COMPUTATIONAL INFRASTRUCTURE FOR GEODYNAMICS

2013-2014 STRATEGIC PLAN & Annual Report

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COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

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Executive Summary

The Computational Infrastructure for Geodynamics (CIG) is a Geoinformatics project funded by the National Science Foundation (NSF) to support and promote development, dissemination, and use of high-quality software for modeling geodynamical and seismological processes. Each year, CIG undertakes a strategic planning process, in which CIG's staff, governing committees, and working groups assess CIG's status, progress, and impact; develop goals for the coming year and beyond, and outline the strategy and work plans for allocating resources to achieve these goals.

This year, CIG's new activities included initiating new software development for geodynamo research based on community definition of the needed capabilities, hosting several new donated codes, outreach to potential partners at high performance computing centers, a new webinar series and quarterly newsletter, and an EarthCube workshop on modeling needs. CIG continued to advance software development in mantle convection, crustal dynamics, long-term tectonics, magma migration, seismology, and evaluated future directions for these codes. CIG supported community development and knowledge transfer through workshops, in person and online tutorials, e-mail distribution lists, and joint workshops with other organizations. We tracked various metrics aimed at measuring the impact of of CIG's activities, including participation in events, downloads of software (Figure 1), and (when available) presentations and publications that use CIG software.

Our plans for the coming year include ongoing development of codes across the scientific domains represented by geodynamics, including release of new codes and new versions of established codes. CIG working groups plan to establish new community benchmarks in geodynamo and mantle convection, define scientific goals and capabilities in long-term tectonics. CIG will continue to develop partnerships with national computing facilities, other partner organizations, and EarthCube. CIG plans to continue community activities and development (especially for early-career scientists) through workshops, meetings, tutorials and webinars, and through outreach by partnerships with educational institutions.

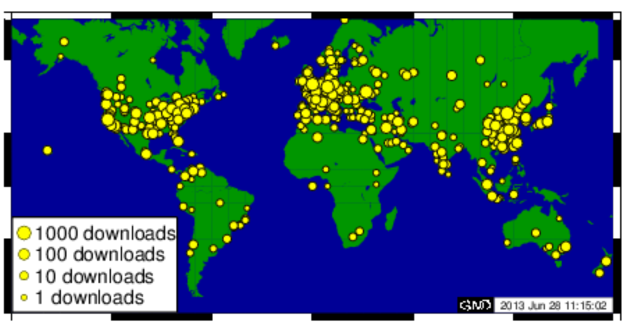

Figure 1. Downloads of codes from CIG's software repositories: July 2012-June 2013

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1. CIG Overview

The Computational Infrastructure for Geodynamics (CIG) supports computation and research in geodynamics. CIG achieves this by developing, supporting, and disseminating high-quality software for the geoscience community and enabling better access to and use of cyberinfrastructure including high-performance computing. This cyber-enabled geosciences community is maintained and grows through workshops, training, outreach, and partnerships with other organizations. The software maintained and developed by CIG addresses research problems that range widely through the earth sciences and includes mantle convection; the geodynamo; magma, crustal and earthquake dynamics; and seismology. With 68 member institutions including 13 international affiliates, CIG is a member-governed organization with a high level of community participation.

CIG publishes annually a rolling 5-year strategic plan. This report updates CIG operational status and covers the period from July 1, 2012 through June 30, 2013 unless otherwise noted. This report also serves as a management and communication tool, designed to support community research and planning and coordination throughout the geosciences.

Prior reports and documents can be found at geodynamics.org.

2. CIG Management and Governance

To remain a nimble and relevant organization, CIG relies on the expertise, vision, and guidance of the community. Its community-centric management structure draws upon features of other successful NSF-supported community infrastructure projects in the Earth sciences. Goals and directions are determined through community input from topical Working Groups and suggestions coming from the scientific community. A Science Steering Committee (SSC) considers and recommends CIG activities, which are then considered and approved by an Executive Committee (EC). The collective charge of the SSC and EC is to identify and balance common needs across disciplines, balancing activities between ongoing support and development of established codes and infrastructure, responding to community needs for new codes and infrastructure, and supporting community development of the CIG community. The management plan, outlined here, has been codified in a set of by-laws available on our web site: http://geodynamics.org/cig/community/documents/bylaws2012.

2.1 Membership

CIG is an institutionally-based organization governed by an Executive Committee. CIG recognizes educational and not-for-profit member institutions with a sustained commitment to CIG objectives in geodynamics and computational science. Foreign affiliate members are accepted but only United States members have voting rights. Each member institution elects one member representative to the electorate. The number of member Institutions continue to increase and currently stands at 68 member institutions including 13 foreign affiliates. This year, CIG welcomed the University of Houston, National Center for Atmospheric Research, and the Singapore Earth Observatory to the community. See Appendix A for a complete list.

2.2 Executive Committee

The Executive Committee (EC) is the primary decision-making body of CIG. The EC meets at least monthly by phone to discuss administration and organization activities. In conjunction with the Director, the EC oversees day-to-day operations through its regular meetings, teleconferences, and electronic mail. The EC approves the annual science plan, management plan, and budget; reviews priorities for software development with input from the electorate and the Science Steering Committee, and creates and appoints committees, such as the Nominating Committee, as needed. The EC has the authority to approve proposal submissions and contractual arrangements for CIG.

The EC has 7 members, of which 5 are voting members: the Chairman, the vice Chairman, and three members at-large. These members are elected by representatives of member institutions for staggered three-year terms. The two *ex officio* members are the Director, and the Chair of the Science Steering Committee.

Current members of the EC and the term end dates are:

- *Chair,* Gary Glatzmaier (2013), University of California, Santa Cruz
- *Vice-Chair,* Mousumi Roy (2013), University of New Mexico
- Wolfgang Bangerth (2014), Texas A&M University
- Scott King (2015), Virginia Polytechnic Institute
- Matt Knepley (2013), University of Chicago
- *Ex officio*, Marc Spiegelman (2013), Columbia University
- *Ex officio,* Louise Kellogg, Director CIG

2.3 Science Steering Committee

The Science Steering Committee (SSC) prioritizes CIG software development from the perspective of the earth science and computational science discipline. The SSC assesses the competing objectives and needs of all the sub-disciplines covered by CIG, provides initial assessment of proposals submitted to CIG, and provides recommendations on the allocation of development resources .The SSC evaluates proposed CIG activities at least once a year formulating a prioritized list of tasks, and developing a yearly strategic plan for CIG. Recommendations from the SSC are forwarded to the EC and are part of the planning process.

The SSC works in consultation with the software development team and the Director to assess how tasks are inter-related and related to the broader needs of the community. To make this process as productive as possible, the Director and SSC look out for opportunities and new activities and work with those who are in the process of proposing a new effort to ensure that it is within the scope of CIG's mission.

The SSC consists of 9 elected members including a chairperson and 2 *ex officio* members - the CIG Director and the Chairman of the EC. The committee includes expertise in both the geosciences and computational sciences and provides guidance within all of the sub-disciplines of computational geodynamics.

Current members of the SSC and the term end dates are:

- *Chair,* Marc Spiegelman (2013), Columbia University
- Jon Aurnou, (2014), University of California, Los Angeles

- Magali Billen, (2015), University of California, Davis
- Jed Brown, (2014), Argonne National Lab
- Roger Buck (2014), Columbia University
- Nadia Lapusta, (2013), California Institute of Technology
- Carl Tape (2014), University of Alaska, Fairbanks
- Peter Van Keken, (2013), University of Michigan
- Jolante van Wijk (2015), University of Houston
- *Ex officio,* Gary Glatzmaier (2013), University of California, Santa Cruz
- *Ex officio,* Louise Kellogg, Director CIG

2.4 Working Groups

Working groups (WG) provide the EC and SSC with domain expertise. WG's, appointed by the EC, provide input on science drivers, technical challenges and resources necessary for research in their domain. CIG's 7 active working groups include:

Computational Science
Seismology
Geodynamo
Long-Term Tectonics
Magma Migration
Mantle Convection
Short-Term Crustal Dynamics

Approximately 7 % of the community (as determined from mailing list subscriptions) is actively involved in governance, drawing from more than 2/3 of the member institutions. Appendix B provides a list of working groups and the 49 working group members who are actively engaged with the CIG community.

2.5 CIG Operations and Administration

CIG is headquartered at the University of California, Davis (UCD). UCD houses CIG in the Earth & Physical Sciences (EPS) building and in the adjacent Mathematical Sciences Building (MSB). These locations provide easy accessibility to expertise in numerical methods, gridding, high-performance computing, networking, scientific visualization, geophysics, and tectonics, as well as access to administrative support staff in the Geology Department (EPS). MSB houses CIG servers and UCD supported HPC resources that are available to local CIG developers. CIG has access to high-speed networking and state-of-the art scientific visualization facilities through KeckCAVES, a visualization facility dedicated to the geosciences.

CIG Headquarters is led by the CIG Director who is supported by 4 full time employees – an Associate Director, Lead Programmer, and 2 Software Developers, and several partial FTE staff. The Director is the Chief Executive Officer of the organization and Principal Investigator on the CIG Cooperative Agreement; she bears ultimate responsibility for its programs and budget. The Director's responsibilities include: (a) devising a fair and effective process for the development of the Strategic Plan, based on proposals or work plans such as those submitted to the Executive Committee by the Science Steering Committee, and overseeing the plan's implementation, (b) acting as the Principal Investigator on proposals submitted by the core CIG facility, retaining final authority to make and implement decisions on grants awarded to the core facility and contracts, (c) ensuring that funds are properly allocated to various CIG activities, and (d) overseeing the preparation of technical reports.

The Associate Director supports day-to-day operations and coordination between CIG units. The Associate Director leads and supports strategic initiatives and all aspects of contract management, personnel and administrative tasks. The Associate Director may act on the behalf of the Director when designated.

CIG's team of dedicated software engineers is headed by the Lead Programmer. The Lead Programmer directs the work of software development team both in-house and sub awardees under direction of the Director and as guided by scientific objectives formulated by the geodynamics community. The software development team provides software services to the community in the form of programming, documentation, training, and support.

CIG Staff Members are:

- *Director,* Professor Louise Kellogg
- *Associate Director,* Dr. Lorraine Hwang
- *Lead Programmer,* Dr. Eric Heien
- *Software Developer,* Dr. Rajesh Kommu
- *Software Developer, Dr. Hiroaki Matsui*
- *HPC Support,* Bill Broadley
- *HPC Support,* Terri Knight
- *Website Administration & Visualization,* Braden Pellett
- *Executive and Event Support,* Gilda Garcia

2.6 The Planning Process

Concepts and plans for CIG activities come directly from the community, member institutions, working groups and their elected committees. As members of the scientific community, WG and SSC members, and the Director are conduits for formal and informal dialog among the CIG community. Formally, users from Member Institutions can submit brief (one page) proposals to suggest new CIG software development tasks, workshops, tutorials, and projects. These proposals can be submitted at any time and are provided to the SSC and EC to read and evaluate.

At least once a year and as part of the development of the strategic planning process, the SSC review these proposals and other ideas, formulate a prioritized list of tasks for software development for the coming year, consider how these tasks are both inter-related and related to the broader needs of the community, and then transmits these as a recommendation to the EC. The EC decides on the allocation of resources based on SSC recommendations.

In practice, new CIG activities are developed iteratively; CIG typically works closely with community members throughout this process, so that proposed activities are relevant to and appropriate for CIG. In turn, the SSC and EC review proposed activities as they come in, provide feedback, and ask questions, again to ensure that proposed activities mesh with CIG's mission and goals.

2.7 Augmented Funding

CIG, upon approval by the EC, can agree to develop additional software or adopt additional tasks upon receipt of augmented funding. The EC will determine whether the activity is within scope of the CIG mission and whether adequate resources are available that would not jeopardize current CIG priorities. Activities can be in the form of new software development using only CIG resources or in collaboration with other organizations. Activities may also support program outreach efforts.

2.8 Communications

CIG employs a variety of methods to keep its own and other communities informed.

2.8.1 geodynamics.org

The website is the home of CIG as seen by most of the community, and serves multiple purposes:

- To highlight research being accomplished by scientists using CIG codes;
- To disseminate news of activities of interest;
- To announce CIG events, including workshops and meetings and to support functions such as workshop registration;
- To disseminate and archive CIG documents including annual reports, strategic plans, by-laws, policies, manuals, tutorials etc.;
- To provide access to CIG software including most recent releases and documentation;
- To provide a portal to XSEDE resources allowing the community access to preinstall software on HPC resources; and
- To provide committees and working groups a centralized site for organization of community activities.

2.8.2 E-mail

CIG maintains a number of electronic mailing lists. E-mail lists for general information (CIG-ALL) and domain-specific information and discussion are open and accessible through the CIG website. Any member of the public may subscribe. These are used to distribute information about software releases, bug fixes, workshops and tutorials, and other general news about activities and programs relevant to the CIG community.

For the period of January 1, 2012 through December 31, 2012, CIG's open e-mail lists distributed information to 877 unique individuals. Figure 2 displays activity by scientific domain, showing the number of members for each list and number of messages sent. The domain-specific lists for groups that have released codes are used frequently for community support. Anyone may post a question or request for help; questions are wide-ranging from scientific application of a particular code to a problem, scientific methodology, to interpretation of error messages at compile or run time. Anyone may also respond. For active codes, developers and active users usually respond within a short time. CIG staff monitor the lists and will answer or redirect emails that remain unanswered. E-mail traffic for the year totaled over 1100 messages, with the most active domain-specific list, Short-Term Crustal Dynamics, accounting for about 37% of the traffic.

E-mail lists for elected or appointed committees, member representatives, and working groups are closed; only members of each group may subscribe or post. These lists support the specific governance-related responsibilities of these smaller groups (for example, voting by the member representatives.).

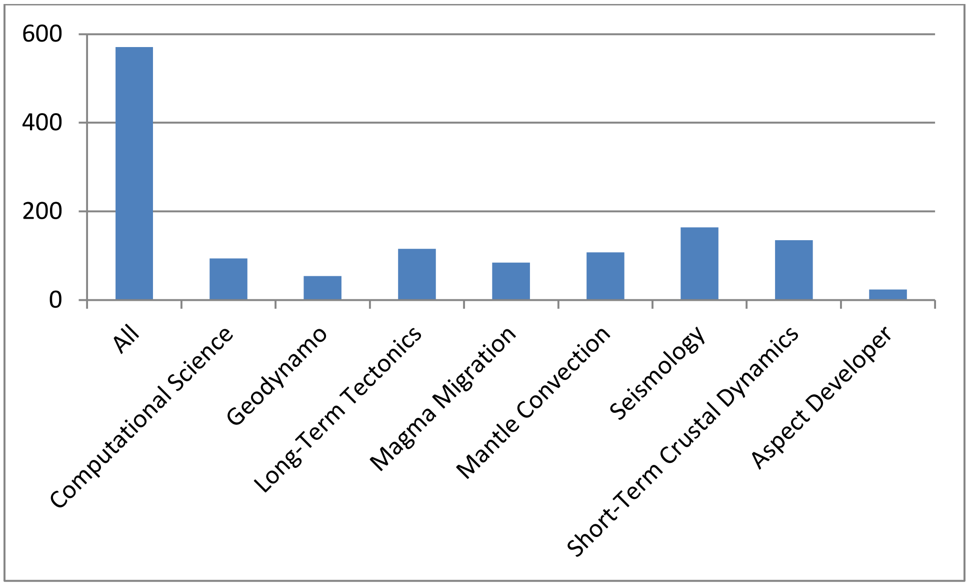


Figure 2a. Number of e-mail list subscribers.

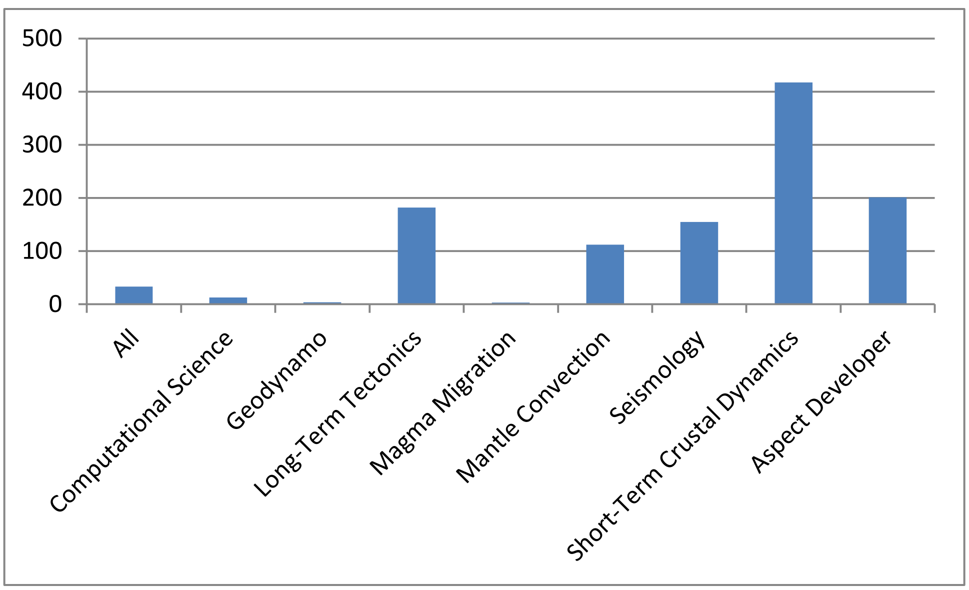


Figure 2b. Number of messages sent through each topical e-mail list and the CIG-ALL announcement list.

