Set the Default to Reproducible

Jonathan Borwein, **FRSC FAAAS FAA FAMS**
www.carma.newcastle.edu.au/jon
Director CARMA (Computer Assisted Research Mathematics and Applications)
Laureate Professor University of Newcastle, NSW

"We have a habit in writing articles published in scientific journals to make the work as finished as possible, to cover up all the tracks, to not worry about the blind alleys or describe how you had the wrong idea first, and so on. So there isn't any place to publish, in a dignified manner, what you actually did in order to get to do the work."

(Richard Feynman, 1918-1988)

THE UNIVERSITY OF NEWCASTLE AUSTRALIA

Revised 29/10/15

Publishing Standards for Computational Science:

"Setting the Default to Reproducible"

Fpr

Mathematical Aspects of Behavioural Economics and Finance

November 13-14 2015

Publishing Standards for Computational Science:

"Setting the Default to Reproducible"

BY VICTORIA STODDEN, JONATHAN BORWEIN, & DAVID H. BAILEY

"'Setting the Default to Reproducible' in Computational Science Research," *SIAM News*, vol. 46, no. 5 (June 2013), pg. 4-6.

Also

D.H. Bailey, J.M. Borwein and Victoria Stodden, ``Set the default to 'open'," *Notices of the AMS*. **60** (6) (2013), 679-680.

D. Bailey, J. Borwein, and V. Stodden. ``Facilitating Reproducibility in Scientific Computing: Principles and Practice." Chapter in *Reproducibility - Principles, Problems, Practices.* Harald Atmanspacher and Sabine Maasen editors. John Wiley & Sons, New York 2015. In Press.

From *SIAM News*, Volume 46, Number 5, June 2013

"Setting the Default to Reproducible" in Computational Science Research

Following a late-2012 workshop at the Institute for Computational and Experimental Research in Mathematics, a group of computational scientists have proposed a set of standards for the dissemination of reproducible research.

By Victoria Stodden, Jonathan Borwein, and David H. Bailey

Computation is now central to the scientific enterprise, and the emergence of powerful computational hardware, combined with a vast array of computational software, presents novel opportunities for researchers. Unfortunately, the scientific culture surrounding computational work has evolved in ways that make it difficult to verify findings, efficiently build on past research, or even apply the basic tenets of the scientific method to computational procedures.

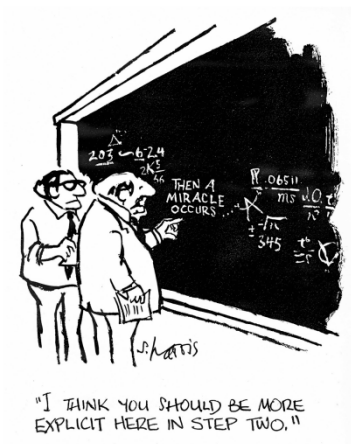
As a result, computational science is facing a credibility crisis [1,2,4,5]. The enormous scale of state-of-the-art scientific computations, using tens or hundreds of thousands of processors, presents unprecedented challenges. Numerical reproducibility is a major issue, as is hardware reliability. For some applications, even rare interactions of circuitry with stray subatomic particles matter.

In December 2012, more than 70 computational scientists and stakeholders, such as journal editors and funding agency officials, gathered at Brown University for the ICERM Workshop on Reproducibility in Computational and Experimental Mathematics (http://icerm.brown.edu/tw12-5-rcem). This workshop gave a broad cross section of computational scientists their first opportunity to discuss these issues and brainstorm ways to improve on current practices; the result was a series of recommendations for establishing really reproducible computational science as a standard [13]. Three main recommendations emerged from the workshop discussions:

1. It is important to promote a culture change that will integrate computational reproducibility into the research process.
2. Journals, funding agencies, and employers should support this culture change.
3. Reproducible research practices and the use of appropriate tools should be taught as standard operating procedure in relation to computational aspects of research.

