

Reproducible Research for Computer Scientists

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Performance Evaluation Lecture
UFRGS, Porto Alegre, August 2015

Course Organization

Scientific Methodology and Performance Evaluation for Computer Scientists

5 lectures of 3 hours

- ① Reproducible research
- ② Data visualization/presentation
- ③ Introduction to probabilities/statistics
- ④ Linear regression
- ⑤ Design of Experiments

Stuff to know about this course

- Way too much stuff for so little time. The slides are extremely dense and I speak very fast. **Don't panic!** Feel free to interrupt
- Slides are self-contained with many *links* and code examples
- Try to **put into practice asap** to get the most out of it and **do not worry about the grade**

Outline

- ① A Few Motivating Examples
- ② The Reproducible Research Movement
 - How does it work in other sciences?
 - Is CS Concerned Really With This?
 - Reproducible Research/Open Science
 - Interesting Approaches for [PD]C Reproducible experiments
 - Many Different Alternatives for Replicable Analysis
- ③ Reporting Results
 - An IMRAD Report
 - Good Practice for Setting up a Laboratory Notebook
- ④ R/knitr Crash Course
 - General Introduction
 - Reproducible Documents: knitR
 - Introduction to R
- ⑤ Emacs Demo of How to Keep Things Tidy
- ⑥ To do for the Next Time

Frustration as an Author

- I thought I used the same parameters but I'm getting different results!
- The new student wants to compare with the method I proposed last year
- My advisor asked me whether I took care of setting this or this but I can't remember
- 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?
- It worked yesterday!
- 6 months later: why did I do that?

Frustration as a Reviewer

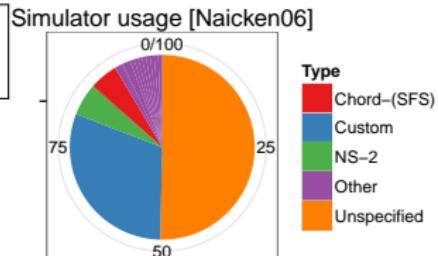
This may be an interesting contribution but:

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

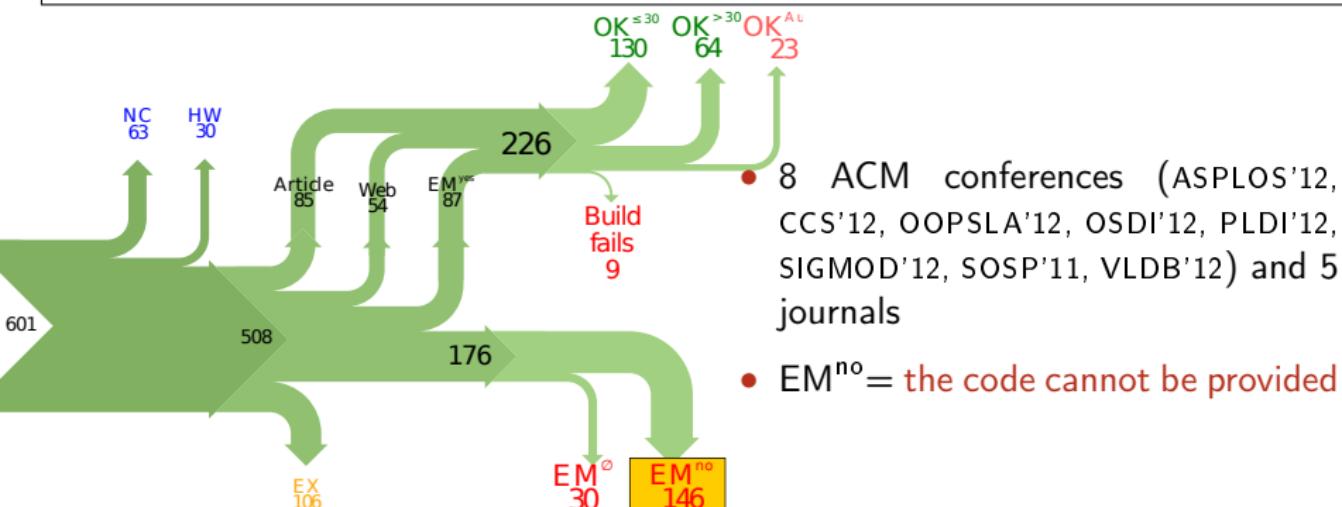
A Few Edifying Examples

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

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/>



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 <system> 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.

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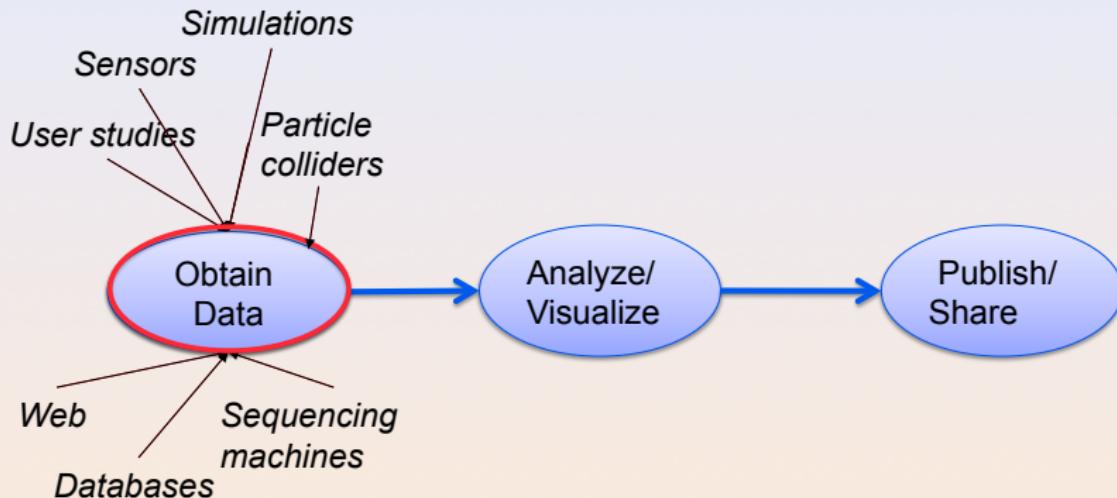
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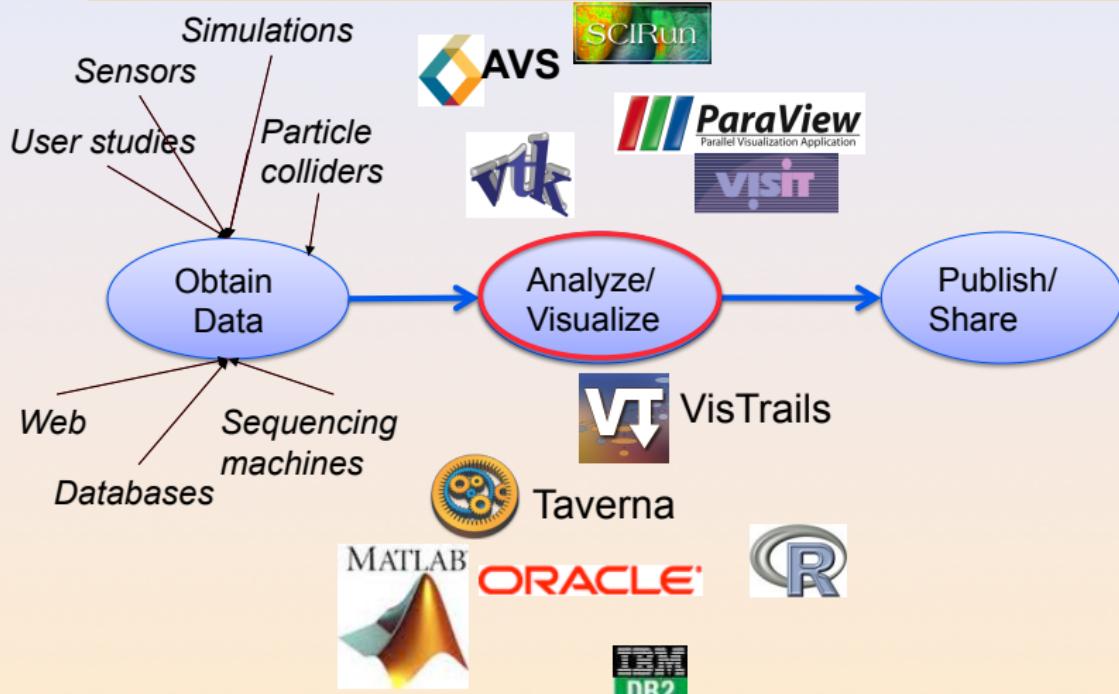
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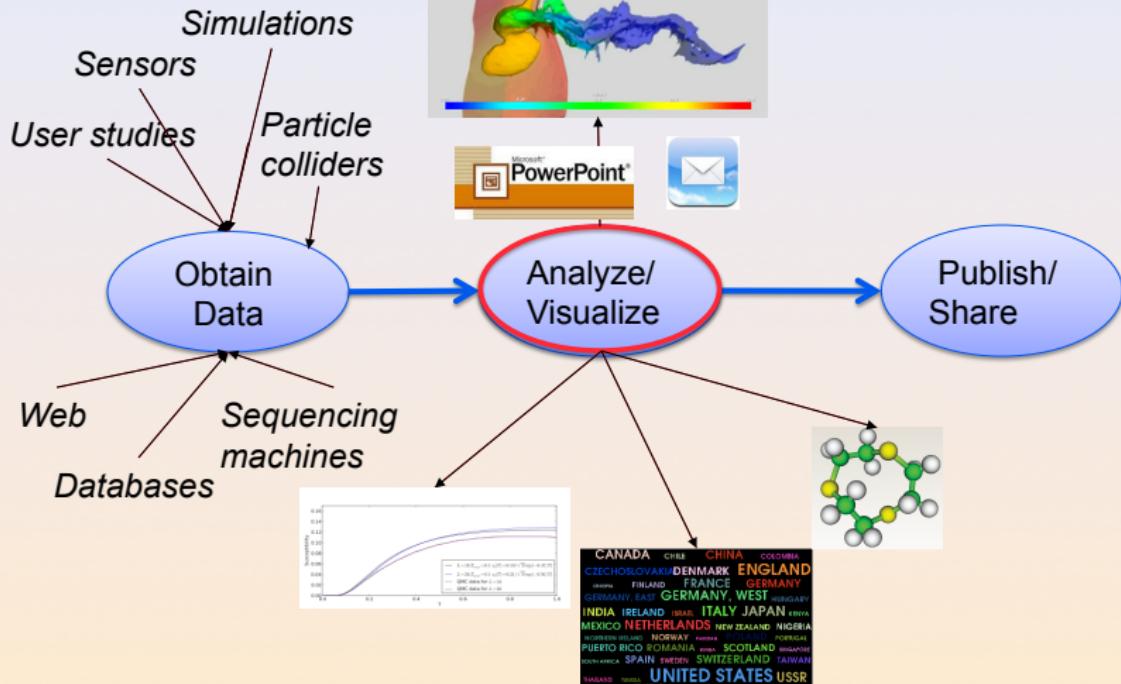
Science Today: Data Intensive



