

Reproducible Research, Open Science Motivation, Challenges, Approaches, . . .

Arnaud Legrand
CNRS, Inria, University of Grenoble

December 3, 2015 – Orléans

Atelier R⁴: Retour d'expéRiences sur la Recherche Rproductible

① A Few Motivating Examples

② The Reproducible Research Movement

How does it work in "real" sciences?

Reproducible Research/Open Science

Many Different Alternatives for Replicable Analysis

Good Practice for Setting up a Laboratory Notebook

③ Where are we now?

Frustration



As an Author

- Advisor: "Did you take care of setting this?" Me: "Uh?"
- I thought I used the same parameters but I'm getting different results! I swear it worked yesterday!
- A new student wants to compare with the method I proposed last year
- The damned fourth reviewer asked for a major revision and wants me to change figure 3 :(Which code and which data set did I use to generate this figure?
- 6 months later: Why did I do that?

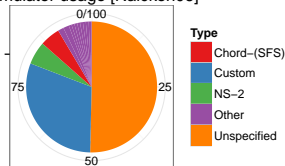
As a Reviewer This may be an interesting contribution but:

- There is no label/legend/... What is the meaning of this graph? If only I could access the generation script
- Why is this graph in logscale? How would it look like otherwise?
- This average value must hide something. As usual, no confidence interval... I wonder whether the difference is significant at all
- That can't be true, I'm sure they removed some points or decided to show only a subset of the data. I wonder what the rest looks like

A Few Edifying Examples

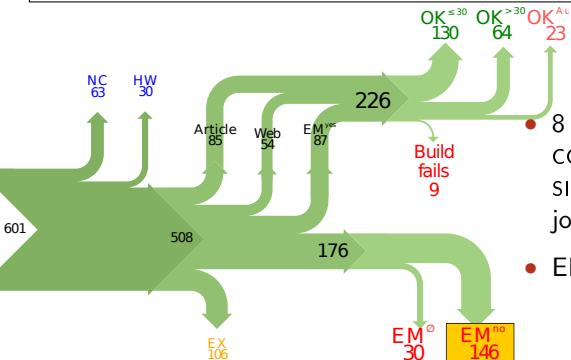
Naicken, Stephen *et Al.*, *Towards Yet Another Peer-to-Peer Simulator*, HET-NETs'06.

Simulator usage [Naicken06]



From 141 P2P sim.papers, 30% use a custom tool,
50% don't report used tool

Collberg, Christian *et Al.*, *Measuring Reproducibility in Computer Systems Research*, <http://reproducibility.cs.arizona.edu/> 2014,2015



- 8 ACM conferences (ASPLOS'12, CCS'12, OOPSLA'12, OSDI'12, PLDI'12, SIGMOD'12, SOSP'11, VLDB'12) and 5 journals
- EM^{no} = the code cannot be provided

The Dog Ate my Homework !!!

- Versioning Problems

*Thanks for your interest in the implementation of our paper. The good news is that I was able to find some code. I am just **hoping** that **it** is a stable working version of the code, and **matches the implementation we finally used for the paper**. Unfortunately, I have **lost some data** when **my laptop was stolen** last year. The bad news is that the code is not commented and/or clean.*

*Attached is the \langle system \rangle source code of our algorithm. I'm **not** very **sure** **whether it is the final version of the code used in our paper**, but it should be at least 99% close. Hope it will help.*

The Dog Ate my Homework !!!

- Versioning Problems
- Bad Backup Practices

*Unfortunately, the server in which my implementation was stored had a **disk crash in April and three disks crashed simultaneously**. While the help desk made significant effort to save the data, my entire implementation for this paper was not found.*

The Dog Ate my Homework !!!

- Versioning Problems
- Bad Backup Practices
- Code Will be Available Soon

*Unfortunately the current system is **not mature enough at the moment**, so it's not yet publicly available. We are actively working on a number of extensions and **things are somewhat volatile**. However, once things stabilize we plan to release it to outside users. At that point, we would be happy to send you a copy.*

The Dog Ate my Homework !!!

- Versioning Problems
- Bad Backup Practices
- Code Will be Available Soon
- No Intention to Release

*I am afraid that the source code was never released. The code was **never intended to be released so is not in any shape for general use.***

The Dog Ate my Homework !!!

- Versioning Problems
- Bad Backup Practices
- Code Will be Available Soon
- No Intention to Release
- Programmer Left

*⟨STUDENT⟩ was a graduate student in our program but **he left a while back** so I am responding instead. For the paper we used a prototype that included many moving pieces that only ⟨STUDENT⟩ knew how to operate and we did not have the time to integrate them in a ready-to-share implementation before he left. Still, I hope you can build on the ideas/technique of the paper.*

*Unfortunately, the author who has done most of the coding for this paper has **passed away** and the code is no longer maintained.*

The Dog Ate my Homework !!!

- Versioning Problems
- Bad Backup Practices
- Code Will be Available Soon
- No Intention to Release
- Programmer Left
- Commercial Code

Since this work has been done at <COMPANY> we don't open-source code unless there is a compelling business reason to do so. So unfortunately I don't think we'll be able to share it with you.

The code owned by <COMPANY>, and AFAIK the code is not open-source. Your best bet is to reimplement :(Sorry.

The Dog Ate my Homework !!!

- Versioning Problems
- Bad Backup Practices
- Code Will be Available Soon
- No Intention to Release
- Programmer Left
- Commercial Code
- Proprietary Academic Code

*Unfortunately, the \langle SYSTEM \rangle sources are **not meant to be opensource** (the code is partially **property of \langle UNIVERSITY 1 \rangle , \langle UNIVERSITY 2 \rangle and \langle UNIVERSITY 3 \rangle .)***

If this will change I will let you know, albeit I do not think there is an intention to make the \langle SYSTEM \rangle sources opensource in the near future.