Changing the Culture

Early in their careers, bench scientists and experimental researchers are taught to maintain notebooks or computer logs of every work detail—including design, procedures, equipment, raw results, processing techniques, statistical methods of analysis. Unfortunately, few computational experiments are documented so carefully. Typically, there is no record of workflow, computer hardware and software configuration, parameter settings, or function invocation sequences. Source code is often either lost or revised with no record of the revisions. These practices not only cripple the reproducibility of results; ultimately, they impede the researchers' own productivity.



Courtesy of S. Harris, ScienceCartoonsPlus.com.

The research system must offer institutional rewards for producing reproducible research at every level, from departmental decisions to grant funding and journal publication. The current academic and industrial research system places primary emphasis on publication and project results, with little attention to reproducibility. It penalizes those who devote the time needed to produce really reproducible research. It is regrettable that software development is often discounted. It has been compared to, say, constructing a telescope, rather than doing *real science*. Thus, scientists are discouraged from writing or testing code. Sadly, NSF-funded projects on average remain accessible on the web only about a year after funding ends. Researchers are busy with new projects and lack the time or money to preserve the old. With the ever-increasing importance of computation and software, such attitudes and practices must change.

Support from Funding Agencies, Journals, and Employers

Software and data should be "open by default," in the absence of conflicts with other considerations, such as confidentiality. Grant proposals involving computational work should be required to provide such details as standards for: dataset and software documentation, including reuse (some agencies already have such requirements [11]); persistence of resulting software and dataset preservation and archiving; standards for sharing resulting software among reviewers and other researchers.

Funding agencies should add "reproducibility" to the specific examples, such as "Broader Impact" statements, that proposals could include. Software and dataset curation should be explicitly included in grant proposals and recognized as a scientific contribution by funding agencies. Templates for data management plans that include making software open and available could be provided, perhaps by funding agencies, or by institutional archiving and library centers [7].

Editors and reviewers must insist on rigorous verification and validity testing, along with full disclosure of computational details [6]. Some details might be relegated to a website, with assurances that this information will persist and remain accessible. Exceptions arise, as in the case of proprietary, medical, or other confidentiality issues, but authors need to state this upon submission, and reviewers and editors must agree that the exceptions are reasonable. Better standards are needed for including citations of software and data in the references of a paper, instead of inline or as footnotes. Proper citation is essential both for improving reproducibility and for ensuring credit for work done in developing software and producing data, which is a key component in encouraging the desired culture change [10].

The third source of influence on the research process stems from employers—tenure and promotion committees and re-search managers at research labs. Software and dataset contributions, as described above, should be rewarded as part of expected research practices. Data and code citation practices should be recognized and expected in computational research.

Teaching and Tools for Reproducible Research

Proficiency in the skills required to carry out reproducible research in the computational sciences should be taught as part of the scientific methodology, along with modern programming and software engineering techniques. This should be a standard part of any computational research curriculum, just as experimental or observational scientists are taught to keep laboratory notebooks and follow the scientific method. Students should be encouraged and formally taught to adopt appropriate tools. Many tools are available or under development to help in replicating earlier results (of the researcher or others). Some tools ease literate programming and publishing of computer code, either as commented code or notebooks. Others capture the provenance of a computation or the complete software environment. Version control systems are not new, but current tools facilitate their use for collaboration and archiving complete project histories. For a description of current tools, see the workshop report [13] or wiki [8].

One of us teaches a graduate seminar that requires students to replicate results from a published paper [9]. This is one way to introduce tools and methods for replication into the curriculum, and it gives students first-hand appreciation for the importance of incorporating principles of reproducibility into the scientific research process.

Conclusions

Recent events in economics and psychology illustrate the current scale of error and fraud in scientific research [3]. Following the lead of the United Kingdom, Australia, and others, the United States recently mandated public release of publicly funded research, including data [12]. We hope that this will help bring about the needed cultural change in favour of consistently reproducible computational research. While different types and degrees of reproducible research were discussed at the ICERM workshop, an overwhelming majority argued that the community must move to "open research": research that uses accessible software tools to permit (a) auditing of computational procedures, (b) replication and independent verification of results, and (c) extension of results or application of methods to new problems.

References

[1] A. Abbott and Nature Magazine, *Disputed results a fresh blow for social psychology*, Scientific American, April 30, 2013; http://www.scientificamerican.com/article.cfm?id=disputed-results-a-fresh-blow-for-social-psychology.

