

Reproducible research

Lessons from the open source world

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SIAM CSE 2011, Reno, NV
March 4, 2011

Outline

- 1 A contrast of cultures
- 2 Technical ideas: tools matter
- 3 Incentives and rewards: changing our practices

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- 1 A contrast of cultures
- 2 Technical ideas: tools matter
- 3 Incentives and rewards: changing our practices

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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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 $\mu \geq 0$ 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

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

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

$$r_{ii'}^{j;l} = 2^{-j} \sum_{k=i'-i}^{i'+i} c_{ii'}^k \int_0^1 \Phi_{k,0}^+(x) (\cot(\pi 2^{-j}(x+l)) + (-1)^{i+i'} \cot(\pi 2^{-j}(-x+l))) dx,$$

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.

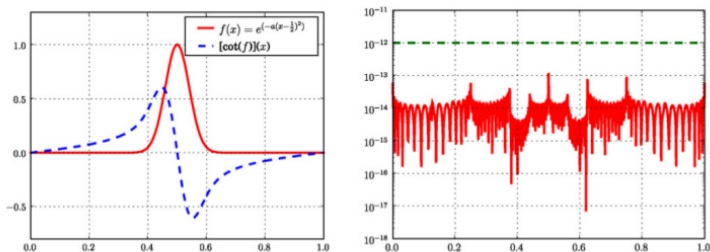


Fig. 3. Results of applying the cotangent kernel to a periodized Gaussian using basis of order $p = 14$ (the last row in Table 1). The pointwise error is shown on the right for a requested accuracy of $\epsilon = 10^{-12}$.

Chance of reproducing results for third parties?

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

[STRFPak](#)[Challenge](#)

STRFlab

Spatio-temporal receptive field lab

Download STRFlab

Please register to download STRFlab:

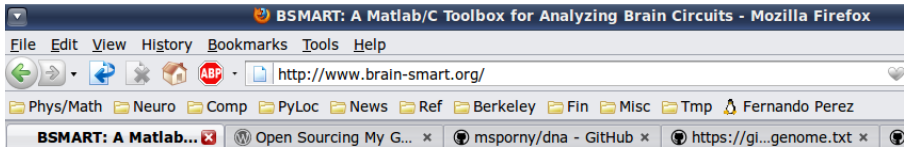
Comments

Sign up for mailing list:

☐

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BSMART: A Matlab/C Toolbox for Analyzing Brain Circuits

BSMART, an acronym of Brain-System for Multivariate AutoRegressive Timeseries, is an open-source software package for analyzing that was born out of a collaborative research effort between Dr. Hualou Liang at Drexel University, Dr. Steven Bressler at Florida Atlantic University of Florida. BSMART can be applied to a wide variety of neuroelectromagnetic phenomena, including EEG. A unique feature of the BSMART package is Granger causality that can be used to assess causal influences and directions of flow.

The backbone of the BSMART project is Multivariate AutoRegressive (MAR) analysis that has been long developed for statistical analysis at different time scales. Based upon a MAR model, a plethora of spectral quantities such as auto power, partial power, coherence and Granger causality can be immediately derived. The approach has been fruitfully used to characterize, with high resolution, functional relations within large scale brain networks.

The BSMART is currently undergoing beta test, freely available under the GNU public license ([download BSMART](#)). It is supported by the National Institute of Neurological Disorders and Stroke (NINDS) through the NIH Neuroinformatics / Human Brain Projects.

The BSMART is described in:

Jie Cui, Lei Xu, Steven L. Bressler, Mingzhou Ding, Hualou Liang, BSMART: a Matlab/C toolbox for analyzing neural time series, *Neural Networks, Special Issue on Neuroinformatics*, 21:1094 - 1104, 2008. ([doi](#))

Please refer to this article when publishing results obtained from the BSMART toolbox. For requesting comments, please contact Hualou Liang at <http://www.brain-smart.org/download/bsmart0p5b105.zip>

Contrast: FOSS better than scientific research?

FOSS: Free and Open Source Software


Public distributed version control: provenance tracking

The screenshot shows a web browser window displaying the GitHub commit history for the `ipython/ipython` repository. The browser's address bar shows the URL `https://github.com/ipython/ipython/commits/master`. The page header includes the GitHub logo and navigation links like `Dashboard`, `Inbox`, `Account Settings`, and `Log Out`. The repository name `ipython / ipython` is prominently displayed, along with statistics for 187 watchers and 103 forks. Below this, tabs for `Source`, `Commits`, `Network`, `Pull Requests (12)`, `Fork Queue`, `Issues (176)`, and `Graphs` are visible. The `Commits` tab is active, showing a list of commits. Two specific commits are highlighted:

- 2011-02-17**: A commit by `minrk` (author) titled `README.txt -> README.rst`, made 1 day ago. The commit details show the commit hash `ebe563dc3431d5aa7e6f`, the tree hash `e74866522c5e030fb128`, and the parent hash `3d86a4157c0cb06c7d1f`.
- 2011-02-16**: A commit titled `Merge remote branch 'origin/pyside-support'`.

