Reproducible research

Lessons from the open source world

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Outline

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Who am I?

Background

- **Particle physics** (theory/computation): numerical QCD
- **Applied mathematics**: algorithm development for PDEs
- **Neuroscience**: algorithms and tools for brain imaging

A common thread: open source computational tools

- **IPython**: interactive Python
- **Matplotlib**: visualization
- **Numpy**: numerics
- **Scipy**: scientific algorithms
- **Nipy**: neuroimaging tools

What does it take to get reproducible research *results?*

Reproducible research practices!

Reproducibility at publication time?
It's already too late.

Learn from a community (open source) where reproducibility is an everyday practice (by necessity)

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Mea culpa: a typical computational publication

ELSEVIER

Available online at www.sciencedirect.com

ScienceDirect

Appl. Comput. Harmon. Anal. 24 (2008) 354–377

Applied and Computational Harmonic Analysis

www.elsevier.com/locate/acha

Fast adaptive algorithms in the non-standard form for multidimensional problems ☆

Gregory Beylkin *, Vani Cheruvu, Fernando Pérez

Department of Applied Mathematics, University of Colorado, Boulder, CO 80309-0526, USA

Received 6 June 2007; accepted 2 August 2007

Available online 14 August 2007

Communicated by Vladimir Rokhlin

Abstract

We present a fast, adaptive multiresolution algorithm for applying integral operators with a wide class of radially symmetric kernels in dimensions one, two and three. This algorithm is made efficient by the use of separated representations of the kernel. We discuss operators of the class $(-\Delta + \mu^2 I)^{-\alpha}$, where $\mu \geqslant 0$ and $0 < \alpha < 3/2$, and illustrate the algorithm for the Poisson and Schrödinger equations in dimension three. The same algorithm may be used for all operators with radially symmetric kernels

Pages of algorithmia as equations or vague methods descriptions

a periodic analogue of the Hilbert transform. In order to find its representation in multiwavelet bases, we compute

$$r_{ii'}^{j;l} = 2^{-j} \int_{-1}^{1} K\big(2^{-j}(x+l)\big)\Phi_{ii'}(x)\,\mathrm{d}x = 2^{-j} \int_{-1}^{1} \cot\big(\pi 2^{-j}(x+l)\big)\Phi_{ii'}(x)\,\mathrm{d}x, \tag{12}$$

where $\Phi_{ii'}(x)$, $i, i' = 0, \ldots, k-1$ are cross-correlation functions described in Appendix A.4 and $l = 0, \pm 1, \pm 2, \ldots, 2^j - 1$. We compute $r_{ii'}^{j;l}$ using the convergent integrals

$$r_{ii'}^{j;l} = 2^{-j} \sum_{k=i'-i}^{i'+i} c_{ii'}^{k} \int_{0}^{1} \Phi_{k,0}^{+}(x)\Big(\cot\big(\pi 2^{-j}(x+l)\big) + (-1)^{i+i'} \cot\big(\pi 2^{-j}(-x+l)\big)\Big)\,\mathrm{d}x,$$

where $\Phi_{k,0}^{+}$ is a polynomial described in Appendix A.4. In our numerical experiment, we apply (11) to the periodic function on [0, 1],

$$f(x) = \sum_{k \in \mathbb{Z}} e^{-a(x+k-1/2)^2},$$

Tables and pretty figures. Now in color!

Table 1
Results from evaluating (13) with our algorithm

p	Scales	N_{blocks}	ϵ	E_2
5	[2,3,4]	8	10^{-3}	1.5×10^{-4}
8	[2,4,5]	12	10^{-6}	1.3×10^{-7}
11	[2,4,5]	14	10^{-9}	1.1×10^{-10}
14	[3,4,5]	16	10^{-12}	4.4×10^{-13}

Notes. The order of the basis p is adjusted as a function of the requested precision ϵ. The second column indicates scales present in the adaptive tree for the input. The third column shows the total number of blocks of coefficients in this tree. The last column (E_2) shows the actual error of the computed solution in the ℓ^2 norm.

