.6/matplotlib	0.99.1.1
mpl_toolkits	/usr/lib/pymodules/python2.6/mpl_toolkits	unknown
numpy	/usr/lib/python2.6/dist-packages/numpy	1.3.0
pytz	/usr/lib/python2.6/dist-packages/pytz	2010b
scipy	/usr/lib/python2.6/dist-packages/scipy	0.7.0
wx	/usr/lib/python2.6/dist-packages/wx-2.8-gtk2-unicode/wx	2.8.10.1 (gtk2-unicode)

Platform information

Name	IP address	Processor	Architecture	System type	Release	Version
Ubuntu01	127.0.1.1	i686	32bit ELF	Linux	2.6.32-24-generic	#39-Ubuntu SMP Wed Jul 28 06:07:29 UTC 2010

Stdout & Stderr

```
/usr/lib/python2.6/dist-packages/numpy/lib/function_base.py:272: DeprecationWarning:
        The histogram semantics being used is now deprecated and
        will disappear in NumPy 1.4.  Please update your code to
        use the default semantics.

  """, DeprecationWarning)
1699.875 65.0
```

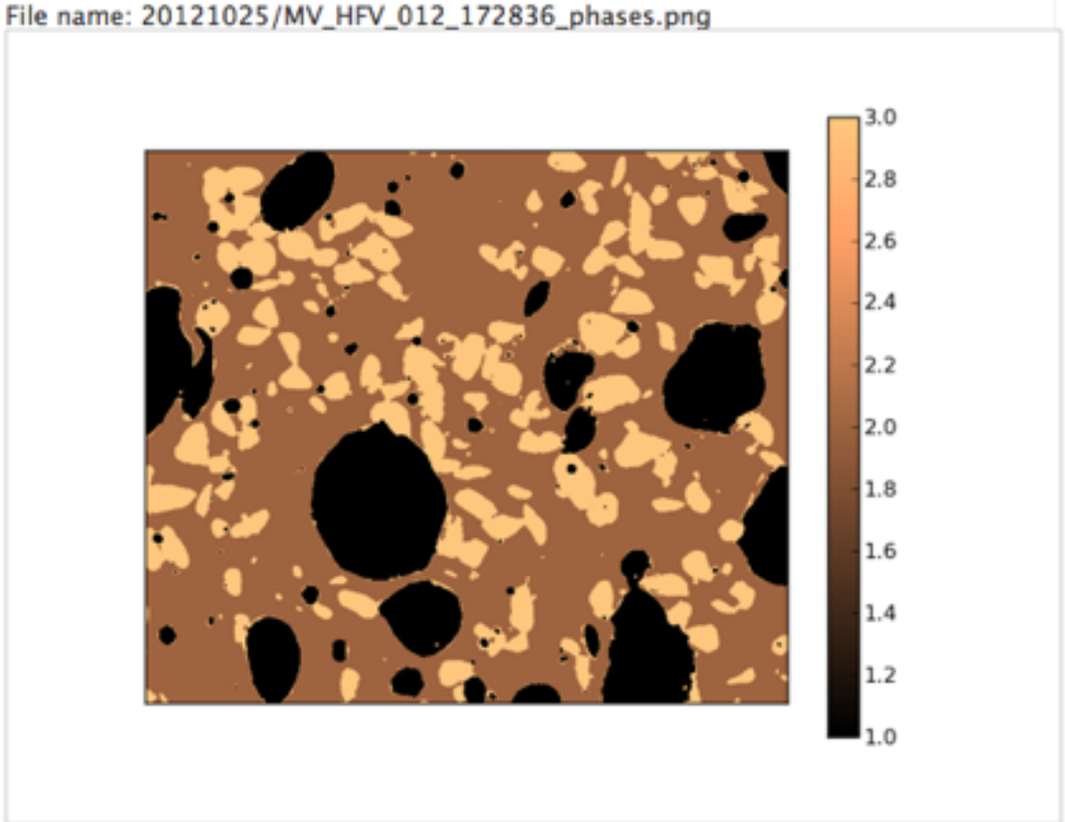
Comparison of records

Click the records you would like to compare:

20121026-174545 20121025-172833

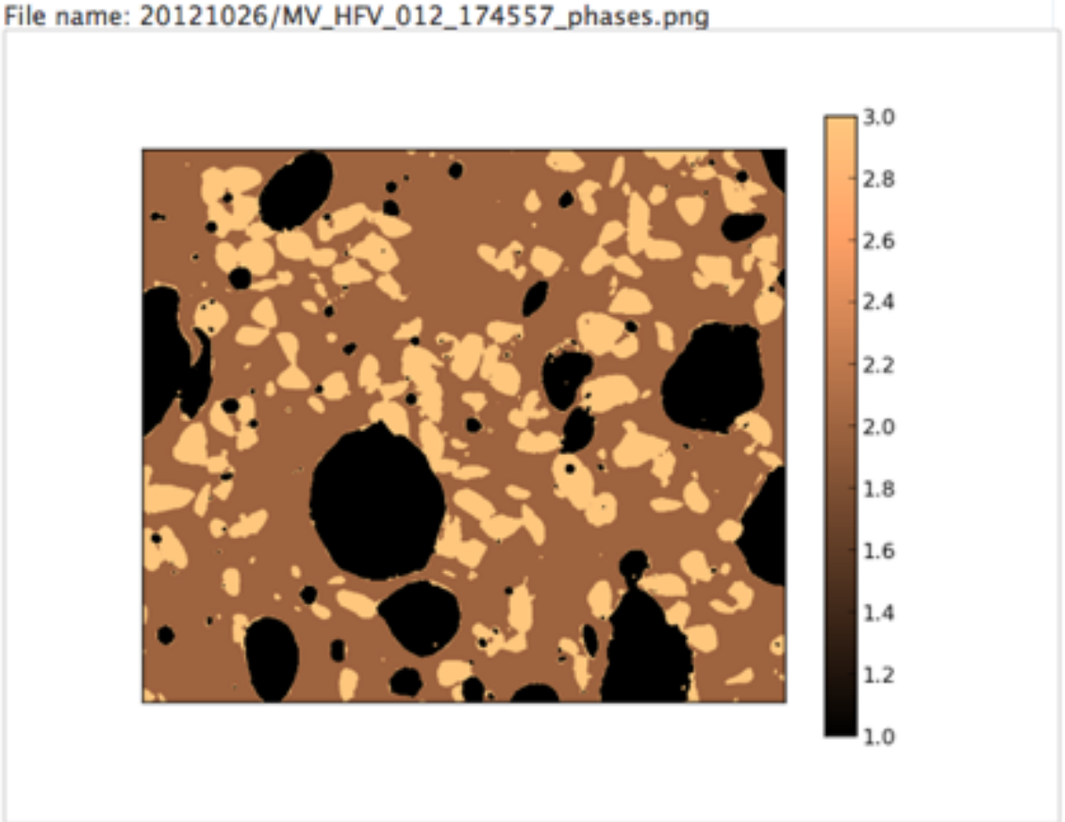
	20121025-172833	20121026-174545
Reason:	Parameters are now in a separate file	Fixed to work with the new numpy.histogram() function
Outcome:		
Timestamp:	25/10/2012 17:28:33	26/10/2012 17:45:45
Duration:	3.85s	3.85s
Executable:	Python version 2.6.5 (/usr/bin/python)	Python version 2.7.3 (/usr/bin/python)
Launch mode:	serial	serial
Repository:	/home/bob/Projects/Glass	/home/bob/Projects/Glass
Main file:	glass_sem_analysis.py	glass_sem_analysis.py
Version:	432ff7ef3f45	924a39a0d24c

