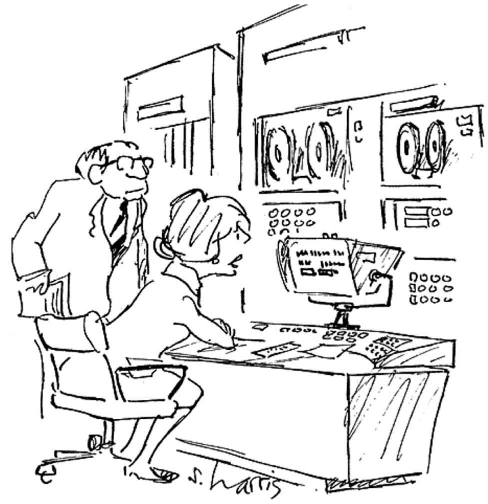
Opinion

Set the Default to "Open"

Reproducible Science in the Computer Age. Conventional wisdom sees computing as the "third leg" of science, complementing theory and experiment. That metaphor is outdated. Computing now pervades all of science. Massive computation is often required to reduce and analyze data; simulations are employed in fields as diverse as climate modeling and astrophysics. Unfortunately, scientific computing culture has not kept pace. Experimental researchers are taught early to keep notebooks or computer logs of every work detail: design, procedures, equipment, raw results, processing techniques, statistical methods of analysis, etc. In contrast, few computational experiments are performed with such care. Typically, there is no record of workflow, computer hardware and software configuration, or parameter settings. Often source code is lost. While crippling reproducibility of results, these practices ultimately impede the researcher's own productivity.

The State of Experimental and Computational Mathematics. Experimental mathematics[1]—application of high-performance computing technology to research questions in pure and applied mathematics, including automatic theorem proving—raises numerous issues of computational reproducibility.[2] It often pushes the bounds in very high precision computation (hundreds or thousands of digits), symbolic computation, graphics, and parallel computation. As with all computational science, one should carefully document algorithms, implementation, computer environments, experiments, and results. Even more emphasis needs to be placed on unique aspects of the discipline: (a) Are precision levels (hundreds or thousands of digits) adequate? (b) What independent consistency checks were employed to validate results? (c) If symbolic manipulation software was employed (e.g., Mathematica or Maple), which version was used? What precise functions were called? What parameter values and environmental settings were used? (d) Have numeric spot checks been performed for derived identities, etc.? (e) Have symbolic manipulations been validated, say, using two different packages? Such checks are crucial, because even the best symbolic and numerical computation packages have bugs and limitations, often exhibited only during hard computations.

The ICERM Workshop on Reproducibility in Computational and Experimental Mathematics. Such concerns motivated a workshop in December 2012, held at the Institute for Computational and Experimental Research in Mathematics at Brown University.[3] Participants included computer scientists, mathematicians, computational



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

physicists, legal scholars, journal editors, and funding agency officials representing academia, government labs, industry research, and all points in between. While different types and degrees of reproducible research were discussed, an overwhelming majority argued that the community must move to "open research": research using accessible software tools to permit (a) "auditing" computational procedures, (b) replication and independent verification of results, and (c) extending results or applying methods to new problems. Of course, the level of validation should be proportional to the importance of the research and strength of claims made.

Workshop Conclusions. *First, researchers need persuasion that efforts to ensure reproducibility are worthwhile*, leading to increased productivity, less time wasted recovering data or code, and more reliable conversion of results from data files to published papers.

Second, the research system must offer institutional rewards at every level, from departmental decisions to grant funding and journal publication. Current academic and industrial research systems place primary emphasis on publication and project results and little on reproducibility. These systems penalize those devoting time to developing or just following community standards.

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.

It is regrettable that software development is often discounted. It is typically compared to, say, constructing a telescope rather than doing real science. Thus, scientists are discouraged from spending time writing or testing code. Sadly, Web projects funded by the National Science Foundation remain accessible only about a year after

[1] *Exploratory experimentation and computation, by David H. Bailey and Jonathan M. Borwein,* Notices, *November 2011.*

[2] Mathematics by Experiment*, CRC Press, 2008.*

[3] *See* `http://icerm.brown.edu/tw12-5-rcem.`

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funding stops. Researchers are busy running new projects without time or money to preserve the old. Given the ever-increasing importance of computation and software, such attitudes and practices must change.

Finally, standards for peer review must be strengthened. Editors and reviewers must insist on rigorous verification and validity testing, along with full disclosure of computational details.[4] Some details might be relegated to a 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 present such issues upon submission, and reviewers and editors must agree such exceptions are reasonable.

Many tools help in replicating past results (by the researcher or others). Some ease literate programming and publishing computer code either as commented code or as 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.

The U.S. has followed the UK, Australia, and others in mandating public release of publicly funded research, including data.[5] We hope this brings a cultural change in favor of consistently reproducible computational research.[6]

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[4] *Redefine misconduct as distorted reporting, by Daniele Fanelli,* Nature*, February 13, 2013.*

[5] *Increasing access to the results of federally funded scientific research, memorandum of the Office of Science and Technology Policy, February 22, 2013.*

[6] *See the workshop report at* http://www.davidhbailey.com/dhbpapers/icerm-report.pdf *and on Wiki at* http://wiki.stodden.net.

Letters to the Editor

Who Should Teach Mathematics Courses?

I was both pleased and dismayed by the article in the October 2012 *Notices* about the PCAST report, and the accompanying Opinion piece. Pleased, because both articles say good things at the end about how to move forward. Dismayed, because the dominant message is one of outrage that we, the only experts in town, weren't consulted.

Yes, mathematicians are entitled to a seat at the table; we should have been part of PCAST, and we should be "actively engaged" in the process of improving all STEM education, not merely in mathematics. But please, let's acknowledge reality. Of course faculty from "mathematics-intensive disciplines other than mathematics" can teach such mathematics courses as calculus, linear algebra, and differential equations. Quite possibly better than we can—they're bilingual, having mastered our treatment of the mathematics as well as the treatment appropriate to their own discipline. They know better than we do what's important for the vast majority of our students, who do not aspire to become professional mathematicians.

Does this mean we should cede control over these courses, or over the training of future mathematics teachers? Of course not. But we should acknowledge not only that others have a right to be at the table, but also that we have failed to adequately meet their needs. What is needed is true collaborative discourse, treating the PCAST report as a wakeup call and making an honest effort to explore all reasonable solutions. And yes, involving those pesky physicists and engineers in the teaching of our courses is reasonable.

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Is Your Journey Really Necessary?

"Is your journey really necessary?", asked the posters in wartime Britain. This question has to be asked again now that catastrophic climate change has become an imminent threat. Trips to meetings and conferences are, of course, good for mathematicians and for mathematics, but the health of the planet is more important. In the last two years I did not go to any conferences involving otherwise unnecessary air travel. In a sense this is easy for me: I am at the end of my career. Yet I feel an intense regret each time I turn down such an invitation, especially when it is coming from good friends.

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Fellows Program

It is with great sorrow that I resign my membership in the AMS. I have been a member for many years but I cannot stomach the silly, elitist Fellows Program which was rammed down the throats of the members despite having been initially voted down. The theory as originally proposed was that mathematicians have not received the respect they deserve from the rest of the scientific community and having a Fellows Program should help the profession and its members to be taken more seriously. I feel certain that this will not happen. Mathematicians have not received the respect and recognition they deserve for a variety of historic reasons, one of which is surely