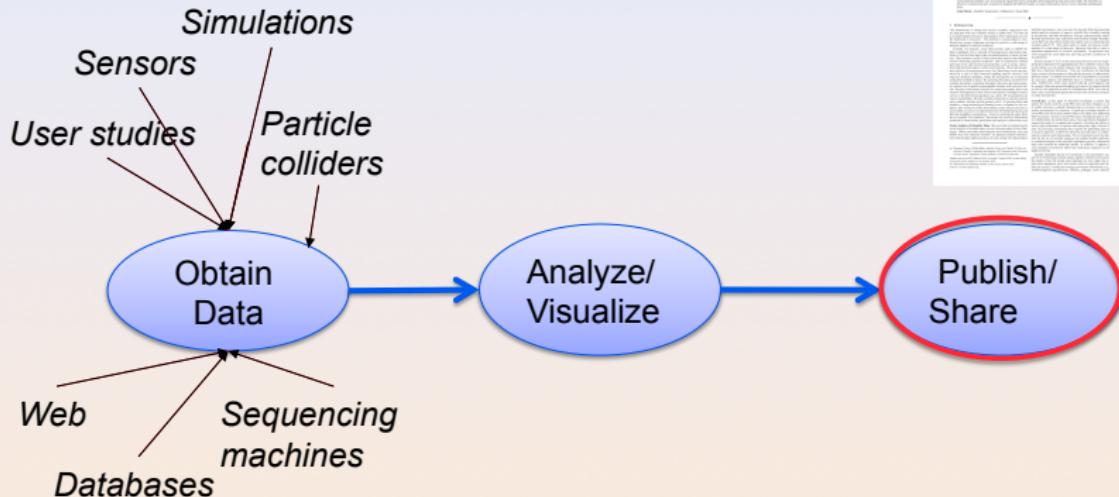
Science Today: Data + Computing Intensive



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Science Today: Data + Computing Inte



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



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- ◆ Publications are just the tip of the iceberg
 - “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
- ◆ Can’t really validate it
 - 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]



A few Words on Scientific Foundation

- Falsifiability or **refutability** of a statement, hypothesis, or theory is an inherent possibility to prove it to be false (not "commit fraud" but "*prove to be false*").
- Karl Popper makes falsifiability the demarcation criterion to **distinguish the scientific from the unscientific**

It is not only not right, it is not even wrong!

– Wolfgang Pauli

- Theories cannot be proved correct but they can be disproved. Only a few stand the test of batteries of **critical experiments**.
- It is not all black and white. There are many stories where scientists stick with their theories despite evidences and sometimes, they were even right to do so...

Testing and checking is thus one of the basis of science

Further readings: **A Summary of Scientific Method**, Peter Kosso, Springer

Why Are Scientific Studies so Difficult to Reproduce?

- Copyright/competition issue
- Publication bias (only the idea matters, not the gory details)
- Rewards for positive results
- Experimenter bias
- Programming errors or data manipulation mistakes
- Poorly selected statistical tests
- Multiple testing, multiple looks at the data, multiple statistical analyses
- ~~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. 2010, Nov.
- Increase in retracted papers:
 - Steen RG, *Retractions in the scientific literature: is the incidence of research fraud increasing?* J Med Ethics 37: 249–253.

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**

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 approximately \$19 million in grant money from the National Institutes of Health.
- 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

Scientific fraud is sooo bad... 😊 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* entries at *having fun with h-index*

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My Feeling

Computer scientists have an incredibly poor training in probabilities, statistics, experiment management

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’m tired of awful combination of tools (perl, gnuplot, sql, . . .) and bad methodology

Common practice in CS

Computer scientists tend to either:

- vary **one factor at a time**, use a very fine sampling of the parameter range,
- **run millions of experiments** for a week varying a lot of parameters and then try to get something of it. Most of the time, they (1) don't know how to analyze the results (2) realize something went wrong...

Interestingly, most other scientists do **the exact opposite**.

These two flaws come from poor training and from the fact that C.S. experiments are **almost** free and very fast to conduct

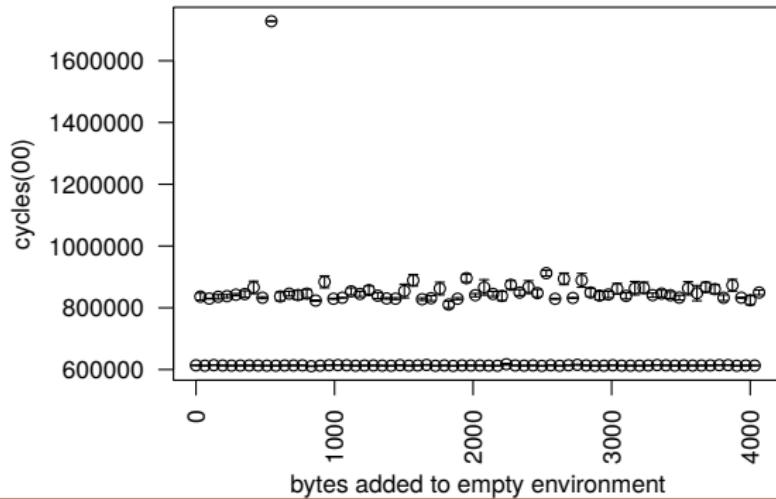
- Most strategies of experimentation (DoE) have been designed to **provide sound answers despite all the randomness and uncontrollable factors**
- **Maximize the amount of information** provided by a given set of experiments
- **Reduce as much as possible the number of experiments** to perform to answer a given question under a given level of confidence

Takes a few lectures on **Design of Experiments** to improve. But anyone can start by reading **Jain's book on The Art of Computer Systems Performance Analysis**

But do we **really** have to care?