[2] D.H. Bailey and J.M. Borwein, *Exploratory experimentation and computation*, Notices Amer. Math. Soc., 58:10 (2011), 1410–1419.

[3] D.H. Bailey and J.M. Borwein, *Reliability, reproducibility and the Reinhart Rogoff error*, April 19, 2013; http://experimentalmath.info/blog/2013/04/reliability-reproducibility-and-the-reinhart-rogoff-error/.

[4] J.M. Borwein and D.H. Bailey, *Mathematics by Experiment*, 2nd edition, AK Peters, Natick, MA, 2008.

[5] D. Donoho, A. Maleki, M. Shahram, V. Stodden, and I. Ur Rahman, *Reproducible research in computational harmonic analysis*, Comput. Sci. Engin., 11:1 (2009), 8–18.

[6] D. Fanelli, *Redefine misconduct as distorted reporting*, Nature, February 13, 2013; http://www.nature.com/news/redefine-misconduct-as-distorted-reporting-1.12411.

[7] For examples see http://scholcomm.columbia.edu/data-management/data-management-plan-templates/ and http://www2.lib.virginia.edu/brown/data/NSFDMP.html and http://www2.lib.virginia.edu/brown/data/NSFDMP.html.

[8] ICERM Reproducibility Workshop Wiki, http://wiki.stodden.net/ICERM_Reproducibility_in_Computational_and_Experimental_Mathematics:_Readings_and_References.

[9] D. Ince, *Systems failure*, Times Higher Education, May 5, 2011; http://www.timeshighereducation.co.uk/416000.article.

[10] R. LeVeque, I. Mitchell, and V. Stodden, *Reproducible research for scientific computing: Tools and strategies for changing the culture*, Comput. Sci. Engin., 14:4 (2012), 13–17.

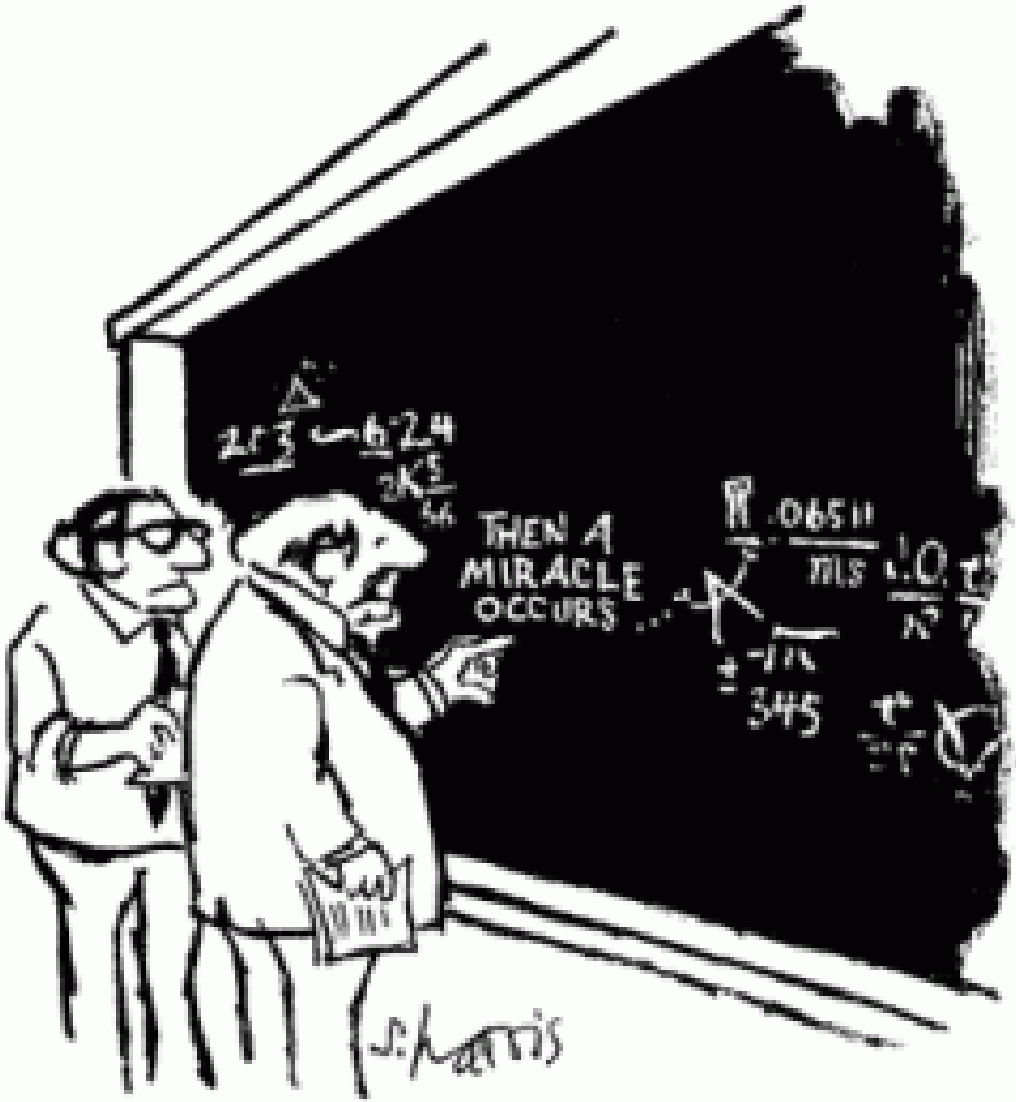
[11] B. Matthews, B. McIlwrath, D. Giaretta, and E. Conway, *The significant properties of software: A study*, 2008; http://www.jisc.ac.uk/media/documents/programmes/preservation/spsoftware_report_redacted.pdf.

