

Computational Infrastructure for  
**Geodynamics**

**Making software the CIG way**

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CIG

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# Big Problems in Geophysics

**Mantle Convection** How are subduction zones created?

**Seismology** How do we image the deep interior?

**Long time-scale tectonics** How do shear zones form and evolve?

**Short time-scale tectonics** How do earthquakes start and stop?

Many of these problems can be profitably explored with simulation.

# CIG's Mission

- Unfortunately, the software needed to investigate these problems is increasingly complicated. As geoscientists strive to investigate more complicated problems in greater detail, they can end up spending all of their time on computer science issues, and little on the physics.
- CIG's mission is to develop, support, and distribute software for the geoscience community.
- My talk will cover CIG's strategy for building useful, reliable, high performance geophysics codes.

# How CIG Builds New Software

1. Get requirements from the community
2. Build on other people's work
3. Use modern software tools
4. Iterate with the community
5. Release

# 1) Get Requirements

- CIG runs a number of workshops for different areas of geophysics. These workshops are the primary source of recommendations directly from the users.

2005 Mantle Convection Workshop: Boulder, CO, 2005/06/19

Geodynamic Modeling of Tectonics Processes: Breckenridge, CO, 2005/06/10

CIG/IRIS Workshop on Computational Seismology: Stevenson, WA, 2005/06/08

Workshop on Community Finite Element Models for Fault Systems and Tectonic Studies:  
Los Alamos, NM, 2005/07/11

CIG-MC Workshop West Lafayette, IN, 2006/03/27

2006 Workshop on Community Finite Element Models for Fault Systems and Tectonic  
Studies: Golden, CO, 2006/06/26

Mantle Dynamics Training - CIDER Workshop: Santa Barbara, CA, 2006/07/16

Magma Migration Workshop: Columbia University, NY, 2006/08/01

Studies of Earth's Deep Interior: Prague, Czech Republic, 2006/07/09

Imaging Science and CIG Computational Seismology Workshop: 2006/09/21

Scientific Computing Workshop: Austin, TX, 2006/10/16

# 1) Get Requirements

- CIG also has a governing body elected from representatives of affiliated institutions - new ones are free to join

Argonne National Laboratory (MSC)  
Brown University  
California Institute of Technology  
Colorado School of Mines  
Colorado State University  
Columbia University  
Cornell University  
Georgia Institute of Technology  
Harvard University  
Johns Hopkins University  
Lawrence Livermore National Laboratory  
Los Alamos National Laboratory (ES)  
Massachusetts Institute of Technology  
Oregon State University  
Pennsylvania State University

Princeton University  
Purdue University  
Rensselaer Polytechnic Institute  
State University of New York at Buffalo  
State University of New York at Stony Brook  
U.S. Geological Survey (Menlo Park)  
University of California, Berkeley  
University of California, Davis  
University of California, Los Angeles  
University of California San Diego  
University of Colorado  
University of Hawaii  
University of Maine  
University of Maryland  
University of Michigan

University of Minnesota  
University of Missouri–Columbia  
University of Nevada, Reno  
University of Oregon  
University of Southern California  
University of Texas at Austin  
University of Washington  
Washington University  
Woods Hole Oceanographic Institution  
Australian National University  
Monash University  
Geological Survey of Norway (NGU)  
University of Science and Technology of China  
University of Sydney  
Victorian Partnership for Advanced Computing

## 2) Build on Other People's Work

Once we have a goal, we look around to see what we can reuse

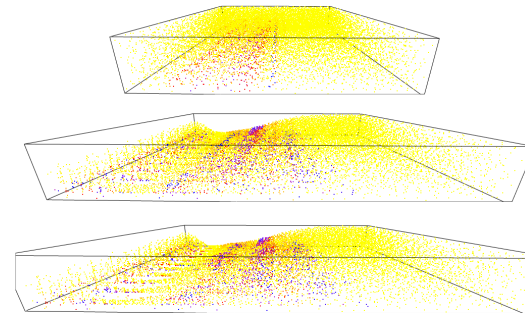
- Linear Algebra: PETSc, BLAS, Lapack
  - In this day and age, no one should be writing their own solvers.
- Data Formats: HDF5
  - Well supported by a number of tools



- Frameworks: Pyre
  - This makes it easy to handle all of the bookkeeping associated with a program (IO, input validation, running a job, etc.), so that the code can concentrate on the physics.