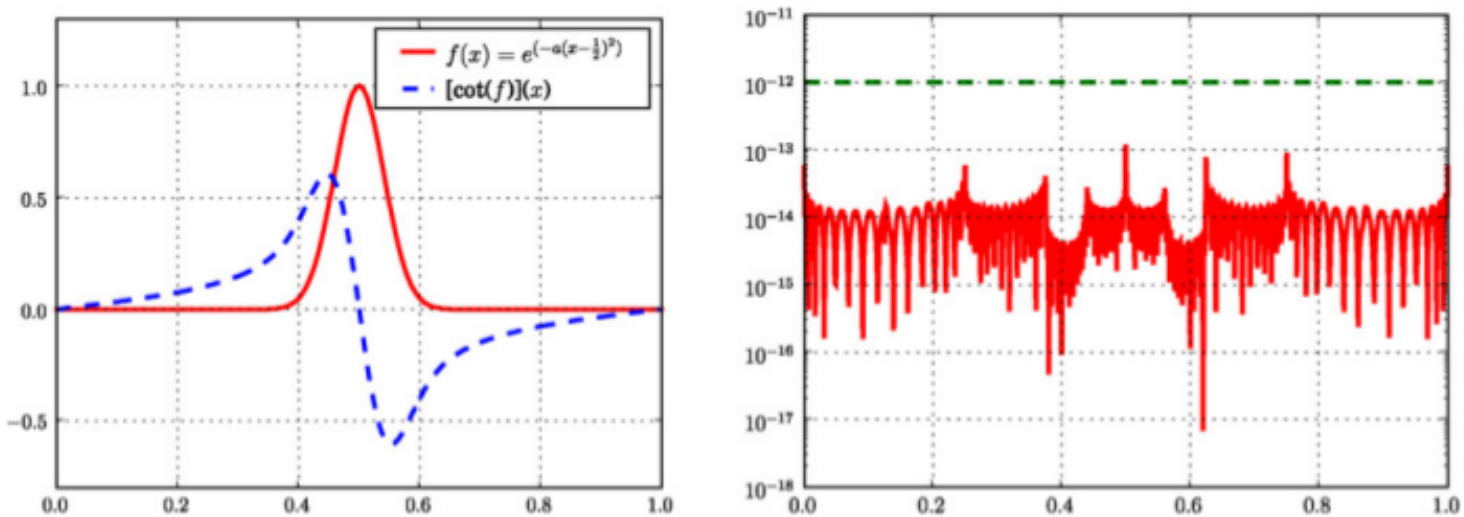
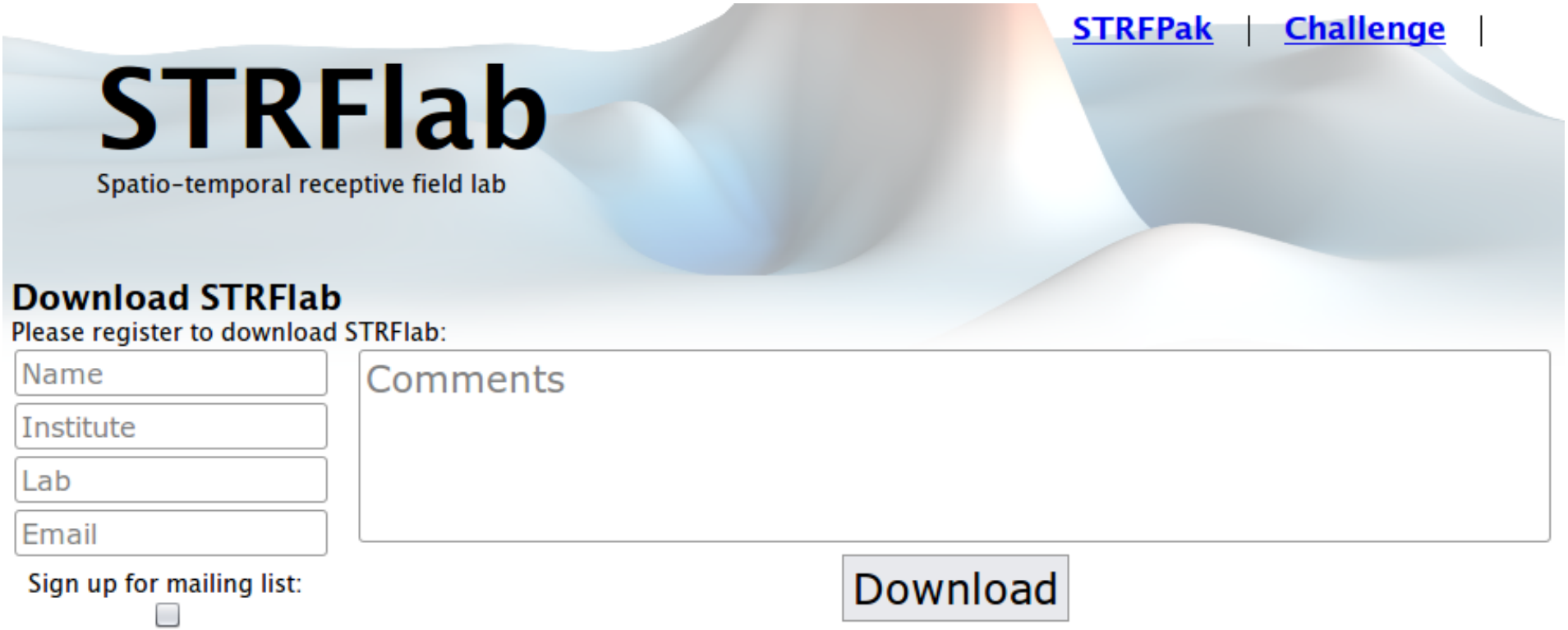


Fig. 3. Results of applying the cotangent kernel to a periodized Gaussian using basis of order $p = 14$ (the last row in Table 1). The pointwise error is shown on the right for a requested accuracy of $\epsilon = 10^{-12}$.

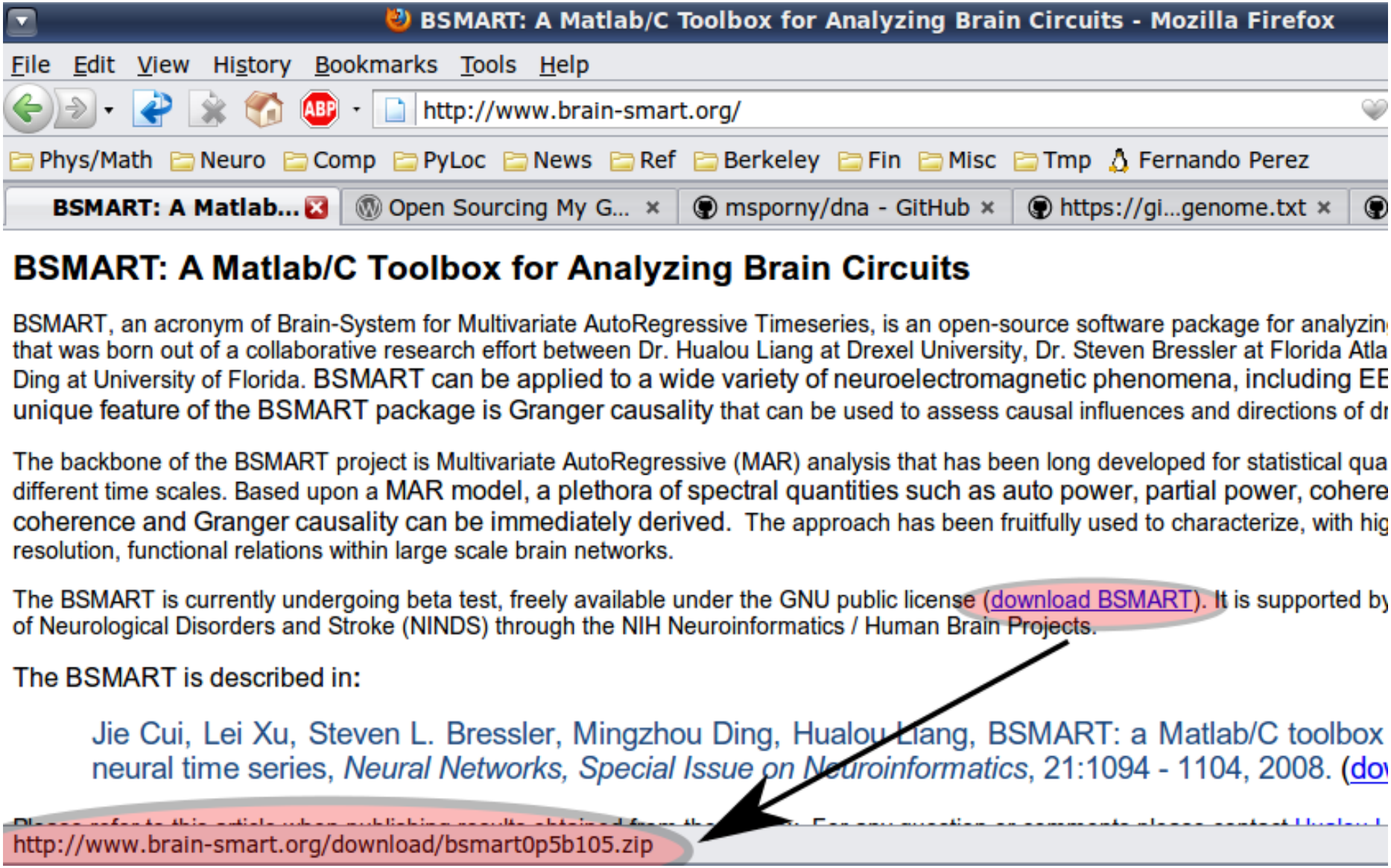
Chance of reproducing results for third parties?