Yes, although designed and built by human beings, computers are **so complex** that mistakes are easy to do...

- T. Mytkowicz, A. Diwan, M. Hauswirth, and P. F. Sweeney. **Producing wrong data without doing anything obviously wrong!**. SIGPLAN Not. 44(3), March 2009



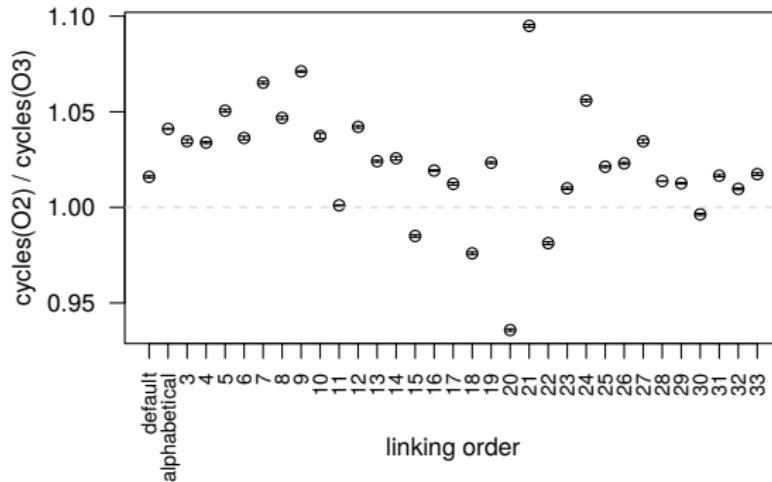
Key principles of experiment design

- Randomize to reduce bias
- Replicate (possibly in a smart way) to increase reliability

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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) (2014 edition)
- 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

Should be seen as opportunities to share experience.

Reproducibility: What Are We Talking About?

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

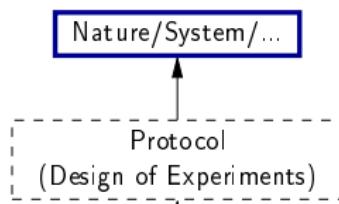
Completely independent reproduction based only on text description, without access to the original code

