Issues in Reproducibility

ICERM Workshop on

Reproducibility in Computational and Experimental Mathematics

December 10-14, 2012

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

Randall J. LeVeque Applied Mathematics University of Washington 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

Many different things...

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Connections to Verification and Validation (V&V), Uncertainty Quantification (UQ).

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(Or results used in engineering analysis / decision making.)

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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).

Archiving code (and data) used to generate published results.

(Or results used in engineering analysis / decision making.)

Public Reproducibility...

Allowing others to reproduce your results. (Readers, referees, researchers down the hall...) Archiving code (and data) used to generate published results.

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- Verifying scientific integrity of results.
- Aid in understanding your ideas and increase impact.

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

Tools to facilitate reproducibility

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Collaboration on open source projects,

Archiving code used for publications.

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 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.

Workflow Management Systems

VisTrails, Madagascar, Sumatra, Taverna, Galaxy, etc.

Capture the workflow used to generate figures, tables, etc. Facilitate tracking the provinance of individual results. Often work together with VCS for source code.

• Literate Programming tools

CWEB, Doxygen, Sphinx, Sweave, etc.

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Notebooks / Publishing tools

Mathematica, Maple, Matlab,

Sage, IPython, knitr, RStudio, etc.

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

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• Web platforms for running code

E.g. Sage Notebook, RunMyCode.org

Policy Issues

Should journals require data/code sharing?

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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 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/

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- Mathematical Programming Computation,
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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

What do/should funding agencies require of grant recipiants?

What can agencies do to encourage/fund reproduciblity?

Panel discussion tomorrow...

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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.

Schedule of the workshop

Lots of time for open discussion — please participate.

Lightning talks Wednesday and Thursday

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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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- 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.