$$\mathcal{O}(10^{-\text{something very big}})$$

Registration-wall software



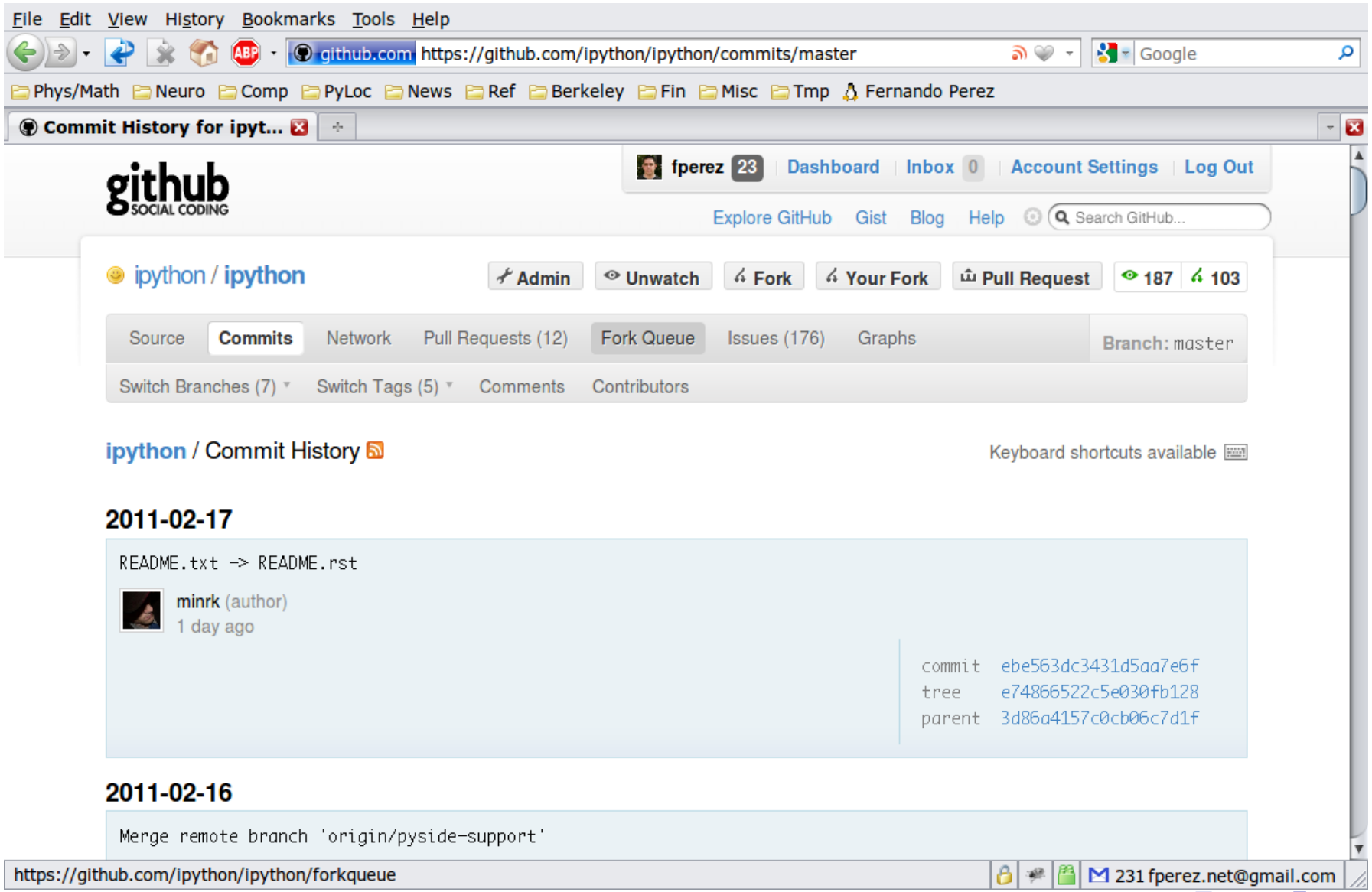
Zip file/tarball dumps



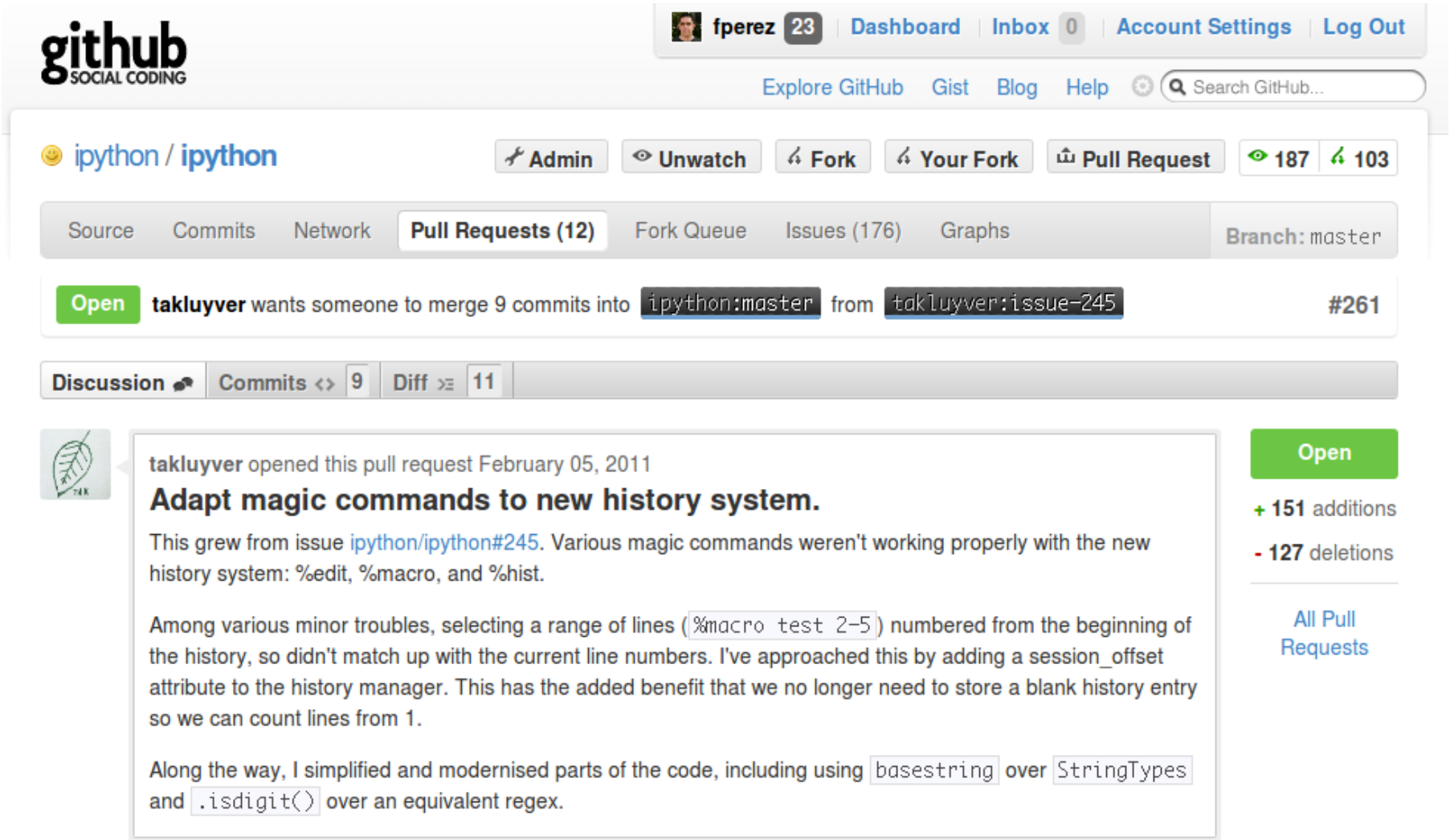