[12] OSTP, *Expanding public access to the results of federally funded research*, February 22, 2013; http://www.whitehouse.gov/blog/2013/02/22/expanding-public-access-results-federally-funded-research.

[13] V. Stodden, D.H. Bailey, J. Borwein, R.J. LeVeque, W. Rider, and W. Stein, *Setting the default to reproducible: Reproducibility in computational and experimental mathematics*, February 2, 2013; http://www.davidhbailey.com/dhbpapers/icerm-report.pdf.

Victoria Stodden is an assistant professor of statistics at Columbia University. Jonathan Borwein is Laureate Professor of Mathematics at the University of Newcastle, Australia. David H. Bailey is a senior scientist in the Department of Computational Research at Lawrence Berkeley National Laboratory and a research fellow in the Department of Computer Science at the University of California, Davis.

CARMA



"I think you should be more explicit here in step two."

ABSTRACT

Recent research scandals in Economics, Medicine, and Social Psychology [2,3] all reinforce the point that

Secret science is bad science

- I will discuss these and the rationale for, events and outcomes of a December 2012 workshop on *Reproducibility in Computational and Experimental Mathematics* held at the **Institute for Research in Computational and Experimental Mathematics** (ICERM) at Brown University [1]
- In particular, I discuss the meeting's primary recommendations for a more accountable, reliable, open practice of computational science

1. *Set the Default to "Open": Reproducible Science in the Computer Age:* http://www.huffingtonpost.com/david-h-bailey/set-the-default-to-open-r_b_263
2. *Scientific fraud, sloppy science – yes, they do happen* https://theconversation.com/profiles/jonathan-borwein-jon-101/articles
3. *The train wreck continues: another social science retraction* (May 2015) https://theconversation.com/the-train-wreck-continues-another-social-science-retraction-42404

ABSTRACT

A group of computational scientists has developed a set of standards to guide the dissemination of reproducible research.