File name: 20121025/MV_HFV_012_172836_phases.png



Digest: c9955f84ca3c19123d24ccc4c87d197514d9e01e

File name: 20121026/MV_HFV_012_174557_phases.png

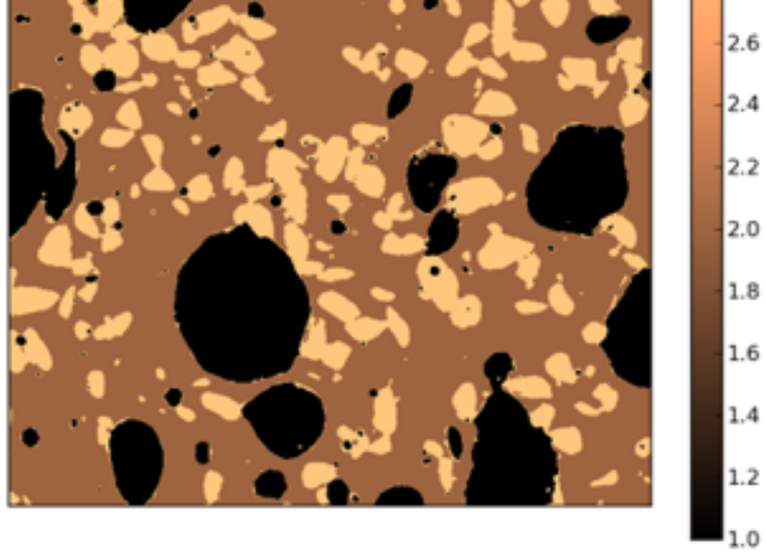


Digest: 7f8ed0c6ef97b8317af8e2d9ab9f856a193c2687

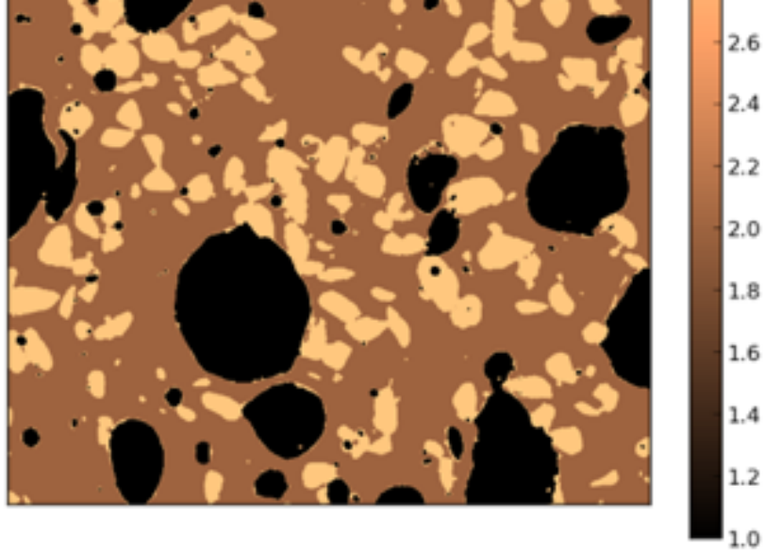
Dependencies:

Name	Path	Version
dateutil	/usr/lib/pymodules/python2.6/dateutil	1.4.1
glib	/usr/lib/pymodules/python2.6/gtk-2.0/glib	unknown
gobject	/usr/lib/pymodules/python2.6/gtk-2.0/gobject	unknown
matplotlib	/usr/lib/pymodules/python2.6/matplotlib	0.99.1.1

Name	Path	Version
PIL	/usr/lib/python2.7/dist-packages/PIL	unknown
PyQt4	/usr/lib/python2.7/dist-packages/PyQt4	unknown
apport	/usr/lib/python2.7/dist-packages/apport	unknown
apt	/usr/lib/python2.7/dist-packages/apt	unknown
dateutil	/usr/lib/python2.7/dist-packages/dateutil	1.5
glib	/usr/lib/python2.7/dist-packages/glib	unknown



Digest: c9955f84ca3c19123d24ccc4c87d197514d9e01e



Digest: 7f8ed0c6ef97b8317af8e2d9ab9f856a193c2687

Dependencies:

Name	Path	Version
dateutil	/usr/lib/pymodules/python2.6/dateutil	1.4.1
glib	/usr/lib/pymodules/python2.6/gtk-2.0/glib	unknown
gobject	/usr/lib/pymodules/python2.6/gtk-2.0/gobject	unknown
matplotlib	/usr/lib/pymodules/python2.6/matplotlib	0.99.1.1
mpl_toolkits	/usr/lib/pymodules/python2.6/mpl_toolkits	unknown
numpy	/usr/lib/python2.6/dist-packages/numpy	1.3.0
pytz	/usr/lib/python2.6/dist-packages/pytz	2010b
scipy	/usr/lib/python2.6/dist-packages/scipy	0.7.0
wx	/usr/lib/python2.6/dist-packages/wx-2.8-gtk2-unicode/wx	2.8.10.1 (gtk2-unicode)

Name	Path	Version
PIL	/usr/lib/python2.7/dist-packages/PIL	unknown
PyQt4	/usr/lib/python2.7/dist-packages/PyQt4	unknown
apport	/usr/lib/python2.7/dist-packages/apport	unknown
apt	/usr/lib/python2.7/dist-packages/apt	unknown
dateutil	/usr/lib/python2.7/dist-packages/dateutil	1.5
glib	/usr/lib/python2.7/dist-packages/glib	unknown
gobject	/usr/lib/python2.7/dist-packages/gobject	unknown
matplotlib	/usr/lib/pymodules/python2.7/matplotlib	1.1.1rc
mpl_toolkits	/usr/lib/pymodules/python2.7/mpl_toolkits	unknown
nose	/usr/lib/python2.7/dist-packages/nose	1.1.2
numpy	/usr/lib/python2.7/dist-packages/numpy	1.6.1
pytz	/usr/lib/python2.7/dist-packages/pytz	2011k
scipy	/usr/lib/python2.7/dist-packages/scipy	0.9.0
setuptools	/usr/lib/python2.7/dist-packages/setuptools	0.6
wx	/usr/lib/python2.7/dist-packages/wx-2.8-gtk2-unicode/wx	2.8.12.1 (gtk2-unicode)

Platform information:

1. **Name:** Ubuntu01
2. **IP address:** 127.0.1.1
3. **Processor:** i686
4. **Architecture:** 32bit
5. **System type:** Linux
6. **Release:** 2.6.32-24-generic