Contrast: FOSS better than scientific research?

FOSS: Free and Open Source Software

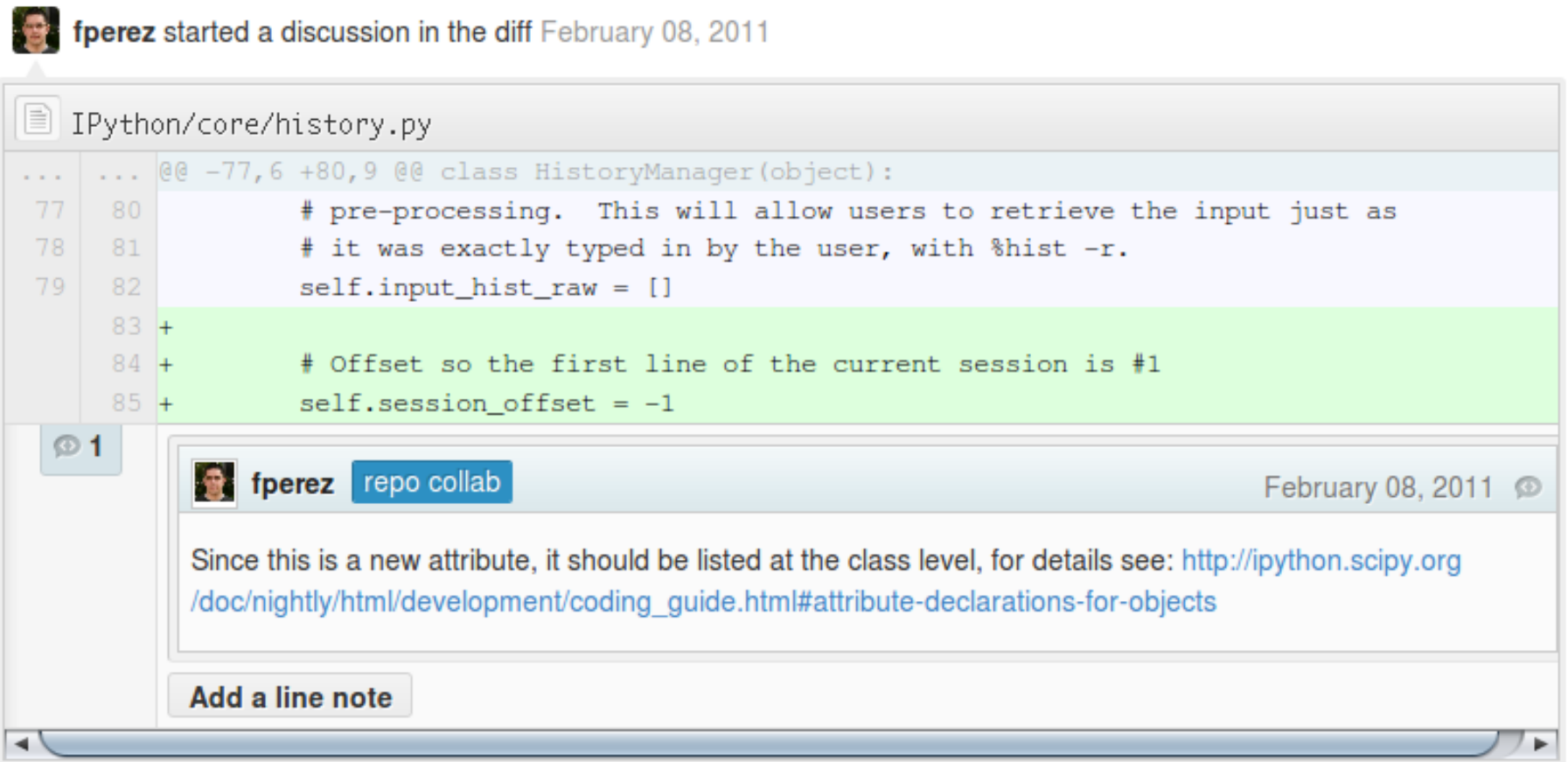
Public distributed version control: provenance tracking