*If you're interested in obtaining the code, **we only ask for a description of the research project** that the code will be used in (**which may lead to some joint research**), and we also have a software license agreement that the University would need to sign.*

The Dog Ate my Homework !!!

- Versioning Problems
- Bad Backup Practices
- Code Will be Available Soon
- No Intention to Release
- Programmer Left
- Commercial Code
- Proprietary Academic Code
- Research vs. Sharing
- ...
- ...

In the past when we attempted to share it, we found ourselves spending more time getting outsiders up to speed than on our own research. So I finally had to establish the policy that we will not provide the source code outside the group.

My Feeling

Computer scientists have an incredibly **poor training in probabilities, statistics, experiment management, Design of Experiments**

Why should we? Computer are **deterministic** machines after all, right? 😊

Ten years ago, I've started realizing how **lame** the articles I reviewed (as well as those I wrote) were in term of experimental methodology.

- Yeah, I know, your method/algorithm is better than the others as demonstrated by the figures
- Not enough information to **discriminate real effects from noise**
- Little information about the **workload**. Would the “conclusion” still hold with a slightly different workload?
- I got tired of awful combination of tools (perl, gnuplot, sql, ...) and **bad methodology**

I got sick of struggling in vain when trying to build on the work of others

① A Few Motivating Examples

② The Reproducible Research Movement

How does it work in "real" sciences?

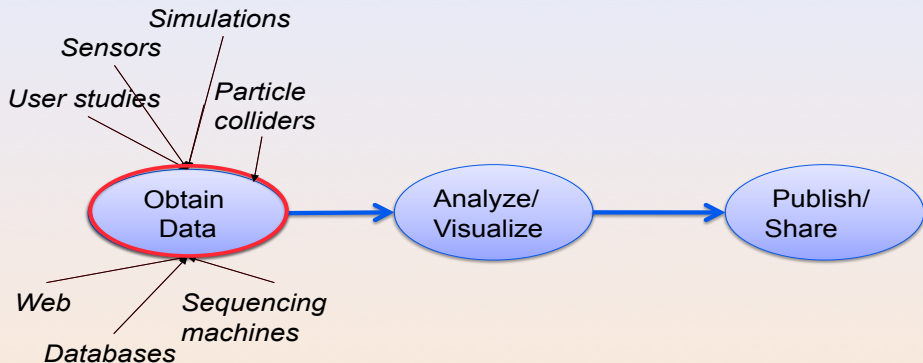
Reproducible Research/Open Science

Many Different Alternatives for Replicable Analysis

Good Practice for Setting up a Laboratory Notebook

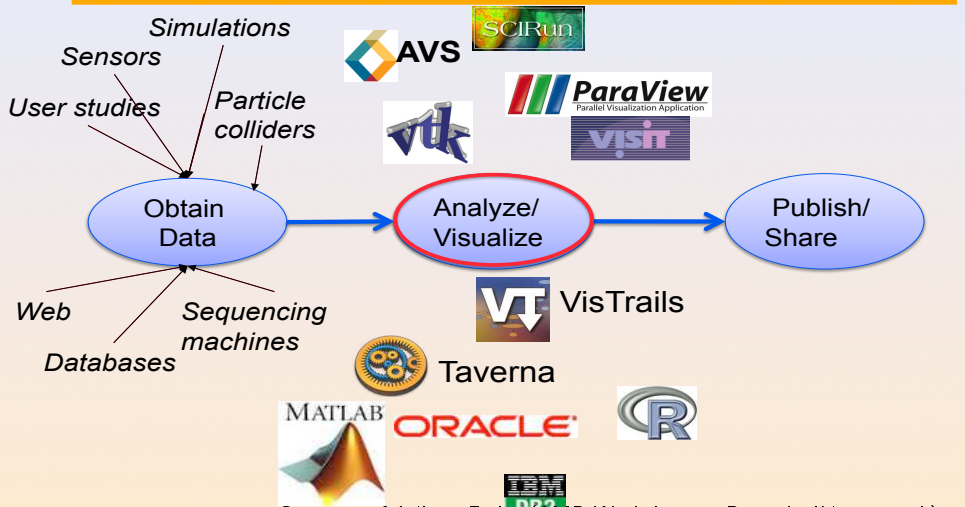
③ Where are we now?

Science Today: Data Intensive



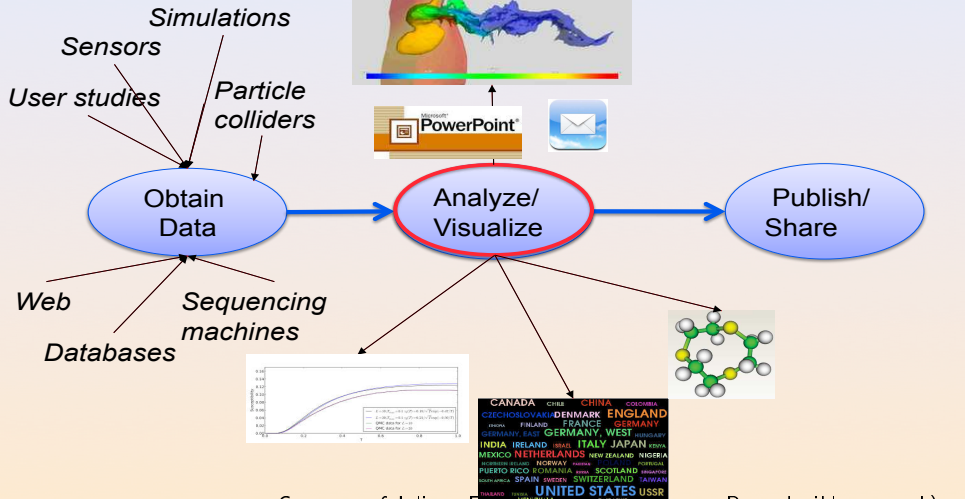
Courtesy of Juliana Freire (AMP Workshop on Reproducible research)

