Automated tracking of computational experiments using Sumatra

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Reproducibility

attack of the clone santas by slowburn, http://www.flickr.com/photos/36266791@N00/70150248/

Replicability ⟷ Reproducibility

Reproduction of the original results using the same tools

- by the original author on the same machine
- by someone in the same lab/using a different machine
- by someone in a different lab

Reproduction using different software, but with access to the original code

Completely independent reproduction based only on text description, without access to the original code

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Replicability

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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
- memory limitations
  - forgetting, implicit knowledge not passed on

What can we do about it?

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
- memory limitations
  - record everything

What do we need to record?

- the code that was run
- how it was run (parameter files, input data, command-line options)
- the platform on which it was run
- why was it run?
- what was the outcome? (output data, figures, qualitative interpretation)

Recording the code that was run

- store a copy of the executable
- or of the source code
- including that of any libraries used
- as well as the compiler used
- and the compilation procedure

Recording the code that was run

- the version of the interpreter
- and any options used in compiling it
- a copy of the simulation script
- and of any external modules or packages that are imported/included

Recording the code that was run

- instead of storing a copy of the code we can store the repository URL and version number

Recording platform information

- processor architecture
- operating system
- number of processors

Recording all this by hand is tedious
and error-prone

A STORY TOLD IN FILE NAMES:

Location: C:\user\research\data

Filename	Date Modified	Size	Type
data_2010.05.28_test.dat	3:37 PM 5/28/2010	420 KB	DAT file
data_2010.05.28_re-test.dat	4:29 PM 5/28/2010	421 KB	DAT file
data_2010.05.28_re-re-test.dat	5:43 PM 5/28/2010	420 KB	DAT file
data_2010.05.28_calibrate.dat	7:17 PM 5/28/2010	1,256 KB	DAT file
data_2010.05.28_huh??.dat	7:20 PM 5/28/2010	30 KB	DAT file
data_2010.05.28_WTF.dat	9:58 PM 5/28/2010	30 KB	DAT file
data_2010.05.29_aaarrrgh.dat	12:37 AM 5/29/2010	30 KB	DAT file
data_2010.05.29_#$@*&!!.dat	2:40 AM 5/29/2010	0 KB	DAT file
data_2010.05.29_crap.dat	3:22 AM 5/29/2010	437 KB	DAT file
data_2010.05.29_notbad.dat	4:16 AM 5/29/2010	670 KB	DAT file
data_2010.05.29_woohoo!!.dat	4:47 AM 5/29/2010	1,349 KB	DAT file
data_2010.05.29_USETHISONE.dat	5:08 AM 5/29/2010	2,894 KB	DAT file
analysis_graphs.xls	7:13 AM 5/29/2010	455 KB	XLS file
ThesisOutline!.doc	7:26 AM 5/29/2010	38 KB	DOC file
Notes_Meeting_with_ProfSmith.txt	11:38 AM 5/29/2010	1,673 KB	TXT file
JUNK...	2:45 PM 5/29/2010		Folder
data_2010.05.30_startingover.dat	8:37 AM 5/30/2010	420 KB	DAT file

Type: Ph.D Thesis Modified: too many times

Recording all this by hand is tedious
and error-prone

let's automate it

What should this automated lab notebook look like?

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

- automate as much as possible, prompt the user for the rest
- interact with version control systems (Subversion, Git, Mercurial, Bazaar ...)
- support serial, distributed, batch simulations/analyses
- link to data generated by the simulation/analysis
- support all and any (command-line driven) simulation/analysis programs
- support both local and networked storage of simulation/analysis records

Requirements

- Be very easy to use, or only the very conscientious will use it

Sumatra

- a Python package to enable systematic capture of the environment of numerical simulations/analyses
- can be used directly in your own code
- or as the basis for interfaces

Current

- a command line interface, `smt`
- a web interface, `smtweb`

Future

- could be integrated into existing GUI-based tools
- or new desktop/web-based GUIs written from scratch