Reproducible Research: Trying to Bridge the Gap

Author



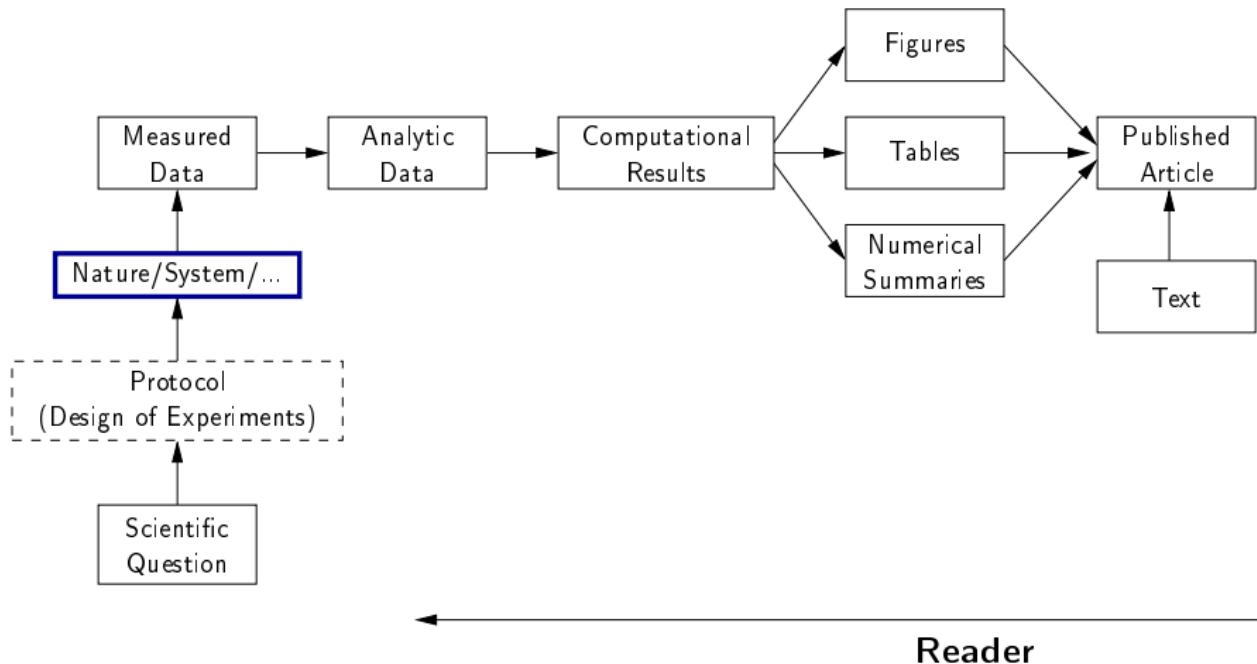
Published Article



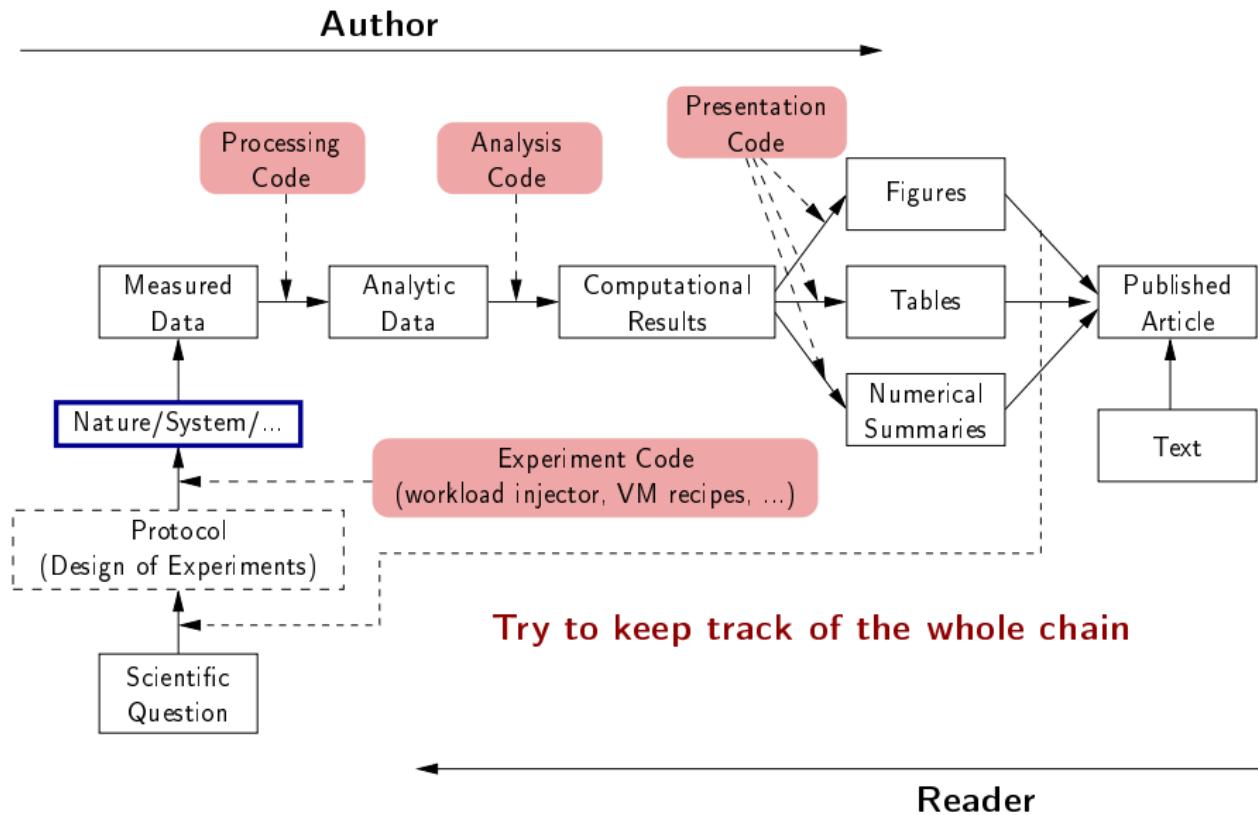
Reader

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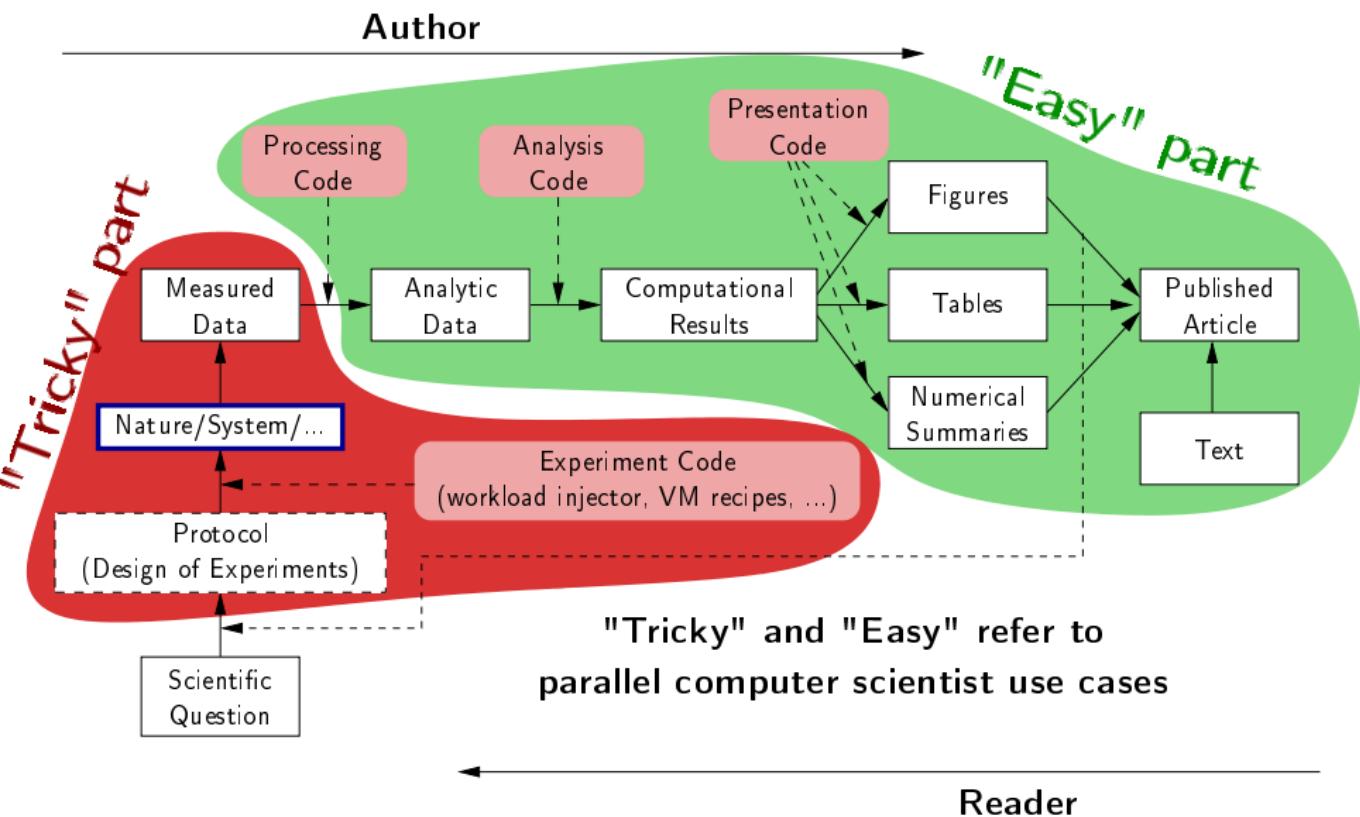
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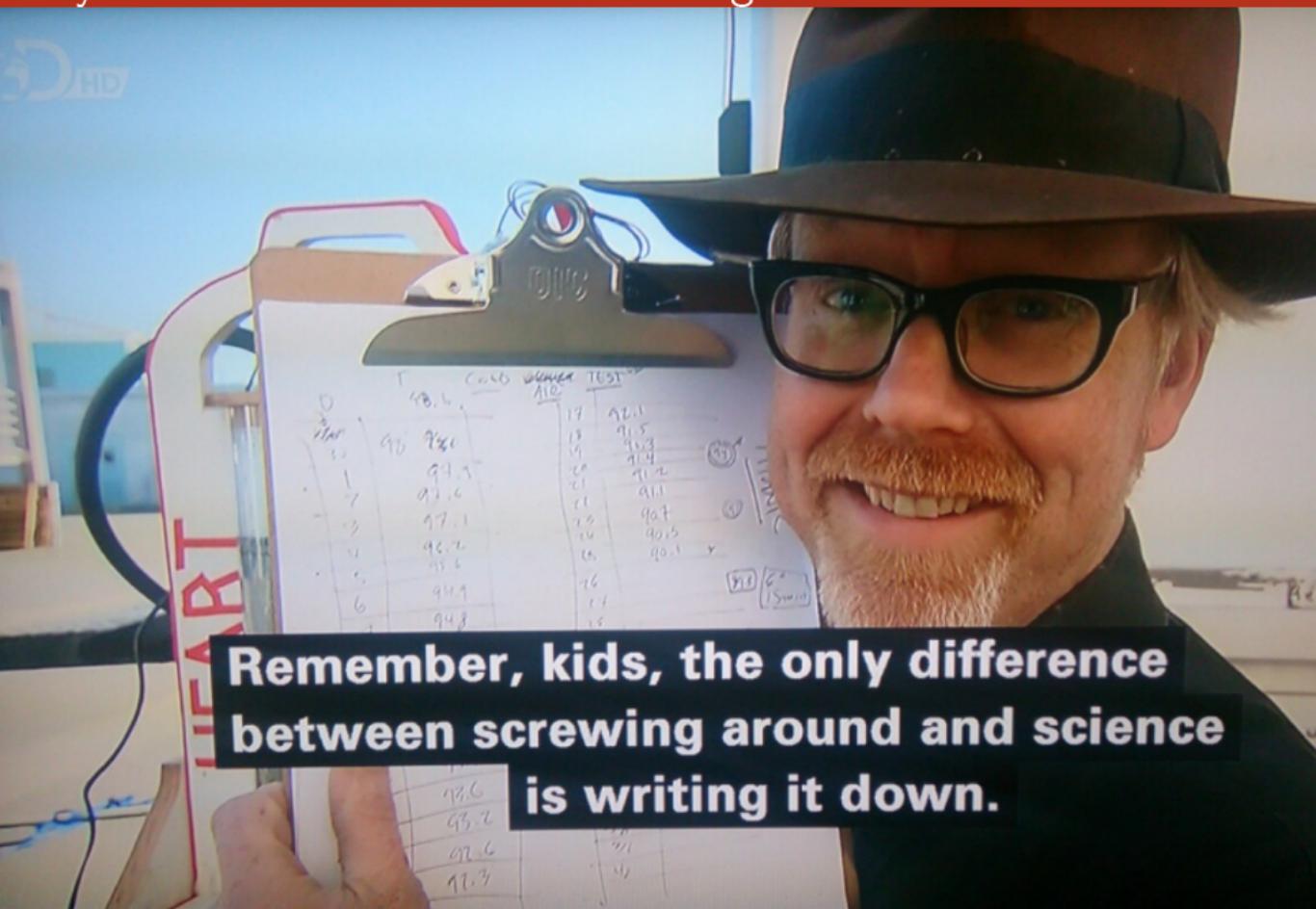
Reproducible Research: Trying to Bridge the Gap



Reproducible Research: Trying to Bridge the Gap



Mythbusters: Science vs. Screwing Around



**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

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

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A few Experiment Management Tools

- Naive way: sh + ssh + ...
 - **Expo** (2007-, G5K)
 - **XPflow** (2012-, G5K)
 - **Execo** (2013-, G5K)
- }
- although nothing
specific to G5K
- Plush (2006-, PlanetLab)
 - OMF (2009-, Wireless testbeds and Planetlab)
 - Splay (2008, distributed algorithm comparison)
 - ...