Science Today: Data + Computing Intensive



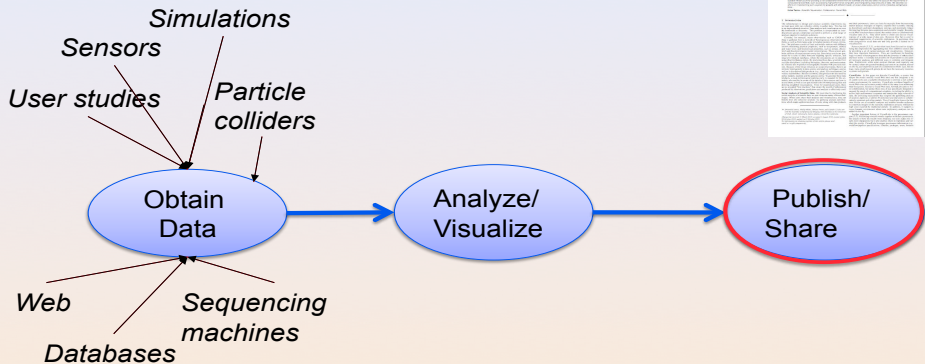
Courtesy of Juliana Freire (AMP Workshop on Reproducible research)

Science Today: Data + Computing Intensive



Courtesy of Juliana Freire (AVIN workshop on Reproducible research)

Science Today: Data + Computing Inte



Courtesy of Juliana Freire (AMP Workshop on Reproducible research)

Science Today: Incomplete Publications

- ◆ Publications are just the tip of the iceberg
 - Scientific record is incomplete---to large to fit in a paper
 - Large volumes of data
 - Complex processes
- ◆ Can't (easily) reproduce results



Courtesy of Juliana Freire (AMP Workshop on Reproducible research)

Science Today: Incomplete Publications

- ◆ Publications are just the tip of the iceberg
 - Scientific results are often incomplete
 - Large volumes of data
 - Complex processes
- ◆ Can't verify results
 - "It's impossible to verify most of the results that computational scientists present at conference and in papers."* [Donoho et al., 2009]
 - "Scientific and mathematical journals are filled with pretty pictures of computational experiments that the reader has no hope of repeating."* [LeVeque, 2009]
 - "Published documents are merely the advertisement of scholarship whereas the computer programs, input data, parameter values, etc. embody the scholarship itself."* [Schwab et al., 2007]

Courtesy of Juliana Freire (AMP Workshop on Reproducible research)

Why Are Scientific Studies so Difficult to Reproduce?

Human error:

- Experimenter **bias**
- Programming **errors** or data manipulation **mistakes**
- Poorly selected statistical tests

There is just no real incentive in doing so:

- Legal barriers, **copyright** (*many ongoing thoughts on this in the US*)
- **Competition** issue (*researchware, bibliometry, . . .*)
- Publication **bias** (only the idea matters, not the gory details)
- Rewards for **positive results**, not for consolidating results

Technical difficulty:

- ~~Hardware and software evolve too quickly. It's not worth it~~
- ~~No resources for storing so much data/information~~
- ~~Lack of easy-to-use tools~~

Evidence for a Lack of Reproducibility

- Studies showing that scientific papers commonly leave out experimental details essential for reproduction and showing difficulties with replicating published experimental results:
 - J.P. Ioannidis. *Why Most Published Research Findings Are False* PLoS Med. 2005 August; 2(8)
- High number of failing clinical trials.
 - *Do We Really Know What Makes Us Healthy?*, New-York Times — September 16, 2007
 - *Lies, Damned Lies, and Medical Science*, The Atlantic. Nov, 2010
- Increase in retracted papers:
 - Steen RG, *Retractions in the scientific literature: is the incidence of research fraud increasing?* J Med Ethics 37: 249–253.



Courtesy V. Stodden, SC, 2015

A Reproducibility Crisis?

The Duke University scandal with scientific misconduct on lung cancer

- *Nature Medicine* - 12, 1294 - 1300 (2006) **Genomic signatures to guide the use of chemotherapeutics**, by Anil Potti and 16 other researchers from Duke University and University of South Florida
- Major commercial labs licensed it and were about to start using it before two statisticians discovered and publicized its faults

Dr. Baggerly and Dr. Coombes found errors almost immediately. Some seemed careless — moving a row or a column over by one in a giant spreadsheet — while others seemed inexplicable. The Duke team shrugged them off as “clerical errors.”

The Duke researchers continued to publish papers on their genomic signatures in prestigious journals. Meanwhile, they started three trials using the work to decide which drugs to give patients.

- Retractions: January 2011. Ten papers that Potti coauthored in prestigious journals were retracted for varying reasons
- Some people die and may be getting worthless information that is based on **bad science**

Courtesy of Adam J. Richards

Definitely

A recent scandal In 2013, *Dong-Pyou Han*, a former assistant professor of biomedical sciences at Iowa State University was disgraced:

- Falsified blood results to make it appear as though a vaccine he was working on had exhibited anti-HIV activity
- Han and his team received \approx \$19 million from NIH
- Retraction and resignation of university
- Han was sentenced in 2015 to 57 months imprisonment for fabricating and falsifying data in HIV vaccine trials. He was also fined US \$7.2 million!