Sumatra

http://neuralensemble.org/sumatra

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

Sumatra

Simulation Management Tool

http://neuralensemble.org/sumatra

Sumatra

~~Simulation~~/Management Tool
Computational Experiment

http://neuralensemble.org/sumatra

Sumatra

Nothing to do with Java

Dependencies

- Python bindings for your preferred version control system (`pysvn`, `mercurial`, `PyGit`, `bzrlib`)
- Django (only needed for web interface)
- mpi4py (if running distributed computations), httplib2

Installation

```
> easy_install sumatra
```

smt

```
$ cd myproject
```

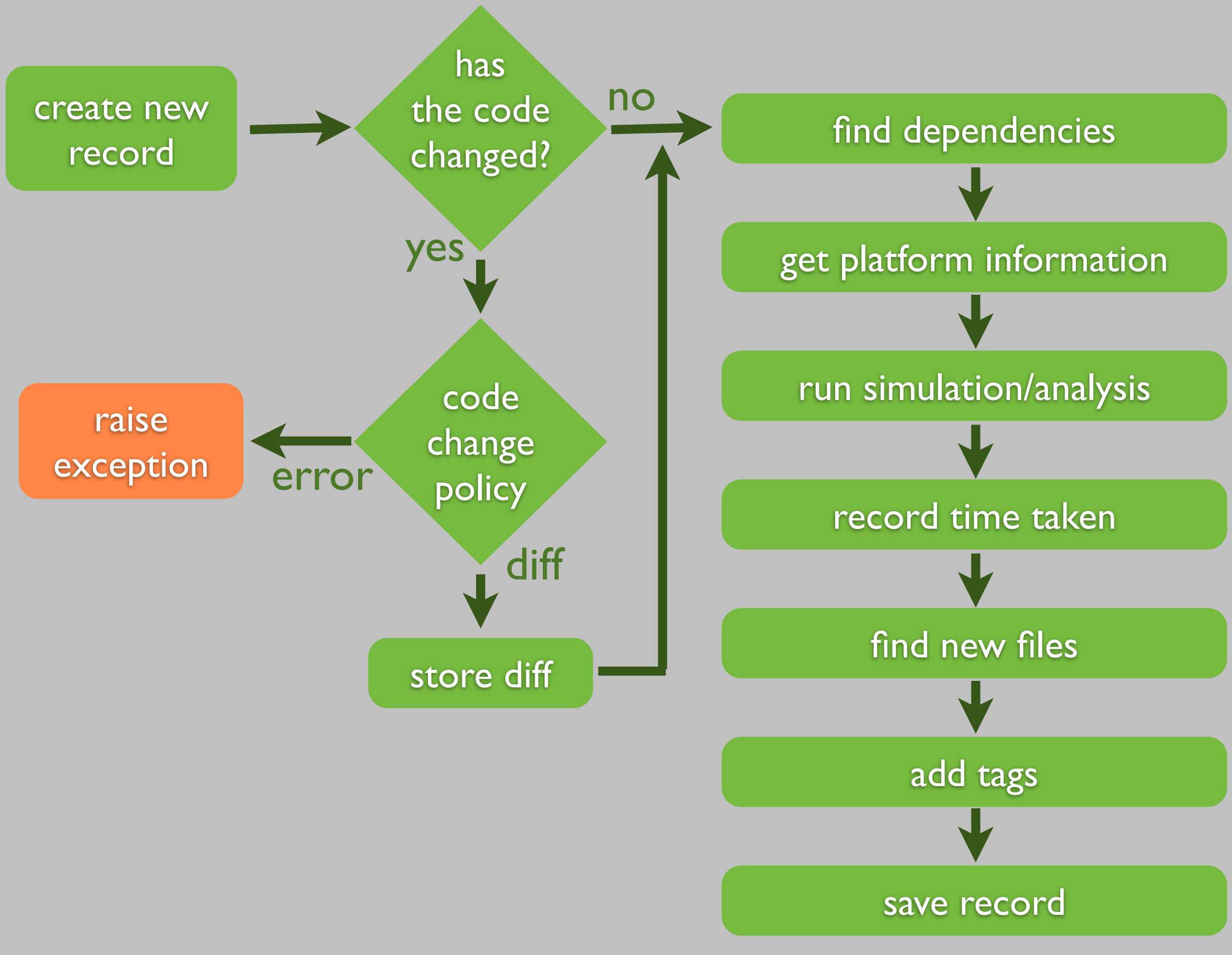
```
$ smt init MyProject
```

```
$ python main.py default.param

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

$ smt run default.param

$ smt run --simulator=python --main=main.py 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! Nobel prize
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 info
Sumatra project
---------------
Name                   : MyProject
Default executable     : Python (version: 2.6.2) at /usr/bin/python
Default repository     : MercurialRepository at /path/to/myproject
                         rf9ab74313efe (main file is main.py)
Default main file      : main.py
Default launch mode    : serial
Data store (output)    : ./Data
.          (input)     : /
Default launch mode    : serial
Record store           : Relational database record store using the
                         Django ORM (database file=.smt/records)
Code change policy     : error
Append label to        : None
```

```
$ 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
```

```
$ smtweb -p 8002 &
```

