The Digitization of Science and the Degradation of the Scientific Method

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Scientific Research is Changing

Scientific computation is becoming central to the scientific method:

- Changing how research is conducted in many fields,
- Changing the nature of how we learn about our world.

Today's academic scientist probably has more in common with a large corporation's information technology manager than with a philosophy or English professor at the same university.

I. Examples of Pervasiveness of Computational Methods

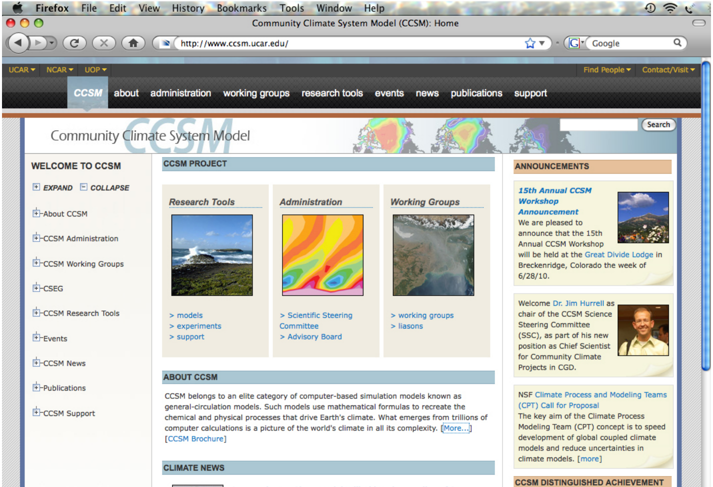
- For example, in statistics:

JASA June	Computational Articles	Code Publicly Available
1996	9 of 20	0%
2006	33 of 35	9%
2009	32 of 32	16%

- Social network data and the quantitative revolution in social science (Lazier et al. 2009);
- Computation reaches into traditionally nonquantitative fields: e.g. Wordhoard project at Northwestern examining word distributions by Shakespearian play.

II. Examples of the Changing Nature of Scientific Discovery

1. Climate Simulation: Community Climate Models (e.g. NCAR),

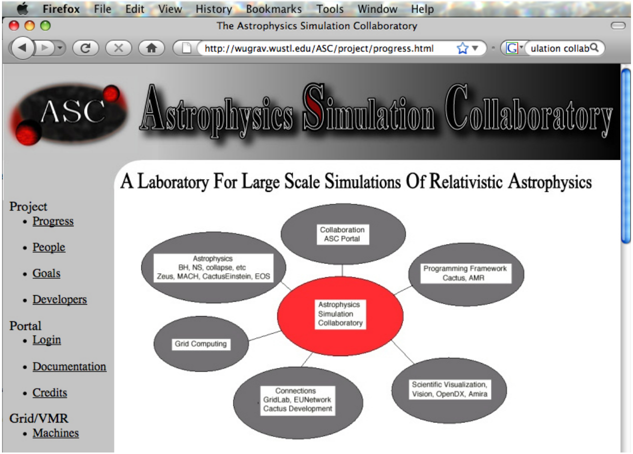


II. Examples of the Changing Nature of Scientific Discovery

2. High Energy Physics: Large Hadron Collider
   - 4 LHC experiments at CERN: 15 petabytes produced annually
   - Data shared through grid to mobilize computing power
   - Director of CERN (Heuer): "Ten or 20 years ago we might have been able to repeat an experiment. They were simpler, cheaper and on a smaller scale. Today that is not the case. So if we need to re-evaluate the data we collect to test a new theory, or adjust it to a new development, we are going to have to be able reuse it. That means we are going to need to save it as open data." Computer Weekly, August 6, 2008

II. Examples of the Changing Nature of Scientific Discovery

3. Astrophysics Simulation Collaboratory, University of Washington



II. Examples of the Changing Nature of Scientific Discovery

4. Dynamic modeling of macromolecules: SaliLab UCSF

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Available online at www.sciencedirect.com
ScienceDirect