They differ in the underlying paradigms and the platforms for which they have been designed

- A taxonomy of experiment management tools for distributed systems,
T. Buchert, C. Ruiz , L. Nussbaum, O. Richard, FGCS, 2014

Expo

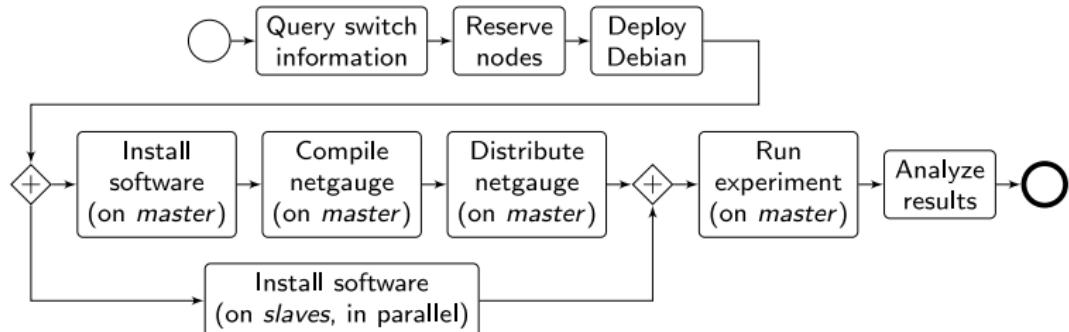
- Grenoble (B. Videau, C. Ruis, O. Richard) <http://expo.gforge.inria.fr/>
- **DSL** (Domain Specific Language) derived from **Ruby** and adapted to the management of experiment (based on **taktuk**, i.e., sh + ssh)
- At the moment Expo interacts with **Planetlab** and **Grid5000** testbeds
- Resource and task abstractions, client-server organization, **interactive** or **batch** mode
- **Native logging and archiving capabilities**
 - every action performed on tasks, error flows, dates, ...
 - lets you know **what** was run, **when**, **where** and **how**

```
1 reserv=ExpoEngine::new(@connection)
2 reserv.site=["bordeaux","lille","luxembourg","nancy","sophia"]
3 reserv.resources=["nodes=50","nodes=10","nodes=4","nodes=4","nodes=30"]
4 reserv.name = "Expo Scalability"
5 reserv.walltime=600
6
7 reserv.run!
8 ptask $all, "hostname"
9 reserv.stop!
```

- Inspired similar tools like **Execo** that provides a **Python-based API**. Script-oriented, fork+sh+ssh or taktuk

XPflow

- Nancy (T. Buchert, L. Nussbaum) <http://xpflow.gforge.inria.fr/>
- **DSL** (Domain Specific Language) derived from **Ruby** and adapted to the management of experiment
- Resources, process, and activities
- Top-down rather than bottom-up: **business process management**
- Cope with **failures** through **snapshots** and **retry policy**



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```
process :exp do |site, switch|
  s = run g5k.switch, site, switch
  ns = run g5k.nodes, s
  r = run g5k.reserve_nodes,
    :nodes => ns, :time => '2h',
    :site => site, :type => :deploy
  master = (first_of ns)
  rest = (tail_of ns)
  run g5k.deploy,
    r, :env => 'squeeze-x64-nfs'
  checkpoint :deployed
  parallel :retry => true do
    forall rest do |slave|
      run :install_pkgs, slave
    end
    sequence do
      run :install_pkgs, master
      run :build_netgauge, master
      run :dist_netgauge,
        master, rest
    end
  end
  end
  checkpoint :prepared
  output = run :netgauge, master, ns
  checkpoint :finished
  run :analysis, output, switch
end
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Activity :install_pkgs

```
activity :install_pkgs do|node|
  log 'Installing packages on ', node
  run 'g5k.bash', node do
    aptget :update
    aptget :upgrade
    aptget :purge, 'mx'
  end
end
```

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end
```

Activity :build_netgauge

```
activity :build_netgauge do |master|
  log "Building netgauge on #{master}"
  run 'g5k.copy', NETGAUGE, master, '-'
  run 'g5k.bash', master do
    build_tarball NETGAUGE, PATH
  end
  log "Build finished."
```

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end
```

Activity :dist_netgauge

```
activity :dist_netgauge do |m, s|
  master, slaves = m, s
  run 'g5k.dist_keys', master, slaves
  run 'g5k.bash', master do
    distribute BINARY,
      DEST, 'localhost', slaves
  end
end
```

- Nancy (T. Buchert, L. Nussbaum) <http://xpflow.gforge.inria.fr/>
- **DSL** (Domain Specific Language) derived from **Ruby** and adapted to the management of experiment
- Resources, process, and activities
- Top-down rather than bottom-up: **business process management**
- Cope with **failures** through **snapshots** and **retry policy**

```
process :exp do |site, switch|
  s = run g5k.switch, site, switch
  ns = run g5k.nodes, s
  r = run g5k.reserve_nodes,
    :nodes => ns, :time => '2h',
    :site => site, :type => :deploy
  master = (first_of ns)
  rest = (tail_of ns)
  run g5k.deploy,
    r, :env => 'squeeze-x64-nfs'
  checkpoint :deployed
  parallel :retry => true do
    forall rest do |slave|
      run :install_pkgs, slave
    end
    sequence do
      run :install_pkgs, master
      run :build_netgauge, master
      run :dist_netgauge,
        master, rest
    end
  end
  checkpoint :prepared
  output = run :netgauge, master, ns
  checkpoint :finished
  run :analysis, output, switch
end
```

Activity :netgauge

```
activity :netgauge do |master, nodes|
  log "Running experiment..."
  out = run 'g5k.bash', master do
    cd PATH
    mpirun nodes, "./netgauge"
  end
  log "Experiment done."
end
```

A few Environment Management Tools

CDE automatically tracks and packages up the Code, Data, and Environment

Providing **not only VMs or binaries but also recipes** is **good!**

E.g., the Kameleon project

- Univ. Grenoble (C. Ruiz, S. Harrache, M. Mercier, O. Richard, . . .)
<http://kameleon.readthedocs.org/>
- Generate customized **appliances** (kvm, LXC, Virtualbox, iso, . . .)
- Ruby-based, **YAML** description of **recipes** with **steps** and **aliases**, execution in **contexts**
- Automatically **checkpoints** to rebuild only what is required

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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
 - 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?

Support different approaches

Vistrails: a Workflow Engine for Provenance Tracking

An Provenance-Rich Paper: ALPS2.0

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. Gamper¹ J. Gukelberger⁶ E. Gulf⁷ S. Guertler⁸
A. Hehn⁹ R. Igashiri¹⁰ S.V. Isakov¹ D. Koop² P.N. Ma¹¹
P. Mates^{1,2} H. Matsuo¹¹ O. Parcollet¹² G. Pawłowski¹³
J.D. Picon¹⁴ L. Pollet¹⁵ E. Santos¹⁶ V.W. Scarola¹⁶
U. Schollwöck¹⁷ C. Silva¹⁸ B. Surer¹⁹ S. Todo^{11,20} S. Trebst¹⁶
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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

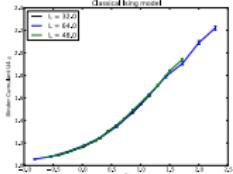
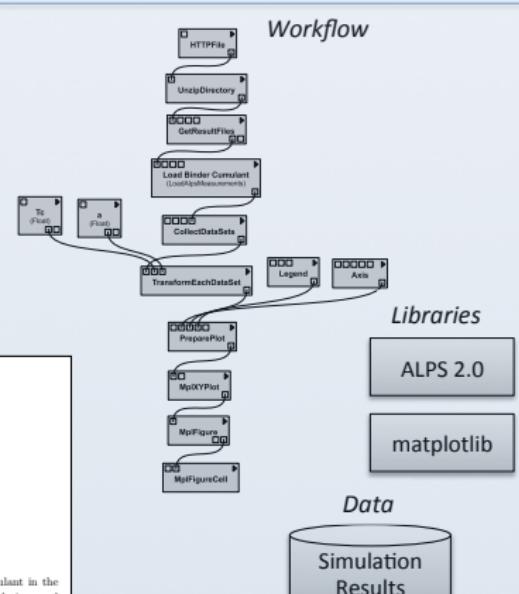


Figure 3 shows a plot of the relative cumulant versus temperature T for the classical Ising model. The x-axis ranges from -0.5 to 0.5, and the y-axis ranges from 1.0 to 2.0. Three data series are plotted for system sizes L = 32, 64, and 128. The L = 32 curve (red) shows significant deviation from the others at low temperatures. As the system size increases, the curves converge towards a single blue line, which represents the critical behavior of the model.



Workflow diagram illustrating the data processing pipeline:

- Data** (Simulation Results) feeds into **ALPS 2.0**.
- ALPS 2.0** feeds into **Libraries**.
- Libraries** feed into **Workflow**.
- Workflow** produces **ALPS 2.0** (which generates **Transformed Data** and **Final Plot**) and **matplotlib**.