The browser's status bar at the bottom shows the full URL `https://github.com/ipython/ipython/forkqueue` and the email address `231 fperez.net@gmail.com`.

Pull requests: ongoing peer review



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ipython / ipython

[Admin](#) | [Unwatch](#) | [Fork](#) | [Your Fork](#) | [Pull Request](#) | [187](#) | [103](#)

[Source](#) | [Commits](#) | [Network](#) | **[Pull Requests \(12\)](#)** | [Fork Queue](#) | [Issues \(176\)](#) | [Graphs](#) | [Branch: master](#)

Open takluyver wants someone to merge 9 commits into `ipython:master` from `takluyver:issue-245` **#261**

[Discussion](#) | [Commits](#) <> 9 | [Diff](#) >= 11



takluyver opened this pull request February 05, 2011


Adapt magic commands to new history system.

This grew from issue [ipython/ipython#245](#). Various magic commands weren't working properly with the new history system: %edit, %macro, and %hist.

Among various minor troubles, selecting a range of lines (%macro test 2-5) numbered from the beginning of the history, so didn't match up with the current line numbers. I've approached this by adding a session_offset attribute to the history manager. This has the added benefit that we no longer need to store a blank history entry so we can count lines from 1.

Along the way, I simplified and modernised parts of the code, including using `basestring` over `StringTypes` and `.isdigit()` over an equivalent regex.

Open
+ 151 additions
- 127 deletions
[All Pull Requests](#)



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

The screenshot shows the Git GUI interface for the 'ipython' repository on the 'master' branch. The top menu bar includes 'File', 'Edit', 'View', 'Repository', and 'Help'. Below the menu is a toolbar with 'History' and 'Commit' buttons. The 'Branch:' dropdown is set to 'master'. The main area displays a list of commits with columns for 'Subject', 'Author', and 'Date'. A commit graph on the left shows the branching structure, with 'origin/master' and 'epatters-pyside-support' branches highlighted. The commit details pane at the bottom shows the SHA, author, date, and subject of the selected commit, along with its parent commit and a diff preview.

Subject	Author	Date
master origin/master README.txt -> README.rst	MinRK	Thu 17 Feb 2011 12:03:09 PM
Merge remote branch 'origin/pyside-support'	epatters	Wed 16 Feb 2011 11:22:17 AM
Merge branch 'ready_cProfile' of https://github.com/tomspur/ipython	Thomas Spura	Wed 16 Feb 2011 12:21:07 AM
Merge branch 'maglc-examples'	Thomas Kluyver	Tue 15 Feb 2011 03:46:10 PM
Skip doctests where necessary.	Thomas Kluyver	Tue 15 Feb 2011 02:34:40 PM
Add example for %cpaste	Sathesh Chandra	Tue 15 Feb 2011 02:27:38 PM
Wrote example for 'colors' command	vankayala sowjanya	Tue 15 Feb 2011 02:12:44 PM
Wrote an example for 'pdef'	vankayala sowjanya	Tue 15 Feb 2011 02:07:59 PM
Tweaks to RST formatting.	Thomas Kluyver	Tue 15 Feb 2011 01:59:38 PM
BUG: Do not store class-specific state on TraitTypes since they may be shared through subcl.	Robert Kern	Tue 15 Feb 2011 12:55:37 PM
epatters-pyside-support PySide fix: PySide's QByteArray constructor does not overload for unicode	epatters	Tue 15 Feb 2011 11:37:47 AM
Improved error message for Qt API switcher.	epatters	Tue 15 Feb 2011 11:21:35 AM
kernel sends reply on the right side of std<x>.flush	MinRK	Tue 15 Feb 2011 01:17:20 AM
fix+test %who_is type checking, skip %who doctests	MinRK	Mon 14 Feb 2011 04:36:30 PM

Details Tree

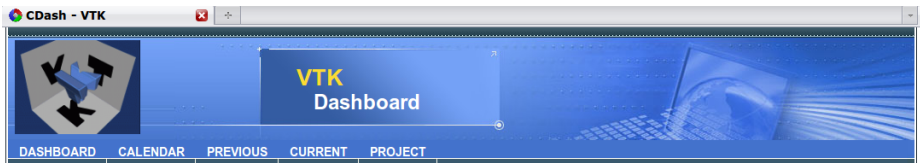
SHA: 3d86a4157c0cb06c7d1fa12ee97bdd5c83f6e712
Author: epatters
Date: Wed 16 Feb 2011 11:22:17 AM EST
Subject: **Merge remote branch 'origin/pyside-support'**
Parent: [604c8e1ef5e5bf07cf48a82eb2acc07b10b9a42b](#) (Merge branch 'ready_cProfile' of https://github.com/tomspur/ipython)
[12ee02612522e257a80fc803c082ce394030e853](#) (PySide fix: PySide's QByteArray constructor does not overload for unicode.)