2.8.3 Annual CIG Business Meeting

The CIG Annual Business meeting is open to all. The meeting reports on CIG activities of the past year and is a forum for open discussions of past and future CIG activities including strategic planning. This meeting is held in conjunction with the AGU Fall meeting in December, when many members of the community are gathered in one place.

2.8.4 CIG Quarterly Newsletter

Launched in August 2012, the CIG Quarterly Newsletter provides information on community and headquarters' activities and news, computational resources, upcoming meetings, current initiatives, and research highlights, along with news of activities from related organizations. The newsletter is available online and distributed to CIG's general e-mail list.

2.9 Metrics for Success

Critical success factors to fulfill CIG's mission fit into three broad categories: software, people and research. Use of these metrics is incorporated throughout the remainder of this strategic plan.

Software

CIG is a community open source software repository and development community. As such its impact to the community is largely measured by usage. Activity can be measured by number of:

- donated codes,
- # of code downloads,
- HPC cycles used,
- repository commits, and
- lines of code.

People

CIG is community organization that must be responsive to its users at the same time grow its user base. As such, its impact is largely measured by community involvement and outreach. This can be measured by the number of:

- governance participants,
- workshop participants and diversity,
- mailing list membership,
- webinar and online tutorial participants,
- YouTube views,
- education products developed,
- website traffic, and
- users of CIG HPC resources.

Research

CIG resources are used to advance research. As such, its impact is largely measured by its ability to enable research and research outcomes. These can be measured by the number of:

- publications (abstracts, thesis, papers) and readership,
- invited presentations,
- special sessions of national meetings organized around CIG resources or codes,
- proposals that draw on or use CIG resources, and
- partnerships with other organizations.

3. Facility Status

CIG's primary focus is the creation, training and distribution of open-source software via its website geodynamics.org. As an NSF Facility, CIG is now regularly cited in the data management plan (DMP) of scientists writing proposals to NSF. CIG's own data management plan focuses on:

- preservation and availability of software and algorithms,
- incorporation of current technology in the dissemination and distribution of code,
- documentation of code, workshops, meetings, and technical reports; and
- ongoing evaluation and assessment of workshops, training sessions, and other program elements.

CIG utilizes modern software tools to continue to harden its software engineering practice and maintains a robust repository to facilitate sharing of validated open source software. CIG's servers are continuously backed up to protect information in the case of catastrophic loss. Full version control protection has been implemented through use of open source repositories such as svn, git and Mercurial. Doxygen generates documentation from source code on a regular basis. CIG partially supports shared technical staff, who are responsible for server upgrades, software version control, and other related issues.

Facility statistics below cover the periods January 1 – December 31, 2012.

3.1 CIG Code Repository

CIG encourages members to donate codes that have scientific value for the geosciences community. Codes come to CIG from two sources:

- Third-party codes –independently developed codes from small research groups or individuals, and
- Community Codes – codes developed via collaborations with CIG staff.

CIG has established a baseline of required elements for the acceptance of third-party code contributions. These requirements and process of accepting our code can be found at:

http://www.geodynamics.org/cig/community/developer

Currently, CIG offers 3 levels of support:

- Level 1 (Highest Support). A Level 1 code is in active development or enhancement. CIG supports, maintains, and provides technical assistance or training in its use, including documentation updates. A Level 1 code may be installed on the XSEDE Community Software Area for the geodynamics community.
- Level 2 (Middle). A Level 2 code is developed independently from CIG, or is no longer undergoing substantial development. CIG facilitates minor changes such as bug fixes, creating and upgrading of binaries.
- Level 3 (Lowest). A Level 3 code is donated or developed by members of the community; CIG does not provide resources for their development, maintenance, or support, other than incidental assistance, i.e. templates for documentation; help creating binaries, and so on.

CIG formally collaborates with individual and groups of researchers, often as part of their proposal submissions to U.S. and international funding organizations, either in an advisory capacity or as a code repository.

Table 1. CIG Repository Software

	Version	# downloads	Lines of Code	Level of Support
Short-Term Crustal Dynamics				
Pylith	1.8.0	5329	289,209	1
Relax	1.0.4	962	12,962	1
LithoMop	0.7.2	97	56,458	3
Long-Term Tectonics				
Gale	2.0.1	1498	3,763,485	3
Plasti	1.0.0	91	7,375	3
SNAC	1.2.0	106	169,885	3
Mantle Convection				
Aspect	-	-	17,322	1
CitcomCU	1.0.3	209	14,323	1
CitcomS	3.2.0	741	79,305	1
ConMan	2.0.0	100	5,945	2
Ellipsis3d	1.0.2	138	34,726	3
HC	1.0.0	424	12,917	3
Seismology				
Specfem3D	2.0.2	217	185,969	1
Specfem3D Globe	5.1.5	676	94,233	1
Specfem3D Geotech	1.1b	1026	8,709	1
Specfem2D	7.0.0	691	142,080	3
Specfem1D	1.0.3	338	771	3
Mineos	1.0.2	838	13,473	3
Flexwin	1.0.1	142	8,953	3
Seismic CPML	1.2	488	7,438	3
Finite-Frequency Tomography Software	-	-		3
Geodynamo				
MAG	1.0.2	86	8,830	3
Computational Science				
Cigma	1.0.0	377	54,646	3
Exchanger	1.0.1	70	35769	3
Pythia/Pyre	8.1.15	1042	-	3

CIG code spans 6 scientific domains and is written in 40 different languages. Of the over 5 million lines of source code kept in the repository, the majority is comprised of shell & scripting languages, C, C++ and Fortran77/90.

Currently, 9 codes receive active support from CIG staff, subawardees or cooperative efforts with other agencies and working groups. All actively supported codes had major releases this year. Table 1 lists current repository holdings including software version number, number of total lifetime downloads, lines of code[1], and current level of support. The CIG Subversion (svn) repository logged 2488 software commits for the past year.

Level 1 supported codes remain the most downloaded as well as the most complex (measured by total lines of code) software packages. Internal code documentation varies, with source averaging 75% of the nonblank lines. Relax, which computes quasi-static relaxation of stress perturbations, is new to the repository this year, and has garnered much interest with nearly 1000 downloads.

In the upcoming year, CIG expects to accept several new codes in the domains of geodynamo, short-term crustal deformation, geodesy, and magma dynamics.

3.2 Web Portal Statistics

Over the past year the website www.geodynamics.org had 63,563 unique visitors, 162,921 visits, and 1,842,705 hits. The majority of visitors are from United States educational institutions. Other domains are well represented (e.g., .net, .com, .org, .gov) as are our international partners. Approximately 20 countries contributed over 1,000 hits each. For the year, downloads exceeded 7600 files. Most downloads are software and manuals (Table 1). Materials from working groups, including presentations and reports, are also frequently downloaded.

3.3 Supercomputing Statistics

CIG successfully applied for supercomputing cycles under two different NSF programs (Table 2.)

Yellowstone-NCAR-Wyoming and XSEDE-Stampede are two NSF-supported Petascale high performance resources launched at the end of 2012. Ranger, a previous XSEDE HPC resource, has been retired. Eight users from the domains of geodynamo, mantle convection, seismology and long term tectonics have consumed 160,860 SUs.

Table 2. Supercomputing Resources.

	SUs	Resource
NCAR	490,000	Yellowstone
XSEDE	840,000	Ranger & Stampede

[1] Statistics compiled using cloc February 2013: http://cloc.sourceforge.net

3.4 Knowledge Transfer

CIG builds and sustains its community through both virtual and in-person events. The Director, Associate Director, or Lead Programmer, and Committee members represent the organization at numerous meetings, conferences and invited talks throughout the year. In addition, CIG actively sponsors outreach through workshops, training, webinars and a booth at AGU.

3.4.1 Workshops, Training and Engagement with Other Communities

CIG has a long tradition of leveraging its resources and community connections with other organizations for educational and strategic planning efforts. Workshops are community driven and organized. CIG-sponsored workshops are typically held biennially for each domain. Joint workshops and tutorial sessions attached to have been held historically in conjunction with annual meetings of the Southern California Earthquake Center (SCEC), Incorporated Research Institutions for Seismology (IRIS), Geological Society of America (GSA), EarthScope, and Cooperative Institute for Dynamic Earth Research (CIDER).

Figure 3. **Participants at the 2012 CDM Workshop, Golden, Colorado**

Special workshops for community planning reach across government agencies including national labs, other NSF branches and the U.S. Geological Survey. An upcoming major new initiative seeks to define and leverage HPC resources from National Labs to solve problems of interest to DOE and the CIG community.

Table 3. 2012-2013 Workshops and Tutorials

Date	Title	Codes	# Participants
June 18-22, 2012	2012 Crustal Deformation Modeling Workshop	Pylith, Relax	63
July 29 – August 2, 2012	Mantle Convection and Lithospheric Dynamic Workshop	Aspect, Gale	73
July 15 – 28, 2012	CIDER	CitcomS	>40
October 8-10, 2012	Geodynamo Developer Meeting	-	31
November 8-9, 2012	Advancing Seismology and Geodynamics through High Performance Computing	-	30
April 22-24, 2013	EarthCube Modeling Workshop for the Geosciences	-	62

Increasingly, CIG is offering virtual tutorials. Virtual offerings help balance time demands for organizers and participants, are recorded and available for later viewing, and are cost effective. The format allows for offering tutorials across multiple time zones and allows extended time to work on tutorials. Workshops vary target early career scientists and vary from beginning to advance levels.

Upcoming workshops and training are posted online and advertised through CIG e-mail lists and those of our partner organizations. In the past year CIG has offered 6 workshops and tutorials (Table 3), involving more than 259 participants from educational institutions, US agencies, and international partners with other organizations to expand our reach. Table 3 lists the workshops and tutorials offered by CIG in the past year.

3.4.2 EarthCube Modeling for the Geosciences Workshop

CIG convened the EarthCube Modeling Workshop for the Geosciences held on April 22-24, 2013 in Boulder, CO. Our co-convenors were two NSF-supported organizations whose communities also have an interest in modeling in the geosciences: CUAHSI and CSDMS. The workshop brought together over 60 geo- and computational scientists, both virtually and in person, to discuss the common needs of modelers. The participants spanned the communities of geophysics, hydrology, surface processes, and oceans and included early career as well as senior scientists. An advance survey of participants conducted and analyzed by an EarthCube-supported social scientist, provided information about the communities aspirations related to EarthCube. The community outlined the need for continued support for continued interdisciplinary support, advanced computing, training and education, and needs for societal and cultural changes to facilitate open access and to ensure scientists receive credit for their efforts to develop high quality models and software. The EarthCube workshop was funded with a supplement from the EarthCube program. The meeting report can be viewed at:
http://geodynamics.org/cig/community/workshops/Earthcube13/ExecSummary

3.4.3 Webinars

The CIG Webinar Series draws from a pool of experts including applied mathematicians, computer scientists, and geoscientists, to both inform and disseminate knowledge on the tools and methodologies employed to further the study of problems in geodynamics. We note that most of the webinars this year were offered by early-career scientists. The one hour webinars are recorded for later viewing on the CIG YouTube channel and linked to CIG website. A full listing is given in Table 4.

Table 4. 2012- 2013 Webinar Schedule

October 11	Wolfgang Bangerth	*Using Existing Libraries to Improve and Solve Computational Problems*
November 15	Timo Heister	*Modern Numerical Methods for Modeling Convection in the Earth's Mantle*
December		NONE (AGU)
January 10	Jed Brown	*High Performance Implicit Solvers for Geodynamics*
March 21	Sylvain Barbot	*Using Relax to probe the rheology of the lithosphere*
April 11	Sarah Minson	*Bayesian Earthquake Modeling*
May 9	Nick Featherstone	*Stellar Scalable Pseudospectral Methods and the Geodynamo*

3.4.4 YouTube

CIG's YouTube channel, *CIG Geodynamics*, hosts videos of simulations from the community, recordings of past webinars and tutorials, and links to playlists of other community members (such as recorded lectures). Traffic is directed to the site mainly as a watched page and through geodynamics.org and comes from an international community. Recently reinvigorated after a hiatus of several years, the page has 24 subscribers and approximately 6000 views. The most popular videos, on the geomagnetic field and CIG visualizations have over 1800 views. The YouTube channel has recently benefitted by the addition of Professor Wolfgang Bangerth's 43 video lectures on Finite Elements in Scientific Computing, part of his Math 676 course taught at Texas A&M.

3.4.5 AGU Presence

We hold the annual CIG meeting in conjunction with the American Geophysical Union (AGU) meeting each year, taking advantage of the presence of more than 20,000 geophysicists in one place. The evening meeting provides a forum for information exchange and discussion about CIG operations.

CIG operates a booth annually at AGU (located on "NSF Street" with other NSF-supported efforts) in collaboration with the UC Davis KeckCAVES visualization center. At the booth, CIG developers are available to answer questions from the community and to demonstrate software.

In addition, we invite the community to provide us with AGU abstracts that they wish to see highlighted on the CIG website for research presentations featuring CIG software. Community members submitted 47 abstracts for posting for the 2012 Fall AGU Meeting. See Appendix C.

3.4.6 Collaborations with Museums and Science Centers

Earthquakes, volcanoes, plate tectonics are only a few of the science subjects addressed by CIG and of interested to the general public. Museum directors seek accurate, visually compelling information to convey the current state of knowledge to the public. In Fall 2012, CIG-enabled research was featured in the exhibit *Earthquake* at the California Academy of Sciences. For the Morrison Planetarium show (Figure **4**), scientists at Lawrence Livermore National Laboratory computed earthquake ground motions of the 1906 San Francisco M7.9 earthquake and a hypothetical M7.05 Hayward Fault scenario. This exhibit was seen by more than 1 million visitors.

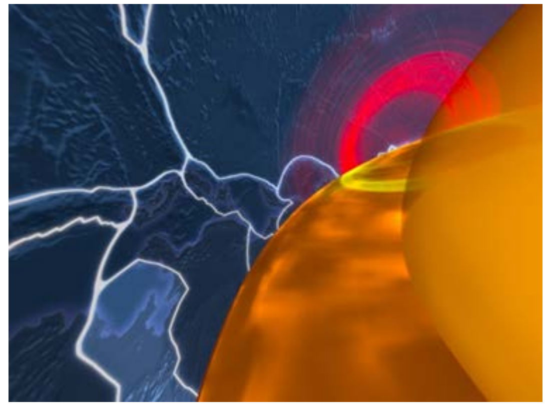


Figure 4. A scene from the CAS "Earthquake" show viewing ground motions at the surface (red) and along a radial cross-section of the Earth (yellow) for the M 7.9 1906 San Francisco earthquake. The view is from the interior looking outward with the Aleutian and Kuril Islands in the center of the view. Plate boundaries are shown as white lines and the outer core is visible in the lower right. Temperature variations in the mantle are indicated by orange shading, inferred from seismic tomography. *Courtesy A. McGarr.*

3.4.7 Publications

CIG scientists published over 36 journal articles in over 22 journals and special volumes the past year using CIG codes. See Appendix D for a selected bibliography.

4. Working Group Progress and Science Plans

CIG's support of the computational needs of the geodynamics community is guided by the working groups, which represent the main scientific domains active in CIG. The following sections provide more specific planning details for the individual communities.

In addition, CIG staff and the SSC and EC make an effort to identify overlapping needs in both scientific and computational functionality from the different domains, in order to support infrastructure for flexible, reusable and interoperable software. This includes a role as a clearing house for best practices in computational solid-Earth Science by developing and implementing a public benchmarking site for code and method evaluation, regression testing and education/training that is consistent across disciplines.

4.1. Geodynamo

The CIG Geodynamo Working Group's primary goal is to develop a next-generation community code. The current code MAG, last updated in 2007, is a serial version of a rotating spherical convection/magnetoconvection/dynamo code (Figure 5). The next generation code must be capable of simulating core dynamics and magnetic field generation processes on massively parallel machines at extreme parameter values to better characterize the highly complex and dynamic state of Earth's core. To achieve this goal, a two phase approach has been identified:

Phase1. Development of the massively parallel community code, and

Phase 2. Incorporation of additional capabilities such as subgrid-scale dynamics and chemistry – a "local code"

As a long term goal, the geodynamo group envisions Phase 3, developing a new dynamo code that will be able to run efficiently on up to 100,000 processors.

