Sharing is Caring

Open Science Initiatives

Presented by Andy R. Terrel

Scientific Software Days 2012

THE UNIVERSITY OF TEXAS AT AUSTIN

Texas Advanced Computing Center

Outline

- Why I support sharing code.

- Sharing code and the economy (both financial and academic)

- Efforts to build a sharing community

Lost Arts

"In truth use is no longer made of it because in neither apartments nor even churches do people want anything that might diminish the light. "

King's Buildings superintendent Charles Nicholas Cochin in 1764 on the petition of Jean-Adolph Dannecker, a gingerbread baker in Strasbourg, to reestablish the stained glass craft.

http://stainedglass.org/?page_id=169

Image credit:

(interior of Saint Denis, stained glass at Amiens Cathedral, window at Chartres, window of the crucifixion at Chartres, rose window at Saint Denis)

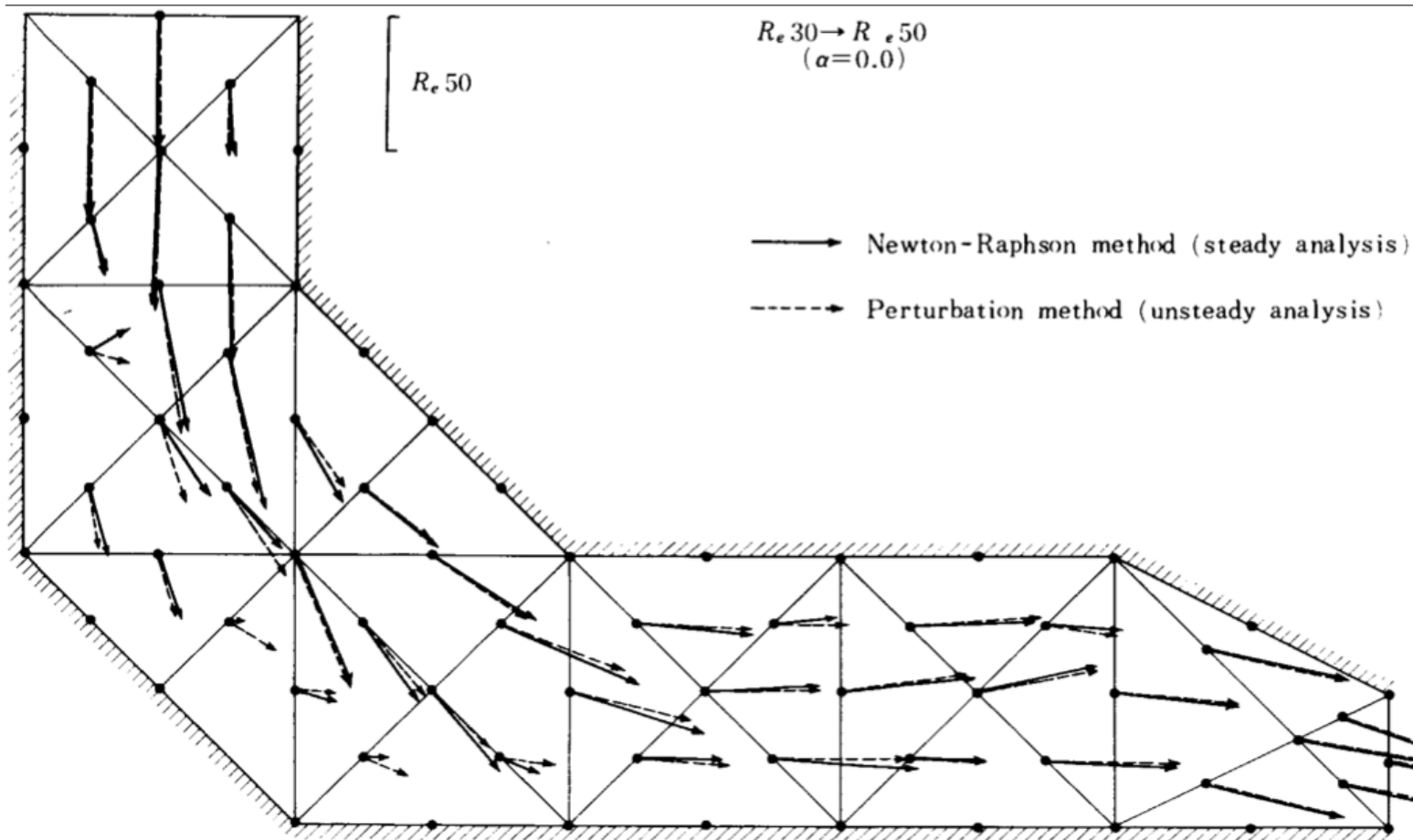Courtesy Mark Bussell/Providence Pictures