Current Opinion in
Cell Biology

The structural dynamics of macromolecular processes

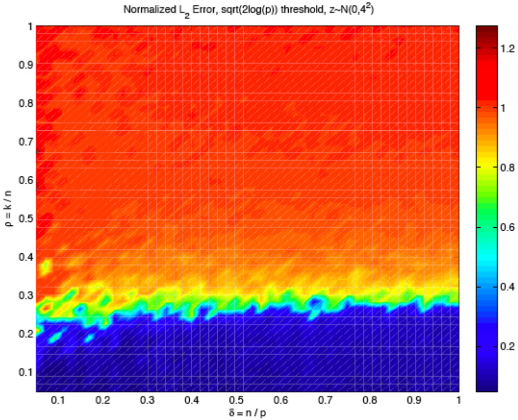
Daniel Russel[1], Keren Lasker[1,2], Jeremy Phillips[1,3],
Dina Schneidman-Duhovny[1], Javier A Velázquez-Muriel[1] and Andrej Sali[1]

Dynamic processes involving macromolecular complexes are essential to cell function. These processes take place over a wide variety of length scales from nanometers to micrometers, and over time scales from nanoseconds to minutes. As a result, information from a variety of different experimental and computational approaches is required. We review the relevant sources of information and introduce a framework for integrating the data to produce representations of dynamic processes.

No single technique, computational or experimental, is able to span all relevant spatial and temporal scales (Figure 3). For static complexes, for example, X-ray crystallography can generate atomic structures of the components, while single particle cryo-electron microscopy (cryo-EM) can provide average mass density maps of the whole assembly at nanometer resolution for the whole assembly. For processes, computer simulations are beginning to reach the microsecond time scale, while

II. Examples of the Changing Nature of Scientific Discovery

5. Mathematical proof by simulation and exhaustive grid search



(Stodden 2006)

Evidence of a problem..

Relaxed practices regarding the communication of computational details is creating a credibility crisis in computational science, not only among scientists, but as a basis for policy decisions and in the public mind.

Recent prominent examples,

- Climategate 2009,
- Microarray-based clinical trials underway at Duke University.

Climategate

- 19 Nov: Emails and documents from CRU appear illegally on the internet; Climate skeptics say the e-mails show that data is being manipulated; HARRY_README.txt
- 22 Nov: Professor Mike Mann under (continuing) internal investigation at Penn
- 1 Dec: Man at centre of controversy, Professor Phil Jones, stands down while inquiry is conducted
- 3 Dec: Saudi chief negotiator says row proves climate change is not caused by humans
- 3 Dec: UEA commissions Sir Muir Russell to chair an independent inquiry
- 4 Dec: Head of UN climate science body says matter cannot be swept "under the carpet"
- 4 May: Virginia AG demands UVA documents related to Mann

Clinical trials based on flawed genomic studies

Timeline:

- Potti et al (2006), Nature Medicine: Main conclusion is that microarray data from cell lines can be used to define drug response "signatures," that predict whether patients will respond,
- Coombes, Wang, Baggerly at M.D. Anderson Cancer Center cannot replicate, and find simple flaws: genes misaligned by one row, column labels flipped, genes repeated and missing from analysis..
- Clinical trials initiated in 2007 (Duke), 2008 (Moffitt).
- Baggerly & Coombes (2009) conducts "forensic bioinformatics" to replicate studies on a particular studies for drugs in clinical trials,

Clinical trials based on flawed genomic studies

Timeline continued:

- Duke launches internal investigation Sept 2009; all three trials suspended in Oct 2009,
- Oct 2009: results reported validated, regardless of errors, because data blinded,
- Baggerly finds data is not blinded as submitted to EORTC investigators, published in *Cancer Letter*, 2009,
- Jan 2010: Duke clinical trials resume, patients allocated to treatment and control groups. "*Neither the review nor the raw data are being made available at this time.*" A future paper will explain their methods.

A Credibility Crisis on Computational Science..

Other examples come to light..

- Geoffrey Chang retractions 2006,
- fMRI correlation analysis 2005,
- Editorial Expression of Concern from *Science* in January 2010,
- more...

Controlling Error is Central to Scientific Progress

"The scientific methods central motivation is the ubiquity of error - the awareness that mistakes and self-delusion can creep in absolutely anywhere and that the scientists effort is primarily expended in recognizing and rooting out error."
David Donoho et al. (2009)

The Third Branch of the Scientific Method

- Branch 1: Deductive/Theory: e.g. mathematics; logic
- Branch 2: Inductive/Empirical: e.g. the machinery of hypothesis testing; statistical analysis of controlled experiments
- Branch 3? Large scale extrapolation and prediction, using simulation and other data-intensive methods.