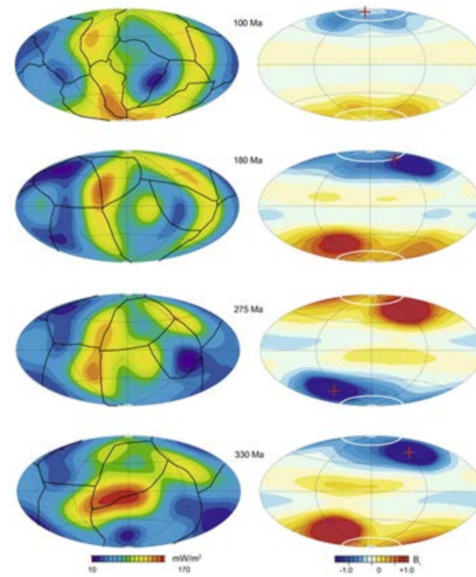


Figure 5. Combining CItcomS and MAG to investigate core evolution. The figure to the left shows CMB heat flux (left) with plate boundaries superimposed (black lines) and the corresponding time average dynamo radial magnetic field on the CMB (right). (Olson, Deguen, Hinnov, and Zhong, 2013, Phys. Earth & Planet. Int., 214, 87-103, doi: 10.1016/j.pepi.2012.10.003)

Outreach & Professional Development

To launch Phase I, a workshop was held in October 2012. The Dynamo Development Workshop focused on surveying both spectral and local numerical methods. Well attended by both geodynamo and solar dynamo community members, the workshop showed that "standard" spectral transform dynamo models can, with care, be made to have good scaling to 30,000 processors. Hence, the Working Group proposes to develop a massively parallelized, well documented community spectral transform dynamo model for broad usage by the dynamo community. By utilizing high performance computing in these dynamo models, the goal is to decrease the fluid viscosity by roughly two orders of magnitude. This will enable transformative studies of fully-developed turbulent dynamo action as occurs in Earth's core.

Software Development

To accomplish this, an existing parallelized spectral transform code, Calypso, will be released for public usage in the upcoming year; and a new public code taking advantage of the advanced parallelization presently implemented in the Anelastic Spherical Harmonic (ASH) code use to study the solar dynamo will be developed. In addition, the community will benchmark (validate and verify) existing codes in order to determine how to best develop a future Level 1 code that will incorporate realistic conditions and include geophysical processes not present in current spectrally-based dynamo models. The plan is for each contributor to first do cases 0 and 1 of the established Boussinesq benchmark originally published by Christensen et al. in 2001, plus another case with a magnetic boundary condition that will be easier for non-spherical-harmonic codes to solve. Then the results of these accuracy benchmarks will be reported to CIG (Dr. Hiroaki Matsui) and each code will be ported to the CIG allocation on XSEDE's Stampede system. Dr. Matsui will then run a series of performance benchmarks for each code, using the spatial resolution each code required to get at least a 1% agreement in the accuracy benchmark. The purpose of this performance benchmark is to decide on a numerical method for phase 3, the long term goal of developing a new dynamo code that will be able to run efficiently on up to 100,000 processors.

Details of the Geodynamo Working Group's 3 year plan are given in Appendix E.1

4.2. Mantle Convection

Activity with mantle dynamics focuses on developing, supporting and maintaining CIG Level 1 codes: ASPECT, and CitComS and CitComCU.

Software Development

The primary long term goal for Mantle Convection is the development of the next generation mantle convection code, ASPECT, an AMR code built on the deal.II finite element library. The past year has seen additions to functionality, documentation and training components. This includes the implementation of compositional fields, development of a GPlates interface, addition of a non-linear solver, generalization of mesh refinement, additions to deal. II functionality, additions to Cookbooks, more internal documentation, and video lectures. This activity resulted in two major software releases: Deal.II v7.3 released Feb 2013, and Aspect 0.2, released May 2013, and the addition of 43 video lectures on deal.II and computational science. In addition, the deal.II team continued general support activities including enhanced testing and community support.

The ASPECT team work will continue towards implementing more realistic models to be implemented in an HPC environment. More details of the ASPECT's team upcoming work plan is given in Appendix E.2

CIG will also continue to support and maintain CitCom (Figure 6). In the past year, improvements have been made to the Stokes solvers and additional functionality is being added by incorporating the PETSc library. These activities will continue in the upcoming year.

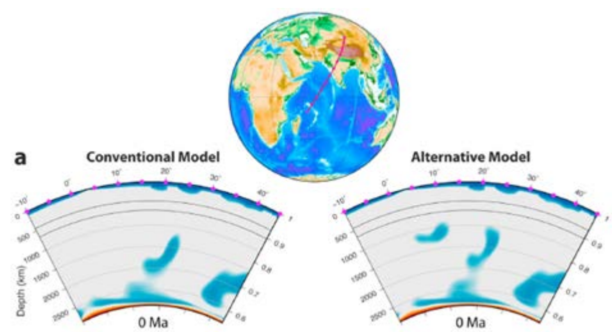


Figure 6. Present-day temperature field predicted by numerical models along a vertical profile with slabs defined as thermal anomalies colder than 10% of the ambient mantle temperature as modeled by CitcomS. Zahirovic, S., R. D. Müller, M. Seton, N. Flament, M. Gurnis, and J. Whittaker (2012), Insights on the kinematics of the India-Eurasia collision from global geodynamic models, *Geochem. Geophys. Geosyst.,* 13, Q04W1, 25, doi:10.1029/2011GC003883.

CitCom is actively reaching out to increase its user base by offering tutorials, most recently, at the 2012 CIDER Summer Program. Similar training will be provided at the 2013 CIDER program.

The July 2012 Mantle and Lithospheric Dynamics workshop highlighted the need for ongoing benchmarking of convection codes, both to demonstrate performance on larger parallel systems and to verify and validate codes as new functionality is added and new methods developed. CIG will support these efforts by developing and disseminating test cases.

4.3. Long-Term Tectonics

The Long-Term Tectonics (LTT) Working Group's primary goal is to converge towards a community-initiated and maintained 2-D and 3-D lithospheric deformation computational code with guided flexibility, modularity, and the ability to model a range of geologic processes. Broadly speaking, the LTT community has little tradition of open source codes; the CIG code GALE was the first to be made widely available to the community, and it has proven challenging for most scientists to use effectively. Historically, codes were usually developed by individual or small groups of researchers to address a narrow range of LTT-related scientific problems. Scientific progress, however, would benefit from repeatability and open sourced, flexible codes (as has been demonstrated by CIG's efforts and impact on LTT and other scientific subdisciplines.)

Outreach & Professional Development

At the Mantle Convection and Lithospheric Dynamics Workshop held in July 2012, the community expressed a need to identify or develop a new, flexible, open source code that can be used for a wide range of scientific problems. With the stabilization and publication of the final version of the lithospheric deformation code GALE, now receiving Level 3 support, the LTT community is without an actively developed open source code.

To address this issue, the LTT Working Group plans a workshop focusing on the current state of computational modeling of lithospheric deformation/processes as well as to define future directions. The workshop will also offer an opportunity for developers of existing codes to demonstrate capabilities and compare functionalities. A prime goal will be the development of use cases to help define community needs.

A hoped-for outcome of the workshop will be the donation of 3rd party codes to the CIG Repository so the community can assess codes and their usage. As these codes are used and evaluated, the community hopes to select one or more for further support and development.

More details of the Long-Term Tectonics Working Group upcoming work plan are given in Appendix E.3.

4.4. Short-Term Crustal Dynamics

The Short-Term Crustal Dynamics Group (STCD) goals are to create numerical models for observationally constrained and internally consistent physics for the 1) entire seismic cycle, 2) tectonics of magmatic systems, geothermal systems, and the cryosphere; and 3) crustal deformation associated with surface loads.

PyLith Development

PyLith development continues to be the main focus of the working group activities. The PyLith development team completed two releases with new features as well as a bugfix release since June 1, 2012. These releases provided (1) a user-friendly interface for computing static Green's functions for use in geodetic inversions with lateral variations in Earth structure, (2) the ability to output the displacement or velocity interpolated to arbitrary locations within the domain, (3) support for PETSc GPU solvers, (4) spatial and temporal variations in tractions for spontaneous earthquake rupture simulations, (5) a post-processing utility to compute fault slip information, such as seismic potency, seismic moment, and moment magnitude directly from PyLith fault output, (6) computation of the stable time step for explicit-time stepping based on the CFL condition and distortion of the finite-element cells from their ideal shapes, and (7) new CUBIT meshing example illustrating how to use a field over the domain to specify the discretization size. The releases fixed over ten minor bugs identified through benchmarking, full scale tests, and user feedback.

Additional bug fixes were released in Spring 2013 with a new feature release targeted for Summer 2013. The new release involves a major reimplementation of the finite-element data structures which will provide tighter integration with PETSc, (2) improve efficiency, and (3) lay the foundation for support of multiphysics capabilities, such as coupling elasticity with heat and/or fluid flow.

Continued development plans for Pylith supports the STCD Group objectives. The primary goal for the coming year will be supporting earthquake cycle simulations via seamlessly coupling quasi-static simulations of interseismic deformation with dynamic simulations of earthquake rupture to bridge the time scales between tectonic loading over hundreds to thousands of years and fault slip in earthquakes over a few to tens of seconds. The second development goal will support multiphysics simulations coupling elastic behavior with heat and fluid flow and span several release cycles. The third development goal, support for a more sophisticated surface loads, will require community input to define computational needs. Lastly, additional development goals are focused on computational science features to support faster and larger simulations, thereby facilitating achieving the geodynamics science objectives.

Development of an Inversion Framework

The geodetic and seismic communities lack an extensible, well-documented, open-source modern framework for inversions of fault slip. Ongoing efforts to benchmark geodetic and seismic source inversions within the Southern California Earthquake Center community highlight many of the complex computational issues and common errors in these underdetermined inversions. The short-term crustal dynamics community envisions development of an inversion framework focused on geodetic and seismic inversions that provides plug-ins for a variety of common inversion methods, including Bayesian approaches. Such a development effort would be independent of PyLith development and should be coordinated with the Computational Seismology working group. This effort requires identifying a scientist to lead this effort followed by refining the software requirements, obtaining funding, and assembling a development team.

Outreach & Professional Development

The STCD Group offers in alternating years, virtual and in person workshops. These meetings continue an ongoing series of workshops held over the past 10 years. The focus of these workshops is physically based models of the distribution of lithospheric stress in space and time via simulation of the strain accumulation, dynamic rupture propagation, and postseismic relaxation over multiple earthquake cycles. This past year, the Crustal Deformation Modeling workshop was held June 18-22, 2012 on the campus of Colorado School of Mines in Golden, CO. The agenda, presentation materials, and list of participants are available at: ~geodynamics.org/cig/community/workinggroups/short/workshops/CDM2012. The group offered a virtual tutorial June 24-28, 2013 and anticipates returning to Colorado for an in-person workshop in 2014.

More details of the Long-Term Tectonics Working Group upcoming work plan and Workshop Activities are given in Appendix E.4.

4.5. Seismology

The main priority for the Seismology Working Group is the continued advancement in capabilities for high performance computing. CIG currently maintains SPECFEM as a tool for both global and regional analysis of seismic observations.

SPECFEM Development

During the past year the SPECFEM suite of software has had major releases. The SPECFEM3D team released a production version and added adjoint capabilities. Work is progressing towards adding GPU capability to SPECFEM3D_GLOBE and will continue in the next year. A beta version that incorporates P and S waves is complete in SPECFEM 2D and will be incorporated in future releases of SPECFEM 3D, allowing better imaging of the crust and upper mantle.

In the short term, SPECFEM will continue to optimize its codes for HPC performance and added functionalities to study a larger suite of imaging problems.

Outreach & Professional Development

SPECFEM will participate in the upcoming CIG-QUEST-IRIS Joint Workshop on Seismic Imaging of Structures July 14-17, 2013 in Fairbanks, Alaska. Developers will be giving invited talks and holding a tutorial.

In the current year, CIG has collaborated with IRIS to identify the needs for high performance computing in the solid earth sciences, and to plan strategic partnerships with federal agencies to improve access to large scale computing. Possible partners include Argonne National Lab, Oak Ridge National Lab, NCAR-Wyoming-Yellowstone, XSEDE, and Lawrence Livermore National Lab. We will continue to explore these possible partnerships, also in conjunction with IRIS.

More details of the coming work plan for development of SPECFEMS are given in Appendix E.5.

4.6. Magma Migration

The Magma Migration Working group's long term goal is to provide flexible multi-physics modeling capability and training for the exploration of coupled fluid-solid mechanics with an emphasis on the dynamics of magmatic plate-boundaries. Problems in magma dynamics are fundamentally coupled multi-physics problems with considerable uncertainties in coupling and basic physics. Significant advances in the understanding of magma physics and available computational infrastructure for multi-physics problems can lead the way to developing a flexible open source code for exploring mantle magnetism that can be made available to the community with Level 1 support.

TeraFERMA Development

A building block in developing a magma migration code is TerraFERMA (the Transparent Finite Element Rapid Model Assembler), a multi-physics model building toolkit. TerraFERMA (TF) has undergone major development including benchmarking in the past year and has been applied to explore coupled fluid-solid flow in subduction zones. TF will be documented and released as a Level 3 code in the upcoming year. Added planned enhancements include integrating TF with core PETSc development to improve performance for large coupled systems.

Outreach & Professional Development

Of importance towards developing a community code, is to cultivate a core group of alpha users to begin exploring a variety of user driven problems to expand the user base. This will help refine the overall design and usability of TF and determine if it is a viable model for design of a flexible public code. In the process, a template for developing best practice for documentation and training in TF will be developed.

A series of workshops is anticipated for 2014 and 2015. Two virtual workshops in 2014 will offer training in TF focusing on magma-dynamics and general multi-physics problems culminating in an in person workshop in 2015. The initial workshop will also serve to demonstrate the activities of the alpha users group as well as begin more general training for other users. Additional short courses especially in computational math could be held in conjunction with other meetings, e.g. CIDER.

Lastly, educational models will be developed. Both a set of tutorial demonstration models will be developed as part of the code distribution and regression testing. As TF is by nature self-documenting, any published model should include access to the metadata so the work is fully reproducible and can be archived by CIG as a modeling resource.

5. 2013-2014 Goals and Resource Allocation

2013-2014 goals will continue to build on 2012-2013 with some notable changes. 2013-2014 goals and progress towards those goals are summarized in Appendix F.

5.1 Geodynamo

Progress towards the development of next generation geodynamo code will be achieved in the upcoming year by:

- Developing a basic dynamo code with full ASH parallelization.
- Community benchmarking on high performance machines for accuracy and performance

Development work will be undertaken by CIG Staff and under subcontract to Colorado University Boulder. Benchmarking definition will be undertaken by a working group from the community. The design of the benchmark is essentially complete and will be distributed in July, 2013 with the hope that the performance benchmark will be complete by late 2013 or early 2014.

5.2 Mantle Convection

ASPECT

Ongoing development of ASPECT will extend the functionality required by the community. This will be achieved by:

- Working with the geodynamics community to implement realistic models. This includes generalizing geometry, material models, as well as extending the passively or actively advected fields, and surface velocities derived from GPlates models, both implemented during the past year.
- Continuing the implementation and verification of numerical methods for compressible models, their documentation, and benchmarking of a variety of approaches for solvers and preconditioners.
- Implementing and verifying numerical methods for fully nonlinear models in which viscosity, density, and a variety of other coefficients depend nonlinearly on temperature, pressure and strain rate. The operator-splitting approach (using a fixed-point method) implanted this past year will be extended, for example using quasi-Newton methods. These methods will be documented and benchmarked.
- Augmenting the existing, 116-page manual by additional material, as well as the development of more cookbooks that can guide new users through the use of ASPECT.
- Improving usability and scalability on large machines by improving portability to clusters where front end nodes run different systems than the compute nodes. The underlying deal.II library will be converted to the cmake build system which will make such cross-compiling simpler, and similarly for the conversion of ASPECT.
- Documenting the methods for publications.

This work will be under taken by subcontract to Texas A&M and Clemson University.

5.3 Long-Term Tectonics

All current LTT codes are now being supported at Level 3 status. No new development is planned.

5.4 Seismology

SPECFEM

Ongoing SPECFEM development will extend its capabilities by:

- Developing the Intel MIC-accelerated versions of SPECFEM3D and SPECFEM3D_GLOBE. MIC is a serious competitor to the GPU and new HPC machines are under development with MIC-accelerated nodes.
- Implementing the ADIOS file format to optimize IO and processing. Implementation will reduce the crippling number of files associated with typical seismological datasets and speed up the parallel pre- and post-processing as part of the adjoin tomography workflow.
- Adding full gravity in SPECFEM3D_GLOBE. This will open up the possibility of applications to free oscillation seismology.
- Working beta version of P and S teleseismic sources for SPECFEM3D.

This work will be undertaken by subcontract to Princeton University and will leverage other ongoing SPECFEM development efforts.

5.5 Short-Term Crustal Dynamics

Pylith

Additional development goals are focused on computational science features to support faster and larger simulations, thereby facilitating achieving the geodynamics science objectives. The PyLith development team plans to add support for higher order basis functions to allow much greater resolution for a given finite-element mesh. This feature facilitates resolving physics across a broader range of scales using a given finite-element mesh to run a simulation at a higher resolution or using a coarser mesh over a larger domain to run a simulation with the same accuracy. Other efforts are focused on reducing simulation runtime. PyLith currently supports use of GPU solvers through integration with PETSc solvers. Adding GPU implementations of the finite-element integration routines, which account for a significant fraction of the overall runtime, would allow users to further accelerate their computations using GPUs.

This work will be undertaken by the PyLith development team at the USGS and GNS Science focused on the geodynamical features, and under subcontract to the University of Chicago for computational science support. However, while PyLith development maintains a steady pace with multiple releases a year, the planned features are becoming more sophisticated and computationally challenging. Additionally, the number of features requested by the community outpaces the rate at which the current development team can implement. In this respect PyLith development is significantly inhibited by a lack of development resources.