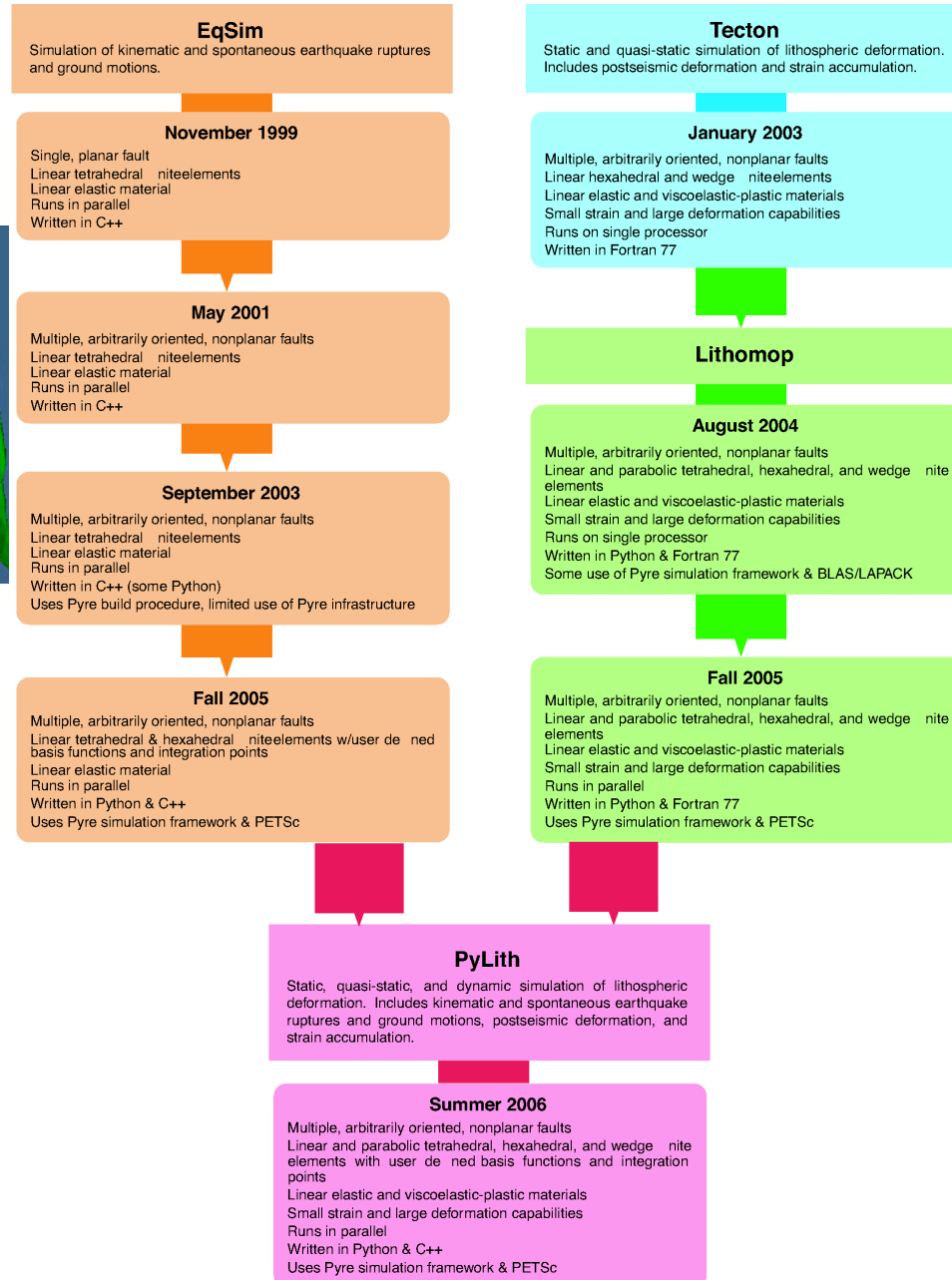
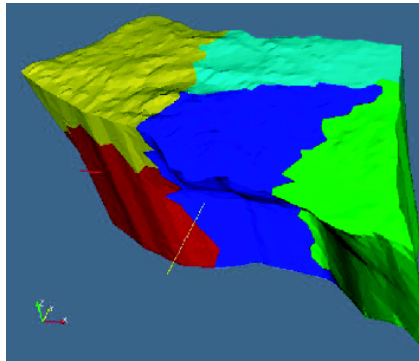


- Large Deformation models (Gale): StGermain, Underworld
  - These libraries provide a rich foundation for Finite Element Analysis using particles. They allowed us to quickly put together a code.