We should avoid witch-hunt

- August 5, 2014, Yoshiki Sasai (stem cell, considered for Nobel Prize) hanged in his laboratory at the RIKEN (Japan). Fraud suspicion...
- In 1986, a young postdoctoral fellow at MIT accused her director, Thereza Imanishi-Kari, of falsifying the results of a study published in *Cell* and co-signed by the Nobel laureate David Baltimore. [...] Declared guilty, Univ. presidency resignation, and finally cleared. This put the careers of two outstanding researchers on hold for ten years based on unfounded accusations.

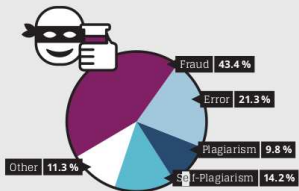
Scientific fraud is bad but let's be careful Have a look at the wikipedia *list of academic scandals*. On a totally different aspect, do not forget to also have a look at the *plagiarism* and *paper generation* wikipedia entries and at *having fun with h-index*

The Battle against Scientific Fraud in the CNRS International Magazine

Is Fraud a new phenomenon?

Biomedical fraud in figures

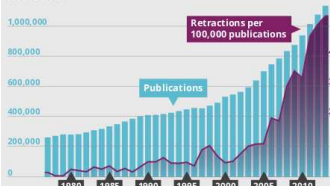
Cause of retraction 1977 to 2012



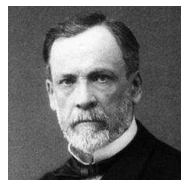
SOURCE: FANG ET AL (2012) PNAS

Number of publications and retractions

1977 to 2013



SOURCE: PUBMED VIA PAMIRETRACT.HERIQU.COM



- Galileo (data fabrication), Ptolemy (plagiarism), Mendel (data enhancement), Pasteur (rigorous but hid failures), ...

① A Few Motivating Examples

② The Reproducible Research Movement

How does it work in "real" sciences?

Reproducible Research/Open Science

Many Different Alternatives for Replicable Analysis

Good Practice for Setting up a Laboratory Notebook

③ Where are we now?

Reproducible Research: the New Buzzword?

H2020-EINFRA-2014-2015

*A key element will be capacity building to link literature and data in order to enable a more transparent evaluation of research and **reproducibility** of results.*

More and more workshops

- Workshop on Duplicating, Deconstructing and Debunking (WDDD) (2002-2014 edition)
- **AMP Workshop. Reproducible Research: Tools and Strategies for Scientific Computing** (2011)
- Working towards Sustainable Software for Science: Practice and Experiences (2013)
- **REPPAR'14: 1st International Workshop on Reproducibility in Parallel Computing**
- Reproducibility@XSEDE: An XSEDE14 Workshop
- Reproduce/HPCA 2014
- TRUST 2014, 2015
- Talk at SC by V. Stodden two weeks ago

Should be seen as **opportunities to share experience**

Reproducibility: What Are We Talking About?

1934: Karl Popper introduces the notion of **falsifiability** and **crucial experiment** and puts **reproducing the work of others** at the core of science

Reproducibility of experimental results is the hallmark of science
[Drummond, 2009]

⚠ Terminology varies ⚠



Inspired by Andrew Davison (AMP Workshop on Reproducible research) and [Feitelson, 2015]

Reproducible Research: Trying to Bridge the Gap

Author



Published
Article

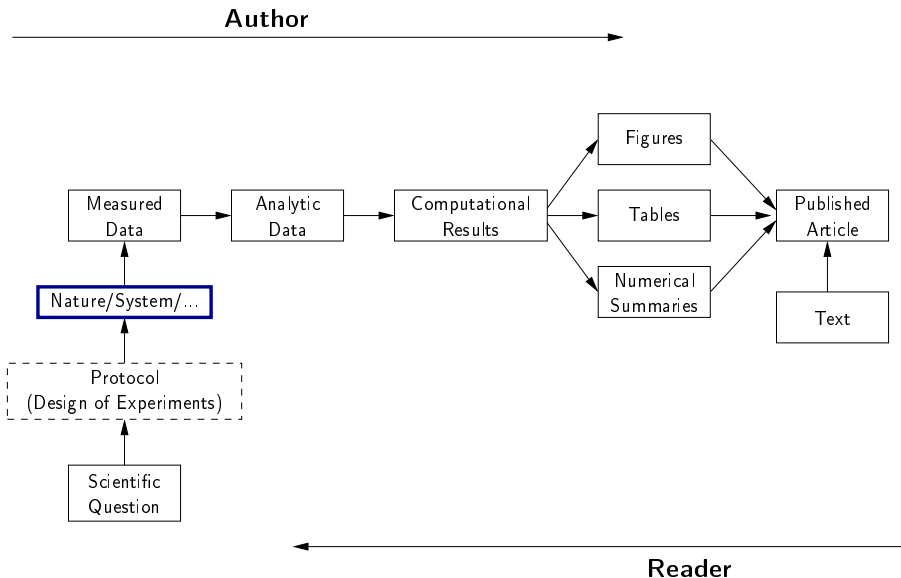
Nature/System/...