5.6 Magma Migration

TerraFERMA

Towards achieving a magma dynamics code, the community will:

- Release TerraFERMA in Summer or Fall 2013 with full documentation.
- Build a core alpha-users group who will collaborate with principal developers to develop example problems and document. These will be archived by CIG.
- Investigate moving key components of Assembly from Dolfin to PETSc to improve performance and memory usage.
- Investigate improvements in PETSc block-preconditioners, e.g. add functionality for Variational inequalities to FieldSplit preconditioners.

PETSc integration will be undertaken by subcontract to the University of Chicago. Activity of the core alpha-users will be partly supported by CIG Staff.

5.7 Infrastructure

CIG plans to continue on several initiatives to harden its infrastructure as well as several new ones:

- Completing migration of the software repository to github. The current Subversion based system used by CIG suffers from several limitations that inhibit code development. The move to Github will allow a more flexible development environment, including: 1) fine grained control of who can read/write each code and creation of development teams for better administrative control, 2) better support for branching which allows scientists to develop functionality for their research and easily incorporate it back into the public release, 3) faster operations on source code and repositories to enable faster work, 4) free hosting and support through Github for public repositories.
- Continuing to build an automated test and build framework with nightly regression testing allowing regular testing of changes submitted to the repository and their underlying libraries.

5.8 Knowledge Transfer

Workshops & Training

CIG plans to organize the following community workshops in the upcoming year:

Working Group	Description	Location	Date
Geodynamo	Geodynamo Benchmarking Workshop	TBD	Winter 2014
Mantle Dynamics	Joint Conference with Canadian Geophysical Union	Banff, Alberta Canada	May 4-7, 2014
Long Term Tectonics	Community Workshop	TBD	Winter 2014
Short Term Crustal Dynamics	Pylith	Golden, Colorado	June 2014
Seismology	CIG/Quest/IRIS	Fairbanks, Alaska	July 14-17, 2013
Magma Dynamics	TerraFERMA Training	Virtual	Winter 2014

Continuing Education

CIG Staff plans to continue to participate in HPC Community activities, e.g. XSEDE conferences and workshops as a means to further their skills and reach out to other communities. This summer one of the CIG Staff will be attending the ANL Sponsored workshop on Extreme Computing to further knowledge on code optimization and usage for HPC.

CIG will continue to provide opportunities to train scientists on HPC by maintaining allocations on HPC resources on community machines.

CIG's lead programmer has joined the XSEDE Campus Champion program. This is a an outreach program of XSEDE, in which representatives of projects with XSEDE allocations receive training, participate in monthly conference calls to learn methods for improving performance on XSEDE resources, and form a cohort of experts who can consult with one another. The Campus Champion in turn is expected to disseminate information to local users of XSEDE resources. As the name implies, XSEDE bases this program on the campus model; we are expanding this model in that our participation is expected to improve outreach to the entire CIG community.

Miscellaneous

To aid knowledge transfer, CIG plans to initiate significant improvements to geodynamics.org by:

- Creating a Reference database. CIG has been collecting and soliciting relevant publications utilizing CIG software. A searchable publications database will aid researchers to discover what research has been published using CIG software and how the software has been used.
- Upgrading Website. CIG's last major website redesign, in 2010, kept the underlying software (Plone). Plone has some limitations in functionality; to take advantage of newer technology, the site will be moved to concrete5, and in the process be redesigned and reorganized to ease navigation to the most frequently visited content and to make information more easily discoverable.

6. NSF Facility Budget

CIG 5 year Budget

A.&B.	**Salaries and Wages**	2,640,527
C.	**Fringe**	721,968
D.	**Equipment**	0
E.	**Travel**	234,181
F.	**Participant Support**	780,606
G.	**Other Direct Costs**	1,900,829
H.	**Total Direct Costs**	6,278,111
I.	**Indirect Costs**	2,214,965
	Total Costs	$8,493,076

Additional Participant Support of $99,262 was received in January 2013 to run the EarthCube Modeling in the Geosciences Workshop in April 2013 bringing the total budget to $8,592,338.

NSF has requested a reduction for 2013-2014 of $200,000 reducing the overall budget to $8,392,338.

Appendix A: Institutional Membership

U.S. Academic Institutions

1. Boston University
2. University of California, Berkeley
3. Brown University
4. University of California, Davis
5. California Institute of Technology
6. University of California, Los Angeles
7. California State University, Northridge
8. University of California, San Diego
9. Colorado School of Mines
10. University of California, Santa Cruz
11. Colorado State University
12. University of Colorado
13. Columbia University
14. University of Connecticut
15. Cornell University
16. University of Hawaii
17. Georgia Institute of Technology
18. University of Houston*
19. Harvard University
20. University of Maine
21. Indiana University
22. University of Maryland
23. Johns Hopkins University
24. University of Michigan
25. Massachusetts Institute of Technology
26. University of Minnesota
27. Northwestern University
28. University of Missouri-Columbia
29. Oregon State University
30. University of Nevada, Reno
31. Pennsylvania State University
32. University of New Mexico
33. Princeton University
34. University of Oregon
35. Purdue University
36. University of Rochester
37. Rensselaer Polytechnic Institute
38. University of Southern California
39. Rice University
40. University of Texas at Austin
41. State University of New York at Buffalo
42. University of Washington
43. State University of New York at Stony Brook
44. Virginia Polytechnic Institute and State
45. Texas A&M University
46. Washington State University
47. University of Alaska, Fairbanks
48. Washington University in St. Louis
49. University of Arizona
50. Woods Hole Oceanographic Institution

U.S. Federal Organizations

1. Argonne National Laboratory (MSC)
2. National Center for Atmospheric Research*
3. Lawrence Livermore National Laboratory
4. U.S. Geological Survey (Menlo Park)
5. Los Alamos National Laboratory (ES)

International Affiliates

1. Australian National University
2. University of Bristol, UK
3. Cardiff University
4. University College London
5. Earth Observatory of Singapore*
6. University of Science and Technology of China
7. Geological Survey of Norway (NGU)
8. University of Sydney
9. GNS Science
10. University of Tuebingen, Germany
11. Monash University
12. Victorian Partnership for Advanced Computing
13. Munich University LMU

*New Members since last strategic plan

Appendix B: CIG Working Group Members

Computational Science

Seismology (5)
- *Lead,* Alan Levander, Rice
- Tim Ahern, IRIS Data Management System, Seattle
- Arthur Rodgers, Lawrence Livermore National Lab
- Carl Tape, University of Alaska at Fairbanks
- Michael Wysession, Washington University at St. Louis

Geodynamo (5)
- *Lead,* Jon Aurnou, UC Los Angeles
- Bruce Buffett, University of California, Berkeley
- Nick Featherstone, University of Colorado, Boulder
- Gary Glatzmaier, UC Santa Cruz
- Hiro Matsui, UC Davis (CIG staff)
- Peter Olson, Johns Hopkins University

Long-Term Tectonics (11)
- *Co-Chair,* Jolante van Wijk, University of Houston
- *Co-Chair*, Katie Cooper, Washington State
- *Co-Chair*, Claire Currie, University of Alberta
- Todd Ehlers, University of Tuebingen, Germany
- Dennis Harry, Colorado State University
- Mousumi Roy, University of New Mexico
- Thorsten Becker, University of Southern California
- Ritske Huismans, Bergen University
- Carolina Lithgow-Bertelloni , University College, London
- Dietmar Muller, University of Sydney
- Patrice Rey, University of Sydney

Magma Migration (8)
- *Lead,* Marc Spiegelman, Columbia University
- Mark Behn, Woods Hole Oceanographic Institution
- Marc Hesse, University of Texas, Austin
- Garrett Ito, University of Hawaii
- Richard Katz, Oxford University
- Matt Knepley, University of Chicago
- Ikuko Wada, Woods Hole Oceanographic Institution
- Cian Wilson, Columbia University

Mantle Convection (13)
- *Lead*, Scott King, Virginia Polytechnic Institute

- *Lead*, Shijie Zhong, University of Colorado, Boulder
- *Lead*, Thorsten Becker, University of Southern California
- Clint Conrad, University of Hawai'i at Manoa
- Carolina Lithgow-Bertelloni, University College, London
- Michael Gurnis ,California Institute of Technology
- Louis Moresi , Monash University
- Rick O'Connell, Harvard University
- Craig O'Neill, Rice University
- Mark Richards, University of California, Berkeley
- Peter van Keken, University of Michigan
- Bernhard Steinberger, Geological Survey of Norway
- Eh Tan, Academia Sinica, Taiwan

Short-Term Crustal Dynamics (7)

- *Lead*, Brad Aagaard, U.S. Geological Survey
- Andy Freed, Purdue University
- Eric Hetland, University of Michigan
- Rowena Lohman, Cornell University
- Brendan Meade, Harvard University
- Mark Simons, California Institute of Technology
- Charles Williams, GNS Science

Appendix C: Fall 2012 AGU Presentations by CIG Scientists

A self-reported list of AGU 2012 presentations that relate to CIG.

Monday, December 3, 2012

P11D-1847. Numerical studies on the structure of Venusian mantle convection constrained by the geoid and topography, An Yang; Jinshui Huang; Shijie Zhong

DI13A-2421. Finite-Frequency Simulations of Core-Reflected Seismic Waves to Assess Models of General Lower Mantle Anisotropy, Andy Nowacki; Andrew Walker; James Wookey and J-Michael Kendall

DI13A-2422. Modeling Mantle Mixing in 3D with Adaptive Mesh Refinement and Implications for Mantle Reservoirs, Louise H. Kellogg; Eric M. Heien; Timo Heister; Wolfgang Bangerth

DI13C-2434. Adaptive coarse space construction and nonlinear smoothers for heterogeneous Stokes problems, Jed Brown; Matthew G. Knepley; Barry Smith

DI13C-2435. An Analysis of ASPECT Mantle Convection Simulator Performance and Benchmark Comparisons, Eric M. Heien; Timo Heister; Wolfgang Bangerth; Louise H. Kellogg

DI13C-2438. A Parallel, Adaptive Modelling Code for Geophysics, Walter Landry; Sylvain Barbot

DI13C-2441. Accelerating forward and adjoint simulations of seismic wave propagation on large GPU-clusters, Daniel Peter; Max Rietmann; Joseph Charles; Peter Messmer; Dimitri Komatitsch; Olaf Schenk; and Jeroen Tromp

DI13C-2444. an open source modeling code for crust and lithosphere dynamics, Jolante W. Van Wijk; Catherine M. Cooper; Claire A. Currie; Walter Landry; Louis N. Moresi

S13B-08. Factors Contributing to Multi-Fault Rupture in the 2010 M7.1 Darfield, New Zealand, Earthquake, Brad Aagaard; Charles Williams; Bill Fry

T13E-2659. Insight from 2D and 3D numerical simulations, Luigi Vadacca; Emanuele Casarotti; Lauro Chiaraluce; Francesco Mirabella

Tuesday, December 4, 2012

DI21A-2348. Intraplate volcanism at the edges of the Colorado Plateau sustained by shear-driven upwelling, Maxim D. Ballmer; Clinton P. Conrad; Eugene I. Smith; Racheal L. Johnsen

NG21A-05. Differential Rotation and Magnetic Field Generation in Giant Gas Planets, Gary A Glatzmaier

S21B-2503. Modeling rupture segmentations on the Cascadia megathrust, Hongfeng Yang; Yajing Liu; and Jeff McGuire

T21E-2629. Constrains on the visco-elastic structure beneath the Tibetan Plateau from deformation induced by variations in hydrological surface loading over multiple time scales, Kristel Chanard; Sylvain Barbot; Jean-Philippe Avouac; William H. Amidon; Guillaume Ramillien

DI22A-01. Meshing, wavefield simulations, and adjoint tomography, Carl Tape; Emanuele Casarotti

DI22A-04. Harnessing Advanced Computational Libraries in Earth Science (Invited), Cian R. Wilson; Marc Spiegelman; Peter van Keken

S22A-07. Earthquake Source Inversion with Dense Networks, Surendra Somala; Jean-Paul Ampuero and Nadia Lapusta

DI23A-2376. Three-dimensional Numerical Models of the Cocos-northern Nazca Slab Gap, Margarete Jadamec; Karen M. Fischer

DI23A-2379. influence of the width ratio between plateau and slab, Pierre-Andre Arrial; Magali I. Billen

DI23A-2380. Insights form 3D Numerical Models, Juan Rodríguez-González; Magali I. Billen; Ana M. Negredo

H23D-1400. Coupled Modeling of Fault Poromechanics During Geologic CO2 Storage, Birendra Jha 1; Bradford H. Hager 2; Ruben Juanes 1

T23D-2709. Using a Geophysical Model to Estimate the Static Coefficient of Friction and Cohesion on a Central Portion of the North Anatolian Fault East of the Marmara Sea, Karimi; Bobak; McQuarrie Nadine

T23H-04. Toward Predictive Modeling of the Earthquake Cycle (Invited, Sylvain Barbot

Wednesday, December 5, 2012

T31D-2619. Application to faults and earthquakes in Tibet, G. Zhang and E. Hetland

T31D-2621. Postseismic Deformation Following the 1999 Chi-Chi Earthquake, Taiwan: Implication for Lower-Crust Rheology Baptiste Rousset; Sylvain Barbot; Jean-Philippe Avouac; Ya-Ju Hsu

T31D-2624. Mechanisms of Postseismic Deformation Following the 2010 El Mayor-Cucapah Earthquake John C. Rollins; Sylvain Barbot; Jean-Philippe Avouac

S33A-2516. Modeling Dynamic Source Rupture with Slip Reactivation and Near-Source Ground Motion of the 2012 Mw 9.0 Tohoku earthquake, P. Galvez; L.Dalguer and J-P Ampuero

T33G-2740. Implications for Craton Stability, Joost van Summeren; Clinton P. Conrad; Mark D. Behn

T33J-02. Past Mantle Dynamics Revealed by Net Characteristics of Surface Plate Motions, Clinton P. Conrad; Bernhard M. Steinberger; Trond H. Torsvik

ED34A-06. Seismic rate changes associated with seasonal, annual and decadal changes in the cryosphere., Jeanne Sauber; Scott Luthcke; Dorothy Hall

S34B-03. Validation of 3D Seismic Velocity Models Using the Spectral Element Method, Monica Maceira; Carene S. Larmat; Robert W. Porritt; David Higdon; Richard M. Allen

S34B-08. Towards global adjoint tomography, Ebru Bozdag; Hejun Zhu; Daniel Peter; Jeroen Tromp

T34B-02. Mantle Convection beneath the Aegir Ridge, a Shadow in the Iceland Hotspot; Samuel M. Howell; Garrett Ito; Asbjorn J. Breivik; Barry B. Hanan; Rolf Mjelde; Kaan Sayit; Peter R. Vogt

T34B-03. New constraints on the origin of the Hawaiian swell from wavelet analysis of the geoid to topography ratio Cecilia Cadio; Maxim D. Ballmer; Isabelle Panet; Michel Diament; Neil M. Ribe

Thursday, December 6, 2012

S41A-2360. 3D resolution tests of two-plane wave approach using synthetic seismograms, Savas Ceylan; Carene S. Larmat; Eric A. Sandvol

S41A-2363. A three-dimensional seismic velocity reference model for Alaska, Carl Tape

S41A-2397. Full waveform tomography of the lithosphere and mantle beneath China, Min Chen; Fenglin Niu; Qinya Liu and Jeroen Tromp

S41A-2415. Ambient-noise Tomography of the Southern California Litosphere, Piero Basini; Qinya Liu; Carl Tape

S41A-2419. Global Seismic Tomography Based on a Sensitivity Database, Elliott Sales de Andrade; Qinya Liu

T43F-2753. Numerical models of the Scotia Sea with globally consistent boundary and initial conditions, Rainer Nerlich; Dr. Christoph Moder; Dr. Stuart R. Clark; Prof. Dr. Hans-Peter Bunge

DI43A-08. Double Layering and Bilateral Asymmetry of a Thermochemical Plume in the Upper Mantle beneath Hawaii Garrett Ito; Maxim D. Ballmer; Cecily J. Wolfe; Sean C. Solomon

DI44A-03. Seismic Velocity Structure of the Mantle beneath the Hawaiian Hotspot and Geodynamic Perspectives (Invited) Cecily J. Wolfe; Gabi Laske; Maxim D. Ballmer; Garrett Ito; John A. Collins; Sean C. Solomon; Catherine A. Rychert

Friday, December 7, 2012

DI51B-05. Lower Mantle Structure from Paleogeographically Constrained Dynamic Earth Models, Dan J. Bower; Michael Gurnis; Maria Seton

NG51D-1788. Improving Particle Integration Efficiency in Mantle Convection Simulation by Combining Numerical Integration Techniques, Emily M. Javan; Ted H. Studley; Eric M. Heien; Louise H. Kellogg

P51C-06. The consequences of melting and melt segregation in the overturned ilmenite-bearing cumulates at the CMB of the Moon, Nan Zhang; E. Marc Parmentier; and Yan Liang

G53A-1126. Salton Trough Post-seismic Afterslip, Viscoelastic Response, and Contribution to Regional Hazard, Jay Parker; Andrea Donnellan; Gregory Lyzenga

T53B-2701. Recent achievements in real-time computational seismology in Taiwan, Shiann-Jong Lee; Wen-Tzong Liang; Bor-Shouh Huang

Appendix D: Publications

Selected list of publications that either were self-reported or mentioned the usage of CIG codes from July 1, 2012 through June 30, 2013.