- Finite Element Earthquake Code (PyLith)



- As a rule, CIG partners with other groups to reduce the workload

- PETSc

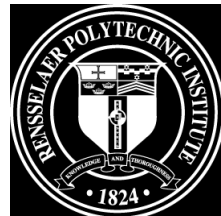


- Gale



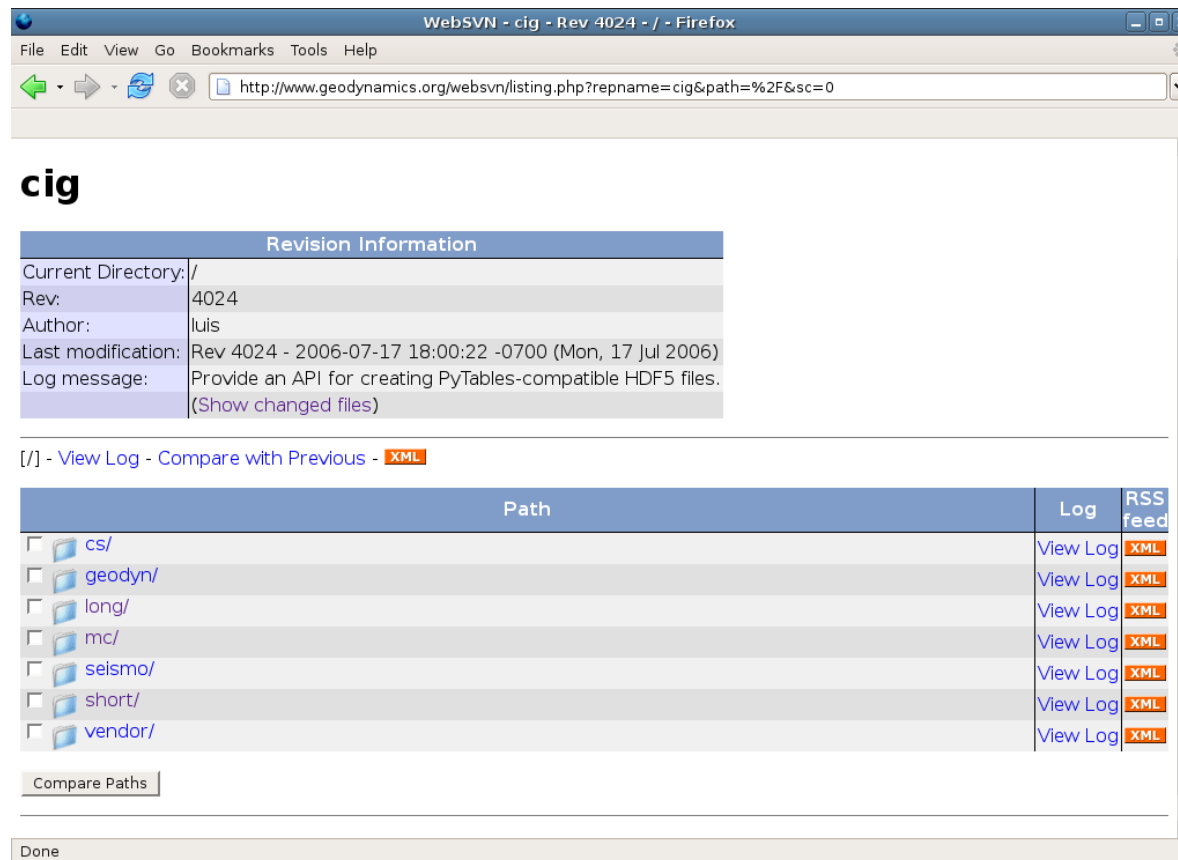
MONASH University

- Pylith



# 3) Use Modern Software Tools

## Version Control



The screenshot shows a Firefox browser window titled "WebSVN - cig - Rev 4024 - / - Firefox". The address bar contains the URL "http://www.geodynamics.org/websvn/listing.php?repname=cig&path=%2F&sc=0". The main content area displays the following information:

### cig

Revision Information	
Current Directory:	/
Rev:	4024
Author:	luis
Last modification:	Rev 4024 - 2006-07-17 18:00:22 -0700 (Mon, 17 Jul 2006)
Log message:	Provide an API for creating PyTables-compatible HDF5 files. ( <a href="#">Show changed files</a> )

[/] - [View Log](#) - [Compare with Previous](#) - [XML](#)

