Dissemination and Management of Computational Science Software

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Sharing Data and Code in Computational Science
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Barriers to Sharing

What are the barriers
to reproducible computations
with large scientific codes?

Transparency is more than Open source

- Installation
  - Dependencies
- Analysis of output
  - Often partially proprietary
- Understanding the algorithm
  - Knuth
  - PETSc

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Workability is more than Repeatability

- Alter parameters
- Change model
- Looking for limits of the method

Credit

- “Code citation”
- Potentially use version control information
- Like the polymath model
- What about good judgment?

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Technology

- Good tools
- Installed infrastructure
- Good user support

Outline

Location and Retrieval

"Where's the Tarball"

- Version Control
  - Mercurial, Git, Subversion
- Hosting
  - BitBucket, GitHub, Launchpad
- Community involvement
  - arXiv, PubMed

Configuration and Build

"It won't run on my iPhone"

- Portability
  - PETSc BuildSystem, autoconf
- Dependencies
  - Does this work with UnsupportedGradStudentAMG?
- Configurable build
  - Build must integrate with the configuration system
  - CMake, SCons

Testing

"They are identical in the eyeball norm"

- Unit tests
  - cppUnit
- Regression tests
  - buildbot
- Benchmarks
  - Cigma

Big Picture

- Usability is paramount
  - Need community by-in
  - Need complete workflow
- Leverage existing systems
  - Adoption is much easier with the familiar
  - arXiv, package managers