1. **Name:** Ubuntu01
2. **IP address:** 127.0.0.1
3. **Processor:** i686 i686
4. **Architecture:** 32bit
5. **System type:** Linux
6. **Release:** 3.2.0-32-generic

Interface with documentation systems

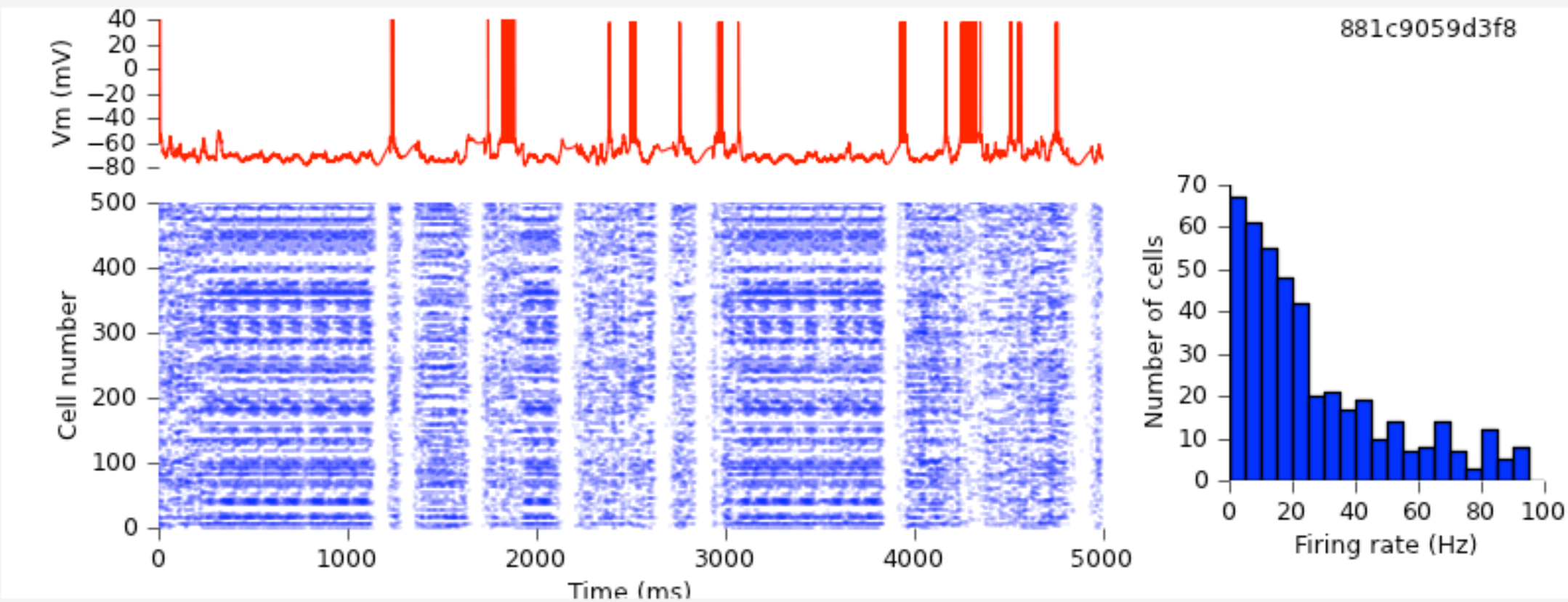
```
advantage that the network can be parallelized using MPI. Otherwise, the
only important difference between ``multiAMPAexp`` and ``NetCon`` is that
the former has a dead time of one millisecond after a conductance step in
which any incoming spikes have no effect.

::

  $ hg update -r 7                        # replaced multiAMPAexp with ExpSyn
  $ python demo_cx05_N=500b_LTS.py
  $ python plot.py spiketimes_cx05_LTS500b.dat numspikes_cx05_LTS500b.dat ..

:smtlink:`20120919-172444`
:smtlink:`20120919-173558`

Despite this difference, the models give comparable results.

.. smtimage:: 20120919-173558
   :digest: 26f6ad85aab0ef1e995042c0a3b3029e303a90a6
```

Interface with documentation systems

dynamics uses NEURON's `NetCon` mechanism to communicate, which has the advantage that the network can be parallelized using MPI. Otherwise, the only important difference between `multiAMPAexp` and `NetCon` is that the former has a dead time of one millisecond after a conductance step in which any incoming spikes have no effect.

```
$ hg update -r 7  # replaced multiStimexp, multiAMPAexp and multiGABAAexp with ExpSyn
$ python demo_cx05_N=500b_LTS.py
$ python plot.py spiketimes_cx05_LTS500b.dat numspikes_cx05_LTS500b.dat Vm170_cx05_LTS500b.dat
```

Despite this difference, the models give comparable results.



