Reproducibility in Computational Science

Randall J. LeVeque
Applied Mathematics
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Reproducibility of one’s own results

- Version control,
- Automated regression testing,
- Workflow software,
- Etc.

All this is important, but not the focus of this talk.

Want to concentrate on reproducing results of others.
• Top 10 reasons not to share your code (and why you should anyway).

• What does reproducibility mean?
• What do/can/should journals do?
• What do/can/should funding agencies do?
• Code and data repositories?
• Scaling to Petascale/Exascale?

• Discussion
Top 10 Reasons to Not Share Your Code
(and why you should anyway)

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Talk from SIAM CSE Conference
March, 2011
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- No proofs
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Suppose a group of cranks started suggesting papers should contain proofs...

Many objections would be raised...
Alternate reality (no proofs in papers)

Some objections...

1. The proof is too ugly to show anyone else.
   1a. It would be too much work to rewrite it neatly so others could read it.
   1b. It's a one-off proof for this particular theorem, not intended for others to see or use.
   1c. My time is much better spent proving another result and publishing more papers rather than putting more effort into this one, which I've already proved.
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And... the student has since disappeared, along with the proof, but I’m sure it was correct!
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3d. The idea is so great I can commercialize and sell the proof. (see Dijkstra’s Mathematics, Inc.)
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4b. Referees would never want to have to read proofs. It would be too hard to determine correctness of long proofs and finding referees would become impossible.
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4d. My proof uses other theorems with unpublished (proprietary) proofs, so it won’t help to publish my proof — readers still will not be able to fully verify correctness.
Back to the real world...
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Let’s examine some code issues...
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- People understand that not all code is software. Much more embarrassing things appear on the web.
Publish your computer code: it is good enough

Freely provided working code — whatever its quality — improves programming and enables others to engage with your research, says Nick Barnes.

Nick Barnes
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INT Exascale Workshop, June 30, 2011
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(Codes developed in industry of labs may be different.)
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Lack of credit:

People will use parts of my code without attribution.

• If culture changes so all publications are accompanied by code, this will be impossible to hide.
• Publishing it with a paper gives it a timestamp and provenance.
• Making your algorithms more understandable leads to more users and citations.
• Trying to use a research code for a new problem is often impossible without involvement of the authors.

⇒ new collaborations.
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- Require proprietary software, or
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- Techniques like Virtualization can help with some technical issues.
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- Set a good example and push for change.
Meaning of **reproducible** computational science?

Some people mean: (replicable a better term?)

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Can obtain exactly the same results as in paper.
(And this will be true forever.)
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Technical problems:  (Not to mention social ones...)

- Code has many dependencies...
  Compilers, software packages, visualization tools, ...
- Some of these may be commercial/proprietary
- May only run on special hardware (e.g. Leadership class)
- All software evolves...
  Even compiler changes can affect results.
Another possible definition (as in experimental science):

Paper describes the algorithm sufficiently well that a reader can implement and obtain \textit{essentially the same} results.
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Middle ground:

Encourage sharing portions of code directly related to the new work being published.

The ability to inspect code greatly improves chances of reproducing results, or using ideas effectively in future work.
Some journals require sharing of data and/or code.

For example Science, as of February, 2011:

“All data necessary to understand, assess, and extend the conclusions of the manuscript must be available to any reader of Science. All computer codes involved in the creation or analysis of data must also be available to any reader of Science. After publication, all reasonable requests for data and materials must be fulfilled.”

http://www.sciencemag.org/site/feature/contribinfo/prep/gen_info.xhtml#dataavail
Funding agency policies

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**NIH** requires access to data and publications.
Many journal allow supplementary material or other on-line resources.

Often only for animations, datasets, etc.

Sometimes also for code.
Supplementary materials in journals

(e.g. SIAM, Society for Industrial and Applied Mathematics)

Possible approach:

• Allow authors to upload static snapshot of code with submission of article.

• Possibly choose whether or not to be refereed.

• Can also include link to another website for evolving code, bug fixes, wiki for feedback, etc.
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Available repositories:

• Authors’ website (not stable!)

• Open source / commercial hosting services, such as
  www.sourceforge.net, code.google.com,
  bitbucket.org, github.com,

May disappear, or change business model.
Could be used by all journals, rather than many different solutions.

Include version control?

Include wiki for posting bugs, comments, etc.?  
“Reputation system” to complement peer review 
Works very well for large open source projects.
Stable Public Data Repositories?

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Note: open source infrastructure already exists!

See...

www.sourceforge.net, code.google.com, bitbucket.org, github.com,
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One approach to archiving full software environment

For example/\www.virtualbox.org runs on Linux, Mac, Windows.

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Problem: VM is large (≥ 1GB), even if code of interest is small.

Possible solution: Provide standard VMs that can be used for broad classes of code?
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How stable is VirtualBox? Need open source version?
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