Protocol
(Design of Experiments)

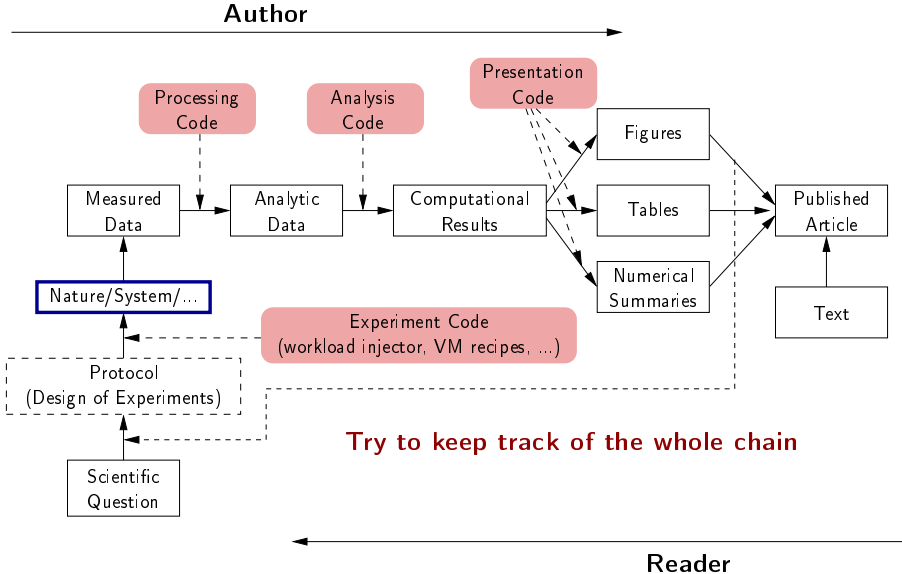
Scientific
Question

Reader

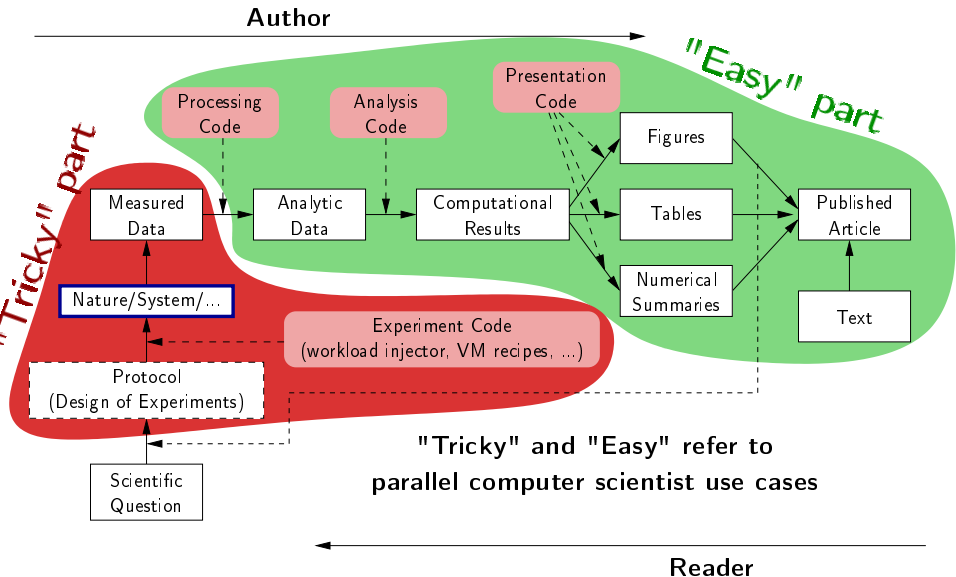
Reproducible Research: Trying to Bridge the Gap



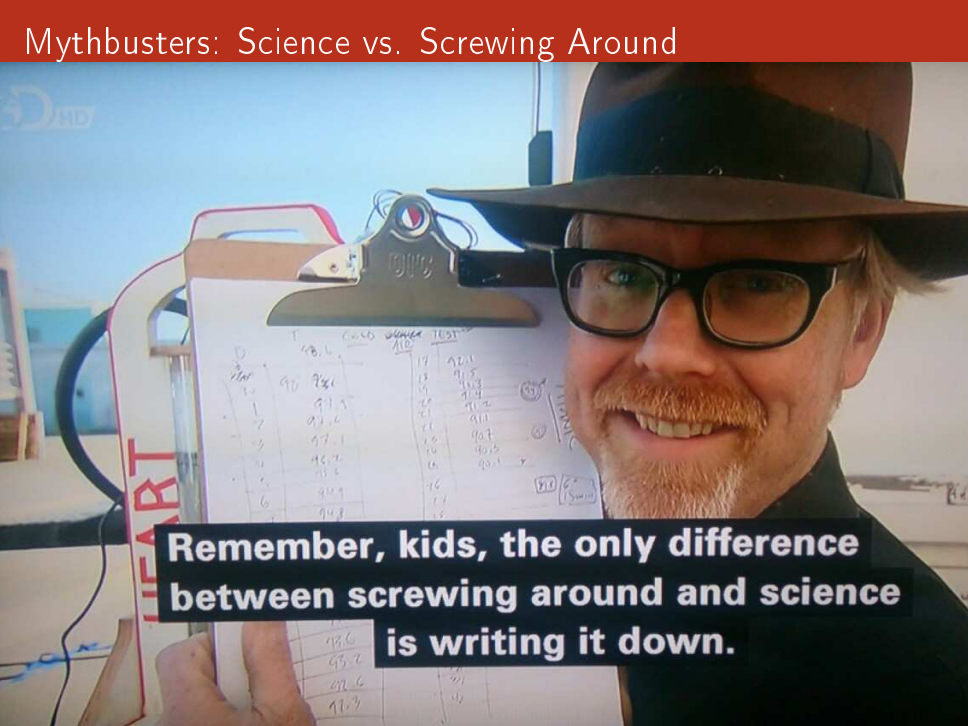
Reproducible Research: Trying to Bridge the Gap



Reproducible Research: Trying to Bridge the Gap



Mythbusters: Science vs. Screwing Around



The man is holding a clipboard with a handwritten table. The table has columns labeled 'D', 'T', 'COLD WATER', and 'TEST'. The 'D' column contains numbers 1 through 6. The 'T' column contains values like 98.4, 98.0, 97.1, 97.6, 96.2, 95.2, 94.9, 94.8. The 'COLD WATER' column contains the number 10. The 'TEST' column contains numbers 17 through 25. There are also some circled numbers and a box labeled 'S'.