Toward a Resolution of the Credibility Crisis

- Typical scientific communication doesnt include code, data, test suites.
- Most published computational science near impossible to replicate.

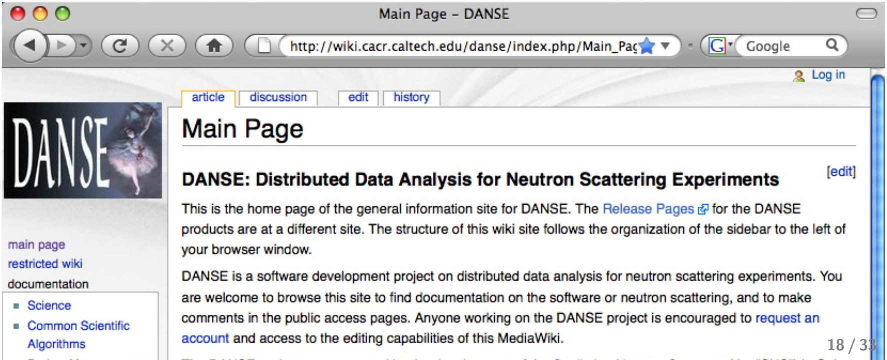
Thesis: Computational science cannot be elevated to a third branch of the scientific method until it generates *routinely verifiable knowledge*. (Donoho, Stodden, et al. 2009)

Sharing of underlying code and data is a necessary part of this solution, enabling *Reproducible Research*.

Question: How do we share computational work?

Goal: encourage reproducibility and verifiability, and permit others to build on the work.

Prototypical example, the Caltech-based DANSE project seeks to share neutron scattering data and code among researchers:



Surveying the Machine Learning Community (Stodden 2010)

Question: Why isn't reproducibility practiced more widely? Answer builds on literature of free revealing and open innovation in industry, and the sociology of science.

Hypothesis 1: Scientists are motivated to share or not share work by perceptions of personal gain or loss.

Hypothesis 2: The willingness to reveal work reflects a scientists desire to belong to a community and gain feedback on work.

- Sample: American academics registered at the Machine Learning conference NIPS.
- Respondents: 134 responses from 593 requests ($\sim$23%).

Top Reasons Not to Share

Code		Data
77%	Time to document and clean up	54%
52%	Dealing with questions from users	34%
44%	Not receiving attribution	42%
40%	Possibility of patents	-
34%	Legal barriers (ie. copyright)	41%
-	Time to verify release with admin	38%
30%	Potential loss of future publications	35%
30%	Competitors may get an advantage	33%
20%	Web/Disk space limitations	29%

"Behind one door is tenure - behind the other is flipping burgers at McDonald's."

Top Reasons to Share

Code		Data
91%	Encourage scientific advancement	81%
90%	Encourage sharing in others	79%
86%	Be a good community member	79%
82%	Set a standard for the field	76%
85%	Improve the caliber of research	74%
81%	Get others to work on the problem	79%
85%	Increase in publicity	73%
78%	Opportunity for feedback	71%
71%	Finding collaborators	71%

Findings

Not surprising:

- Reasons for not revealing reflect private incentives.
- Reasons for revealing include community membership and opportunities for feedback.

Several surprises:

- Computational scientists motivated to share by communitarian ideals.
- Computational scientists not that worried about being scooped.
- Computational scientists quite worried about Intellectual Property issues when sharing data and code.
- Attribution matters for those who share vs those who do not share.

Legal Barriers to Reproducibility: Copyright

To promote the Progress of Science and useful Arts, by securing for limited Times to Authors and Inventors the exclusive Right to their respective Writings and Discoveries. (U.S. Const., art. I, §8, cl. 8)

- Original expression of ideas falls under copyright *by default* (papers, code, figures, tables..)
- Copyright secures exclusive rights vested in the author to:
  - reproduce the work
  - prepare derivative works based upon the original
  - limited time: generally life of the author + 70 years

Exceptions and limitations: Fair Use: "the fair use of a copyrighted work . . . for purposes such as criticism, comment, news reporting, teaching (including multiple copies for classroom use), scholarship, or research, is not an infringement of copyright." 17 U.S.C. §107.