$R_e\,30 \rightarrow R_e\,50$
$(\alpha=0.0)$

$R_e\,50$

———→ Newton-Raphson method (steady analysis)

----→ Perturbation method (unsteady analysis)

Fig. 4. Comparison of computed steady velocity between by steady analysis and by unsteady analysis.
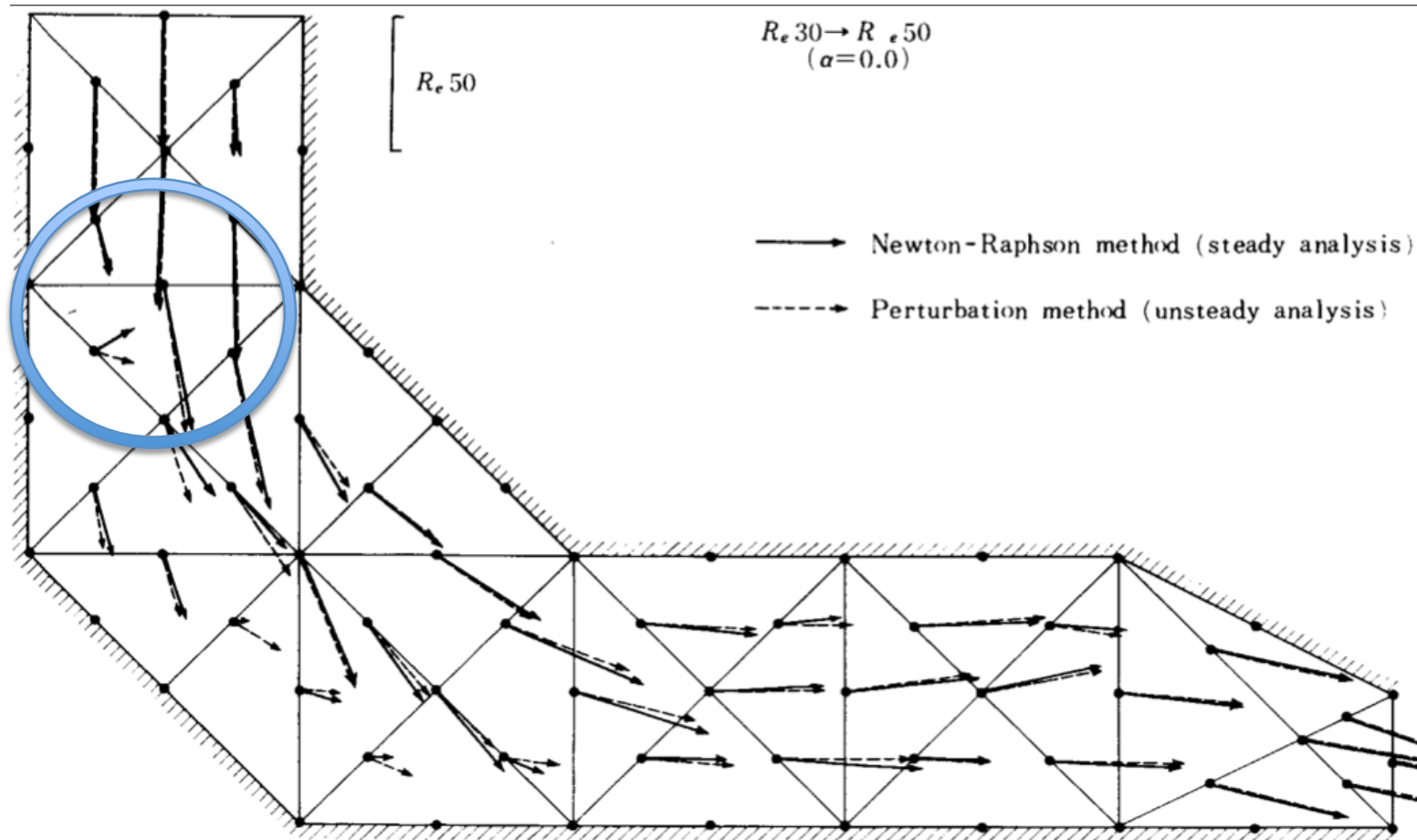
Image credit: [Kawahara Takeuchi 1977]