Sumatra: TestProject: List of records

http://127.0.0.1:8002/

Google

TestProject: List of records

Delete include data	Label	Reason	Outcome	Duration	Processes	Simulator		Script			Date	Time	Tags
						Name	Version	Repository	Main file	Version			
☐	20100709-154255		'Eureka! Nobel prize here we come.'	0.59 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:42:55	
☐	20100709-154309			0.59 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:43:09	
☐	haggling	'determine whether the gourd is worth 3 or 4 shekels'	'apparently, it is worth NaN shekels.'	0.59 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:43:20	foobar
☐	20100709-154338	'test effect of a smaller time constant'		0.59 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:43:38	
☐	haggling_repeat	Repeat experiment haggling	The new record exactly matches the original.	0.58 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:43:47	

Sumatra: TestProject: haggling

http://127.0.0.1:8002/haggling/

Google

TestProject: *haggling*

Save changes | Delete

Return to record list

Label: haggling

Reason: 'determine whether the gourd is worth 3 or 4 shekels'

Outcome: 'apparently, it is worth NaN shekels.'

Timestamp: 09/07/2010 15:43:20

Duration: 0.59 s

Executable: Python version 2.5.2 (/usr/local/bin/python)

Launch mode: serial

Repository: /Users/andrew/tmp/SumatraTest

Main file: main.py

Version: 396c2020ca50

Tags: foobar

Data files

/Users/andrew/tmp/SumatraTest/Data

example2.dat 1.2 KB

Parameters

n = 50
seed = 34326
distr = normal

Dependencies

Name	Path	Version
Carbon	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/plat-mac/Carbon	unknown
Finder	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/plat-mac/lib-scriptpackages/Finder	unknown

Dependencies

Name	Path	Version
Carbon	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/plat-mac/Carbon	unknown
Finder	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/plat-mac/lib-scriptpackages/Finder	unknown
PyQt4	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/site-packages/PyQt4	unknown
Pyrex	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/site-packages/Pyrex-0.9.8.5.0001-py2.5.egg/Pyrex	unknown
StdSuites	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/plat-mac/lib-scriptpackages/StdSuites	unknown
_builtinSuites	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/plat-mac/lib-scriptpackages/_builtinSuites	unknown
_xmlplus	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/site-packages/PyXML-0.8.4.0003-py2.5-macosx-10.3-fat.egg/_xmlplus	0.8.4
dateutil	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/site-packages/python_dateutil-1.4.0001-py2.5.egg/dateutil	1.4
enthought	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/site-packages/TraitsGUI-3.0.2-py2.5.egg/enthought	unknown
matplotlib	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/site-packages/matplotlib-0.98.3.0001-py2.5-macosx-10.3-fat.egg/matplotlib	0.98.3
mpl_toolkits	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/site-packages/matplotlib-0.98.3.0001-py2.5-macosx-10.3-fat.egg/mpl_toolkits	unknown
numarray	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/site-packages/numarray-1.5.2.0001-py2.5-macosx-10.3-fat.egg/numarray	1.5.2
numpy	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/site-packages/numpy-1.1.1.0001-py2.5-macosx-10.3-fat.egg/numpy	1.1.1
pytz	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/site-packages/pytz-2008c.0001-py2.5.egg/pytz	2008c
setuptools	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/site-packages/setuptools-0.6c8.0002-py2.5.egg/setuptools	0.6c8
wx	/Library/Frameworks/Python.framework/Versions/4.0.30002/lib/python2.5/site-packages/wxPython-2.8.7.1.0001_s-py2.5-macosx-10.3-fat.egg/wx	2.8.7.1 (mac-unicode)