Using `sumatra` directly in Python scripts

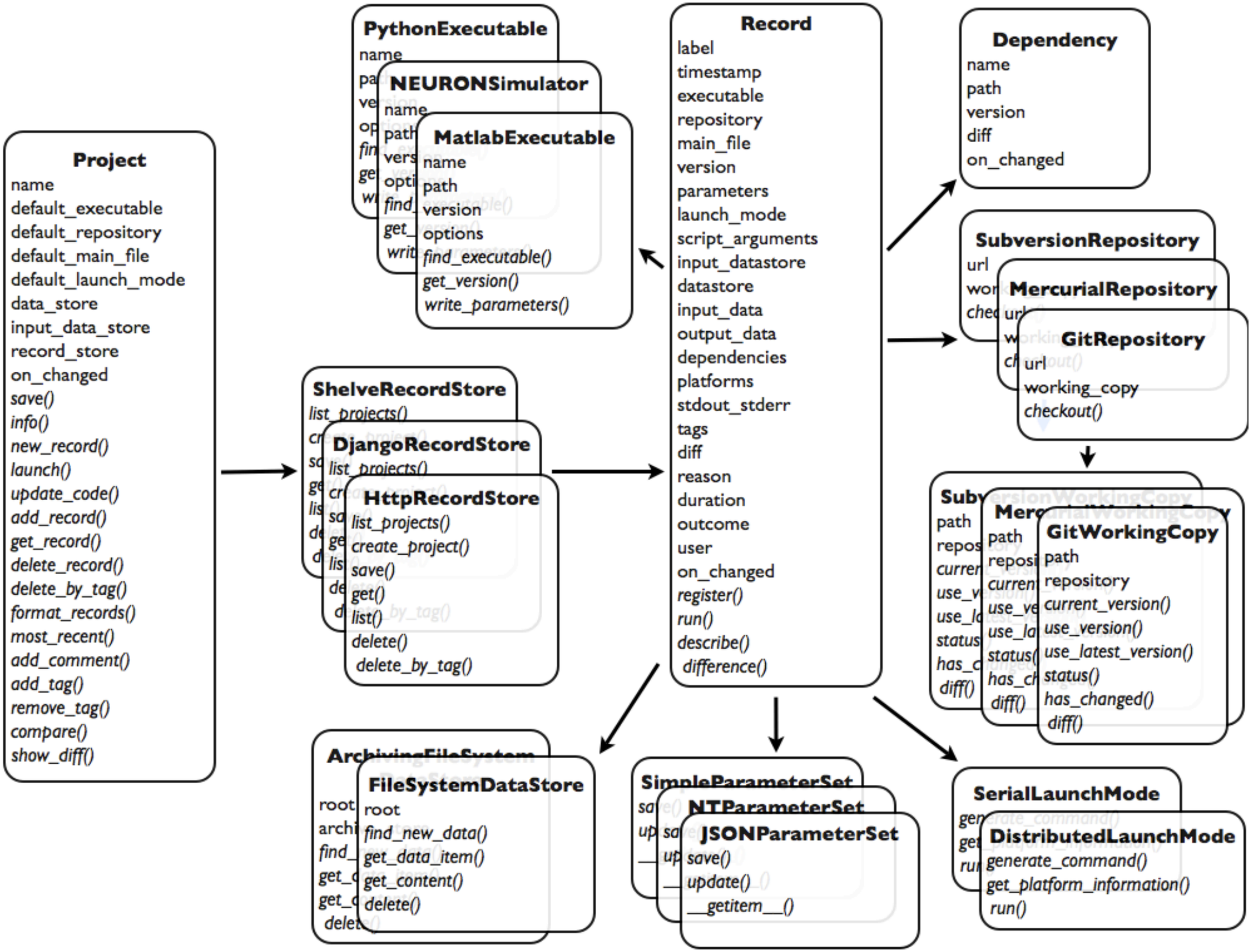
```
import numpy
import sys

def main(parameters):
    numpy.random.seed(parameters["seed"])
    distr = getattr(numpy.random, parameters["distr"])
    data = distr(size=parameters["n"])
    output_file = "Data/example.dat"
    numpy.savetxt(output_file, data)

parameter_file = sys.argv[1]
parameters = {}
execfile(parameter_file, parameters) # this way of reading parameters
                                     # is not necessarily recommended
