Obtaining Faithful/Reproducible Measurements on Modern CPUs

Arnaud Legrand and Tom Cornebize
Univ. Grenoble Alpes, CNRS, Inria, Grenoble INP

Journée SIF – Reproductibilité de la recherche
May 2021
Reproducible Research and Computer Science
The processing steps between raw observations and findings have gotten increasingly numerous and complex
The processing steps between raw observations and findings have gotten increasingly numerous and complex.
The processing steps between raw observations and findings have gotten increasingly numerous and complex.
The processing steps between raw observations and findings have gotten increasingly numerous and complex.
The processing steps between raw observations and findings have gotten increasingly numerous and complex.
The processing steps between raw observations and findings have gotten increasingly numerous and complex.

Reproducible Research = Bridging the Gap by working Transparently.
"Reproducible Research": First Appearance

Claerbout & Karrenbach, meeting of the Society of Exploration Geophysics, 1992

Electronic Documents Give Reproducible Research a New Meaning

Jon F. Claerbout and Martin Karrenbach, Stanford Univ.

SUMMARY

A revolution in education and technology transfer follows from the marriage of word processing and software command scripts. In this marriage an author attaches to every figure caption a pushbutton or a name tag usable to recalculate the figure from all its data, parameters, and programs. This provides reproducibility in both the electronic document and the computational analysis.

In 1990, we set this sequence of goals:

• Learn how to merge a publication with its underlying computational analysis.

• Teach researchers how to prepare a document in a form where they themselves can reproduce their own research results a year or more later by “pressing a single button”.

• Learn how to leave finished work in a condition where coworkers can reproduce the calculation including the final illustration by pressing a button in its caption.

• Prepare a complete copy of our local software environment so that graduating students can take their work away with them to other sites, press a button, and reproduce their Stanford work.

• Merge electronic documents written by multiple authors (SEP reports).

• make incremental improvements in electronic-document software

• seek partners for broadening standards (and making incremental improvements).

Our basic goal is reproducible research. The electronic document is our means to this end. In principle, reproducibility in research can be achieved without electronic documents and that is how we started. Our first nonelectronic reproducible document was a textbook in which the paper document contained the name of a program script in every figure caption. The program scripts were organized by book chapter and section so they could be correlated to an accompanying magnetic tape dump of the file system. The magnetic tape also contained all the necessary data to feed the program script.

Now that we have begun using CD-ROM publication, we can go much further. Every figure caption contains a pushbutton that jumps to the appropriate science directory (folder) and initiates a figure rebuild command and then displays the figure, possibly as a movie or interactive program. We normally display seismic images of the earth’s interior, but to reach wider audiences, Figure 1 shows a satellite weather picture which the pushbutton will animate as seen on commerical television. We include all our plot software as well as freely available software from many sources, including compilers and the LaTeX word processing system. Naturally we cannot include licensed software, but with the exception...
Existing Tools, Emerging Standards

Notebooks and workflows

Software environments

Sharing platforms

Notebooks and workflows

Software environments

Sharing platforms
Scientific practices have greatly evolved, in particular since we rely on computers

How computers broke science – and what we can do about it

– Ben Marwick, The conversation, 2015

1. Computational science concerns:
   - Genomics software engineering, computational reproducibility, provenance
   - Computational fluid dynamics numerical issues

2. Statistical concerns:
   - Social Psychology, Medical sciences, ... methodology, statistics, pre-registration

What about Computer Science?
All this is about Computational Sciences. Should we care?

Computer Science is young and inherits from Mathematics, Engineering, Linguistic, Nat. Sciences, ...

Purely theoretical scientists whose practice is close to mathematics may not be concerned (can’t publish a math article without releasing the proofs).

- Have a look at talk by Vladimir Voevodsky in 2014 at Princeton

Les quatre concepts de l’informatique, Gilles Dowek 2011:

- Algorithm, Machine, Language, Information
Well, I design algorithms!