Legend and axes are part of the **Final Plot**.

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

¹ Correspondence

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.

VCR: A Universal Identifier for Computational Results

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  
>
```

VCR: A Universal Identifier for Computational Results

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
```

VCR: A Universal Identifier for Computational Results

Word-processor plugin App

LaTeX source

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

LaTeX source with VCR package

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

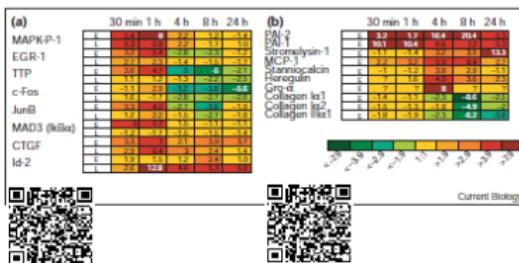
Permanently bind printed graphics to underlying result content

VCR: A Universal Identifier for Computational Results

Research Paper Analysis of replicative senescence Shelton et al. 943

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 a natural progression of events in senescence. In contrast, transcripts were hyper-induced in serum-stimulated senescent cells, suggesting that the transition to senescence is associated with a dramatic increase in gene expression. The genes that are induced in senescent cells include those that are involved in the regulation of the extracellular matrix, such as collagenases, cathepsins, and proteases, as well as those that are involved in the regulation of the immune system, such as TLR-4 and NF- κ B.

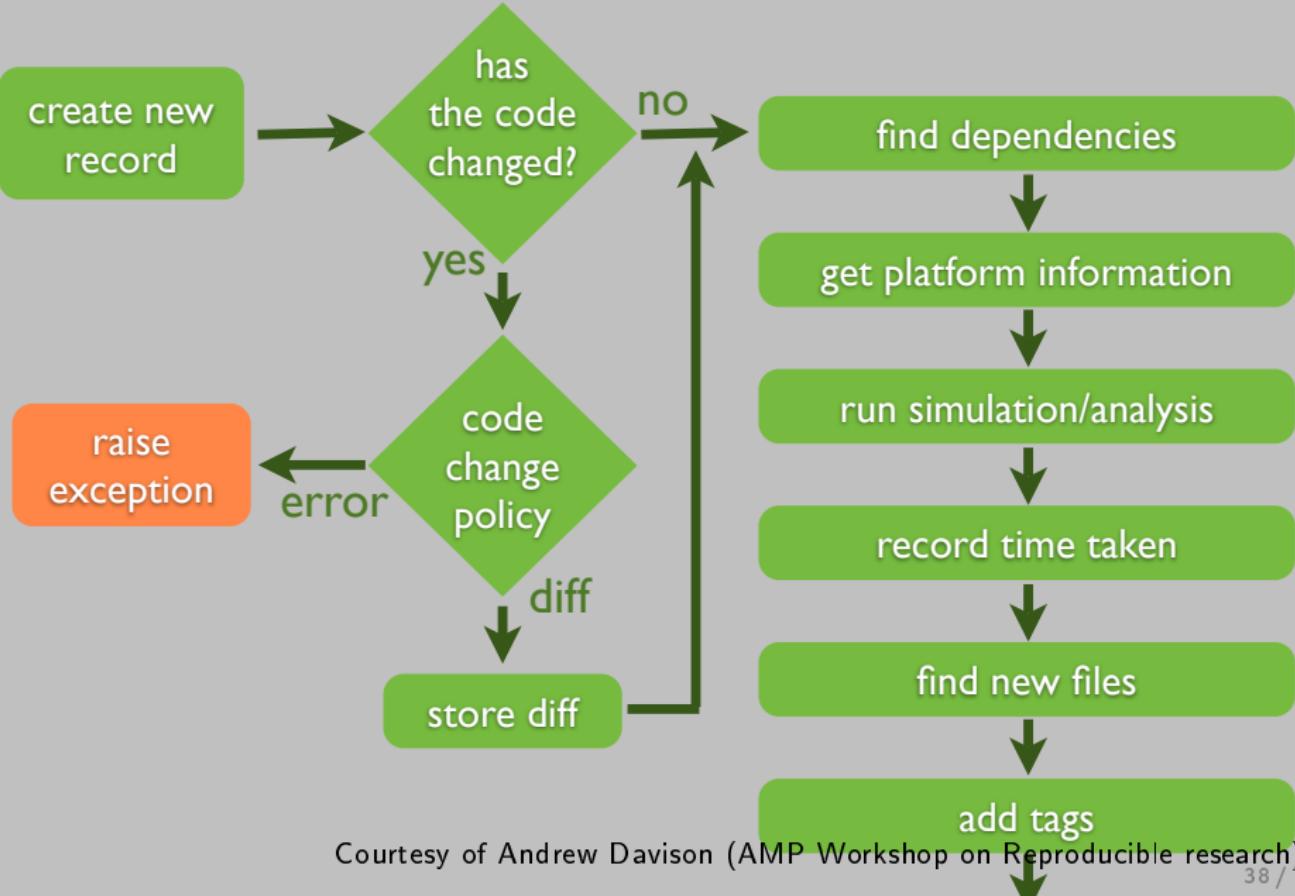
states overlap substantially with those in telomere-induced senescence (W.F., D.N.S., R. Allsopp, S. Lowe, and G. Ferbeyre, unpublished observations) and thus are likely to use many of the same activation processes.

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].

surprisingly, early-passage cells also overexpress many of the markers associated with senescence in dermal fibroblasts, including TLR-4, NF- κ B, and cathepsins. These

Courtesy of Manoj Gavish and David Donoho (AMP Workshop on Reproducible research)

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

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"/>	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
<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"/>	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	

So many new tools

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: **Figshare**, **ActivePapers**, **Elsevier executable paper**, ...

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Structure

Research articles are often structured in this basic order:

Introduction Why was the study undertaken? What was the research question, the tested hypothesis or the purpose of the research?

Methods When, where, and how was the study done? What materials/hardware were used? How was it configured?

Results What answer was found to the research question; what did the study find? Was the tested hypothesis true? **Present useful results in a synthetic way with a logical order.**

Discussion What might the answer imply and why does it matter? How does it fit in with what other researchers have found? What are the possible bias and points to improve? What are the perspectives for future research?

Such structure **facilitates literature review** and is a very effective way to convey information.

If the report is a few pages long then **an abstract is required.**

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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 can be either structured **by dates** (\sim add tags) or **by experiment campaigns** (\sim add date/time)

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. More detailed links are given in slide 69.

Last but not least:

Provide links to Raw Data!!!

When/How Often Should I Use it?

I have a very intense usage (demo to **general journal** and specific **BOINC journal**) and I tend to capture a lot of information but you do not have to be as extreme as I am. Here are a few advices:

- Spending **more than an hour without** at least **writing** what you're working on **is not right**...
 - **Take a 5 minutes** break and ask yourself what you're doing, what is keeping you busy and where all this is leading you
- While working on something, you will often notice/think about something you should fix/improve but you just don't want to do it now. Take 20 seconds to write a **TODO** entry.
- There are moments where you have to **wait for something** (compiling, deployment, ...). It is generally the perfect time for improving your notes (e.g., detail the steps to accomplish a TODO entry).
- **By the end of the day**: daily (and weekly) **review!**
 - Update your lists, write what the next steps are
 - **Summarize in a 2-4 lines** (for your advisor) what you did, what was difficult, what you learnt.

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 3133t 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 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)

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Why R?

R is a great language for data analysis and statistics

- Open-source and multi-platform
- Very expressive with high-level constructs
- Excellent graphics
- Widely used in academia and business
- Very active community
 - Documentation, FAQ on <http://stackoverflow.com/questions/tagged/r>
- Great integration with other tools

Why is such R a pain for computer scientists?

- R is **not** really a **programming** language
- Documentation is for statisticians
- Default plots are **cumbersome** (meaningful)
- Summaries are **cryptic** (precise)
- **Steep learning curve** even for us, computer scientists whereas we generally switch seamlessly from a language to another! That's frustrating!
;)

Do's and dont's

~~R is high level, I'll do everything myself~~

- CTAN comprises 4,334 \TeX , \LaTeX , and related packages and tools.
Most of you do not use plain \TeX .
- Currently, the CRAN package repository features 4,030 available packages.
- How do you know which one to use??? Many of them are highly exotic
(not to say useless to you).