main(parameters)
```

```python
import numpy
import sys
from sumatra.parameters import build_parameters
from sumatra.decorators import capture

@capture
def main(parameters):
    numpy.random.seed(parameters["seed"])
    distr = getattr(numpy.random, parameters["distr"])
    data = distr(size=parameters["n"])
    output_file = "Data/%s.dat" % parameters["sumatra_label"]
    numpy.savetxt(output_file, data)

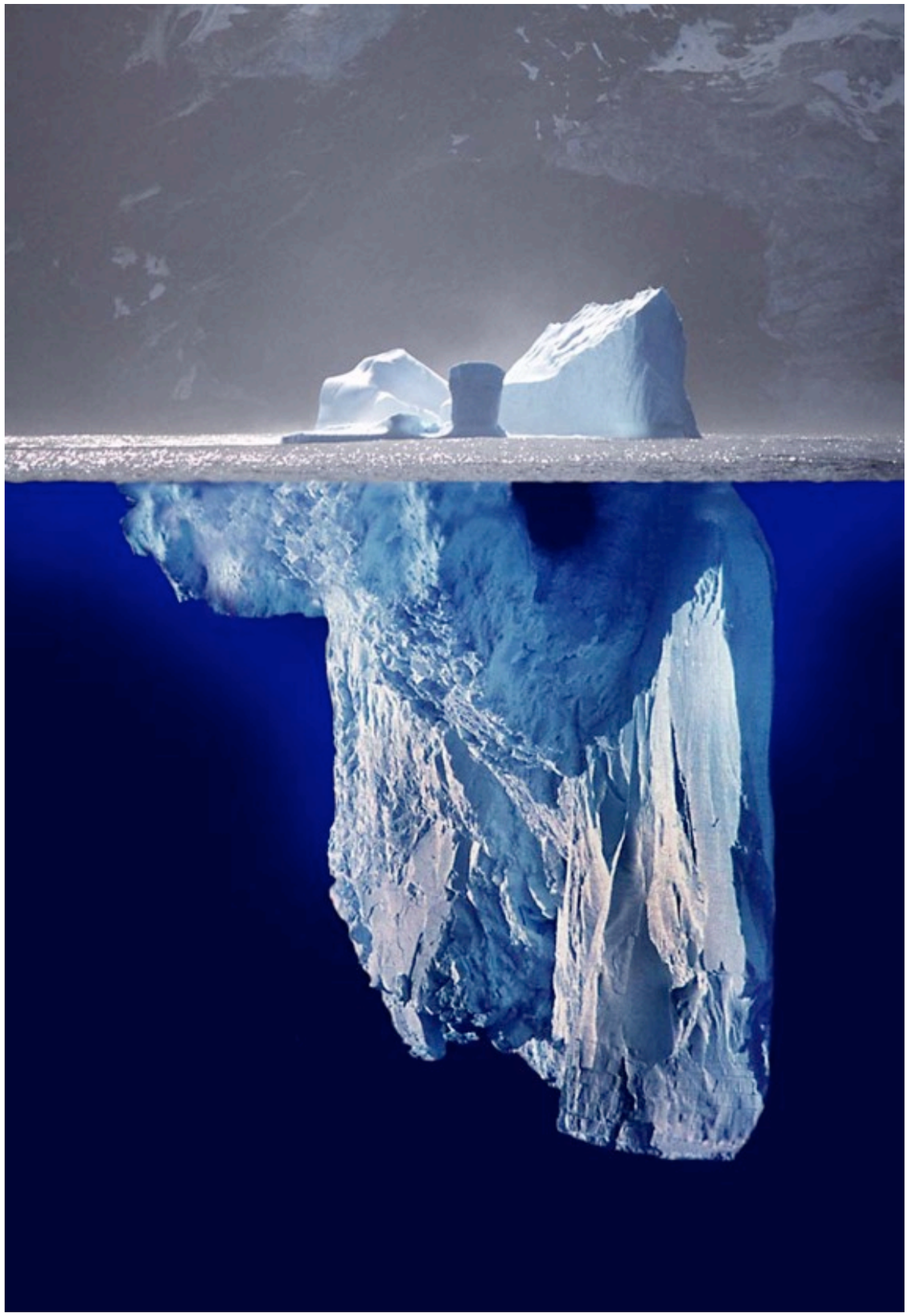
parameter_file = sys.argv[1]
parameters = build_parameters(parameter_file)
main(parameters)
```