- "Real" problems are all NP-hard, Log-APX, etc.
- Real workload = NP-completeness proof widgets, regularities and properties (difficult to formally state but that should be exploited)

Algorithms are evaluated on particular workloads that impact both their running time and the quality of the solutions
Well, I design algorithms!

- "Real" problems are all NP-hard, Log-APX, etc.
- Real workload = NP-completeness proof widgets, regularities and properties (difficult to formally state but that should be exploited)

Algorithms are evaluated on particular workloads that impact both their running time and the quality of the solutions

**Image Processing:** True horror stories, E. Meinhardt-Llopis, CANUM 2016

- The proposed multigrid algorithm converges to the solution of the problem in $O(N)$ using biharmonic functions
- Surprisingly, our naive multi-scale Gauss-Seidel converges much faster
"Real" problems are all NP-hard, Log-APX, etc.

Real workload = NP-completeness proof - widgets, regularities and properties (difficult to formally state but that should be exploited)

Algorithms are evaluated on particular workloads that impact both their running time and the quality of the solutions

Image Processing: True horror stories, E. Meinhardt-Llopis, CANUM 2016

- The proposed multigrid algorithm converges to the solution of the problem in $O(N)$ using biharmonic functions
- Surprisingly, our naive multi-scale Gauss-Seidel converges much faster
**I design Machine Learning Algorithms**

**Machine Learning:** Trouble at the lab, The Economist 2013

According to some estimates, three-quarters of published scientific papers in the field of machine learning are bunk because of this "overfitting".

– Sandy Pentland (MIT)

**NeurIPS, ICLR:** open reviews, reproducibility challenges

→ Joelle Pineau @ NeurIPS’18

Every month in CACM, there is an article about the ethical consequences of Machine Learning on:

- Car driving, Autonomous guns, Law enforcement (risk assessment, predictive policing), ...  
  **It’s Not the Algorithm, It’s the Data** (CACM, Feb. 2017)
- Advertising, Loan attribution, Selection at University, Organ transplant

Increasing society concern about **fairness** and **transparency**
Computer science is not more related to computers than Astronomy to telescopes

– Dijkstra (mis-attributed)

Right, why should we care about computers? They are deterministic machines after all, right? 😊
Computer science is not more related to computers than Astronomy to telescopes

– Dijkstra (mis-attributed)

Right, why should we care about computers? They are deterministic machines after all, right? 😊

Model ≠ Reality. Although designed and built by human beings, computer systems are so complex that mistakes easily slip in...

Our reality evolves!!! The hardware keeps evolving so most results on old platforms quickly become obsolete (although, we keep building on such results 😏).

We need to regularly revisit and allow others to build on our work!

Key Concerns for our Community (Room for Improvement)

P1: Repeated experiments
P2: Workload and cfg. coverage
P3: Experimental setup description
P4: Open access artifact
P5: Prob. result descr. of meas. perf.
P6: Statistical evaluation

Key DoE principles:

1. **Replicate** to increase reliability.
2. **Randomize** to reduce bias. **Evaluate** statistical confidence.
Horror Stories when Measuring CPU Performance
Measuring performance is difficult

Producing wrong data without doing anything obviously wrong!

Mytkowicz et al. in ACM SIGPLAN Not. 44(3), March 2009

Changing the size of environment variables can trigger performance degradation as high as 300%; simply changing the link order of object files can cause performance to decrease by as much as 57%.
Producing wrong data without doing anything obviously wrong!

Mytkowicz et al. in ACM SIGPLAN Not. 44(3), March 2009

changing the size of environment variables can trigger performance degradation as high as 300%; simply changing the link order of object files can cause performance to decrease by as much as 57%.


**STABILIZER** forces executions to sample the space of memory configurations by repeatedly rerandomizing layouts of code, stack, and heap objects at runtime. [...] Re-randomization ensures that layout effects follow a Gaussian distribution, enabling the use of statistical tests like ANOVA.
Producing wrong data without doing anything obviously wrong!

Mytkowicz et al. in ACM SIGPLAN Not. 44(3), March 2009
changing the size of environment variables can trigger performance degradation as high as 300%; simply changing the link order of object files can cause performance to decrease by as much as 57%.