I learnt with <http://www.r-bloggers.com/>

- Lots of introductions but not necessarily what you're looking for so I'll give you a short tour.
You should quickly realize though that you need proper training in statistics and data analysis if you do not want tell nonsense.
- Again, you should read Jain's book on **The Art of Computer Systems Performance Analysis**
- You may want to follow online courses:
 - <https://www.coursera.org/course/compdata>
 - <https://www.coursera.org/course/repdata>

Install and run R on debian

```
1 apt-cache search r
```

Err, that's not very useful :) It's the same when searching on google but once the filter bubble is set up, it gets better...

```
1 sudo apt-get install r-base
```

```
1 R
```

```
1 R version 3.2.0 (2015-04-16) -- "Full of Ingredients"
2 Copyright (C) 2015 The R Foundation for Statistical Computing
3 Platform: x86_64-pc-linux-gnu (64-bit)
4
5 R is free software and comes with ABSOLUTELY NO WARRANTY.
6 You are welcome to redistribute it under certain conditions.
7 Type 'license()' or 'licence()' for distribution details.
8
9 R is a collaborative project with many contributors.
10 Type 'contributors()' for more information and
11 'citation()' on how to cite R or R packages in publications.
12
13 Type 'demo()' for some demos, 'help()' for on-line help, or
14 'help.start()' for an HTML browser interface to help.
15 Type 'q()' to quit R.
```

Install a few cool packages

R has its own package management mechanism so just run R and type the following commands:

- ddply, reshape and ggplot2 by Hadley Wickham (<http://had.co.nz/>)

```
1 install.packages("plyr")
2 # or better: install.packages("dplyr")
3 install.packages("reshape")
4 # or better: install.packages("tidyverse")
5 install.packages("ggplot2")
```

- knitr by (Yihui Xie) <http://yihui.name/knitr/>

```
1 install.packages("knitr")
```

IDE

Using R interactively is nice but quickly becomes painful so at some point, you'll want an IDE.

Emacs is great but you'll need *Emacs Speaks Statistics*

```
1 sudo apt-get install ess
```

In this tutorial, I will briefly show you [rstudio](https://www.rstudio.com/) (<https://www.rstudio.com/>)
and later how to use org-mode

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Rstudio screenshot

RStudio screenshot showing the R Markdown interface, workspace, and console.

File menu: File, Edit, Code, View, Project, Workspace, Plots, Tools, Help.

Code Editor: Displays two R Markdown files: `markdown-introduction.rmd` and `example-r-markdown.rmd`. The code in `example-r-markdown.rmd` includes R code for generating a scatter plot and its corresponding data frame.

```
28 v ``{r basicconsole}
29 x <- 1:10
30 y <- round(rnorm(10, x, 1), 2)
31 df <- data.frame(x, y)
32 df
33
34
35
36 ## Plots
37 Images generated by 'knitr' are saved in a figures folder. However,
| they also appear to be represented in the HTML output using a [data
| URI scheme]( http://en.wikipedia.org/wiki/Data_URI_scheme). This
| means that you can paste the HTML into a blog post or discussion
| forum and you don't have to worry about finding a place to store the
| images; they're embedded in the HTML.
38
39 ### Simple plot
40 Here is a basic plot using base graphics:
41
42 ``{r simpleplot}
43 plot(x)
44
45
46 ``{r simpleplot}
47 plot(x)
```

Console: Shows the R session history.

```
> set.seed(1234)
> library(ggplot2)
> library(lattice)
> x <- 1:10
> y <- round(rnorm(10, x, 1), 2)
> df <- data.frame(x, y)
> df
   x   y
1 1 1.31
2 2 2.31
3 3 3.36
4 4 4.27
5 5 5.04
6 6 6.11
7 7 8.43
8 8 8.98
9 9 8.38
10 10 9.27
> plot(x)
```

Workspace: Shows the data frame `df` with 10 observations and 2 variables: `x` (integer[10]) and `y` (numeric[10]).

Plots: A scatter plot of `x` vs `y`, showing a positive linear trend.

x	y
1	1.31
2	2.31
3	3.36
4	4.27
5	5.04
6	6.11
7	8.43
8	8.98
9	8.38
10	9.27

Reproducible analysis in Markdown + R

- Create a new **R Markdown** document (Rmd) in rstudio
- R chunks are interspersed with “`{r}`” and “`
- Inline R code: ‘`r sin(2+2)`’
- You can **knit** the document and share it via **rpubs**
- R chunks can be sent to the top-level with Alt-Ctrl-c
- I usually work mostly with the current environment and only knit in the end
- Other engines can be used (use rstudio **completion**)

```
1 `'{r engine='sh'}
```

```
2 ls /tmp/
```

```
3 `'
```

- Makes **reproducible analysis as simple as one click**
- Great tool for quick analysis for self and colleagues, homeworks, ...

Reproducible articles with L^AT_EX + R

- Create a new R **Sweave** document (Rnw) in rstudio
- R chunks are interspersed with <>>= and @
- You can **knit** the document to produce a pdf
- You'll probably quickly want to **change default behavior** (activate the cache, hide code, ...). In the preembule:

```
1 <<echo=FALSE>>=
2 opts_chunk$set(cache=TRUE,dpi=300,echo=FALSE,fig.width=7,
3                 warning=FALSE,message=FALSE)
4 @
```

- Great for journal articles, theses, books, ...

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Introduction to R

⑤ Emacs Demo of How to Keep Things Tidy

⑥ To do for the Next Time

Data frames

A data frame is a data tables (with columns and rows). `mtcars` is a built-in data frame that we will use in the sequel

```
1 head(mtcars);
```

		mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
1	Mazda RX4	21.0	6	160	110	3.90	2.620	16.46	0	1	4	4
2	Mazda RX4 Wag	21.0	6	160	110	3.90	2.875	17.02	0	1	4	4
3	Datsun 710	22.8	4	108	93	3.85	2.320	18.61	1	1	4	4
4	Hornet 4 Drive	21.4	6	258	110	3.08	3.215	19.44	1	0	3	3
5	Hornet Sportabout	18.7	8	360	175	3.15	3.440	17.02	0	0	3	2
6	Valiant	18.1	6	225	105	2.76	3.460	20.22	1	0	3	1

You can also load a data frame from a CSV file:

```
1 df <- read.csv("http://foo.org/mydata.csv", header=T,  
2 strip.white=TRUE);
```

You will **get help** by using ?:

```
1 ?data.frame  
2 ?rbind  
3 ?cbind
```

Exploring Content (1)

```
1 names(mtcars);  
  
1 [1] "mpg"   "cyl"   "disp"  "hp"    "drat"  "wt"    "qsec" "vs"    "am"  
2 [11] "carb"  
  
1 str(mtcars);  
  
1 'data.frame': 32 obs. of 11 variables:  
2 $ mpg : num  21 21 22.8 21.4 18.7 18.1 14.3 24.4 22.8 19.2 ...  
3 $ cyl  : num  6 6 4 6 8 6 8 4 4 6 ...  
4 $ disp : num  160 160 108 258 360 ...  
5 $ hp   : num  110 110 93 110 175 105 245 62 95 123 ...  
6 $ drat : num  3.9 3.9 3.85 3.08 3.15 2.76 3.21 3.69 3.92 3.92 ...  
7 $ wt   : num  2.62 2.88 2.32 3.21 3.44 ...  
8 $ qsec : num  16.5 17 18.6 19.4 17 ...  
9 $ vs   : num  0 0 1 1 0 1 0 1 1 1 ...  
10 $ am   : num  1 1 1 0 0 0 0 0 0 0 ...  
11 $ gear : num  4 4 4 3 3 3 3 4 4 4 ...  
12 $ carb : num  4 4 1 1 2 1 4 2 2 4 ...
```