1. Arrial, Pierre-André; Billen, Magali I.; (2013) "Influence of geometry and eclogitization on oceanic plateau subduction", Earth and Planetary Science Letters Volume 363 34-43 DOI: 10.1016/j.epsl.2012.12.011
2. Ballmer, Maxim D.; Conrad, Clinton P.; Smith, Eugene I.; Harmon, Nicholas; (2013) "Non-hotspot volcano chains produced by migration of shear-driven upwelling toward the East Pacific Rise", Geology Volume 41 (4) 479-482 DOI: 10.1130/g33804.1
3. Bonaccorso, A.; Currenti, G.; Del Negro, C.; (2013) "Interaction of volcano-tectonic fault with magma storage, intrusion and flank instability: A thirty years study at Mt. Etna volcano", Journal of Volcanology and Geothermal Research Volume 251 127-136 DOI: 10.1016/j.jvolgeores.2012.06.002
4. Bower, Dan J.; Gurnis, Michael; Seton, Maria; (2013) "Lower mantle structure from paleogeographically constrained dynamic Earth models", Geochemistry, Geophysics, Geosystems Volume 14 (1) 44-63 DOI: 10.1029/2012GC004267
5. Bower, Dan J.; Gurnis, Michael; Sun, Daoyuan; (2013) "Dynamic origins of seismic wavespeed variation in", Physics of the Earth and Planetary Interiors Volume 214 74-86 DOI: 10.1016/j.pepi.2012.10.004
6. Burkett, Erin; Gurnis, Michael; (2013) "Stalled slab dynamics", Lithosphere Volume 5 (1) 92-97 DOI: 10.1130/l249.1
7. Cottaar, Sanne; Buffett, Bruce; (2012) "Convection in the Earth's inner core", Physics of the Earth and Planetary Interiors Volume 198–199 67-78 DOI: 10.1016/j.pepi.2012.03.008
8. Ewert, H.; Groh, A.; Dietrich, R.; (2012) "Volume and mass changes of the Greenland ice sheet inferred from ICESat and GRACE", Journal of Geodynamics Volume 59–60 111-123 DOI: 10.1016/j.jog.2011.06.003
9. Faccenna, Claudio; Becker, Thorsten W.; Conrad, Clinton P.; Husson, Laurent; (2013), "Mountain building and mantle dynamics", Tectonics Volume 32 (1) 80-93 DOI: 10.1029/2012TC003176
10. Fenoglio-Marc, L.; Rietbroek, R.; Grayek, S.; Becker, M.; Kusche, J.; Stanev, E.; (2012) "Water mass variation in the Mediterranean and Black Seas", Journal of Geodynamics Volume 59–60 168-182 DOI: 10.1016/j.jog.2012.04.001
11. Flament, Nicolas; Gurnis, Michael; MŸller, R. Dietmar; (2013) "A review of observations and models of dynamic topography", Lithosphere Volume 5 (2) 189-210 DOI: 10.1130/l245.1
12. Forno, G. Dal; Gasperini, P.; Spada, G.; (2012) "Implementation of the Complete Sea Level Equation in a 3D Finite Elements Scheme: A Validation Study", VII Hotine-Marussi Symposium on Mathematical Geodesy Volume 137 393-397 DOI: 10.1007/978-3-642-22078-4_59
13. Ghosh, A.; Becker, T. W.; Humphreys, E. D.; (2013) "Dynamics of the North American continent", Geophysical Journal International DOI: 10.1093/gji/ggt151
14. Groh, A.; Ewert, H.; Scheinert, M.; Fritsche, M.; Rülke, A.; Richter, A.; Rosenau, R.; Dietrich, R.; (2012) "An investigation of Glacial Isostatic Adjustment over the Amundsen Sea sector, West Antarctica", Global and Planetary Change Volume 98–99 45-53 DOI:10.1016/j.gloplacha.2012.08.001
15. Höink, Tobias; Lenardic, Adrian; Richards, Mark; (2012) "Depth-dependent viscosity and mantle stress amplification: implications for the role of the asthenosphere in maintaining plate tectonics", Geophysical Journal International Volume 191 (1) 30-41 DOI: 10.1111/j.1365-246X.2012.05621.x

16. Huang, Jinshui; Yang, An; Zhong, Shijie; (2013) "Constraints of the topography, gravity and volcanism on Venusian mantle dynamics and generation of plate tectonics", Earth and Planetary Science Letters Volume 362 207-214 DOI: 10.1016/j.epsl.2012.11.051
17. Husson, L.; Conrad, C. P.; (2012) "On the location of hotspots in the framework of mantle convection", Geophysical Research Letters Volume 39 (17) L17304 DOI: 10.1029/2012GL052866
18. Jadamec, Margarete A.; Billen, Magali I.; Kreylos, Oliver; (2012) "Three-dimensional simulations of geometrically complex subduction with large viscosity variations", Proceedings of the 1st Conference of the Extreme Science and Engineering Discovery Environment: Bridging from the eXtreme to the campus and beyond 1-8 DOI: 10.1145/2335755.2335827
19. Krishnan, Swaminathan; Casarotti, Emanuele; Goltz, Jim; Ji, Chen; Komatitsch, Dimitri; Mourhatch, Ramses; Muto, Matthew; Shaw, John H; Tape, Carl; Tromp, Jeroen; (2012) "Rapid Estimation of Damage to Tall Buildings Using Near Real-Time Earthquake and Archived Structural Simulations", Bulletin of the Seismological Society of America Volume 102 (6) 2646-2666
20. Le Pourhiet, Laetitia; Huet, Benjamin; May, Dave A.; Labrousse, Loic; Jolivet, Laurent; (2012) "Kinematic interpretation of the 3D shapes of metamorphic core complexes", Geochemistry, Geophysics, Geosystems Volume 13 (9) Q09002 DOI: 10.1029/2012GC004271
21. Nielsen, Karina; Khan, Shfaqat A.; Spada, Giorgio; Wahr, John; Bevis, Michael; Liu, Lin; van Dam, Tonie; (2013) "Vertical and horizontal surface displacements near Jakobshavn Isbræ driven by melt-induced and dynamic ice loss", Journal of Geophysical Research: Solid Earth 1-9 DOI: 10.1002/jgrb.50145
22. Nielsen, Karina; Khan, Shfaqat Abbas; Korsgaard, Niels J.; Kjær, Kurt H.; Wahr, John; Bevis, Michael; Stearns, Leigh A.; Timm, Lars H.; (2012) "Crustal uplift due to ice mass variability on Upernavik Isstrøm, west Greenland", Earth and Planetary Science Letters Volume 353–354 182-189 DOI: 10.1016/j.epsl.2012.08.024
23. Olson, Peter; Deguen, Renaud; Hinnov, Linda A.; Zhong, Shijie; (2013) "Controls on geomagnetic reversals and core evolution by mantle convection in the Phanerozoic", Physics of the Earth and Planetary Interiors Volume 214 87-103 DOI: 10.1016/j.pepi.2012.10.003
24. Quéré S.; Lowman, J. P.; Arkani-Hamed, J.; Roberts, J. H.; Moucha, R.; (2013) "Subcontinental sinking slab remnants in a spherical geometry mantle model", Journal of Geophysical Research: Solid Earth n/a--n/a DOI: 10.1002/jgrb.50102
25. Rey, Patrice F.; Teyssier, Christian; Kruckenberg, Seth C.; Whitney, Donna L.; (2012) "Viscous collision in channel explains double domes in metamorphic core complexes: REPLY", Geology Volume 40 (10) e280 DOI: 10.1130/g33202y.1
26. Richter, A.; Groh, A.; Dietrich, R.; (2012) "Geodetic observation of sea-level change and crustal deformation in the Baltic Sea region", Physics and Chemistry of the Earth, Parts A/B/C Volume 53–54 43-53 DOI: 10.1016/j.pce.2011.04.011
27. Rietmann, Max; Messmer, Peter; Nissen-Meyer,Tarje; Peter, Daniel; Basini, Piero; Komatitsch, Dimitri; Schenk, Olaf; Tromp, Jeroen; Boschi, Lapo; Giardini, Domenico; (2012) "Forward and adjoint simulations of seismic wave propagation on emerging large-scale GPU architectures", Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis 1-11
28. Rousset, Baptiste; Barbot, Sylvain; Avouac, Jean-Philippe; Hsu, Ya-Ju; (2012) "Postseismic deformation following the 1999 Chi-Chi earthquake, Taiwan: Implication for lower-crust rheology", Journal of Geophysical Research: Solid Earth Volume 117 (B12) B12405 DOI: 10.1029/2012JB009571
29. Shephard, G. E.; Liu, L.; Müller, R. D.; Gurnis, M.; (2012) "Dynamic topography and anomalously negative residual depth of the Argentine Basin", Gondwana Research Volume 22 (2) 658-663 DOI: 10.1016/j.gr.2011.12.005

30. Spada, Giorgio; Galassi, Gaia; (2012) "New estimates of secular sea level rise from tide gauge data and GIA modelling", Geophysical Journal International Volume 191 (3) 1067-1094 DOI: 10.1111/j.1365-246X.2012.05663.x
31. Thébaud, N.; Rey, P. F.; (2013) "Archean gravity-driven tectonics on hot and flooded continents: Controls on long-lived mineralised hydrothermal systems away from continental margins", Precambrian Research Volume 229 93-104 DOI: 10.1016/j.precamres.2012.03.001
32. van Summeren, Joost; Gaidos, Eric; Conrad, Clinton P.; (2013) "Magnetodynamo Lifetimes for Rocky, Earth-Mass Exoplanets with Contrasting Mantle Convection Regimes", Journal of Geophysical Research: Planets n/a-n/a DOI: 10.1002/jgre.20077
33. Wallace, Laura M.; Beavan, John; Bannister, Stephen; Williams, Charles; (2012) "Simultaneous long-term and short-term slow slip events at the Hikurangi subduction margin, New Zealand: Implications for processes that control slow slip event occurrence, duration, and migration", Journal of Geophysical Research: Solid Earth Volume 117(B11) B11402 DOI: 10.1029/2012JB009489
34. Whitney, Donna L.; Teyssier, Christian; Rey, Patrice; Buck, W. Roger; (2013) "Continental and oceanic core complexes", Geological Society of America Bulletin Volume 125 (3-4) 273-298 DOI: 10.1130/b30754.1
35. Yang, Hongfeng; Liu, Yajing; Lin, Jian; (2013) "Geometrical effects of a subducted seamount on stopping megathrust rupture", Geophysical Research Letters n/a-n/a DOI: 10.1002/grl.50509
36. Zhu, Hejun; Bozdağ, Ebru; Peter, Daniel; Tromp, Jeroen; (2012) "Seismic wavespeed images across the Iapetus and Tornquist suture zones", Geophysical Research Letters Volume 39 (18) L18304 DOI: 10.1029/2012GL053053

Appendix E: Working Group Plans

The work plans attached below were discussed and recommended by vote of the Science Steering Committee and then discussed and approved by vote of the Executive Committee. Committee members who participated in the development of these plans recused themselves from discussion of the relevant work plan.

E.1 Geodynamo

Community Dynamo Code Development and Benchmark Project

Following the successful Dynamo Development Workshop held in Boulder in October 2012, here we summarize the work plan to develop a massively parallelized, well documented community spectral transform dynamo model that is for broad usage by the dynamo community. With such an HPC model, it should be possible to decrease the fluid viscosity in such dynamo models by roughly two orders of magnitude. This will enable transformative studies of fully-developed turbulent dynamo action as occurs in Earth's core.

The dynamo workshop in October surveyed both spectral and local numerical methods and the prospect of a local code (finite element, finite volume, or spectral element) is still a prime goal in the geodynamo working group; however it's a longer term goal. The outcome of the new dynamo benchmark discussed below will provide guidance for that goal; and work may begin on adopting and modifying a local code in year 3. However, the main focus of this proposal is the shorter term (and likely easier) goal of making an existing parallel, spherical harmonic (spectral) dynamo code scale well to tens of thousands of cores.

We estimate that 20 to 40 US planetary core dynamics researchers (PI's, postdocs and students) will make use of these community codes. A similar number of dynamo researchers would likely adopt it outside the US. Furthermore, many solar dynamo, stellar dynamo, exoplanet and gas planet modelers would be expected to make use it as well. Overall, the number of users will likely range from 40 to 120 researchers. (Detailed **Possible PI User Base** at back of document.)

This document provides the work plan for this project beginning in January 2013.

Task 1: Development of State-of-the-Art Spectral Codes

This project's primary objective is to generate a documented, commented and benchmarked CIG community HPC dynamo code (level 1) that parallelizes with good scaling to over 10,000 processors. Well attended by both geodynamo and solar dynamo community members, it was made clear at the Boulder workshop that "standard" spectral transform dynamo models can, with care, be made to have good scaling to 30,000 processors. In fact, solar dynamo modelers have now parallelized their so-called Anelastic Spherical Harmonic (ASH) code to scale to 30,000 processors. They are now testing its scaling out to 90,000 processors on Kraken.

Task 1 has been defined a) to take an existing parallelized spectral transform code and release it for public usage on a roughly one year timescale and b) to develop a public spectral transform code with the more advanced parallelization presently implemented in the ASH code. All the proposed Tasks will be carried out under review of an Oversight Committee comprised of Jon Aurnou, Bruce Buffett, Gary Glatzmaier and Peter Olson (chair). This committee will act to manage these tasks, test the codes and provide real time feedback on their ease of use, portability, documentation, etc.

<u>Task 1a:</u> The Boussinesq spectral transform code Calypso has recently been donated to CIG by **Dr. Hiro Matsui** for Level 3 support. This code has been validated using the benchmark cases of Christensen et al. (2001). It has also been run on XSEDE and scales well using 200 processors (Figure 1). There is no dynamo code that scales to this level that is presently available in the public domain.

The Task 1a goal would be to release Calypso on a relatively short, one-year time- scale. We are proposing here that Calypso receive **Level 3** CIG support, after making the following modifications: i) improve its documentation; ii) look for simple improvements in its parallelization scheme; iii) provide example files; iv) consider adding anelasticity. Dr. Matsui would be in charge of code development and documentation of this code. We propose that Dr. Matsui join CIG as a full-time programmer/developer in order to carry out this and following tasks.

<u>Task 1b:</u> We also propose the development of a novel public spectral transform code with CIG **Level 1** support that scales to tens of thousands of processors. This new HPC spectral code will have the advanced parallelization of the ASH code, allowing far more realistic, turbulent systems to be studied than are presently accessible to the dynamo community. To carry out this code development project in collaboration with Dr. Matsui, **Postdoctoral Associate Nick Featherstone** (NCAR / High Altitude Observatory) would be hired at the 50% level for one year. This position will be evaluated at the end of the year, with further funding sought depending on the performance benchmarks reached at that time.

In collaboration with Dr. Tom Clune (GSFC), Dr. Featherstone has been a lead developer of the advanced parallelization scheme implemented in the most recent version of the ASH code (Figure 2). Thus, Dr. Featherstone is ideally-suited to port this parallel computing expertise from the solar community to the geodynamo community. Further, the ASH development community is interested in having a public, state-of-the- art dynamo code that it is not in charge of supporting and maintaining.

Drs. Featherstone and Clune have found it is more efficient to start from the parallelization framework and then develop interchangeable coding modules. This framework is relatively flexible, allowing the user to specify, for example, between either spherical shell or Cartesian coordinate systems. Similarly, different governing equation sets can also be solved. Thus, it will be possible to select between Boussinesq, anelastic and low Mach number approximations and to solve either the full dynamo equations or to solve other systems of equations, such as the multi-scale, asymptotically-reduced dynamo equations under development by Keith Julien's group at CU Boulder.

The Calypso code and the proposed, highly optimized, HPC spectral code will be maintained by CIG developers using version control and will be configured to be highly portable and to be able to use a variety of libraries. These codes will have standard and automated tests that will be used to check accuracy and performance while modifications are being made. The developers will also provide a set of example problems that will help users understand the capabilities of each code. It is understood that these conditions are already part of Level 1 support in CIG. Drs. Matsui and Featherstone will consult with current CIG developers on how best to design these capabilities.

The requested 50% level of support would be optimal, as Dr. Featherstone is funded at the 50% level for the next three years on an NSF Astronomy helioseismology modeling project at HAO. This CIG parallelization task would allow Dr. Featherstone to continue with dynamo modeling research and, in doing so, to bridge the gap between the solar and geodynamo modeling communities.

Task 2: Community Performance Benchmark

We are proposing to carry out a concurrent performance benchmark of existing dynamo codes. A previous benchmark study, Christensen et al. (2001), was carried out, which focused on the accuracy of the dynamo solutions provided by various codes. However, a decade later, it is clear that accuracy is not the only significant issue. The dynamo community is now seeking to determine the behavior of planetary dynamo systems under realistic, very low viscosity conditions. The first obvious step is to optimize the widely used spectral transform models (i.e., Tasks 1a, b). In the longer term, we seek to determine how best to develop a future CIG Level 1 code that will parallelize well to many hundreds of thousands of processors. Further, we must consider how best to include geophysical processes not considered in the present spectrally-based dynamo models.

For Task 2, the benchmark definition team (Julien Aubert, Jon Aurnou, Nick Featherstone, Gary Glatzmaier, Ashley Willis and Keke Zhang) have defined two benchmark cases that will focus on both solution accuracy and code performance. Essential to the success of this task will be to compare the results of the various spectral models with those of the local models, specifically the codes from Sandia, Argonne and TAMU that were presented at the Boulder workshop. Towards this end, we have selected boundary conditions that are easily implemented by either method.