Remember, kids, the only difference between screwing around and science is writing it down.

A Difficult Trade-off

Many different tools/approaches developed in various communities

But mainly two approaches:

Automatically keeping track of everything

- the code that was run (source code, libraries, compilation procedure)
- processor architecture, OS, machine, date, ...

VM-based solutions	and	Experiment engines
Virtualbox/kvm/...		Expo, Xpflow, Execo
CDE		Plush/OMF/Splay
Singularity		

Ensuring others can understand/adapt what was done

- Why did I run this?
- Does it still work when I change this piece of code for this one?

Laboratory notebook and recipes

① A Few Motivating Examples

② The Reproducible Research Movement

How does it work in "real" sciences?

Reproducible Research/Open Science

Many Different Alternatives for Replicable Analysis

Good Practice for Setting up a Laboratory Notebook

③ Where are we now?

Our Approach: An Infrastructure to Support Provenance-Rich Papers [Koop et al., ICCS 2011]

- ◆ Tools for *authors* to create reproducible papers
 - Specifications that encode the computational processes
 - Package the results *Support different approaches*
 - Link from publications
- ◆ Tools for testers to repeat and validate results
 - Explore different parameters, data sets, algorithms
- ◆ Interfaces for searching, comparing and analyzing experiments and results
 - Can we discover better approaches to a given problem?
 - Or discover relationships among workflows and the problems?
 - How to describe experiments?

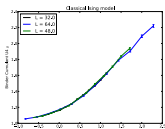
An Provenance-Rich Paper: ALPS2.0

arXiv:1101.2646v4 [cond-mat.str-el] 23 May 2011

The ALPS project release 2.0:
Open source software for strongly correlated
systems

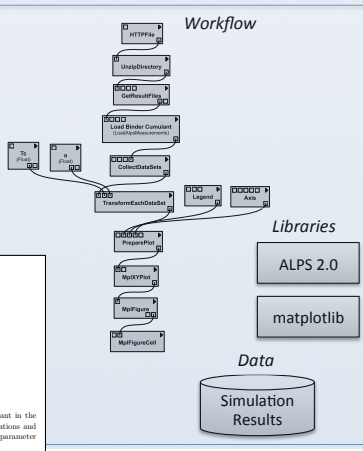
B. Bauer¹ L. D. Carr² H.G. Evertz³ A. Feiguin⁴ J. Freire⁵
S. Fuchs⁶ L. Gamper⁷ J. Gukelberger⁸ E. Gull⁹ S. Guertler⁴
A. Hehn¹⁰ R. Igarashi^{11,10} S.V. Isakov¹ D. Koop¹ P.N. Ma¹
P. Mates¹² H. Matsuo¹³ O. Parcollet¹² G. Pawłowski¹³
J.D. Picon¹⁴ L. Pollet¹⁵ E. Santos⁶ V.W. Scarola¹⁶
U. Schollwöck¹⁷ C. Silva⁸ B. Surer¹ S. Todo^{18,11} S. Trebst¹⁸
M. Troyer¹ M. L. Wall¹ P. Werner¹ S. Wessel^{19,20}

- ¹Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
- ²Department of Physics, Colorado School of Mines, Golden, CO 80401, USA
- ³Institut für Theoretische Physik, Technische Universität Graz, A-8010 Graz, Austria
- ⁴Department of Physics and Astronomy, University of Wyoming, Laramie, Wyoming 82071, USA
- ⁵Scientific Computing and Imaging Institute, University of Utah, Salt Lake City, Utah 84112, USA
- ⁶Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany
- ⁷Columbia University, New York, NY 10027, USA
- ⁸Bethe Center for Theoretical Physics, Universität Bonn, Nussallee 12, 53115 Bonn, Germany



1 Correspond

Figure 3. In this example we show a data collapse of the Binder Cumulant in the classical Ising model. The data has been produced by remotely run simulations and the critical exponent has been obtained with the help of the VisTrails parameter exploration functionality.



Chronicling computations in real-time

VCR computation platform Plugin = Computation recorder

Regular program code

```
figure1 = plot(x)
save(figure1, 'figure1.eps')
```

```
> file /home/figure1.eps saved
>
```

Chronicling computations in real-time

VCR computation platform Plugin = Computation recorder

Program code with VCR plugin

```
repository vcr.nature.com  
verifiable figure1 = plot(x)
```

```
> vcr.nature.com approved:  
> access figure1 at https://vcr.nature.com/ffaaffb148d7
```

Word-processor plugin App

LaTeX source

```
\includegraphics{figure1.eps}
```

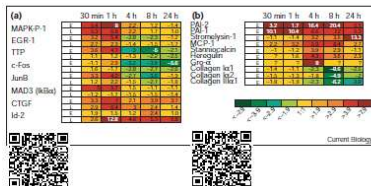
LaTeX source with VCR package

```
\includeresult{vcr.thelancet.com/ffaaffb148d7}
```