Pull requests: ongoing peer review



Pull requests: back and forth discussion



fperez started a discussion in the diff February 08, 2011

IPython/core/history.py

```
...  ...  @@ -77,6 +80,9 @@ class HistoryManager(object):
77   80           # pre-processing.  This will allow users to retrieve the input just as
78   81           # it was exactly typed in by the user, with %hist -r.
79   82           self.input_hist_raw = []
     83   +
     84   +       # Offset so the first line of the current session is #1
     85   +       self.session_offset = -1
```

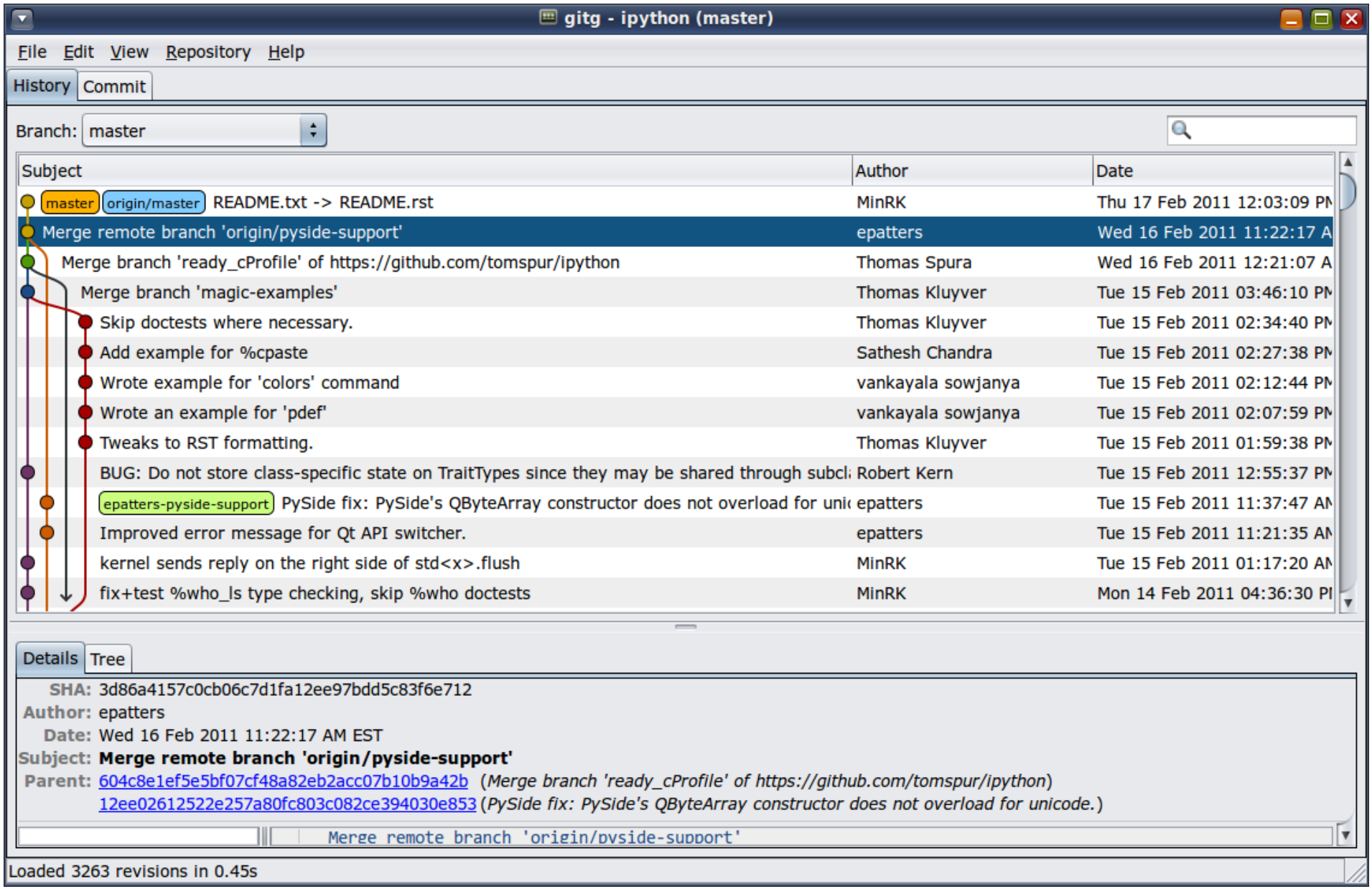
1

fperez repo collab February 08, 2011

Since this is a new attribute, it should be listed at the class level, for details see: http://ipython.scipy.org/doc/nightly/html/development/coding_guide.html#attribute-declarations-for-objects