This benchmarking study will be carried out primarily by a CIG developer, likely Dr. Matsui. This will allow all the codes to be ported to the same machine (e.g., XSEDE allocation), in order to run benchmark cases with as much uniformity as possible. Wherever necessary, the code developers will take part in order to optimize individual code performance.

Task 3: Code Dissemination & Community Feedback

The Oversight Committee is planning to hold further CIG Dynamo Development workshops over the next three years. As part of these, Drs. Featherstone and Matsui will teach the Development community how to port and run their CIG-based codes. This will provide an excellent setting for receive feedback from the user communities.

In Year 3 of this proposal, Drs. Featherstone and Matsui will lead a community code dissemination workshop. This aim of this (virtual?) workshop will be to release the HPC spectral code for public usage, and to solicit feedback from the broadest possible audience.

Three-Year Timeline of Proposed Work and Milestones

Year 1

1. Matsui optimizes and documents the Calypso spectral transform code
   - **a. Target Date: Level 3 supported release July 2013**
2. Featherstone and Matsui develop the new HPC spectral code from the ground up a. Featherstone estimates 6-8 months to have a prototype dynamo code with full-
   ASH parallelization
   - b. **Target Date: Prototype release in October-November 2013**
3. Dynamo community performance benchmark (Task 2)
   - a. We will request computing resources from CIG to have Matsui carry out benchmark cases on a common high performance machine.
     - i. Note that access to a common machine is essential.
     - ii. These benchmark cases will each require at most a few hours of wall clock time. Thus, we will not require a large time allocation for this task.
   - **b. Target Date: Optimized codes, run uniformly; October 2013**
4. CIG Dynamo Development Workshop
   - a. Proposed time **October 2013**; Location: NCAR; Local host: Mark Miesch b.
     Present and discuss Task 2 benchmark results
   - c. Present and teach community to operate i.
     Calypso
     - ii. HPC spectral code prototype
       1. Solicit community feedback
       2. Discuss development of: robust interface; output module; standard data format; standard analysis tools; community data archive
   - d. Include Japanese developers (e.g., Kageyama and Sakuraba)

Year 2

1. Matsui updates Calypso in response to Development Workshop feedback
   - **a. Target Date: New release March 2014**
2. Matsui and Featherstone implementations to the HPC spectral code:
   - a. Robust interface
   - b. Flexible equation sets module (developed already by Featherstone in HPC ASH code variant)
     - i. Spherical vs. Cartesian coordinate systems
       - **1. Target Date: May 2014**
     - ii. Implement Boussinesq, anelastic, and low Mach number approximations
       - **1. Target Date: October 2014**
3. Publication of Performance Benchmark
   - **a. Target Date: August 2014**
4. CIG Dynamo Development Workshop
   - a. Location and goals to be determined
   - b. Feedback on Calypso and HPC spectral code

Year 3

1. Featherstone leads advanced implementations to HPC spectral code:
    a. Solver option for Keith Julien's multi-scale asymptotic dynamo equation sets b. Extend beyond ASH standard, e.g.,
        i. Parallel I/O
        ii. Fault tolerances
        iii. Fast Legendre transform
        iv. GPU, MIC or Cray Cascade compatibility
2. Based on Task 2 Benchmark results, Matsui begins development of Level 1 local HPC dynamo code
    a. Possibly adapting pre-existing HPC local MHD code (e.g., Argonne, Sandia, or TAMU)
3. CIG Community Workshop
    a. Goal: Disseminate HPC spectral code broadly to dynamo user community
4. CIG Dynamo Development Workshop
    a. Location and goals to be determined

Code Descriptions:

Calypso:

The Calypso code (Matsui/Buffett) is based on the community-standard spectral transform method and has been validated using the benchmark of Christensen et al. (2001). It has been run on XSEDE and scales well using several hundred cores (**Figure E.1.1**).

Developed in the last year, Calypso has not been used to date in published studies. At present, though, Matsui and postdoctoral fellow Eric King are using Calypso to study the effects of different thermal boundary conditions and whether large-scale structure persists with constant heat flux when the Rayleigh number is increased. Buffett's team has also used Calypso to develop a stochastic model for the dipole magnetic field (based on the Fokker-Planck equation), which can be compared with geomagnetic field observations. A paper on the application of the Fokker-Planck equation to paleomagnetic observations, made in collaboration with Cathy Constable (UCSD), is expected to be submitted in early 2013. Furthermore, Dr. Matsui is carrying out the benchmark study recently proposed by Prof. Andy Jackson (ETH) (case 1: spherical shell dynamo case subject to pseudo-vacuum magnetic boundary conditions). This benchmark / code comparison study is expected to be submitted for publication in February-March of 2013.

Calypso uses both MPI and OpenMP for the parallelization. The MPI parallelization uses a two-dimensional domain decomposition, so the number of domains does not limit the number of processors that can be used effectively in a calculation. The specific formulation of the spectral equations is based on the curl of the momentum equation and the curl of the vorticity equation. Consequently, there is no direct solution for fluid pressure.

The spherical harmonic transform consists of a Fourier transform in longitude and a Legendre transform in the latitude. Scalar and vector fields on the spherical grid are defined by spherical coordinates (*r*, q, j) and spherical harmonic modes (*l*,*m*). The subdomains are organized to eliminate communication during a particular transform.

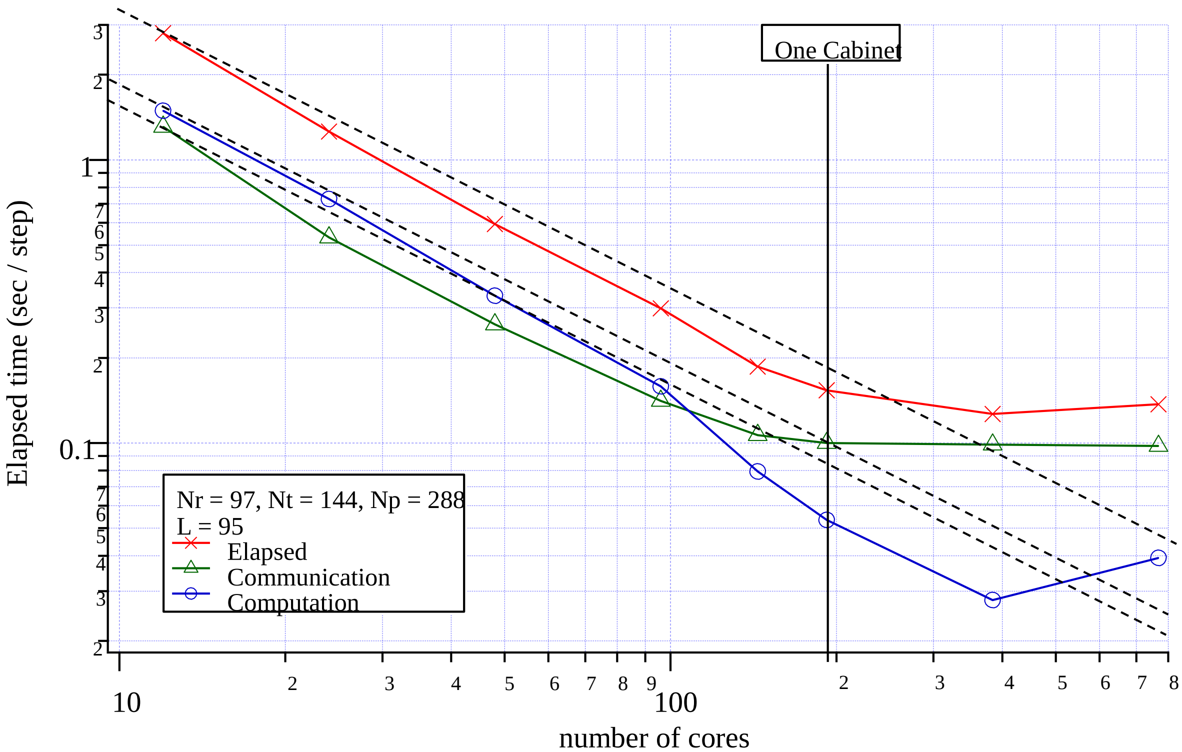


Figure E.1.1: Scaling behavior on XSEDE of the Calypso code. Image courtesy of H. Matsui.

Consider a field *f* on a spherical grid. The Fourier transform pair *f* (*r*, q, j) and *f* (*r*, q, *m*) are decomposed in the radial direction *r* and meridional direction q. The Legendre transform pair *f* (*r*, q, *m*) and *f* (*r*, *l*, *m*) are decomposed in the radial direction *r* and spherical harmonics order *m*. Finally, we decompose the spectral equations for *f* (*r*, *l*, *m*) according to the modes *l* and *m*. The resolution of a calculation is defined by the triangle truncation ($0 < l < L$, $-l < m < l$, where *L* is the truncation level). In order to balance the number of calculations in the Legendre transform, the triangular structure of the transform pair *f* (*r*, q, *m*) and *f* (*r*, *l*, *m*) is reorganized into a rectangle. The resulting rectangle is evenly divided between processors. OpenMP is also used to parallelize the transforms for modes or positions in each subdomain.

Two large data transfers are required for each spherical transform. We use one-to-one communication subroutines (MPI_ISEND, MPI_IRECV, and MPI_WAITALL) with a communication table for the data transfer. The communication table is generated by a separate, preprocessing program. Each communication table is specific for the choice of truncation level and number of processors. The same program also generates indexing data in each spherical transform.

<u>HPC ASH Code:</u>

Recent improvements in the the Anelastic Spherical Harmonics (ASH) code have resulted from the implementation of specific changes to the communications framework. By restructuring ASH in such a way as to minimize the number of collective operations performed per iteration, it has been possible to greatly diminish the accumulated overhead time of these operations (latency). It is this accumulated latency that ultimately inhibits the scalability of many pseudo-spectral codes. For the first step, the ASH code was rewritten such that derivatives are computed and then saved within a larger buffer space that is transposed to the next configuration using one call to ALLTOALLV. In addition to lowering the latency associated with the collective operations, this process increases the efficiency of the Legendre transform and Fourier transform operations. Following each transpose, the entire buffer is transformed using the transform operation appropriate to that space. When multiple fields are transformed at once in this fashion, the computational overhead associated with the transform (allocation/deallocation of temporary arrays, computation of temporary variables, etc.) is lower.

It has been shown that scalability up to 10,000 cores is achievable with the ASH code for relatively large grids (1024^3 points) using vendor provided MPI ALLTOALL libraries specific to each machine (**Figure E.1.2**). However, this can be improved upon using customized tree algorithms for the ALLTOALLV operation that are designed to minimize the number of messages sent. The use of algorithms whose latency footprint scales as sqr (NCPU), rather than NCPU, have proven successful in parallelizing the ASH code on the Kraken supercomputer at NICS.

The communications improvements can be made rather generically to other spectral codes, irrespective of geometry (spherical, cylindrical or Cartesian) and can be implemented in a flexible coding framework that can be modified to solve a variety of dynamo problems relevant to the geo-, solar and laboratory dynamo communities.

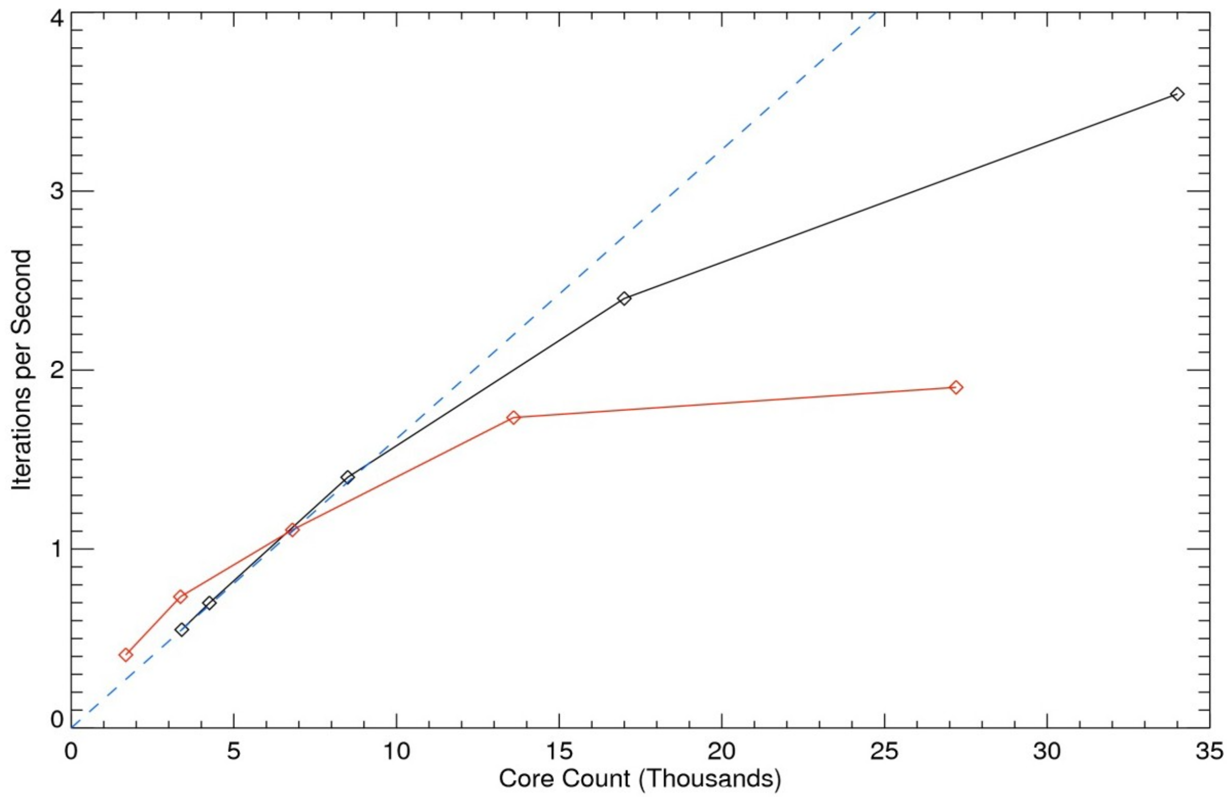


Figure E.1.2: Scaling behavior on Kraken of the optimized ASH code for rotating anelastic spherical shell convection with 400 radial points by 1024 longitudinal points by 2048 azimuthal points. The dashed blue line shows ideal scaling; the red line shows the scaling for a normal ALLTOALLV call; the black line shows custom ALLTOALLV call with dual transpose. Image courtesy of N. Featherstone.

<u>Possible *PI-Level* User Base for Advanced CIG Dynamo Codes:</u>

US: Aurnou, Bergman, Buffett, Bloxham, Brummell, Constable, Forrest, Garaud, Glatzmaier, Julien, Kuang, Lathrop, Miesch, Nimmo, Ogden, Olson, Rogers, Russell, Toomre, Weiss, Zuber
Canada: Dumberry, Gomez Perez, Heimpel, Jellinek, Johnson, Stanley
UK: Chekochihin, Gubbins, Guervilly, Hollerbach, Hughes, Jones, Mound, Simitev, Tobias, Zhang
France: Alboussierre, Amit, Aubert, Brun, Cardin, Deguen, Dormy, Evonuk, Gillet, Hulot, Le Bars, Le Gal, Samuel, Schaeffer
Swiss: Finlay, Jackson, Livermore, Noir
Germany: Busse, Christensen, Hansen, Harder, Stellmach, Tilgner, Wicht
Eastern Europe: Heyjda, Saminichin

<u>ROUGH ESTIMATE: 63 Likely PI Level Dynamo User Groups</u>

E.2 Mantle Convection

Scope of work

The goal of this sub-contract is the development of ASPECT, the next generation, massively parallel, adaptive finite element solver for mantle convection. ASPECT, built on the deal.II finite element library, the p4est library for massively parallel adaptive meshes, and the Trilinos library for linear algebra, has been written in the first years of this sub-contract and has been documented in a publication. Development is now geared towards extending the functionality required by the community.

Our work in year 4 will focus on the following goals:

1. Work with the geodynamics community on providing extensions to ASPECT that are required to implement realistic models. This includes generalizing geometry, material models, as well as extending the passively or actively advected fields, and surface velocities derived from GPlates models, both implemented during year 3.
2. Continuing the implementation and verification of numerical methods for compressible models, their documentation, and benchmarking of a variety of approaches for solvers and preconditioners.
3. Implementation and verification of numerical methods for fully nonlinear models in which viscosity, density, and a variety of other coefficients depend nonlinearly on temperature, pressure and strain rate. During year 3, we have implemented an operator-splitting approach (using a fixed-point method). We will extend this approach, for example using quasi-Newton methods. These methods will be documented and benchmarked.
4. Augmenting the existing, 116-page manual by additional material, as well as the development of more cookbooks that can guide new users through the use of ASPECT.
5. Improve usability and scalability on large machines. We have already tested and documented scalability up to several thousand cores but want to go beyond this. To this end, we will also improve portability to clusters where front end nodes run different systems than the compute nodes. We are in the process of converting the underlying deal.II library to the cmake build system that makes such cross-compiling simpler, and will follow-up by converting ASPECT as well.
6. Document the methods we are developing in ASPECT through further publications.