Permanently bind printed graphics to underlying result content

Figure 3

Time course of serum stimulation. (a) Early passage (E: PD30) or late passage (L: PD89) BJ cultures were held in 0.5% serum for 2 days, then stimulated with 10% FBS. RNA levels from cultures at the indicated time points (Cy5 channel) were compared with the uninduced starting culture (Cy3 channel). Positive values indicate higher expression in induced cells; negative values indicate lower expression in induced cells. Question marks indicate that there was insufficient signal for detection. A complete listing of serum-responsive genes from this analysis is provided in Supplementary material. (b) The serum-responsiveness of select senescence-regulated genes in early passage (PD30) BJ fibroblasts.



senescence response appears to overlap substantially with gene expression patterns observed in activated fibroblasts during wound healing [24–26]. MCP-1, Gro- α , IL-1 β and IL-15 are strong effectors of macrophage and neutrophil recruitment and activation [27,28]. The upregulation of Toll (Tlr-4) in senescent fibroblasts confirms the overall immune response behavior at senescence. Tlr-4 is an IL-1 receptor homolog and is implicated in the activation of the gene regulatory protein NF- κ B, a function proposed to be part of the innate immune response [29]. The induction of IL-15 at senescence is also consistent with an innate immune response, as IL-15 can be induced by NF- κ B-dependent transcription [30] and also participates in inflammatory disease processes [28].

Deficiencies in the response of senescent cells to serum stimulation have been reported, and include an inability to induce the expression of *c-fos* mRNA [31] and markers of late G1 and S phase [32]. In response to serum, expression of inflammatory chemokines, matrix-degrading proteases and their modulators is induced in early-passage dermal fibroblasts, and expression of matrix collagens is reduced.

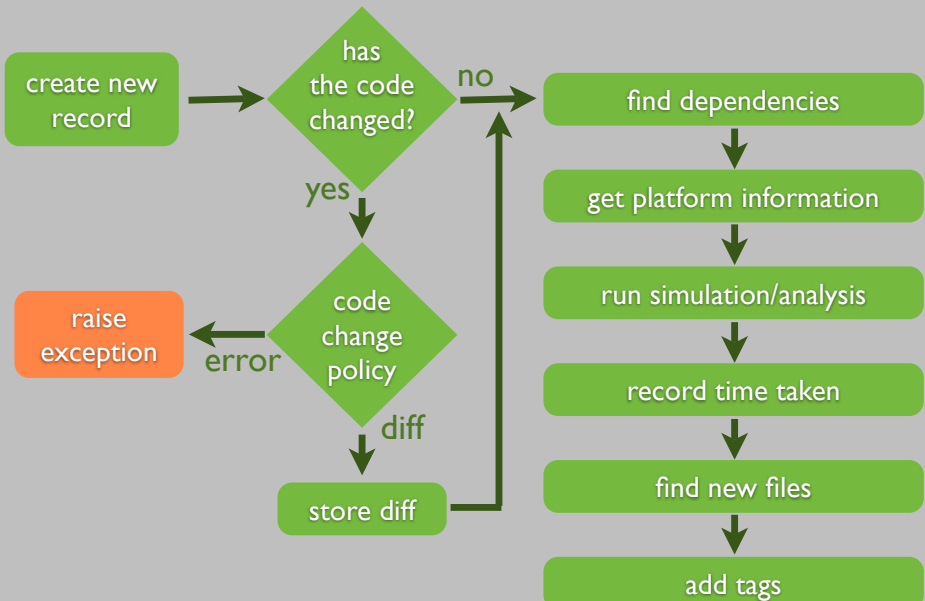
This transient burst of activity may represent the natural response of the VCR and repair [29]. Id-2 is a marker of the markers associated with senescence in dermal fibro-

states overlap substantially with those in telomere-induced senescence (W.F., D.N.S., R. Allsopp, S. Lowe, and G. Ferbeyre, unpublished observations) and thus are likely to use many of the same activation processes.

The pattern of gene expression at senescence varies substantially in different cell types. Although the expression of matrix and structural proteins, such as the collagens, keratins and auxiliary factors, is repressed in RPE cells, inflammatory regulators are not induced, in contrast to dermal fibroblasts. Physiologically, this would make sense, as an acute inflammatory response in a tissue critical for normal vision would be likely to have deleterious consequences. However, as the RPE layer has a central role in the deposition and maintenance of extracellular matrix in the retina, decrements in the ability of senescent RPE cells to maintain appropriate expression patterns, as evidenced by decreased expression of collagens, keratins, aggrecan, transglutaminase and so on, would be predicted to have adverse effects on retinal architecture. Dysfunction of the RPE cell layer is considered to be a substantial factor in the development of age-related macular degeneration [36].

This transient burst of activity may represent the natural response of the VCR and repair [29]. Id-2 is a marker of the markers associated with senescence in dermal fibro-

Sumatra: an "experiment engine" that helps taking notes



Courtesy of Andrew Davison (AMP Workshop on Reproducible research)

Sumatra: an "experiment engine" that helps taking notes

```
$ smt comment 20110713-174949 "Eureka! Nobel prize  
here we come."
```

Sumatra: an "experiment engine" that helps taking notes

```
$ smt tag "Figure 6"
```

Sumatra: an "experiment engine" that helps taking notes

Sumatra: TestProject: List of records

http://127.0.0.1:8002/

TestProject: List of records

Delete Include data	Label	Reason	Outcome	Duration	Processes	Simulator		Script			Date	Time	Tags
						Name	Version	Repository	Main file	Version			
<input type="checkbox"/>	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	
<input type="checkbox"/>	20100709-154309			0.59 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:43:09	
<input type="checkbox"/>	hagling	'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	fooba
<input type="checkbox"/>	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	
<input type="checkbox"/>	hagling_repeat	Repeat experiment hagling	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	