Path	Log	RSS feed
<input type="checkbox"/> <a href="#">cs/</a>	<a href="#">View Log</a>	<a href="#">XML</a>
<input type="checkbox"/> <a href="#">geodyn/</a>	<a href="#">View Log</a>	<a href="#">XML</a>
<input type="checkbox"/> <a href="#">long/</a>	<a href="#">View Log</a>	<a href="#">XML</a>
<input type="checkbox"/> <a href="#">mc/</a>	<a href="#">View Log</a>	<a href="#">XML</a>
<input type="checkbox"/> <a href="#">seismo/</a>	<a href="#">View Log</a>	<a href="#">XML</a>
<input type="checkbox"/> <a href="#">short/</a>	<a href="#">View Log</a>	<a href="#">XML</a>
<input type="checkbox"/> <a href="#">vendor/</a>	<a href="#">View Log</a>	<a href="#">XML</a>

Done

- Undo
- Makes it easy to find when a change (bug) was introduced
- Retains a history of why you made changes
- Answers the question: What have I done lately?
- Eases working with others: Branching and Merging
- Simplifies releases

# Automated Regression Testing

BuildBot: CitcomS Buildbot - Firefox

File Edit View Go Bookmarks Tools Help

http://www.geodynamics.org/buildbot/CitcomS/

CitcomS_Buildbot	failed compile	none	none	none	none	build successful	none	none	
last build									
current activity	idle	offline	offline	offline	offline	idle	offline	offline	
time (PDT)	<a href="#">changes</a>	<a href="#">stress x86 debian unstable</a>	<a href="#">p-wave q5 osx 10.4</a>	<a href="#">s-wave x86 debian nightly</a>	<a href="#">crust x86 debian stable</a>	<a href="#">convection x86 debian stable</a>	<a href="#">dynamo x86 debian stable</a>	<a href="#">compress x86 debian stable</a>	<a href="#">eaton x86 debian unstable</a>
Mon 17 Jul 2006 18:55:07									
18:53:59	compile failed <a href="#">log</a>								
18:53:47	'./configure' <a href="#">log</a>								
	'autoreconf -i' <a href="#">log</a>								
	checkout r4024 <a href="#">log</a>								
	Build 0								
18:53:24	connect bot-stress								
18:02:06									
18:00:51						compile <a href="#">log</a>			
						'./configure' <a href="#">log</a>			
						'autoreconf -i' <a href="#">log</a>			

Done

- We can write tests to prevent bugs from occurring (or recurring)
- Runs tests on platforms that not everyone has easy access to.
- Benchmarking catches cases where there is an error in the equations or boundary conditions.

# Bug Tracker: What needs to be done. What has been fixed

List of issues - Roundup issue tracker - Firefox

File Edit View Go Bookmarks Tools Help

http://www.geodynamics.org/roundup/issues/

## List of issues

Search

ID	Activity	Title	Status	Creator	Assigned To
<b>urgent</b>					
36	2 weeks ago	why Citcoms can't be installed with intel compiler(icc) ?	chatting	anonymous	
<b>bug</b>					
35	1 week ago	CitcomS.py -- inconsistent times in C and Pyre	chatting	Gurnis	tan2
40	1 week ago	libtool: compile: unable to infer tagged configuration	chatting	leif	leif
37	1 week ago	libtool doesn't create DLLs on Windows	chatting	leif	leif
39	1 month ago	Python's distutils is lying/broken	chatting	leif	leif
38	1 month ago	MPI_LIBS broken	unread	leif	leif
34	2 months ago	reconfiguring cached configure doesn't work	unread	leif	leif
28	2 months ago	CitcomS-2.0.2 ENV for openDX scripts	chatting	Gurnis	leif
31	2 months ago	'libdir' vs. 'libexecdir'	unread	leif	leif
25	2 months ago	Fix multigrid check in CitcomCU	testing	anonymous	luis
29	2 months ago	CitcomS: --lsf.queue works, but --launcher.queue doesn't???	unread	leif	leif
27	3 months ago	PyLith 'make check' broken	chatting	leif	leif
1	4 months ago	CitcomS-2.0.1 bug?	testing	luis	luis
2	4 months ago	CitcomCU-1.0.0 warnings with intel compiler	testing	luis	luis
14	5 months ago	possible MPICH2 issue with Pythia	unread	leif	leif
6	5 months ago	pyconfig is not cleaned	unread	leif	leif
<b>feature</b>					
32	1 week ago	"make install" should be optional	chatting	leif	leif
22	3 weeks ago	CitcomCU visualization tools	testing	anonymous	luis