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Image credit: [Kawahara Takeuchi 1977]

Oldroyd-B Fluids

$$\nabla \cdot \mathbf{u} = 0,$$

$$\nabla \cdot \mathbf{T} = \mathbf{f}$$

$$\mathbf{T} \equiv Ip + 2\eta \mathbf{D} + \boldsymbol{\tau},$$

$$\mathbf{D} \equiv \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

Oldroyd-B fluids

- Kawahara Takeuchi 1977 paper on first FEM paper for the Oldroyd-B fluid model

- Andy in his office in 2006 struggled for 6 months to understand why his code didn't work.

- Papers in 1985, 1991 refuting the paper's results

Other People's Writing

- http://bit.ly/ICERM_Notes →
  http://wiki.stodden.net/
  ICERM_Reproducibility_in_Computational_and_Experimental
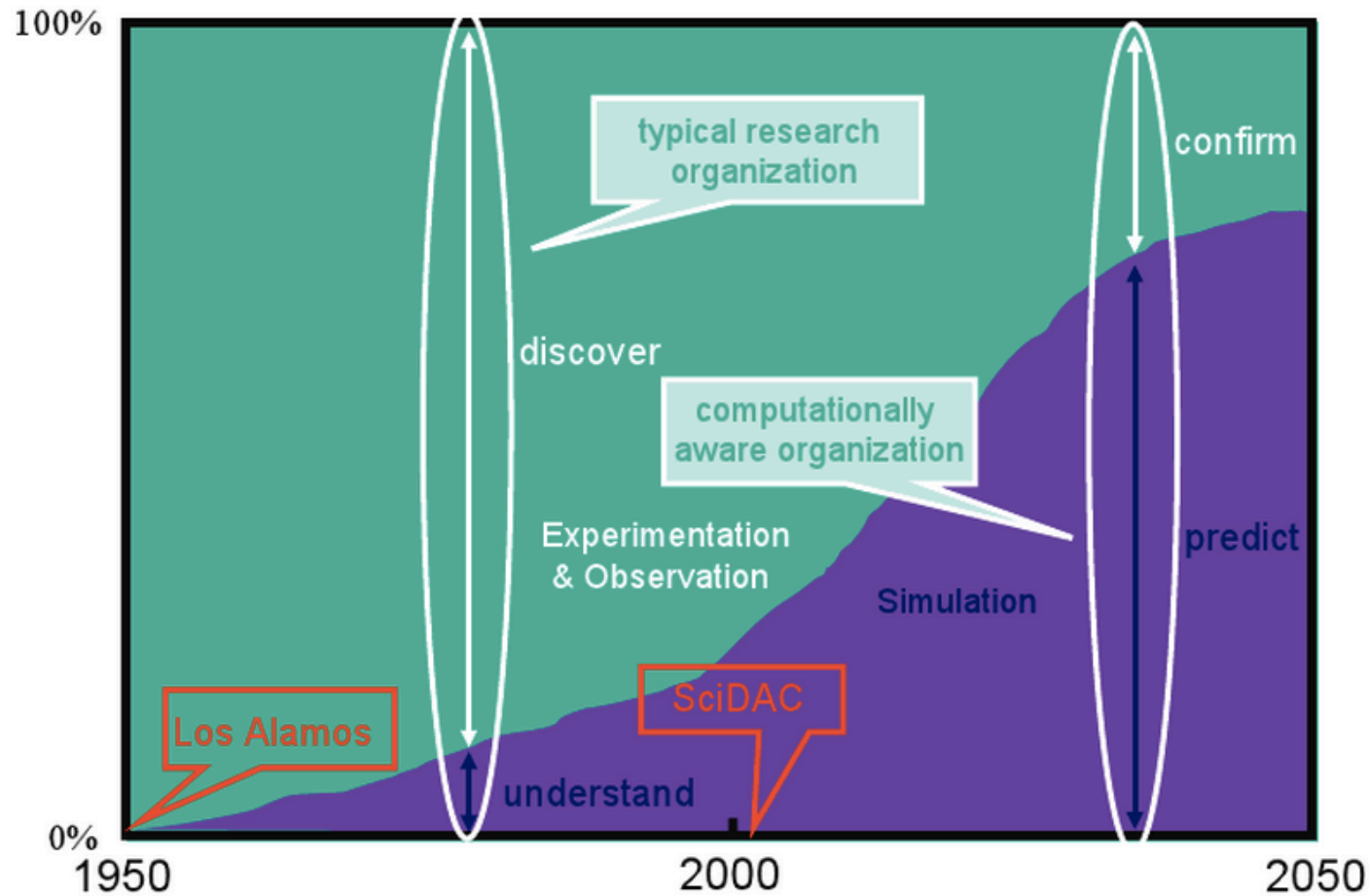 _Mathematics:_Readings_and_References