Courtesy of Andrew Davison (AMP Workshop on Reproducible research)

New Tools for Computational Reproducibility

- Dissemination Platforms:

ResearchCompendia.org

IPOL

Madagascar

MLOSS.org

thedatahub.org

nanoHUB.org

Open Science Framework

The DataVerse Network

RunMyCode.org

- Workflow Tracking and Research Environments:

VisTrails

Kepler

CDE

Galaxy

GenePattern

Synapse

Sumatra

Taverna

Pegasus

- Embedded Publishing:

Courtesy of Victoria Stodden (UC Davis, Feb 13, 2014)

Verifiable Computational Research

Sweave

knitR

Collage Authoring Environment

SHARE

And also: **Org-Mode** 😊, **Figshare**, **Zenodo**, **ActivePapers** 😊, **Elsevier executable paper** 😞, ...

① A Few Motivating Examples

② The Reproducible Research Movement

How does it work in "real" sciences?

Reproducible Research/Open Science

Many Different Alternatives for Replicable Analysis

Good Practice for Setting up a Laboratory Notebook

③ Where are we now?

Step 0: Taking Notes

Document your:

- **Hypotheses**: keep track of your ideas/line of thoughts
- **Experiments**: details on how and why an experiment was run, including failed or ambiguous attempts.
- **Initial analysis or interpretation** of these experiments: was the outcome conform to the expectation or not? does it (in)validate the hypothesis?
- **Organization**: keep track of things to do/fix/test/improve

Structure:

- ① General information about the document and organization **conventions** (e.g., directory structure, notebook structure, experimental result storing mechanism, ...)
- ② Documentation of **commonly used commands** and of how to set up experiments (e.g., git cloning, environment deployment, connection to machines, compiling scripts)
- ③ Experiment results are better structured **by dates** (↪ add tags)

Which format should I use ?

- **Wikis** are encouraged to favor collaboration but I do not find them really effective
- **Blogging** systems are also a way of managing such notebook but they should rather be considered as an effective way to share information with others
- I recommend to use basic **plain-text** format and to **structure it hierarchically**

Here is a **link** to an excerpt of the journal of one of my PhD student, managed with `git/org-mode`.

Last but not least:

Provide links to **Raw Data!!!**

I have a very intense usage of my journal and I'll **demo this tomorrow**.

Moving to replicable articles and reproducible research becomes natural.

Step 1: Sharing Code and Data

What kinds of systems are available?

- "Good" - The cloud (Dropbox 😞, Google Drive, Figshare)
- Better - Version control systems (SVN, Git and Mercurial)
- "Best" - Version control systems on the cloud (GitHub, Bitbucket)

Depends on the level of privacy you expect but you probably already know these tools.

Few handle GB files...

Is this enough?

- 1 Use a workflow that documents both data and process
- 2 Use the machine readable CSV format
- 3 Provide raw data and meta data, not just statistical outputs
- 4 Never do data manipulation and statistical tests by hand
- 5 Use R, Python or another free software to read and process raw data (ideally to produce complete reports with code, results and prose)

Step 2: Literate Programming

Donald Knuth: explanation of the program logic in a natural language interspersed with snippets of macros and traditional source code.

I'm way too stupid to program this way but that's exactly what we need for writing a reproducible article/analysis!

Org-mode (requires emacs)

My favorite tool.

- plain text, very smooth, works both for html, pdf, ...
- allows to combine all my favorite languages even with sessions

Ipython/Jupyter notebook

If you are a python user, go for it! Web app, easy to use/setup...

KnitR (a.k.a. Sweave)

For non-emacs users and as a first step toward *reproducible papers*:

- Click and play with a modern IDE (e.g., Rstudio)

① A Few Motivating Examples

② The Reproducible Research Movement

How does it work in "real" sciences?

Reproducible Research/Open Science

Many Different Alternatives for Replicable Analysis

Good Practice for Setting up a Laboratory Notebook

③ Where are we now?

What is needed?

- Many **legal aspects** about data/code/idea sharing
 - I do not really care as I am a civil servant and I strongly believe research is a team sport
- Changes in **funding agency** requirements
 - Starting ? But I hardly see how they could really enforce things
- Changes in journal/conferences **publication requirements**
 - Several attempts (reproducibility labels)
 - V. Stodden seems confident (progressive policies rapidly adopted, journals with high impact factors)
- **Cultural changes** in our **relation to publication**

What is needed?

- Many **legal aspects** about data/code/idea sharing
 - I do not really care as I am a civil servant and I strongly believe research is a team sport
- Changes in **funding agency** requirements
 - Starting ? But I hardly see how they could really enforce things
- Changes in journal/conferences **publication requirements**
 - Several attempts (reproducibility labels)
 - V. Stodden seems confident (progressive policies rapidly adopted, journals with high impact factors)
- **Cultural changes** in our **relation to publication**

I think the change has to be profound and **cannot be top-down**

- **Train** our researchers and **students** to use better tools, better research methodology, Statistics/Design of Experiments, performance evaluation, ...
- Several computer scientists linked with **Inria** have started working on this subject. Inria asked me to **animate/coordinate** this group and open it way beyond Inria so that our action is effective at national scale

Possible Subjects

Webinars (1/month ?) with interactions, hands on keyboards when relevant.

- 1 Reproducible research, challenges, ethic
- 2 Provenance tracking of experimental data
- 3 Numerical reproducibility
- 4 Large scale experimental platforms
- 5 Code and Data archiving
- 6 Workflows
- 7 Online journals, companion websites
- 8 Evaluation campaign/challenges/benchmarks
- 9 ...

I need your help so set up such organization