Done

**Issues**

[Create New](#)

[Show Unassigned](#)

[Show All](#)

[Search](#)

Show issue:

**Login**

[Register](#)

[Lost your login?](#)

**Help**

[Roundup docs](#)

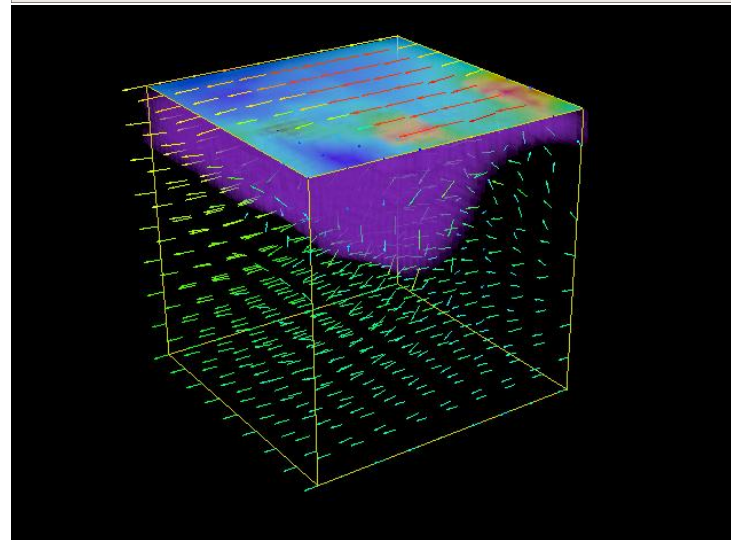
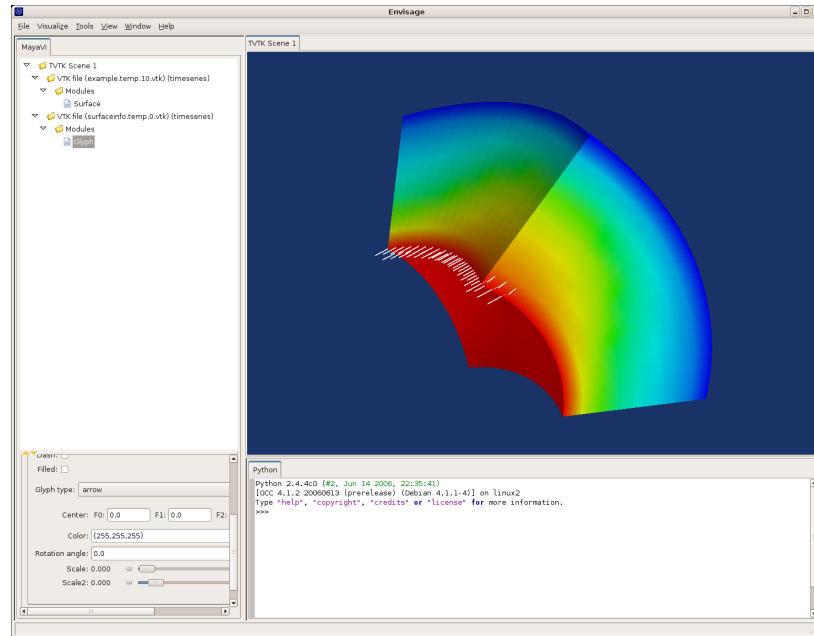
## Cross Platform Build Tools: Autoconf, Automake, BuildSystem, SCons

- They run tests to see what is supported on your platform, so you know ahead of time whether something will work.
- Simplifies the building of libraries and executables on the wide variety of platforms.
- Centralizes the place where changes need to be made. It is much more scalable than a mess of makefiles.
- Sometimes you can have code work on a machine that did not exist when the code was written.



## Visualization Tools

- OpenDX
- Mayavi



# 4) Iterate with the Community

- We release betas of ongoing work: Release early, Release often
- Publicly accessible software repository  
<http://geodynamics.org/websvn>
- Public, archived mailing lists  
<http://geodynamics.org/cig/lists>
- Public Bugtracker  
<http://geodynamics.org/roundup>

- Free software, with no dependency on proprietary tools. So there is sometimes some minor porting
  - Absoft⇒gfortran, g95
  - IDL⇒GDL



# 5) Release

- Tests
- Documentation
- Binaries
- Support
  - Training Sessions
  - Mailing lists