Sumatra components



Code versioning and dependency tracking

the code, the whole code and nothing but the code



1. Recursively find imported/ included libraries
2. Try to determine version information for each of these, using
   1. code analysis
   2. version control systems
   3. package managers
   4. etc.

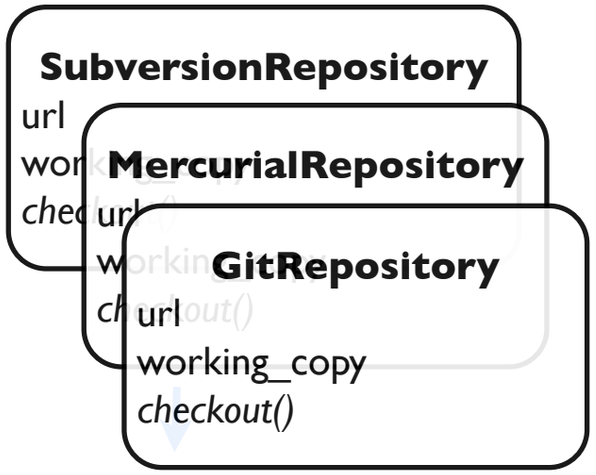
Iceberg by Uwe Kils http://commons.wikimedia.org/wiki/File:Iceberg.jpg

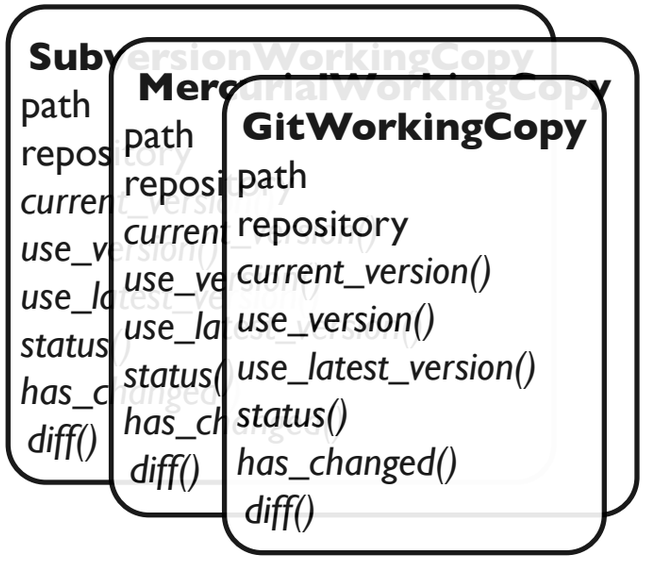
Code versioning and dependency tracking

the code, the whole code and nothing but the code

```
sumatra.dependency_finder.python
sumatra.dependency_finder.matlab
sumatra.dependency_finder.R
sumatra.dependency_finder.fortran

sumatra.versioncontrol.subversion
sumatra.versioncontrol.mercurial
sumatra.versioncontrol.git
sumatra.versioncontrol.bazaar
```





Launching computations

locally, remotely, serial or parallel

`sumatra.launch`

SerialLaunchMode
generate_command()
get_platform_information()
run()

DistributedLaunchMode
generate_command()
get_platform_information()
run()

BatchLaunchMode
generate_command()
get_platform_information()
run()

QueuedLaunchMode
generate_command()
get_platform_information()
run()

Parameter handling

Simple

```
a = 2
b = 3
c = [4, 5, 6]
```

Config

```
[foo]
  a: 2
  b: 3
[bar]
  c: [4, 5, 6]
```

JSON

```
{
  'foo': {
      'a': 2,
      'b': 3
      },
  'bar': {
      'c': [4, 5, 6]
      }
}
```

`sumatra.parameters`

Data handling

telling Sumatra where to find the data generated by your code and what to do with it

- Data generated on local file system
  - ➡ `FileSystemDataStore`
- Data on local file system and automatically archived
  - ➡ `ArchivingFileSystemDataStore`
- Data on local file system and mirrored to web (e.g. DropBox)
  - ➡ `MirroredFileSystemDataStore`
- Data generated in a relational database
  - ➡ `RelationalDataStore`
- Data automatically pushed to FigShare
  - ➡ `FigShareDataStore`

`sumatra.datastore`

Storing provenance information

for solo or collaborative projects

- local filesystem

- remote server

`sumatra.recordstore`

Remote record store

- RESTful API (JSON over HTTP):

/	GET
/<project_name>/[?tags=<tag1>,<tag2>,...]	GET
/<project_name>/tagged/<tag>/	GET, DELETE
/<project_name>/<record_label>/	GET, PUT, DELETE
/<project_name>/permissions/	GET, POST

Remote record store

UNIC – Neuroinformatics: Network simulations of self-sustained activity in networks of adaptive exponential integrate and fire neurons

https smt.andrewdavison.info/records/Destexhe_JCNS_2009/

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Network simulations of self-sustained activity in networks of adaptive exponential integrate and fire neurons

The aim of this project is to convert an original NEURON model written by Alain Destexhe, published in the following article:

> Destexhe, A. (2009) Self-sustained asynchronous irregular states and Up/Down states in thalamic, cortical and thalamocortical networks of nonlinear integrate-and-fire neurons. *Journal of Computational Neuroscience* **27**: 493-506. [arXiv preprint: http://arxiv.org/abs/0809.0654]

from Hoc to PyNN. Using PyNN makes it possible to simulate the model using the NEST and Brian simulators, and using the FACETS / BrainScaleS neuromorphic hardware, as well as NEURON.