Responses Outside the Sciences 1: Open Source Software

Software with licenses that communicate alternative terms of use to code developers, rather than the default assigned by copyright law.

Richard Stallman created the GNU Public License (GPL) in 1989 to ensure distribution of source code, with compiled programs. Majority of open source code under GPL.

Since then hundreds of software licenses have been created with varying terms:

- (Modified) BSD license
- MIT license
- Apache 2.0
- "Lesser" GPL v3
- ... (see http://www.opensource.org/licenses/alphabetical)

Open Source Software: The Movement

Free Software Foundation

- Richard Stallman, Founder, 1985
- "the leading civil liberties group defending your rights in the digital world."

Responses Outside the Sciences 2: Creative Commons

Larry Lessig, Founder, 2001

- Adapts Open Source Software approach to artistic and creative works
- Provides a suite of licenses:
  - BY: if you use the work attribution must be provided,
  - NC: work cannot be used for commercial purposes,
  - ND: derivative works not permitted,
  - SA: derivative works must carry the same license as the original work.

Response from Within the Sciences: The Reproducible Research Standard (Stodden 2009)

- Remove copyright's barrier to reproducible research,
- Realign the IP framework with longstanding scientific norms.
  A suite of license recommendations for computational science:

  1. Release media components (text, figures) under CC BY,
  2. Release code components under Modified BSD or similar,
  3. Release data to public domain (CC0) or attach an attribution license.

Winner of the Access to Knowledge Kaltura Award in 2008.

Releasing Data?

- Raw facts not copyrightable.
- Original "selection and arrangement" of these facts is copyrightable. (Feist Publns Inc. v. Rural Tel. Serv. Co., 499 U.S. 340 (1991)).
- $\Longrightarrow$ the possibility of a residual copyright in data (attribution licensing or public domain certification).
- Law doesn't match reality on the ground: What constitutes a "raw" fact?

Benefits and Difficulties of the RRS

- Focus becomes release of the entire research compendium
- Hook for funders, journals, universities
- Standardization avoids license incompatibilities
- Clarity of rights (beyond Fair Use)
- IP framework supports scientific norms
- Facilitation of research, thus citation, discovery

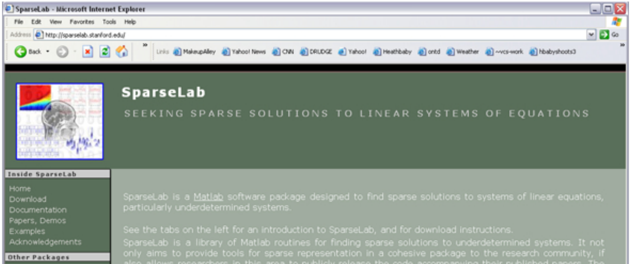
Difficulties:

- Massive codes, software support, streaming data,...
- Tools for ease of implementation (ie. data provenance and workflow),
- "progress depends on artificial aids becoming so familiar they are regarded as natural" I.J. Good, "How Much Science Can You Have at Your Fingertips" 1958.

Publishing, SparseLab, and Reproducible Research

SparseLab: a MATLAB toolbox that makes software solutions for sparse systems available.

- A platform for code/data sharing: 13 papers and 12 authors.
- Standardized tools could advance the research community;
- Demos, exercises, documentation, download and install script, acknowledgments, guidance for contributors included;
- Over 7000 downloads in 2008.



Conclusions

1. Massive computation revolutionizing scientific research, including quantitative social science.
2. New paradigm(s) for publication and verification of results: legal standard and open platforms.
3. Questions emerging regarding adherence to the scientific method, and replicability o our published computational results.
4. Barriers to reproducibility, including Copyright.
5. New directions for improving reproducibility: e.g. software development for provenance and workflow tracking; citation standards; funder and journal requirements.

References:

- "Enabling Reproducible Research: Open Licensing for Scientific Innovation"
- "15 Years of Reproducible Research in Computational Harmonic Analysis"
- "The Legal Framework for Reproducible Research in the Sciences: Licensing and Copyright,"
- "The Scientific Method in Practice: Reproducibility in the Computational Sciences"

`http://www.stanford.edu/~vcs`

Data and Code Sharing Roundtable, Nov 2009:
`http://www.stanford.edu/~vcs/Conferences/RoundtableNov212009/`