Merge remote branch 'origin/pyside-support'

Loaded 3263 revisions in 0.45s

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

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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

[Project Home](#) [Downloads](#) [Wiki](#) **Issues** [Source](#)

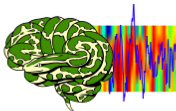
New issue [Advanced search](#) [Search tips](#)

							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 mattmap 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 + 0.1111111111111111*(1.000000000000000 + 2.000000000000000*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 mattmap		
51	Enhancement	Started	Medium	Release0.7.0	matt...@gmail.com	RootOf for polynomial equations Polynomial NeedsReview mattmap		
326	Defect	Started	Medium	Release0.7.0	matt...@gmail.com	sympy.roots_sturm(...) hangs Polynomial EasyToFix NeedsReview mattmap		
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 mattmap		

Documentation: Sphinx

Math, code and validated examples: literate programming

Nitime: time-series analysis for neuroscience



[Nitime Home](#) | [Nitime Documentation](#) » [Examples](#) »

[previous](#) | [next](#) | [modules](#) | [index](#)

Auditory processing in grasshoppers ¶

Extracting the average time-series from one signal, time-locked to the occurrence 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

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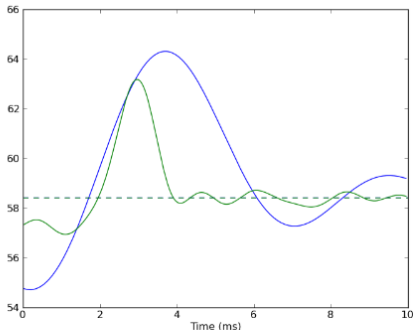
Previous topic

[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

- 1 A contrast of cultures
- 2 Technical ideas: tools matter
- 3 Incentives and rewards: changing our practices

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)

Welcome, **Fernando Perez**. [Sign Out](#) | [Project List](#) | [Forge Management](#) | [Help](#)

Projects

Managed Projects: 17

Student
repos

Public repo

Admin repo

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-  [msc10-hegomez](#)
-  [msc10-hsalinas](#)
-  [msc10-jorgecardona](#)
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- [MSC10 - Estudiante Juan Valdez](#)
- [msc10-mahecha](#)
- [msc10-nmoure](#)
-  [msc10-quarktas](#)
- [Modern Scientific Computing \(UdeA 2010\)](#), Course materials for the 2010 edition at the Universidad de Antioquia
-  [Modern Scientific Computing \(UdeA 2010\) - Admin](#)
- [neutrino mass matrix](#)
- [test-svn](#), test svn support
- [rootmpi](#), Mpi project with cern
- [Semillero DM](#)

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>



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msporny / dna

Watch

Fork

229

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[Source](#)

[Commits](#)

[Network](#)

[Pull Requests \(1\)](#)

[Issues \(8\)](#)

[Graphs](#)

Branch: master

Graph

[Members](#)

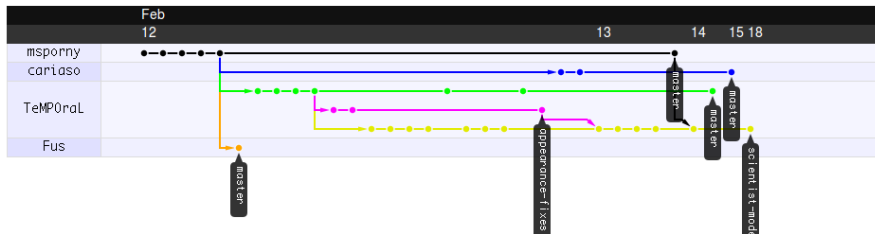
The dna network graph

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?

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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 \iff individual authorship.
- 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 reproducibility

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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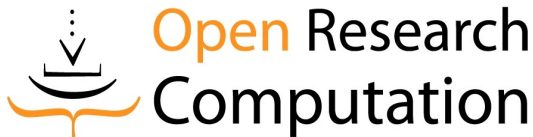
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submissions

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Cameron Neylon (UK)

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