- **Computation is now central to the scientific enterprise**, and the emergence of powerful computational hardware combined with a vast array of computational software, presents novel opportunities for researchers
- Unfortunately the scientific culture surrounding computational work has evolved in ways that make it difficult to
  - verify findings, efficiently build on past research, or even to apply the basic tenets of the *scientific method* to computational procedures

MANY ICERM PARTIPANTS

A CREDIBILITY CRISIS

As a result computational science is facing a large credibility crisis [1-4]

The enormous scale of state-of-the-art scientific computations, using tens or hundreds of thousands of processors, presents unprecedented challenges

- **Numerical reproducibility** is a major issue, as is hardware reliability
- For some applications, even rare interactions of circuitry with stray subatomic particles matter

2012 ICERM MEETING

In December of 2012, more than 70 computational scientists and stakeholders such as journal editors and funding agency officials gathered at Brown University for the ICERM **Workshop on Reproducibility in Computational and Experimental Mathematics**

This workshop provided the first opportunity for a broad cross section of computational scientists to discuss these issues and brainstorm ways to improve on current practices, resulting in a series of recommendations *to establish really reproducible computational science as a standard* [5]

- Main recommendations emerging from the workshop are:

THREE MAIN RECOMMENDATIONS

1. It is important to promote a **culture change** that will integrate computational reproducibility into the research process
2. **Journals, funding agencies, and employers** should support this culture change
3. **Reproducible research practices and the use of appropriate tools should be taught** as standard operating procedure in relation to computational aspects of research

CHANGING THE CULTURE

- Early in their career, **bench scientists and experimental researchers are taught** to maintain notebooks or computer logs of every work detail
  - design, procedures, equipment, raw results, processing techniques, statistical methods of analysis, etc.
- Unfortunately **few computational experiments are documented so carefully**
  - Typically, there is no record of workflow, computer hardware and software configuration, parameter settings, or function invocation sequences.
- Source code is often lost, or is revised with no record of the revisions
  - while crippling reproducibility of results, these practices ultimately impede the researchers' own productivity

INSTITUTIONAL REWARDS

The research system must offer institutional rewards for producing reproducible research at every level from departmental decisions to grant funding and journal publication

- Current academic and industrial research system places primary emphasis on publication and project results and little on reproducibility
- It penalizes those devoting time to producing really reproducible research. It is regrettable that software development is often discounted:
  - It has been compared disparagingly to, say, constructing a telescope, rather than doing *real science*
- Thus, scientists are discouraged from spending time writing or testing code. Sadly, NSF-funded projects on average remain accessible on the web only about a year after funding ends.
  - Researchers are busy with new projects and lack time or money to preserve the old. With the ever-increasing importance of computation and software, such attitudes & practices must change.

FUNDING AGENCIES JOURNALS AND EMPLOYERS

Should Support This Change. Software and data should be "open by default" unless it conflicts with other considerations, such as confidentiality. **Grant proposals** involving computational work should be required to provide details such as standards for:

- **dataset and software documentation**, including reuse (some agencies already have such requirements [6])
- **persistence** of resulting software and dataset **preservation and archiving**
- **standards for sharing** resulting software among reviewers and other researchers

FUNDING AGENCIES

- Agencies should add **"reproducible research"** to the list of specific examples that proposals could include in their requirements
  - such as "Broader Impact" or "value to Australia" statements
- **Software and dataset curation** should be explicitly included in grant proposals and recognized as a scientific contribution by funding agencies
  - templates for data management plans could be made available that include *making software open and available*, perhaps by funding agencies, or by institutional archiving and library centers [7]

EDITORS AND REVIEWERS

Must insist on rigorous verification and validity testing, along with **full disclosure** of computational details [8]

- some details might be relegated to website, with assurances this information will persist and remain accessible
- **exceptions exist**, such as where proprietary, medical, or other confidentiality issues arise, but authors need to state this upon submission, and reviewers and editors *must agree* such exceptions are reasonable

- There is also a need for **better standards** on how to include citations for software and data in the references of a paper, instead of inline or as footnotes
  - **proper citation** is essential both for improving reproducibility and in order to provide credit for work done developing software and producing data, which is a key component in encouraging the desired culture change [9]

EMPLOYERS

The third source of influence on the research process stems from employers – **tenure and promotion committees and research managers at research labs**.

- **Software and dataset contributions**, as described in the previous two subsections, should be rewarded as part of expected research practices.
- **Data and code citation practices** should be recognized and expected in computational research.