E.3 Long-Term Tectonics

Working Group for Strategic Plan 2013-2014 (Year 4)

Science Goals and Objectives

Long term goal:

To converge towards a community initiated and maintained 2- and 3-D lithospheric deformation computational code with guided flexibility (re: numerical methods), modularity, and the ability to solve a range of geologic processes.

Motivation: The LTT community has no tradition of open source codes. Existing codes were usually developed to address a narrow group of LTT-related scientific problems. Scientific progress would benefit from repeatability and open sourced, flexible codes.

Summary of plans for 2013-2014:

Since LTT modeling challenges are very distinctive from mantle convection modeling needs, an LTT focused community workshop will be organized in 2013. Aim of this workshop is to invite several code developers to present their codes, discuss scientific and numerical challenges, and modeling needs of the community. Both users and code developers will be invited to attend the workshop.

In Fall 2013 several groups will be invited to make available their codes online through CIG. These codes can be explored and used by the community. Feedback from the community will guide further code development with the aim to converge toward a community initiated code or set of codes.

The LTT working group will submit a topical session proposal on LTT modeling to AGU.

Activities in Support of Goals and Objectives

Activity 1. LTT Workshop Winter 2014

a. The workshop will invite developers, users and computational specialists to discuss the current state of computational modeling of lithospheric deformation/processes as well as the future directions for the community. To move forward on the long-term goal of a community LTT code, an assessment of the capabilities of current codes is warranted. A number of "hero" codes exist in the community. The workshop will give developers a chance to demonstrate their codes and potential users the opportunity to compare functionality and develop use cases to help define community needs.
   We anticipate that this will be the first in a series of bi-annual meetings. The LTT community does not have a tradition of focused meetings, and such as meeting is expected to facilitate community building as well as modeling issues unique to LTT science problems.
b. Workshop Committee. The committee will be responsible for identifying and engaging participants and setting the agenda. The committee will develop strawman use cases and functionalities for discussion to clarify scientific objectives and computational requirements. During the first LTT meeting, benchmarks will be discussed to enable better compare code capabilities. We will require CIG administration help in event and travel support. We anticipate 20-40 participants, including students.

Activity 2. Support Code Donation into CIG Repository

a. As the community is looking for a platform to potentially build off, the best way to assess available code is through usage. The LTT will reach out to developers to encourage code donation.
b. CIG support is required in reviewing, accepting and making available donated codes through the repository. Some resources maybe requested so codes are usable to the community. This will include support for optimization and development of manuals. We do not anticipate any codes being deposited immediately but perhaps ongoing beginning in early 2014. We anticipate the donation of about 3 codes in the coming year.

Next 5 year plans

a. The LTT community will participate in the combined mantle convection/ LTT workshops that are held bi-annually, and organize focused LTT meetings in alternating years.
b. Donated codes will be used by the scientific community in 2014 and 2015, and further evaluated by the developers and the community. They will be discussed during the 2015 LTT meeting. One or several codes may be selected for further CIG support.
c. CIG support is required in reviewing, accepting and making available donated codes through the repository. Some resources maybe requested so codes are usable to the community. We anticipate codes being deposited ongoing beginning early 2014.

These activities are summarized in the timeline:

	2013		2014				2015				2016				2017				2018	
	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2
LTT workshop								X	X							X	X			
Code donation to CIG repository			X	X	X	X	X	X												
Combined mantle convection/ LTT workshop				X								X								X
Community supported Code development									X	X	X	X	X	X						

Outreach & Professional Development

A. Proposed/Suggested Workshops for the LTT Community:
   2013, 2015, 2017 LTT Workshops
B. We anticipate that training is needed for users of donated codes. Support may be requested for code optimization for the code developers.
C. Development of Educational Modules:
   The LTT working group is developing an educational publication targeted toward undergrad / grad students with limited background in modeling. The publication presents realistic geological problems of increasing complexity. It explains methods and considerations that are needed when developing numerical models. Students can use this as a starting point for learning how to develop models and how to use Gale.

Summary of Past Year's Activities

A stable, final version of Gale was published online. The LTT working group is working on a publication that describes a study where Gale is used for a set of numerical experiments increasing in complexity. The models are thermally-mechanically coupled, using non-linear rheology, and include extension as well as compression experiments. This manuscript can be used for educational purposes, as outlined above. Initial models were presented as a poster at AGU. Each of the LTT co-chairs visited CalTech to work with Walter Landry on Gale and the setup of these models.

A combined LTT/mantle convection workshop was held in Summer 2012. Presentations from the LTT community addressed scientific long-term tectonics problems and a discussion on Gale and alternatives. There was consensus that LTT needs to move forward with finding an open source code that can be used for a range of scientific problems.

A committee was formed to study possible formats of CIG-supported LTT codes and code-developments. Scientific (Buck and Roy) and numerical white papers (Lavier, Choi, Tan and Calo, and Brown, Knepley and May) summarizing the scientific and numerical needs and current status were presented to CIG.

E.4 Seismology

1 Introduction

The main development of SPECFEM2D, SPECFEM3D and SPECFEM3D GLOBE is a collaborative effort involving Dimitri Komatitsch (CNRS, Marseille) and Qinya Liu (University of Toronto). Many other developers make contributions, e.g., Christina Morency (Livermore) continues to develop SPECFEM2D for coupled acoustic-(a)elastic)-poroelastic simulations, Emanuele Casarotti (INGV, Rome) is improving the CUBIT-SPECFEM meshing interface, Roland Martin (Toulouse) works on PML for the 2D and 3D codes, and Carl Tape (Fairbanks) and Min Chen (Rice) work on adjoint capabilities. Many users have made significant contributions to the packages, e.g., Bernard Schubert (Nice) & Ebru Bozdag (Princeton) have added SAC functionality, Brian Savage (Rhode Island) added attenuation, Vala Hjorleifsdottir (UNAM) incorporated kinematic rupture simulations, Piero Basini (Toronto) worked on meshing and the implementation of noise, Hejun Zhu (Princeton) & Yang Luo (Chevron) improved meshing based on CUBIT, Jean-Paul Ampuero & Surendra Somala (Caltech) added a dynamic rupture simulations library, and Hom Nath Gharti (while at NORSAR; currently at Princeton) extended SPECFEM3D to quasi-static problems, such as slope stability analysis.

At Princeton, the main developers are currently me and postdocs Matthieu Lefebvre and Hom Nath Gharti, and, in the context of GPU computing, senior HPC analyst Robert Knight (Princeton Institute for Computational Science & Engineering). Princeton senior Linux systems administrator David Luet is primarily responsible for the southern California and global ShakeMovie systems, which are based on SPECFEM3D and SPECFEM3D GLOBE, respectively, and routinely produce 3D synthetic seismograms for the seismological community.

What I am requesting from CIG is financial support to help cover some of the considerable costs associated with the continued development and maintenance of this very broad array of activities. The requested resources would be used to help cover a fraction of the related Princeton salaries. All work is ultimately supervised by me and Dimitri Komatitsch. We have frequent email, Skype and telephone interactions, plus various members of the development team meet face-to-face on a regular basis. All SVN traffic is seen by the entire group of people with SVN write permissions.

Both SPECFFEM3D and SPECFEM3D GLOBE (which can also perform regional simulations) would benefit from the following scope of work for which we are requesting CIG support.

2 Scope of Work

Over the next year (10/1/2013–9/30/2014) we propose to carry out the following tasks:

1. Continued development of GPU versions of SPECFFEM3D and SPECFEM3D GLOBE. The GPU effort involves an international collaboration with Dimitri Komatitsch, Olaf Schenk in Basel, Daniel Peter at the ETH in Zürich, Jeff Larkin from NVIDIA and located at Oak Ridge National Laboratory (ORNL), and Matthieu Lefebvre, Robert Knight and me at Princeton. For this development, we have access to 'Titan' at ORNL, a GPU-accelerated (NVIDIA K20) Cray (2013 INCITE award of 100 million core hours), and a new SGI at Princeton with 200 graphics cards (NVIDIA K20).

2. Development of Intel MIC-accelerated versions of SPECFFEM3D and SPECFEM3D GLOBE. MIC is a serious competitor to the GPU, and we want to position ourselves to capitalize on either or both types of hardware accelerators in the near term. In this regard, Dimitri and I have established collaboration with the Intel Exascale Lab in Paris (Pierre Thierry and Marie-Christine Sawley). The new SGI at Princeton has 10 MIC-accelerated nodes for code development.

3. Implementation of the ADIOS file format to optimize IO. Like HDF5, netCDF and parallel- netCDF, ADIOS is designed for easy-to-use, fast, scalable, and portable IO. For seismological applications, these attributes are required to reduce the crippling number of files (e.g., in SEED or SAC formats) associated with typical seismological datasets, and to implement fast parallel pre- and post-processing as part of the adjoint tomography workflow. A single run of SPECFFEM3D and SPECFEM3D GLOBE will produce just a single synthetic ADIOS 'event file', and observed data for a given event are combined in a single observed ADIOS event file. Consequently, each earthquake will have just two associated time series files: one for the data and another for the synthetics. Pre- and post-processing operations are performed in parallel on pairs of ADIOS events files, minimizing access to the file system by performing all operations in memory. An additional huge benefit of ADIOS is that it enables one to encode all the meta data associated with a synthetic seismogram, e.g., parameter settings, version of the source code, compile options, etc., thereby ensuring reproducibility of simulations. We have engaged the IRIS DMC in a discussion about the possibility of extracting ADIOS event files directly from the IRIS database.

4. Implementation of the ADIOS file format in the pre- and pos-tprocessing workflows of adjoint tomography. This requires rewriting the adjoint tomography toolkit, motivated by the ADIOS file format. Typical operations on time series — such as detrending, demeaning, cutting, tapering, bandpass filtering, instrument response removal, etc., followed by window selection based on FLEXWIN and the making of measurements, e.g., cross-correlation traveltimes or frequency- dependent phase and amplitude anomalies — need to be performed on pairs of observed and synthetic ADIOS event files, thereby enabling parallel operations on thousands of shots in exploration seismology and thousands of earthquakes in regional and global seismology.

5. Full gravity in SPECFEM3D GLOBE. Currently, the global code uses the so-called Cowling approximation for gravity: incorporating the effects of background gravity, but ignoring gravitational perturbations induced by the motion. Including full gravity is a notoriously difficult problem, because this requires solving Poisson's equation in the solid Earth and —most challenging— Laplace's equation in all of space. By taking advantage of so-called infinite elements in the con- text of the spectral-element method, we are now able to solve Laplace's equation, coupling its solution to conservation of linear momentum. This development opens up the possibility of using SPECFEM3D GLOBE for free oscillation seismology. The next challenge is to improve the accuracy of the time integration scheme to be able to calculate the several-days-long time series used in normal-mode seismology. For this reason, we are investigating fourth-order Runga-Kutta and symplectic time schemes as alternatives to the currently used second-order accurate Newmark scheme.

In an important and exciting symbiotic development, we are working on a quasi-static version of the global code with full gravity for postseismic and postglacial rebound calculations. The resulting software would be of considerable interest to the glacial isostatic adjustment community, thereby significantly broadening our user pool.

6. Working beta version of P and S teleseismic sources in SPECFEM3D. Coda waves arriving after the main teleseismic P and S phases are used extensively to 'image' crustal and upper mantle structure based on 'receiver functions'. The goal is to use the same coda waves for imaging based on full 3D simulations in combination with adjoint methods.

Accommodation of teleseismic waves and receiver functions is a collaborative effort with Qinya and Dimitri. The approach requires prescribing an incident P or S wavefield on the boundaries of a high-resolution model domain that contains the structure of interest, and calculating sensitivity kernels based on adjoint methods within this domain. Qinya and her postdoc Ping Tong have implemented interfacing between a 1D FK solution and SPECFEM2D, and will soon start work on interfacing Tarje Nissen-Meyer's 1D axi-SEM code with SPECFEM3D. As envisioned by the

CIG Seismology Working group, having teleseismic inputs will make SPECFEM3D and (the regional versions of) SPECFEM3D GLOBE more broadly useful for the seismology community.

All software will be open source and freely available via CIG. Software manuals will be updated by

Princeton staff and collaborators to reflect all code modifications and enhancements.

E.5 Short-Term Crustal Dynamics

Working Group for Strategic Plan 2013-2014 (Year 4)

Science Goals and Objectives

Observationally constrained and internally consistent physics for the entire seismic cycle

Our goal is to resolve the entire seismic cycle in numerical models that capture interseismic deformation, rupture nucleation and propagation, and postseismic deformation with realistic Earth models (geometrical complexity, material heterogeneity, and inelastic rheologies). Constraints on fault and bulk rheologies that are consistent with extensive geodetic, seismic, and geologic observations are critical to understanding the behavior of fault systems and improving the accuracy and precision of earthquake hazard assessments.

Observationally constrained and internally consistent physics for tectonics of magmatic systems, geothermal systems, and the cryosphere

Integrate modeling tectonic processes with heat and fluid flow, thereby enabling complex rheologies with temperature dependent parameters. Incorporating heat and fluid flow into tectonic modeling significantly expands the range of scientific problems that can be addressed (such as seismic tremor in geothermal areas) and permits direct application of additional geophysical constraints. Viscoelastic, elastoplastic, and viscoplastic rheologies are important for bridging between seismic and tectonic time scales.

Observationally constrained modeling of crustal deformation associated with surface loads

Constrain the bulk rheologies of the crust using geodetic and geologic observations of deformation arising from glacial rebound, reservoir impounding, and other surface loads. This objective also facilitates separating crustal deformation associated with surface loads from tectonic loading, which is critical in regions where both processes are occurring and interacting.

Activities in Support of Goals and Objectives

Ongoing PyLith Development

PyLith development supports all three of the working group's objectives. Our primary goal for the coming year will be supporting earthquake cycle simulations via seamlessly coupling quasi-static simulations of interseismic deformation with dynamic simulations of earthquake rupture to bridge the time scales between tectonic loading over hundreds to thousands of years and fault slip in earthquakes over a few to tens of seconds. By combining these two types of PyLith simulations, users will be able to include the effects of 3-D elastic, viscoelastic, and elastoplastic bulk rheologies as well as different fault rheologies in self-consistent simulations of deformation over the entire seismic cycle. Because optimal discretizations differ significantly between the quasi-static and dynamic portions, we will first focus on using the same finite-element discretization for the two time scales. A longer term goal will be to overcome the obstacle of using different finite-element discretizations for the different time scales by development of interpolation modules to project the solution from one discretization onto another.

These interpolation modules will be tightly integrated into PETSc, thereby providing these capabilities to the broader scientific community.

Our second development goal involves supporting multiphysics simulations coupling elastic behavior with heat and fluid flow. This will involve refactoring the elasticity portion of PyLith into modules that couple multiple governing equations. This approach also permits formulating efficient implementations of incompressible material response, which is commonly used to estimate deviatoric stresses associated with gravitational loading in materials with 3-D variations in elastic properties, an important ingredient in many crustal deformation problems. Implementing these features is targeted to begin in late 2013 with an initial release of a preliminary implementation in June 2014. We anticipate that implementing extensive support for coupling elasticity to heat and/or fluid flow will span a few releases.

PyLith currently supports a relatively flexible interface for applying surface loads via tractions. Further support for more sophisticated surface loads will require additional engagement with the community to define the computational needs.

Additional development goals are focused on computational science features to support faster and larger simulations, thereby facilitating achieving the geodynamics science objectives. The PyLith development team plans to add support for higher order basis functions to allow much greater resolution for a given finite-element mesh. This feature facilitates resolving physics across a broader range of scales using a given finite-element mesh to run a simulation at a higher resolution or using a coarser mesh over a larger domain to run a simulation with the same accuracy. Other efforts are focused on reducing simulation runtime. PyLith currently supports use of GPU solvers through integration with PETSc solvers. Adding GPU implementations of the finite-element integration routines, which account for a significant fraction of the overall runtime, would allow users to further accelerate their computations using GPUs.

Reaching these development milestones requires ongoing support for Matthew Knepley with additional support for two development meetings per year involving the PyLith developers (Brad Aagaard, Matthew Knepley, and Charles Williams). While PyLith development maintains a steady pace with multiple releases a year, the planned features are becoming more sophisticated and computationally challenging. Additionally, the number of features requested by the community outpaces the rate at which the current development team can implement them. In this respect PyLith development is significantly inhibited by a lack of development resources. CIG currently supports Matthew Knepley, who focuses on the finite-element data structures and computational science features. All of the geodynamics features are implemented by Brad Aagaard and Charles Williams, who are supported by their institutions but only spend a fraction of their time on PyLith development. PyLith development could be significantly accelerated with identification and funding of additional community members that have the necessary computational science skills.

Development of an Inversion Framework

The geodetic and seismic communities lack an extensible, well-documented, open-source modern framework for inversions of fault slip. Ongoing efforts to benchmark geodetic and seismic source inversions within the Southern California Earthquake Center community highlight many of the complex computational issues and common errors in these underdetermined inversions. The short-term crustal dynamics community envisions development of an inversion framework focused on geodetic and seismic inversions that provides plug-ins for a variety of common inversion methods, including Bayesian approaches. Such a development effort would be independent of PyLith development and should be coordinated with the Computational Seismology working group. This effort requires identifying a scientist to lead this effort followed by refining the software requirements, obtaining funding, and assembling a development team.

