Issues in Reproducibility

ICERM Workshop on
Reproducibility in Computational and
Experimental Mathematics

December 10-14, 2012

http://icerm.brown.edu/tw12-5-rcem

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Introduce some of the workshop themes:

- What does “reproducible” mean?
- Why is it hard to achieve?
- Tools for reproducibility
- Policy issues

Workshop schedule and goals
What does Reproducible Research mean?

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Connections to Verification and Validation (V&V), Uncertainty Quantification (UQ).
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Archiving code used to generate published results.

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Version control is highly recommended!

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- Easily modify tables/figures to satisfy referees,
- Or check results in prior publication,
- Ability to build on your own past research of your own (or students / collaborators).
What does Reproducible Research mean?

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Public Reproducibility...

Allowing others to reproduce your results.
(Readers, referees, researchers down the hall...)
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- Verifying scientific integrity of results.
- Aid in understanding your ideas and increase impact.
What does Reproducible Research mean?

What does it mean that others can reproduce your results?

Possible answers...

• Download the code and type `make plots`, see identical plots appear.
• Be able to implement the algorithm from description in paper and other archived sources, and get essentially the same results.
• Various things in between.

Terms such as replicable or repeatable are sometimes used in addition to reproducible.

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Tools to facilitate reproducibility

- **Version control systems (VCS)**
  CVS, Subversion, Mercurial, Git, Bazaar, etc.

- Public hosting sites for VCS repositories
  Github, Bitbucket, Google code, sourceforge, etc.

- Collaboration on open source projects,
  Archiving code used for publications.

- Other archives with stable URLs, DOIs
  Institutional or public data repositories,
  journal supplementary materials, etc.
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- **Workflow Management Systems**
  - VisTrails, Madagascar, Sumatra, Taverna, Galaxy, etc.
  - Capture the workflow used to generate figures, tables, etc.
  - Facilitate tracking the provenance of individual results.
  - Often work together with VCS for source code.
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  CWEB, Doxygen, Sphinx, Sweave, etc.
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- **Notebooks / Publishing tools**
  - Mathematica, Maple, Matlab,
  - Sage, IPython, knitr, RStudio, etc.
Tools to facilitate reproducibility

- **Virtualization**

  Package code along with complete environment (OS, compilers, graphics tools, etc.)

  E.g., VirtualBox, VMware, etc.
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- **Cloud computing**
  
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- **Web platforms for running code**
  E.g. Sage Notebook, RunMyCode.org
Policy Issues

Should journals require data/code sharing?

Some already do, e.g. Science:
Data and materials availability.
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
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After publication, all reasonable requests for data and
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Many journals allow “supplementary materials”.
(But often not code...)
Possible danger of creating new requirements:

Researchers in industry or national labs often find it very difficult to release code, or even fragments...

- Proprietary / copyright issues
- National security
- Export control
Funding agencies

What do/should funding agencies require of grant recipients?

What can agencies do to encourage/fund reproducibility?

Panel discussion tomorrow...
What are the rewards / penalties for attempting to do reproducible research?

Often much more to be gained by moving on to next project than cleaning up and posting code.

Little recognition available vs. many potential downsides of sharing.
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How can we encourage more recognition and better support?

Concerns for young researchers in particular.
Lots of time for open discussion — please participate.
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**Poster session Wednesday evening:**

  Not to late to submit a poster.

  Laptop demos also welcome.
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Wednesday – Friday afternoons: Time for break-out groups...

Discussion groups on topics of interest.

Hands-on demos of reproducibility tools.

Informal talks.
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- Learn cool new stuff from talks and discussions.
- Make new contacts with similar interests.
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- Produce some outcomes that will be useful to others...
  - Wiki with links to resources, articles, tools, policies, etc.
  - Guides to best practices / surveys of tools?
  - Editorials or articles about the workshop or reproducibility more generally that might reach a broad audience.