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Tim O'Reilly at OSCON

- Every big company created in the last 10 years depends on open source software

- http://www.oscon.com/oscon2012/public/schedule/detail/25028

Balance shift in modality of scientific discovery

(dates are somewhat symbolic)

1686 — scientific models

1947 — numerical algorithms

1976 — computer architecture

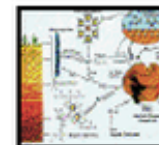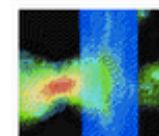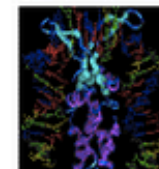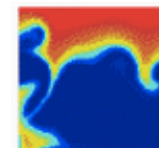1992 — scientific software engineering
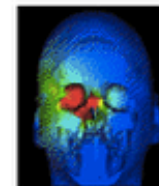
"Computational science is undergoing a phase transition."

David Keyes at NITRD (http://cra.org/ccc/nitrdsymposium-keyes.php)

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NumFOCUS

- Sponsor sprints and conferences

- Provide scholarships and grants

- Provide hardware grants for student developers

- Pay for the creation of publicly-available documentation and basic course development

- Work with domain-specific organizations

- Raise funds from industries using Python and NumPy

http://numfocus.org

Open Science Foundation

We are open source computer scientists, citizen scientists, and scientist-scientists, science writers, journalists, and educators, makers of and advocates for Open Data, Open Access, and Open Source. Our mission is in short: to open science.

http://opensciencefederation.com/

Run My Code

1. A researcher has an idea.

2. The researcher writes a paper based on this idea.

3. Using RunMyCode, the researcher creates a companion website associated with this paper. The companion website allows people to implement the methodology presented in the paper.

http://www.runmycode.org/

Tools

- Github (https://github.com/)
- Bitbucket (https://bitbucket.org/)

- Figshare
- Travis CI

- Building software BIG PROBLEM!
  - NumFOCUS Discussion (https://groups.google.com/d/topic/numfocus/rtG7VkGFVMw/discussion)
  - Third Bit blog (http://third-bit.com/blog/archives/4555.html)

TACC

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