**STABILIZER** forces executions to sample the space of memory configurations by repeatedly rerandomizing layouts of code, stack, and heap objects at runtime. [...] Re-randomization ensures that layout effects follow a Gaussian distribution, enabling the use of statistical tests like ANOVA.

Randomization helps fighting bias incurred by:
1. specific configurations $AA...A \rightarrow A_1A_2...A_n$ (pseudo-replication)
2. temporary perturbations $AA...A BB...B \rightarrow ABBAAAB...$
On the Importance of Content Initialization

- \( C = A \times A \) (2048 \times 2048), independant
- \( A \) initialized with \( 0 \ 1 \ 0.987 \ 1, 2, 3, \ldots \) random
- Time scale = 5 minutes
On the Importance of Content Initialization

- \( C = A \times A \) (2048 \times 2048), independent
- \( A \) initialized with \( 0 \quad 1 \quad 0.987 \quad 1, 2, 3, \ldots \) \( \text{random?} \)
- Time scale = 5 minutes

Evolution of DGEMM performance on some nodes of parasilo (matrices of size 2048 \times 2048)

Matrix content
- 0
- 0.987
- 1
- random
- sequential

Courtesy of T. Cornebize, DGEMM performance is data-dependent https://hal.inria.fr/hal-02401760
On the Importance of Content Initialization

- $C = A \times A \ (2048 \times 2048)$, independant
- $A$ initialized with $0 \ 1 \ 0.987 \ 1, 2, 3, \ldots \ \text{random}$
- Time scale = 5 minutes

Evolution of DGEMM performance on some nodes of parasilo (matrices of size $2048 \times 2048$)

Bit-flips $\Rightarrow$ NRJ Consumption $\Rightarrow$ $T^\circ$ $\uparrow$ + TDP $\Rightarrow$ Frequency $\Rightarrow$ Performance ?!

Courtesy of T. Cornebize, DGEMM performance is data-dependent https://hal.inria.fr/hal-02401760
On the Importance of Content Initialization

- \( C = A \times A \) (2048 \times 2048), independent
- \( A \) initialized with \( \begin{bmatrix} 0 & 1 & 0.987 & 1, 2, 3, \ldots \end{bmatrix} \) random

Time scale = 5 minutes

Evolution of DGEMM performance on some nodes of dahu (matrices of size 2048\times2048)

Courtesy of T. Cornebize, DGEMM performance is data-dependent [https://hal.inria.fr/hal-02401760](https://hal.inria.fr/hal-02401760)
On the Importance of Content Initialization

- \( C = A \times A (2048 \times 2048) \), independant
- \( A \) initialized with \( \begin{bmatrix} 0 & 1 & 0.987 & 1, 2, 3, \ldots \end{bmatrix} \) random

Distribution of DGEMM performance on some nodes of dahu (matrices of size 2048\( \times \)2048)

Courtesy of T. Cornebize, DGEMM performance is data-dependent [https://hal.inria.fr/hal-02401760](https://hal.inria.fr/hal-02401760)
On the Importance of Content Initialization

- $C = A \times A \ (2048 \times 2048)$, independent
- $A$ initialized with $\begin{bmatrix} 0 & 1 & 0.987 & 1, 2, 3, \ldots \end{bmatrix}$
- Time scale = 5 minutes

Evolution of the temperature when running the calibration on dahut

Courtesy of T. Cornebize, *DGEMM performance is data-dependent* https://hal.inria.fr/hal-02401760
On the Importance of Content Initialization

- \( C = A \times A \) (2048 × 2048), independant
- \( A \) initialized with \[ \begin{bmatrix} 0 & 1 & 0.987 & 1, 2, 3, \ldots \end{bmatrix} \] random

Time scale = 5 minutes

Evolution of the frequency when running the calibration on dahu

Mask size (bits)
- 0
- 10
- 20
- 30
- 40
- 50
- 53

Courtesy of T. Cornebize, DGEMM performance is data-dependent

https://hal.inria.fr/hal-02401760
Avoiding "Temporary" Perturbations (Randomizing a Factorial Design)