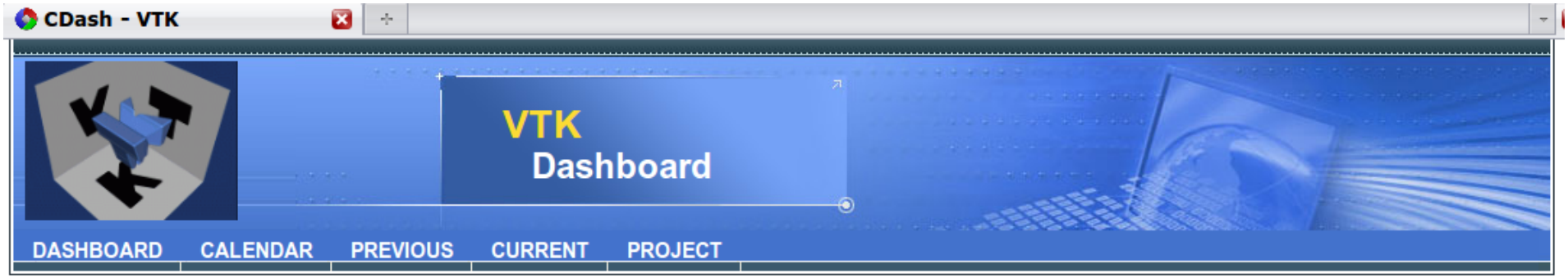
Add a line note

Branches: exploratory work with control



Automated tests: validation

The VTK Build Dashboard: immediate feedback



9 files changed by 5 authors as of **Friday, February 18 2011 20:00:00 EST** Help

[Show Filters]

Nightly Expected

Site	Build Name	Update		Configure			Build			Test				Build Time
		Files	Min	Error	Warn	Min	Error	Warn	Min	NotRun	Fail	Pass	Min	
p90n03.pbm.ihost.com	AIX00F614-xlC	8	0.1	0	0	4.4	0	0	167.7	0	5	835	34.2	2011-02-19T04:01:58 EST
londinium.kitware	Arch-GCC-4.5-x86_64-debug	8	0.2	0	0	1	0	4	11.4	0	8	1356	45.4	2011-02-18T21:53:58 EST
londinium.kitware	Arch-GCC-4.5-x86_64-release	0	0.1	0	0	0.9	0	8	18.1	0	6	1357	27.9	2011-02-18T23:17:26 EST
amber1.kitware	Debian4-x64-gcc	8	0.4	0	0	1.2	0	0	51.4	0	1	518	10.2	2011-02-18T21:06:41 EST

Public bug trackers

sympy

Python library for symbolic mathematics

Search projects

Project Home | Downloads | Wiki | **Issues** | Source

New issue **Search** Open issues **for** Search Advanced search Search tips

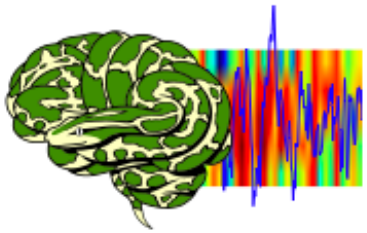
1 - 100 of 891 Next › **List** | Grid

	ID ▼	Type ▼	Status ▼	Priority ▼	Milestone ▼	Owner ▼	Summary + Labels ▼
☆	2018	Defect	Accepted	Critical	Release0.7.0	smi...@gmail.com	terms vs factors NeedsBetterPatch smichr
☆	2126	Defect	Accepted	Critical	Release0.7.0	smi...@gmail.com	fix doctest or quality testing to recognize doctests NeedsBetterPatch smichr Testing
☆	2133	Defect	Started	Critical	Release0.7.0	matt...@gmail.com	Merge new polynomials manipulation module Polynomial NeedsBetterPatch mattpap NeedsReview
☆	2151	Defect	Accepted	Critical	Release0.7.0	Ronan.L...@gmail.com	BasicMeta.keep_sign Series
☆	1276	Defect	Started	High	Release0.7.0	----	solve(-1 + x**2 + 0.111111111111111*(1.00000000000000 + 2.00000000000000*x)**2,x) fails EasyToFix Polynomial Solvers
☆	1721	Defect	Accepted	High	Release0.7.0	Ronan.L...@gmail.com	Rename class 'Real'
☆	1735	Defect	New	High	Release0.7.0	Ronan.L...@gmail.com	Rename .func attribute (.args too?)
☆	1919	Enhancement	Accepted	High	Release0.7.0	Vinzent.Steinberg	unify behavior of var() and symbols() NeedsReview smichr mattpap
☆	51	Enhancement	Started	Medium	Release0.7.0	matt...@gmail.com	RootOf for polynomial equations Polynomial NeedsReview mattpap
☆	326	Defect	Started	Medium	Release0.7.0	matt...@gmail.com	sympy.roots_.sturm(...) hangs Polynomial EasyToFix NeedsReview mattpap
☆	527	Enhancement	Started	Medium	Release0.7.0	----	guessing what functions, like integrate, roots, factor, apart (and many more), should do with the given expression NeedsReview mattpap

Documentation: Sphinx

Math, code and validated examples: literate programming

Nitime: time-series analysis for neuroscience



Auditory processing in grasshoppers ¶

Extracting the average time-series from one signal, time-locked to the occurence of some type of event in another signal is a very typical operation in the analysis of time-series from neuroscience experiments. Therefore, we have an additional example of this kind of analysis in *Event-related fMRI*

In the following code-snippet, we demonstrate the calculation of the spike-triggered average (STA). This is the average of the stimulus wave-form preceding the emission of a spike in the neuron and can be thought of as the stimulus 'preferred' by this neuron.