The project is also intended as a case study of converting a NEURON model to PyNN.

Label	Reason	Outcome	Duration	Date/Time	Executable	Repository	Version	Script	Argu
20120928-114020	Plot data from the last simulation run with NEURON		2.20 s	2012-09-28 11:40:20	Python 2.7.1	https://bitbucket.org/apdavison/destexhe_jcns_2009	5f6221aa3a14	plot.py	spike num Vm_
20120928-113952	Plot data from the last simulation run with NEST		2.26 s	2012-09-28 11:39:52	Python 2.7.1	https://bitbucket.org/apdavison/destexhe_jcns_2009	5f6221aa3a14	plot.py	spike num Vm_
20120928-110307	Plot data from the previous simulation run	Up- and down-states seen. Spike display truncated.	2.49 s	2012-09-28 11:03:07	Python 2.7.1	https://bitbucket.org/apdavison/destexhe_jcns_2009	05644ae81d7c	plot.py	spike num Vm_
20120928-105047	Running pure PyNN version with NEURON backend	Network structure different due to different random number generator. Mean firing	59.93 s	2012-09-28 10:50:47	Python 2.7.1	https://bitbucket.org/apdavison/destexhe_jcns_2009	05644ae81d7c	demo_cx05_N=500b_LTS.py	neur

Remote record store

https://smt.andrewdavison.info/records/Destexhe_JCNS_2009/?format=json

https smt.andrewdavison.info/records/Destexhe_JCNS_2009/?format=json

Porting... | https:/... | reStruc... | Creatin... | web.ar... | WP5T3... | {3} Acti... | PROV-... | Sumatr... | Covera... | Sumatr... | Managi...


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Destexhe, A. (2009) Self-sustained asynchronous irregular states and Up/Down states in thalamic, cortical and thalamocortical networks of nonlinear
integrate-and-fire neurons.  *Journal of Computational Neuroscience* **27**: 493-506. [arXiv preprint: http://arxiv.org/abs/0809.0654]\n\nfrom Hoc to PyNN_.
Using PyNN makes it possible to simulate the model using the NEST_ and Brian_ simulators, and using the FACETS / BrainScaleS_ neuromorphic hardware, as well
as NEURON.\n\nThe project is also intended as a case study of converting a NEURON model to PyNN.\n\n.. _NEURON: http://www.neuron.yale.edu/neuron\n.. _PyNN:
http://neuralensemble.org/PyNN\n.. _NEST: http://www.nest-initiative.org/\n.. _Brian: http://briansimulator.org/\n.. _BrainScaleS:
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```

Remote record store

- **Clients:**
  - browser
  - HttpRecordStore (part of `sumatra` package)
  - curl
- **Server implementations:**
  - Django-based (https://bitbucket.org/apdavison/sumatra_server/)
  - MongoDB-based (https://github.com/btel/Sumatra-MongoDB)

Plans / Ideas

- Dependency finders for R, Fortran, C/C++, Ruby
- Better support for projects with build steps/integration with build tools
- LaTeX package
- Export in W3C PROV-XML or PROV-O format
- Better support for pipelines
- Support for parameter searching (“smt batch”)
- IPython Notebook integration?
- Export of recipes enabling recreation of environment
- Alternative web views, e.g. diary format - more like a traditional lab notebook

Community

- 6 contributors (including 1 GSoC student)
- mailing list has 39 members
- previous version had 1222 downloads in 18 months, current version 248 downloads in two months
- http://neuralensemble.org/sumatra
- (mirror) https://bitbucket.org/apdavison/sumatra

Sumatra

Simulation Management Tool

http://neuralensemble.org/sumatra

Sawahs in West Sumatra by CharlesFred http://www.flickr.com/photos/charlesfred/2869003149/

Sumatra

~~Simulation~~/Management Tool
Computational Experiment

http://neuralensemble.org/sumatra

Sawahs in West Sumatra by CharlesFred http://www.flickr.com/photos/charlesfred/2869003149/


Sumatra
Nothing to do with Java
Sumatra by smysnbrg http://www.flickr.com/photos/87169621@N00/1018131117/


Sumatra
Not a million miles
from Madagascar
Indian Ocean map by Tentotwo https://commons.wikimedia.org/wiki/File:Indian_Ocean_laea_location_map.svg

Conclusions

To be accepted by busy scientists, a tool to assist with making research more reproducible should:

- be part of day-to-day workflow
- be easy to use
- require minimal changes to existing workflows
- provide immediate benefit

As tool developers, we should think about making as much as possible of our functionality available as libraries, so others can find new ways to use it


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http://www.andrewdavison.info
Sumatran orangutan
by BelalangJantan http://www.flickr.com/photos/7164478@N07/3575735482/