- HPL performance (32 nodes, 70 cfg., 5 repetitions)
- Time scale = 3 days

Courtesy of T. Cornebize
Avoiding "Temporary" Perturbations (Randomizing a Factorial Design)

- HPL performance (32 nodes, 70 cfg., 5 repetitions) · Time scale = 3 days

Courtesy of T. Cornebize
Avoiding "Temporary" Perturbations (Randomizing a Factorial Design)

- HPL performance (32 nodes, 70 cfg., 5 repetitions)
- Time scale = 3 days

Courtesy of T. Cornebize
Platform Evolution Over a Long Period

Dahu-14

Outlier
- False
- True

Weird
- False
- Positive
- Negative

Dahu-26

Outlier
- False
- True

Weird
- False
- Positive
- Negative

Courtesy of T. Cornebize, https://cornebize.net/g5k_test/
Platform Evolution Over a Long Period

Dahu overview

Outlier
- False
- True

Probability
- [+] 0% - 0.01%
- [+] 0.01% - 0.1%
- [+] 0.1% - 1.0%
- [+] 1.0% - 10.0%
- 10.0% - 100%
- [-] 1.0% - 10.0%
- [-] 0.1% - 1.0%
- [-] 0.01% - 0.1%
- [-] 0% - 0.01%

Date

2019-08 2019-11 2020-02 2020-05 2020-08 2020-11 2021-02

Node: CPU

Courtesy of T. Cornebize, https://cornebize.net/g5k_test/
Conclusion
1. **A separation of concerns**
   - Transparent Measurement Procedure and Analysis Procedure

2. **Randomized and Designed Experiments** allowing to both:
   - Check the model and Instanciate it

3. Careful recording of all experimental parameters (before and during XPs)
Reproducible Research = Rigor and Transparency

To err is human. **Good research requires time and resources**

1. **Train yourself and your students**: RR, statistics, experiments
   - Beware of checklists and norms
   - Understand what’s at stake

#RRMooc 3rd Edition: ≈ Feb. 2020

A **new MOOC**: "Advanced RR" (Oct 2021?)
   - Managing data (HDF5, archiving)
   - Software environment control (Docker, GUIX)
   - Scientific workflow (snakemake)
To err is human. **Good research requires time and resources**

1. **Train yourself and your students**: RR, statistics, experiments  
   - Beware of checklists and norms  
   - Understand what’s at stake  
   
   #RRMooc 3rd Edition: ≈ Feb. 2020  

   A new MOOC: ”Advanced RR” (Oct 2021?)  
   - Managing data (HDF5, archiving)  
   - Software environment control (Docker, GUIX)  
   - Scientific workflow (snakemake)  

2. **Change the norm**: make publication practices evolve  
   - Require data, code, environment, XP protocol, …  

3. **Incentive**: consider RR/open science when hiring/promoting
To err is human. Good research requires time and resources

1. **Train yourself and your students:** RR, statistics, experiments
   - Beware of checklists and norms
   - Understand what’s at stake
   
   #RRMooc 3rd Edition: ≈ Feb. 2020

   A new MOOC: "Advanced RR" (Oct 2021?)
   - Managing data (HDF5, archiving)
   - Software environment control (Docker, GUIX)
   - Scientific workflow (snakemake)

2. **Change the norm:** make publication practices evolve
   - Require data, code, environment, XP protocol, ...

3. **Incentive:** consider RR/open science when hiring/promoting

4. **Prepare the Future:** How to share Experiments?
   - Reuse, reuse, reuse!
   - Shared and controled testbeds (e.g., Grid’5000/FIT-IoTLab)
   - Toward literate experimentation?
   
   4–8 October, 2021 @ Strasbourg
   16th GDR RSD Fall School: Reproductibilité et recherche expérimentale en réseaux et en systèmes [https://rsd-ecole.cnrs.fr/](https://rsd-ecole.cnrs.fr/)