Platform information

Name	IP address	Processor	Architecture	System type	Release	Version
dhcp-12-56.ens.fr	129.199.12.56	i386 i386	32bit	Darwin	9.8.0	Darwin Kernel Version 9.8.0: Wed Jul 15 16:55:01 PDT 2009; root:xnu-1228.15.4~1/RELEASE_I386

TestProject: *haggling*

Return to record

example2.dat

```
7.907044147908758314e-01
9.477014701088509741e-02
1.675740714241656715e+00
8.087734934749459814e-01
-3.930586588052103481e-01
1.135906247492430410e+00
-3.364521723023050082e-01
-1.618924993187704220e-01
4.502319146511311598e-01
-6.229447130613413597e-01
-8.749602125292015309e-01
-1.022383310028285530e+00
1.631837671625364194e+00
7.071715339639573772e-01
-3.857494957160916838e-01
-1.938590502404218929e+00
-3.840079545304994069e-01
2.543672264647489079e-01
-1.590639681557504126e+00
9.755700771898647705e-01
3.394566100954360954e-01
1.546769138105918984e+00
-5.617409082801874121e-01
-1.863397012724956836e+00
6.564861554841714408e-01
1.053391199630216102e+00
2.709896780028555607e-01
-5.829809662700129458e-01
2.117353834389190226e+00
5.411866008757018065e-01
-6.029287547744773823e-01
-5.801084967982524793e-02
-3.708293525285061842e-01
-1.048902119461476934e+00
-9.423948053155544180e-01
8.458066748157527792e-02
-5.192887844952853715e-01
-9.214658744583642536e-01
5.349458364200462279e-01
```

Using `sumatra` within your own 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)
```

```
import numpy
import sys
import time
from sumatra.projects import load_project
from sumatra.parameters import build_parameters

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)

project = load_project()
record = project.new_record(parameters=parameters,
                            main_file=__file__,
                            reason="reason for running this simulation")
parameters.update({"sumatra_label": record.label})
start_time = time.time()

main(parameters)

record.duration = time.time() - start_time
record.output_data = record.datastore.find_new_data(record.timestamp)
project.add_record(record)

project.save()
```

```
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)
```

Supported parameter file formats

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]
      }
}
```

Finding dependencies

- requires per-language implementation

  currently supported: Python, Hoc, GENESIS script language

  planned: Matlab, Octave, R *(collaborators wanted...)*

- version finding based on various heuristics:

  some language specific (e.g. in Python check for `__version__`, `get_version()`, `...`)

  some generic (where dependency code is under version control system, managed by package manager...)

Linking to input and output data

- Intention to support different data stores (filesystem, relational database, ...)
- Stores SHA1 digest of data to ensure file contents haven't changed
- `smtweb` has 'smart' display for certain data types (e.g. csv is displayed as HTML table)

Record stores

- multiple ways to store experiment records, to support both solo/ local and collaborative/distributed projects:

  - simple (no dependencies, does not support smtweb)
  - Django/SQLite-based (default)
  - remote (HTTP+JSON)

Remote record store & Sumatra Server

- 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`

- Client: HttpRecordStore (part of `sumatra` package)
- Server: Django site including `sumatra_server` app (https://bitbucket.org/apdavison/sumatra_server/)

  (Bartosz Telenczuk has also started to implement a MongoDB-based server https://github.com/btel/Sumata-MongoDB)

Version control

- your code is *required* to be under version control
- currently supports Subversion, Git, Mercurial, Bazaar

Discussion points:

- could just store copy of code, but want to promote best practice
- version control by stealth?