Outreach & Professional Development

Workshops

We plan to continue our series of workshops through a combination of biannual in-person meetings (even years) and biannual virtual workshops (odd years). The in-person five-day workshops include both scientific discussions (three days) and hands-on software user-tutorials (two days). These workshops foster community development by providing opportunities for in-depth presentation and discussions of science topics along with informal interaction among scientists, particularly between those beginning their career (graduate students and postdocs) and more senior scientists (faculty and researchers). We also facilitate collaboration with the broader community by inviting presentations on relevant topics from scientists in other subdisciplines. We plan to continue seeking funding for these biannual workshops from CIG, SCEC, NSF, and NASA.

Following upon our extremely successful initial virtual workshop in 2011, we plan to continue using virtual workshops to provide extensive online training in crustal deformation modeling. Our primary focus is educating users on how to leverage the growing number of features in PyLith for their own research. Archiving the sessions from virtual workshops provides new users with immediate access to training sessions, allowing them to quickly learn content at their own pace without waiting for scheduled training sessions. Additionally, because previous training sessions are archived, subsequent virtual workshops can focus on new features and more advanced topics, rather than repeating content from previous sessions, which have been archived. For example, the 2013 virtual workshop includes sessions on advanced features such as computing static Green's functions for 3-D earth structure for use in geodetic inversions, using fault constitutive models to model aseismic slip and earthquake rupture, and running PyLith in parallel.

Specialized Online Training

We plan to offer additional online training sessions on topics requested by the community. We anticipate offering a couple of these training opportunities per year. They will likely focus on bringing users up to speed on new features following releases of new PyLith versions.

Summary of Past Year's Activities

PyLith Development

PyLith development continues to be the main focus of the working group activities. The PyLith development team completed two releases with new features as well as a bugfix release since June 1, 2012. These releases provided (1) a user-friendly interface for computing static Green's functions for use in geodetic inversions with lateral variations in Earth structure, (2) the ability to output the displacement or velocity interpolated to arbitrary locations within the domain, (3) support for PETSc GPU solvers, (4) spatial and temporal variations in tractions for spontaneous earthquake rupture simulations, (5) a post-processing utility to compute fault slip information, such as seismic potency, seismic moment, and moment magnitude directly from PyLith fault output, (6) computation of the stable time step for explicit-time stepping based on the CFL condition and distortion of the finite-element cells from their ideal shapes, and (7) new CUBIT meshing example illustrating how to use a field over the domain to specify the discretization size. The releases fixed over ten minor bugs identified through benchmarking, full scale tests, and user feedback.

An additional bugfix release is targeted for release in April 2013 with a new feature release in June 2013. The new release involves a major reimplementation of the finite-element data structures. The main objectives from switching from the C++ Sieve data structures to the new C Plex data structures are (1) provide tighter integration with the rest of PETSc through C data structures and functions that build upon the vector (Vec) and Data Management (DM) objects, (2) improve efficiency via reduced memory usage and runtime, and (3) lay the foundation for support of multiphysics capabilities, such as coupling elasticity with heat and/or fluid flow. The new Plex data structures should also provide better memory load balancing in large parallel runs.

Crustal Deformation Modeling workshop

The 2012 Crustal Deformation Modeling workshop was held June 18-22 on the campus of Colorado School of Mines in Golden, CO. The agenda, presentation materials, and list of participants are available at http://www.geodynamics.org/cig/community/workinggroups/short/workshops/CDM2012. This meeting continued an ongoing series of workshops held over the past 10 years. The focus of these workshops is physically based models of the distribution of lithospheric stress in space and time via simulation of the strain accumulation, dynamic rupture propagation, and postseismic relaxation over multiple earthquake cycles. The workshop included participation from 62 scientists. As in previous workshops in this series, nearly two-thirds of the participants were graduate students and postdocs. In this workshop 44% of the participants were graduate students, 21% were postdocs, 18% were faculty, and 18% were researchers. About 80% of the attendees participated in both the tutorials on the first two days of the workshop (Monday and Tuesday) and the science talks and discussions over the following two and one-half days (Wednesday, Thursday, and Friday).

The tutorials focused on Relax and PyLith with some discussion of CUBIT for meshing and ParaView for visualization. The 11 science talks covered a range of topics associated with modeling earthquake deformation, including the role of geodetic modeling in the Uniform California Earthquake Rupture Forecast (UCERF3), elastic block modeling, Bayesian inversion methods, conceptual models of slow slip, the rheology of the lower crust with constraints on crust-mantle interactions, and insights from critical taper analysis on earthquake cycle modeling. The workshop also included two discussion sessions with one focused on the need for an inversion framework and one focused on prioritizing features to be included in PyLith. The participants expressed strong support for a community kinematic inversion code using a highly modular approach. Such a code would target the geodetic modeling community but might support seismic data as well. The main obstacle is finding the appropriate scientist to lead/champion the code development effort. The two hot topics for PyLith development were multiphysics capabilities and earthquake cycle modeling.

E.6 Magma Migration

Working Group for Strategic Plan 2013-2014 (Year 4)

Science Goals and Objectives

Long Term Goal: Provide flexible multi-physics modeling capability and training for the exploration of coupled fluid-solid mechanics with an emphasis on the dynamics of magmatic plate-boundaries.

(From the Magma-Dynamics proposal):

Magmatic plate boundaries (mid ocean ridges, subduction zones) and intra-plate hot spots are among the most important and complex dynamic and chemical systems in the solid earth. While volumetrically small, these regions have global consequences for mantle flow and plate tectonics through the spontaneous localization of weak plate boundaries. Magmatism in these regions also provides the dominant mechanism for geochemical fractionation, mixing and sampling of the Earth's mantle. Many of the observational constraints on both plate-boundary processes and global mantle dynamics come from regional studies of lavas from mid-ocean ridges, subduction zones and oceanic hot spots and form focus areas for many initiatives such as GeoPRISMS, EarthScope and core EAR and MGG Geophysics programs.

Despite the importance of these problems, and a considerable amount of research on their dynamics, there still does not exist a flexible, publicly available, well documented open-source computational toolkit for exploration of mantle magmatism. One reason for this is that magma/mantle dynamics are fundamentally coupled, multi-physics problems with considerable uncertainties in coupling and even basic physics. Years of research demonstrate that small changes in assumptions about coupling (e.g.,~effects of fluids on solid rheology) can dramatically change the underlying physics, length, time scales, and appropriate computational strategies. To make these problems accessible to a larger community requires both flexible tools for model development and working, non-trivial demonstration codes, as templates for new development. Fortunately, there have been significant advances in both our understanding of magma physics and available computational infrastructure for multi-physics problems. Our principal long term objective is to make such infrastructure, and the training and understanding, required to use it available to the general geodynamics community as a level 1 CIG code. Well-designed software tools that are transparent and reusable, can enable a much broader range of users of complex models and greatly enhance the discussion and exploration of complicated (and simple) geodynamic systems.

Short Term Goal. Contribute a general multi-physics modeling capability for plate-boundary scale magma-dynamics problems.

Our immediate goal is to document and release a working multi-physics model building toolkit, TerraFERMA (the Transparent Finite Element Rapid Model Assembler) written by Cian Wilson (LDEO/Columbia) as open-source code and a level 3 contribution to CIG. (See Activity 1 below).

TerraFERMA, leverages multiple advanced libraries (FEniCS, PETSc, Spud) to provide a flexible, reproducible and reusable modeling framework for Finite Element modeling of Multi-physics problems. It is not a “magma-dynamics” code per se, but a much more general system for generating transparent, custom compiled models from a common infrastructure and human readable options file. Unlike traditional geodynamic models, TF provides the user remarkable flexibility in not only solver configuration but in actual high-level description of the underlying PDE’s. TF has been developed using modern software development practices (version control, source hosting, buildbot regression testing etc.) and has been benchmarked against a large range of published geodynamic benchmarks for mantle convection, magma dynamics and subduction zones.

Short-Intermediate Term Goal 1. Develop a core group of alpha users

Using the released code, our second goal is to cultivate a small group of alpha-users to begin exploring a variety of user driven problems to expand the user base and refine the overall design and usability of TF to determine if this is a viable model for design of a flexible public code. This will also provide a template for developing best practice for documentation and training in TF.

Short-Intermediate Term Goal 2. Integrate development of TF with core PETSc development for multi-physics problems

Given a working code base plus a small dedicated user community, the next stage is to start a set of technical improvements to the low-level assembly and solver infrastructure of TF to improve performance for large coupled systems and compatibility with other CIG PETSc based projects (e.g. pylith), while keeping the flexibility of the user interface and design.

Activities in Support of Goals and Objectives

Activity 1: Release C. Wilson’s TerraFERMA and contribute to CIG as a level 3 code.

a) This is a direct response to our short-term goals
b) TerraFERMA will be released as open-source code in conjunction with the submission of the paper documenting its design and features. Estimated release dates are late spring/early summer 2013
c) This part does not require immediate CIG resources. Cian has already developed a full development and testing harness and the code will be made available through a code hosting service (most likely bitbucket).

Activity 2. Build core alpha-users group

a) This is a direct response to our first short-intermediate goals
b) This activity will begin with the open-source release of TF. The initial group will involve members of Magma Dynamics Working group and select users who will collaborate with principal developers for developing example problems and documentation through published manuscripts and archived model problems on the CIG web-site
c) This part will require moderate support from CIG for coordinating projects, making results available and beginning professional user documentation for TF.

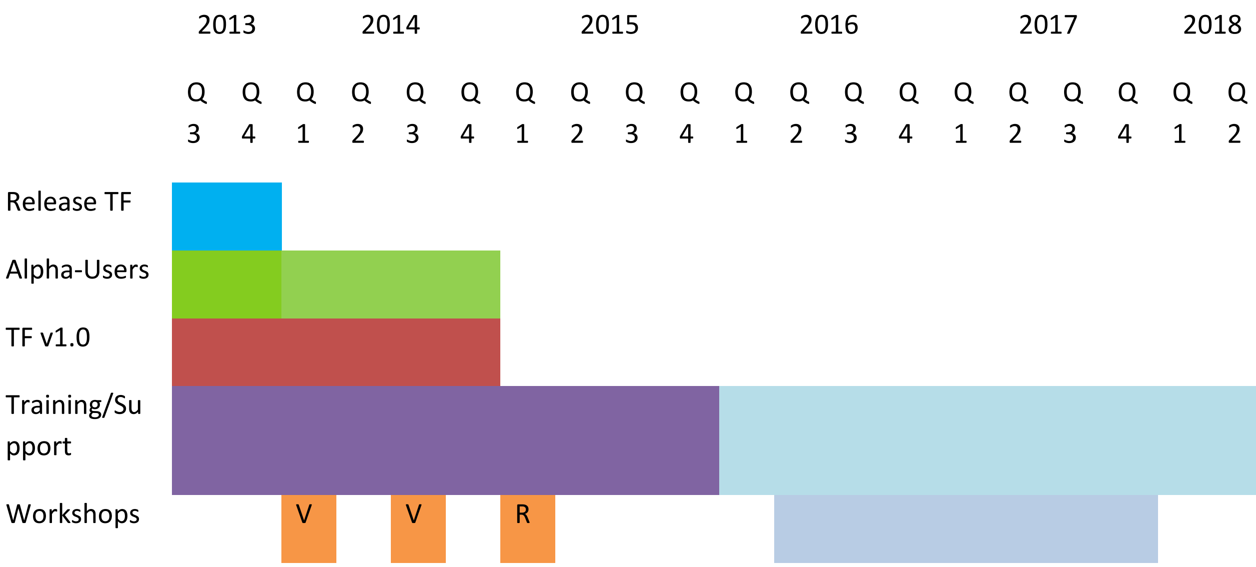
a. In addition we will expect at least one CIG developer to work with the alpha-users group to become familiar with TF and help manage support and questions
b. We might also request help with porting TF to various production machines and XSEDE resources

Activity 3. Begin second phase development with Matt Knepley on Core PETSc Infrastructure

a) This is a direct response to our second short-intermediate goals
b) Simultaneously with the release of TF, we will begin exploring technical improvements to both the assembly and solver infrastructure. This work will be in collaboration with Matt Knepley and Jed Brown and will primarily be exploring the transfer of functionality from dolphin to native PETSc. These developments, however, will be done on a separate development branch of a joint Columbia/CIG code so as not to break the basic functionality of TF.
c) This part will require CIG resources in the form of Matt Knepley's subcontract as spelled out in the original magma dynamics proposal.
    a. Matt will work directly with Cian, Spiegelman and members of the Magma Dynamics Working group to develop the core PETSc infrastructure for native PETSc assembly and sparsity building for nested matrices as well as improvements to the block preconditioners and variational inequality solvers. These improvements will be incorporated directly into PETSc and be available to a wider range of projects including multi-physics modeling in pylith, solver backends potentially for ASPECT as well as general finite volume codes for magma dynamics. Depending on funding available, this part might also require additional support for Cian Wilson and the TF front end.
    b. Continuing support of the new code on XSEDE resources
    c. Continuing development of documentation and training materials

Activity 4. Develop training and support materials for TF (including virtual/in person users workshop)

a) This activity is an essential component of all new code development and is designed to develop solid users documentation for TF as well has hands on tutorials in general and more geo-specific magma-dynamics problems
b) We propose a virtual user's workshop Early in 2014 to demonstrate activities of the alpha-users group and begin more general training for other users
c) This part will require CIG resources in terms of management support for workshops as well as TF developer's time.



Outreach & Professional Development

A. We propose several Virtual workshops/training sessions in 2014 followed by a general multi-physics workshop sometime in 2015, possibly in coordination with other CIG meetings.

B. TF will require considerable training, particular for those without a background in computational math. This training however is common to many of the CIG codes and projects. TF specific training sessions will focus on magma-dynamics and general multi-physics problems however, we also could see having more general training/short courses in computational math possibly in conjunction with CIDER.

C. Development of Educational Modules: TF is by nature partly self-documenting as every model comes with a fully working options file that contains all the information required to compose and solve a model. A set of tutorial demonstration models will be developed as part of the code distribution and regression testing (we already have all of the published convection benchmarks coded up). Moreover a key design criteria of TF is that any published results of a model should also include access to the options file so that the work is reproducible. We request that CIG keep an archive of working TF models as both tutorials and modeling resources.

D. Synergistic activities. Depending on time and interest, we would be happy to run tutorials/short courses in cooperation with other organizations. In particular, we foresee that a summer short course on computational methods in coordination with CIDER would be a very useful mechanism for expanding and disseminating the use of advanced modeling in solid-earth geosciences.

Summary of Past Year's Activities

- General proposal for magma dynamics development was formulated and approved by CIG (but start date depends on initial release of TF)
- Cian Wilson and Marc Spiegelman, previewed TerraFERMA at Mantle convection/Lithospheric Deformation Workshop in Davis.

- Wilson has continued continued major development on TF which will be described in two manuscripts (supported by GeoPrisms). The first is a general description of TF design, implementation and benchmarking to accompany the open-source release. The second is a science paper that uses TF to explore coupled fluid-solid flow in subduction zones.
- Wilson and Spiegelman have begun discussion on next phase of development with Matt Knepley and Jed Brown, including a phased migration of some of the lower level functionality of TF from FEniCS (Dolfin) to PETSc.

Appendix F. Status of Past Year (2012) Goals

c=continuing effort, ip=in progress, d=delayed, ca=cancelled, f=finished

	GOAL	status
I.	**Common Infrastructure**	
a.	Maintain LAN, servers, desktops, notebook computers	c
b.	Maintain Plone website (http://geodynamics.org)	c
c.	Maintain software repository	c
d.	Maintain and expand regression testing	c
e.	Initiate general benchmarking site	d
f.	Maintain and Upgrade Science Gateway and Web Portal	c
II.	**Software Development**	
a.	Short term tectonics code development (*PyLith)*	c
b.	Magma dynamic software TerraFERMA (*FEniCS/PETSc based)*	c
c.	ASPECT (release versions 0.9 and 1.0)	c
d.	Geodynamo code development (goals to be determined at October	ip
e.	Establish tools for mantle convection benchmark	ip
f.	Maintain existing stable software (bug fixes, etc) such as CitcomS and Gale.	c
III.	**Organizing Community Participation**	
a.	Crustal Deformation Workshop, June 2012. Colorado School of Mines, 60	f
b.	Mantle/Lithospheric Dynamics Workshop, UC Davis July-Aug, 2012. 70	f
c.	Geodynamo Developer-User Working Meeting, Fall 2012. Approximately 24	f
d.	Annual CIG Business Meeting, in conjunction with the AGU Fall Meeting,	f
e.	CIG Tutorials at Earthscope 2013 (Location and date TBA)	ca
f.	Joint CIG-QUEST meeting, July 2013 (Fairbanks, Alaska)	ip
IV.	**User Training**	
a.	Self-Training – Web accessible via geodynamics.org	
i.	User manuals available on website for download with code	c
ii.	Cookbooks and Virtual Tutorial sections under main code pages	c
iii.	Benchmarks described on code page for code verification/setup	c
iv.	Active mailing lists for questions/advice/bug reports	c
v.	Contact information for developers posted for direct contact	c
vi.	Help menus built into Seismology portal gateway	d
vii.	Site-specific Instructions for Using CSA Software	d
b.	Developer-led Group Training Sessions	
i.	CDM Virtual Workshop, June 2013	ip
ii.	Gale training, Summer 2012	f
iii.	CitCom training at CIDER summer program, July 2012	f