We start by importing the required modules:

```
import numpy as np

import nitime.timeseries as ts
import nitime.analysis as tsa
import nitime.viz as viz
```

Two data files are used in this example. The first contains the times of action potentials

Site Navigation

Documentation
Development
News

NIPY Community

Community Home
NIPY Projects
Mailing List
License

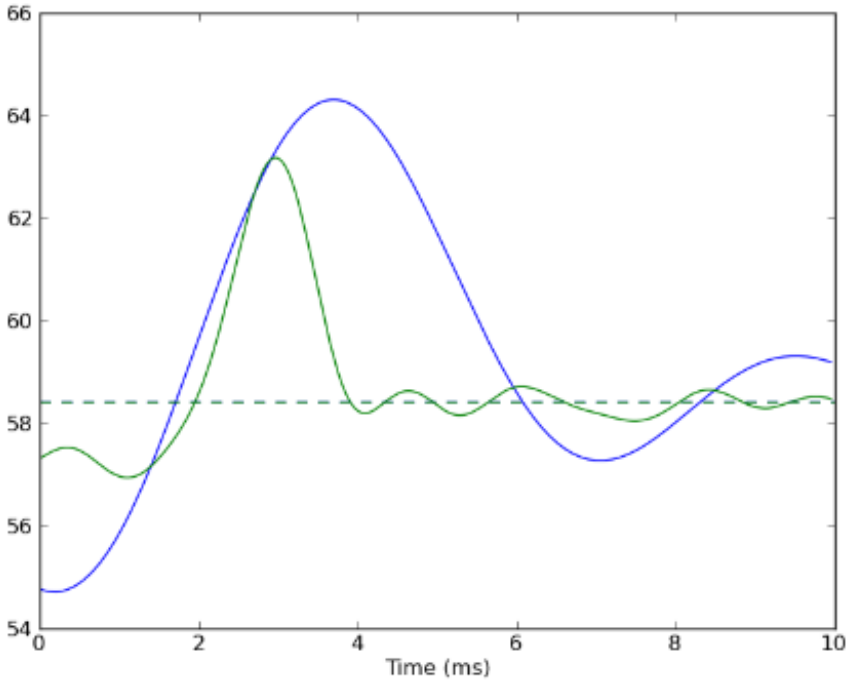
Previous topic

Event-related fMRI

Next topic

Multi-taper coherence estimation

Docs with data, full code and references



plt.show() is called in order to display the figures

```
plt.show()
```

The data used in this example is also available on the CRCNS data sharing web-site.

[Rokem2006] Ariel Rokem, Sebastian Watzl, Tim Gollisch, Martin Stemmler, Andreas V M Herz and Ines Samengo (2006). Spike-timing precision underlies the coding efficiency of auditory receptor neurons. J Neurophysiol, 95:2541-52

Example source code

You can download the full source code of this example. This same script is also included in the Nitime source distribution under the `doc/examples/` directory.

Outline

Version control everywhere

Git: the tool you didn't know you needed

Reproducibility?

- Tracking and recreating every step of your work
- In the software world: it's called Version Control!

Git: an enabling technology. Use version control for everything

- Paper writing (never get `paper_v5_john.tex` by email again!)
- Grant writing
- Everyday research
- Teaching (never accept an emailed homework assignment again!)

Advantages of pervasive distributed version control

- Tracking of everyday results: a "time machine" view.
- Distributed backup.
- Explore lines of research/writing.
- Collaborate with colleagues.

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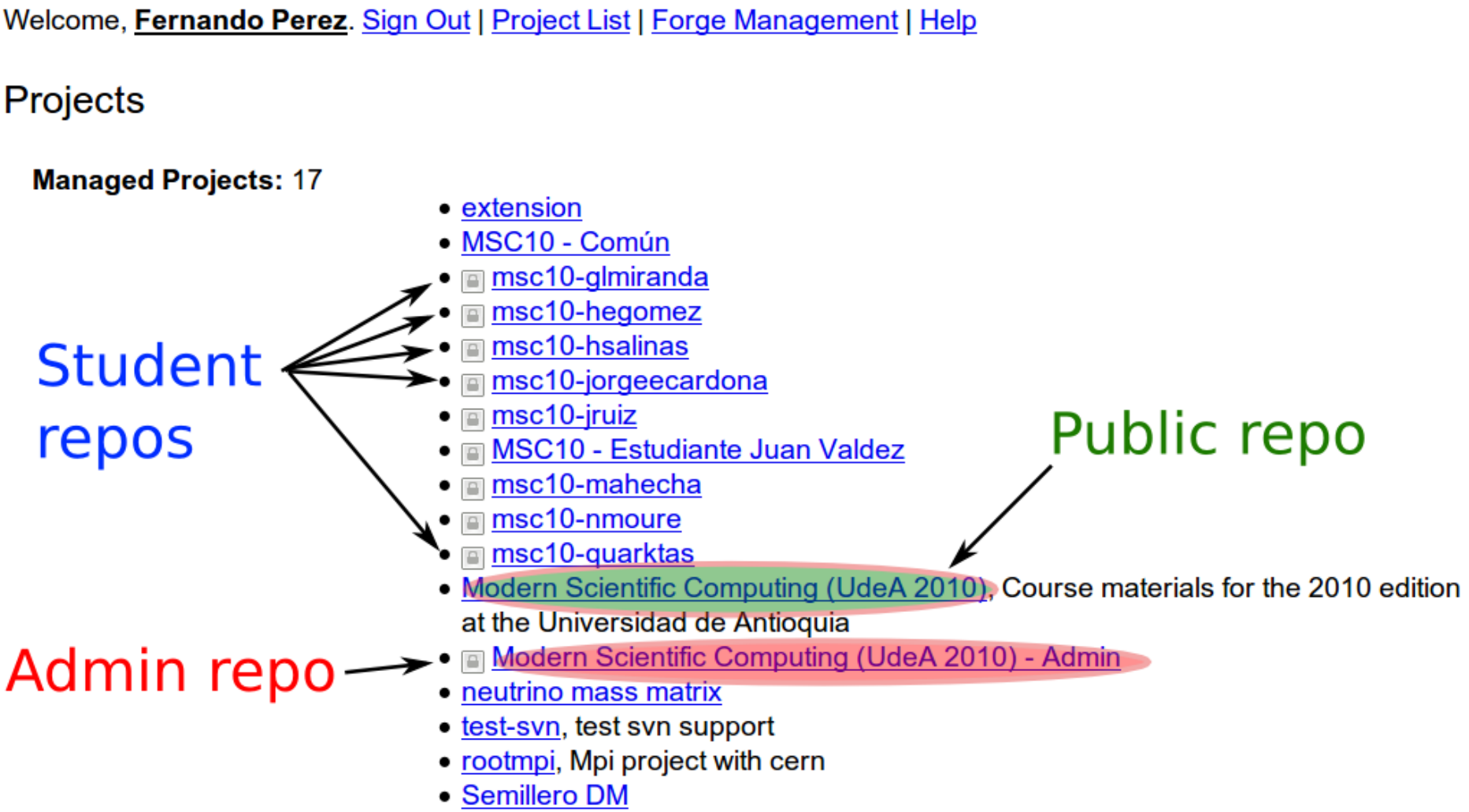
Git for running a course? Yes! Die, email attachments!