Exploring Content (2)

```
1 dim(mtcars);  
2 length(mtcars);
```

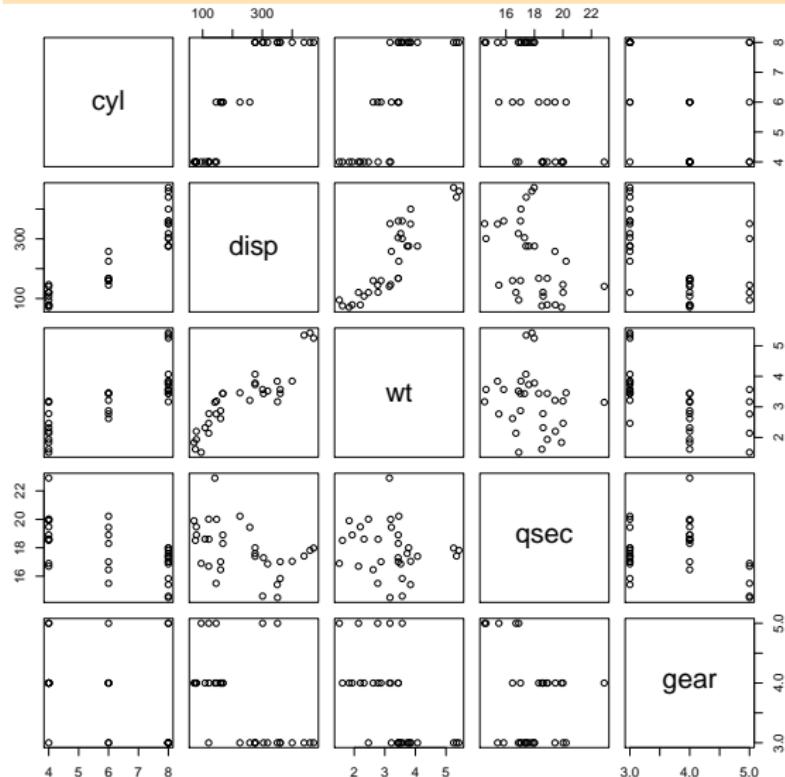
```
1 [1] 32 11  
2 [1] 11
```

```
1 summary(mtcars);
```

	mpg	cyl	disp	hp
Min.	:10.40	Min. :4.000	Min. : 71.1	Min. : 52.0
1st Qu.	:15.43	1st Qu.:4.000	1st Qu.:120.8	1st Qu.: 96.5
Median	:19.20	Median :6.000	Median :196.3	Median :123.0
Mean	:20.09	Mean :6.188	Mean :230.7	Mean :146.7
3rd Qu.	:22.80	3rd Qu.:8.000	3rd Qu.:326.0	3rd Qu.:180.0
Max.	:33.90	Max. :8.000	Max. :472.0	Max. :335.0
	drat	wt	qsec	vs
Min.	:2.760	Min. :1.513	Min. :14.50	Min. :0.0000
1st Qu.	:3.080	1st Qu.:2.581	1st Qu.:16.89	1st Qu.:0.0000
Median	:3.695	Median :3.325	Median :17.71	Median :0.0000
Mean	:3.597	Mean :3.217	Mean :17.85	Mean :0.4375
3rd Qu.	:3.920	3rd Qu.:3.610	3rd Qu.:18.90	3rd Qu.:1.0000

Exploring Content (3)

```
1 plot(mtcars[names(mtcars) %in% c("cyl", "wt", "disp", "qsec", "gear")])
```



Accessing Content

```
1 mtcars$mpg
```

```
1 [1] 21.0 21.0 22.8 21.4 18.7 18.1 14.3 24.4 22.8 19.2 17.8 16.4 17.0  
2 [16] 10.4 14.7 32.4 30.4 33.9 21.5 15.5 15.2 13.3 19.2 27.3 26.0 30.4  
3 [31] 15.0 21.4
```

```
1 mtcars[2:5,]$mpg
```

```
1 [1] 21.0 22.8 21.4 18.7
```

```
1 mtcars[mtcars$mpg == 21.0,]
```

```
1          mpg cyl disp  hp drat    wt  qsec vs am gear carb  
2 Mazda RX4     21   6 160 110  3.9 2.620 16.46  0  1    4    4  
3 Mazda RX4 Wag 21   6 160 110  3.9 2.875 17.02  0  1    4    4
```

```
1 mtcars[mtcars$mpg == 21.0 & mtcars$wt > 2.7,]
```

```
1          mpg cyl disp  hp drat    wt  qsec vs am gear carb  
2 Mazda RX4 Wag 21   6 160 110  3.9 2.875 17.02  0  1    4    4
```

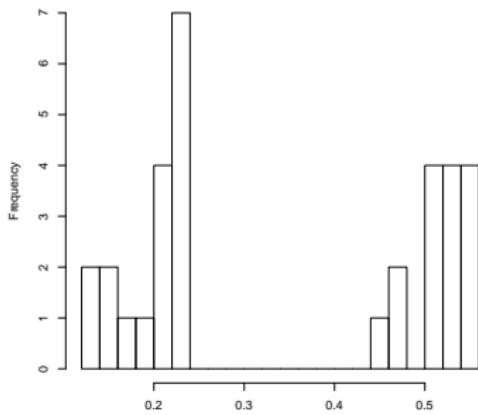
Extending Content

```
1 mtcars$cost = log(mtcars$hp)*atan(mtcars$disp)/  
2   sqrt(mtcars$gear**5);  
3 mean(mtcars$cost);  
4 summary(mtcars$cost);
```

```
1 [1] 0.345994  
2      Min. 1st Qu. Median      Mean 3rd Qu.      Max.  
3 0.1261 0.2038 0.2353 0.3460 0.5202 0.5534
```

```
1 hist(mtcars$cost, breaks=20);
```

Histogram of mtcars\$cost



Take away Message

- R is a great tool but is only a tool. There is no magic. You need to understand what you are doing and get a **minimal training in statistics**
- It is one of the building block of **reproducible research** (the *reproducible analysis* block) and **will save you a lot of time**
- It provides you an access to any statistical method you ever dreamt of
- Read at least Jain's book: **The Art of Computer Systems Performance Analysis**
- There are introductory **online courses** (from John Hopkins university) on coursera which you may want to follow

Outline

① A Few Motivating Examples

② The Reproducible Research Movement

How does it work in other sciences?

Is CS Concerned Really With This?

Reproducible Research/Open Science

Interesting Approaches for [PD]C Reproducible experiments

Many Different Alternatives for Replicable Analysis

③ Reporting Results

An IMRAD Report

Good Practice for Setting up a Laboratory Notebook

④ R/knitr Crash Course

General Introduction

Reproducible Documents: knitR

Introduction to R

⑤ Emacs Demo of How to Keep Things Tidy

⑥ To do for the Next Time

Literate Programming on a Daily Basis

Mastering Emacs

- C-g: get me out of here!
- C-_: undo
- Activate CUA keys in the Options menu

Mastering Org-mode

- Tab will fold/unfold stuff
- C-c C-c: do something (context-sensitive) where you are
- <s + Tab, <b, <l, <r, <h, ... for **creating code blocks**
- C-c C-e: **export**
- C-c c: **capture content**
- C-c C-o / C-c l / C-c C-l: open/store/insert **links**
- C-c C-a: **attach** a file
- C-c C-d: set deadline, C-c C-t: TODO/DONE

Emacs/Org-mode Recap

Key features

- Plain text makes it **very robust** and **human readable**
- Allow to **mix any language** and has a notion of session that makes its use very effective
- Allow to produce both `html` documents, classical `LATEX`articles, beamer slides, `odt` documents, ... Native **pretty printing** on Github

A Few Links to Learn More

- *Org for beginners, my emacs configuration and tricks for Mac OS X users*
- A *script capturing* and gathering many **information** into a *single result document*
- A *laboratory notebook* with notes about all the **experiments** performed since the beginning of the project
- *Litterately conducting experiments* using org-mode

This was way too much information...

... but keep these slides in mind and re-read them later. You will follow many links when you will realize what they can bring to you.

- We need to put all this in practice.
- During this semester, you will learn how to improve your methodology
- You will apply analysis and reporting techniques to a simple use case:

One of your colleague just implemented a multi-threaded version of the quicksort algorithm for multi-core machines. He's convinced his code can save significant time saving but unfortunately, he did not follow the performance evaluation lecture and he would like your help to promote his code.

- After you have tried, we will debrief on what you did and discuss how it could be improved

To do for the Next Time (1/2)

- ① Install R and Rstudio and all the packages I previously mentioned (`plyr`, `dplyr`, `reshape`, `tidyR`, `ggplot2`) on your own machines.
- ② Make sure you know how to `create small reproducible analysis` and publish them on! `rpubs` with Rstudio.
- ③ Start `learning R` with `swirl`: You may want to have a look at *R for Beginners*.
- ④ Setup emacs `org-mode` and start playing with it.

To do for the Next Time (2/2)

- ① Fork on Github and send me corresponding URL
<https://github.com/alegrand/M2R-ParallelQuicksort>
- ② Experiment this code on various environments (laptop, G5K, ...)
- ③ Take notes on what you did and push back your journal on github
- ④ Create a synthetic one page IMRAD report