Plans

(contributions of code and ideas welcome)

- determine compilation options for executable, where possible
- determine version, compilation options for Python C-extensions, shared libraries more generally (interact with Linux package managers?)
- Implement other `DataStores`, e.g. based on FTP, HDF5, SQLite, DropBox
- Add `dependency_finder` sub-modules for Matlab, Octave, R, C/C++
- add remote launch option (ssh-based)
- implement `BatchLaunchMode`
- add support for simple workflows (running multiple computations sequentially)
- enable launching computations from the web interface

Summary

Sumatra

- a toolbox for automated metadata capture for computational experiments
- basic metadata captured for any language, logging dependencies requires language-specific plugin

`smt`

- requires no changes to existing code
- requires minimal changes to workflow
- “Be very easy to use, or only the very conscientious will use it”

http://neuralensemble.org/sumatra

@apdavison

http://www.andrewdavison.info

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

Project
name
description
default_executable
default_repository
default_main_file
default_launch_mode
data_store
record_store
on_changed
data_label
save()
info()
new_record()
launch()
update_code()
add_record()
get_record()
delete_record()
delete_by_tag()
format_records()
most_recent()
add_comment()
add_tag()
remove_tag()
compare()
show_diff()

RecordStore
save()
get()
list()
labels()
delete()
delete_by_tag()
most_recent()

Executable
name
path
version

Record
label
timestamp
reason
duration
executable
repository
main_file
version
parameters
input_data
script_arguments
launch_mode
datastore
outcome
output_data
dependencies
platforms
tags
diff
user
on_changed
register()
run()
describe()
difference()
delete_data()

Dependency
name
path
version
diff

WorkingCopy
path
repository
current_version()
use_version()
use_latest_version()
status()
has_changed()
diff()

Repository
url
checkout()
get_working_copy()

DataKey
path
digest

DataStore
find_new_data()
archive()
get_data_item()
get_content()
delete()

ParameterSet
save()
update()
__getitem__()
pretty()

LaunchMode
generate_command()
get_platform_information()
pre_run()
run()

Project
name
description
default_executable
default_repository
default_main_file
default_launch_mode
data_store
record_store
on_changed
data_label
save()
info()
new_record()
launch()
update_code()
add_record()
get_record()
delete_record()
delete_by_tag()
format_records()
most_recent()
add_comment()
add_tag()
remove_tag()
compare()
show_diff()

PythonExecutable
name
path
version

NEURONSimulator
name
path
version

NESTSimulator
name
path
version

ShelveRecordStore
save()
get()
list()
labels()
delete()
delete_by_tag()
most_recent()

DjangoRecordStore
save()
get()
list()
labels()
delete()
delete_by_tag()
most_recent()

HttpRecordStore
save()
get()
list()
labels()
delete()
delete_by_tag()
most_recent()

Record
label
timestamp
reason
duration
executable
repository
main_file
version
parameters
input_data
script_arguments
launch_mode
datastore
outcome
output_data
dependencies
platforms
tags
diff
user
on_changed
register()
run()
describe()
difference()
delete_data()

Dependency
name
path
version
diff
on_changed

SubversionWorkingCopy
path
repos
current
use_v
use_l
status
has_c
diff()

MercurialWorkingCopy
path
repos
current
use_ve
use_la
status(
has_ch
diff()

GitWorkingCopy
path
repository
current_version()
use_version()
use_latest_version()
status()
has_changed()
diff()

SubversionRepository
url
wo
che

MercurialRepository
url
w
ch

GitRepository
url
working_copy
checkout()

FileSystemDataStore
find_new_files()
archive()
list_files()
get_content()

SimpleParameterSet
save()
update()
__g
pre

NTParameterSet
save()
upd
__g
pre

JSONParameterSet
sav
up
__
pr

ConfigParser ParameterSet
save()
update()

SerialLaunchMode
generate_command()
get
pre
ru

DistributedLaunchMode
generate_command()
get_platform_information()
pre_run()
run()