Self-hosted Indefero (open source tool)



One student's work

msc10-mahecha Updates

Development Team
Admins
- Diego Restrepo
- Diego restrepo
- Fernando Perez

Happy Crew
- jorge mahecha

Age Sort asc/desc	**Change**
Feb 26, 2010	
1 year 6 days	Taller P7
	Commit 5dede49122d65cec185b8777deaae3a8a2f42a31, by Jorge Mahecha
1 year 6 days	Taller P7
	Commit 15dcfa67a75b079fe81f7c4493b22ab4f24c9866, by Jorge Mahecha
Feb 22, 2010	
1 year 9 days	Taller P2
	Commit 3b03586a4b73130d1cfbf4039755e512e529e994, by Jorge Mahecha
Feb 20, 2010	
1 year 11 days	Taller P1
	Commit 09c2530cdc5dbd19af358c637616b3ce5166fb0a, by Jorge Mahecha

Git: publish your genome!

http://manu.sporny.org/2011/public-domain-genome

github SOCIAL CODING

fperez 23 | Dashboard | Inbox 0 | Account Settings | Log Out

Explore GitHub | Gist | Blog | Help | Search GitHub...

msporny / dna

Watch | Fork | 229 | 26

Source | Commits | **Network** | Pull Requests (1) | Issues (8) | Graphs | Branch: master

Graph | Members

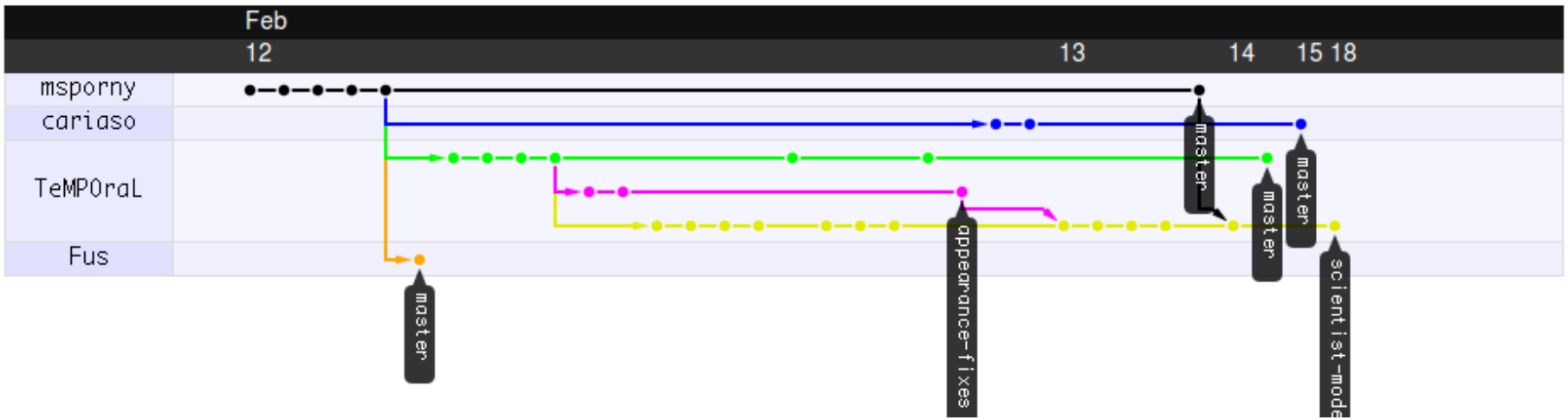
The dna network graph

Keyboard shortcuts available

*All branches in the network using **msporny/dna** as the reference point. Read our blog post about how it works.*

Show Help

Last updated: 1 day ago



Limitations of git (and similar) for our purposes

Written for software development!

- Sub optimal for tracking anything other than source code.
- Not great for **binary files.**
- **No semantic intelligence**
  - Purely line-oriented
  - No understanding of the structure of documents
  - Format-specific change-tracking?
- Hard problem, (or a **good CS research project**)
  - Any CS grad students in the audience?

Outline

Incentives and rewards

In Open Source

- Individual attribution in commit logs.
- Volunteers find reward in community.
- For some, it's part of their job.
- No hidden work before "publication": the **process** is open.

Academia: a naïve transplant won't work

- Success $\Longleftrightarrow$ individual authorhsip.
- Fears of scooping from open development.
- Low/no requirements from journals. But changing!
  - *Biostatistics*, *Open Research Computation*, *SIAM discussions*
  - *Science*, Feb 2011: "To address the growing complexity of data and analyses, Science is extending our data access requirement listed above to include computer codes involved in the creation or analysis of data."
- Similarly for funding agencies.
  - Also changing: new NSF data management requirements.

Adopt a *habit* of reproducibilty

Make version control as routine as email

- Git for your next grant
- Git in your next in-house research project.
- Disk is cheap! Separate repositories for:
  - Libraries: automated tests and docs *during the development process.*
  - In-house tools shared across project but of less generic use.
  - Project/dataset specific repositories.
- **Write** your next paper with a repository that can produce all results/figures.
- **Publish** your next paper with the code/data repository for it
  - Properly licensed, see V. Stodden's standard.

Use your influence to improve the situation

FINAL NIH STATEMENT ON SHARING RESEARCH DATA

...Reviewers will **not** factor the proposed data-sharing plan into the determination of scientific merit or priority score.
[emphasis mine]
`http://grants1.nih.gov/grants/guide/notice-files/NOT-OD-03-032.html`

This must change!

- **Grant review panel**
  - Credit proposals that do a good job on this front, note those that don't.
- **Hiring/tenure/promotion committee**
  - credit good computational work.
- **Teaching:**
  - students must treat computing as rigorously as other parts of the research. `http://software-carpentry.org`

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