TEACHING AND TOOLS FOR REPRODCIBLE RESEARCH

CARMA

Proficiency in the skills required to carry out reproducible research in the computational sciences should be **taught** as part of the scientific methodology, along with teaching modern programming and software engineering techniques

- this should be a standard part of any computational research curriculum, just as experimental or observational scientists are taught to keep a laboratory notebook and follow the scientific method.
- **Adopting appropriate tools should be encouraged, and formally taught**. Many tools exist and are under development to help in replicating past results (by the researcher or others).
  - some ease **literate programming** and publishing of computer code, either as commented code or notebooks.
  - others capture provenance of a computation or the complete software environment. Version control systems are not new, but current tools facilitate use for collaboration and archiving complete project histories.
- For a **description of current tools** see workshop report [5] or wiki [10]
  - VS teaches graduate seminar requiring students to replicate results from a published paper [11]. This is one way to introduce tools and methods for replication into curriculum; students experience first hand how important it is to incorporate principles of reproducibility into the scientific research process.

CONCLUSION

Recent events in medicine, economics and psychology illustrate the current scale of error and fraud [12].

- The United States has recently followed the lead of the United Kingdom, Australia and others in mandating public release of publicly funded research, including data [13]

We hope this helps bring about needed cultural change in favour of consistently reproducible computational research

While different types and degrees of reproducible research were discussed at ICERM, an overwhelming majority argued the **community must move to "open research"**: research using accessible software tools to permit

(a) auditing of computational procedures,

(b) replication and independent verification of results, and

(c) extending results or applying methods to new problems.

THE FUTURE IS BRIGHT

CARMA

"It says it's sick of doing things like inventories and payrolls, and it wants to make some break-throughs in astrophysics."

THANK YOU

REFERENCES

1. D. Donoho, A. Maleki, M. Shahram, V. Stodden, and I. Ur Rahman. "Reproducible research in computational harmonic analysis." *Computing in Science and Engineering*, 11, January 2009.
2. D. H. Bailey and J. M. Borwein, "Exploratory Experimentation and Computation," *Notices of the AMS*, vol. 58 (Nov. 2011), p. 1411-1419.
3. J. M. Borwein and D. H. Bailey, *Mathematics by Experiment*, Edition 2, AK Peters, 2008.
4. A. Abbott and Nature Magazine, "Disputed Results a Fresh Blow for Social Psychology," Scientific American, April 30, 2013. http://www.scientificamerican.com/article.cfm?id=disputed-results-a-fresh-blow-for-social-psychology
5. V. Stodden, D. H. Bailey, J. Borwein, R. J. LeVeque, W. Rider and W. Stein, "Setting the Default to Reproducible: Reproducibility in Computational and Experimental Mathematics," 2 Feb 2013, http://www.davidhbailey.com/dhbpapers/icerm-report.pdf.
6. B. Matthews, B. McIlwrath, D. Giaretta, and E. Conway. "The significant properties of software: A study." 2008. http://www.jisc.ac.uk/media/documents/programmes/preservation/spsoftware_report_redacted.pdf.

REFERENCES

7. For examples see: http://scholcomm.columbia.edu/data-management/data-management-plan- templates/ and http://www2.lib.virginia.edu/brown/data/NSFDMP.html
8. D. Fanelli, "Redefine misconduct as distorted reporting," *Nature*, 13 Feb 2013, available at http://www.nature.com/news/redefine-misconduct-as-distorted-reporting-1.12411.
9. R. LeVeque, I. Mitchell, and V. Stodden. "Reproducible research for scientific computing: Tools and strategies for changing the culture." *Comp in Science and Engin.*, 13–17, July 2012.
10. ICERM Reproducibility Workshop Wiki: http://wiki.stodden.net/ICERM_Reproducibility_in_Computational_and_Experimental_Mathematics:_Readings_and_References
11. D. Ince, System Failure, *Times Higher Education*, May 5, 2011. http://www.timeshighereducation.co.uk/416000.article
12. D. H. Bailey and J. M. Borwein, "Reliability, Reproducibility and the Reinhart-Rogoff error," https://theconversation.com/the-reinhart-rogoff-error-or-how-not-to-excel-at-economics-13646, April 19, 2013.
13. OSTP, "Expanding Public Access to the Results of Federally Funded Research," 22 Feb 2013, available at http://www.whitehouse.gov/blog/2013/02/22/expanding-public-access-results-federally-funded-research