2021-2022

ANNUAL REPORT

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

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Executive Summary

The Computational Infrastructure for Geodynamics (CIG) is 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. During the current reporting period, we have focused on making progress on all aspects of software development, improving CIG's practices and governance, strengthening partnerships, continuing education and training, and building community.

CIG supported community development and knowledge transfer through regular meetings, workshops, webinars, newsletters, tutorials, and our discussion forum. This year, we completed the transition to a new website hosted by HUBzero® at SDSC. We held regular users' meetings and workshops for community supported software projects ASPECT, PyLith, and Rayleigh. Outreach activities included virtual and in person workshops. In person workshops, restarted in the spring with COVID protocols in place. Activities included the ASPECT User workshop, ASPECT Hackathon, CIG Software Developers Workshop, and the Crustal Deformation Modeling Workshop. We had significant international participation in both virtual and in person events. Our webinar series continued highlighting contributions to CIG software by early career researchers. In addition, the new Seismic Cycles Working Group sponsored a 7-webinar series with 14 speakers highlighting a broad spectrum of physics important to earthquakes cycle modeling. The CIG Distinguished Speaker program continues its focus in bringing CIG-supported science to colleges and universities that are underrepresented in the geosciences. Visits occurred both in person and virtually this year.

CIG continued to advance software development in mantle convection, crustal dynamics, dynamo, long-term tectonics, seismology, and evaluated future directions for these codes. The community made great progress in adding new features to codes expanding its application to a wide range of scientific problems including major efforts in the implementation of viscoplastic rheology (ASPECT), poroelasticity (PyLith), and improved code performance (Rayleigh, ASPECT). We supported improvements to World Builder increasing its capabilities to create complex 3D models and AVNI to facilitate rapid prototyping of multi-scale models by reconciling and assimilating features ranging from reservoir to global scales. We initiated a Python base repository, GDMATE, to support the sharing of analyses tools in geodynamics. Our plans for the coming year include continued development of codes across the scientific domains represented by geodynamics, including release of new codes and new versions of established codes.

CIG Staff continue to support code contributions as requests arise during the year through our established approval process. We will continue community activities and career development (especially for early-career scientists) through planned workshops, tutorials, hackathons, and webinars. We continue to develop partnerships with national computing facilities and other partner organizations. These include managing and renewing CIG's allocation on XSEDE and utilizing allocations on Frontera, to continue to optimize community codes for applications in global mantle flow, lithospheric deformation, and core dynamics.

We continued to work with the CIG community and other relevant communities to improve best practices in software development and software repositories and contribute to cross-cutting initiatives in FAIR and FAIR4RS. We held our second CIG Software Developers meeting 28 February & 1 March bringing together our developer community to examine current and best practices in software. The CIG Developers Workshop resulted in a number of recommendations that will help expand the CIG developer community, make software more accessible to new users, increase pathways to acceptance into the CIG community of codes, increase developer productivity through use of common infrastructure and best practices for software development.

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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 geoscience 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 dynamo; magma, crustal and earthquake dynamics; and seismology. With 90 member institutions including 21 international affiliates, CIG is a member-governed organization with a high level of community participation.

This document updates CIG operational status and covers the period from August 1, 2021, through July 31, 2022, unless otherwise noted.

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 updated in 2018 and available on our website [pdf].

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. International affiliate members are accepted, but only United States members have voting rights. Each member institution selects one member-representative to the electorate. The number of member institutions continues to increase and currently stands at 90 member institutions including 21 international affiliates. Of these, 5 are inactive as member representatives have moved to new institutions. In 2022, CIG welcomed University of Oklahoma. See Appendix A.

2.2 Executive Committee

The Executive Committee (EC) is the primary decision-making body of CIG. The EC meets regularly to discuss administration and organizational activities. In conjunction with the Director, the EC oversees day-to-day operations through its regular meetings, web conferences, electronic mail, and forum. 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. See Responsibilities of the EC.

The EC has 7 members, of which 5 are voting members: Chairman, Vice Chairman, and three members at-large. 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,* Claire Currie (2022), University of Alberta
- *Vice Chair,* Alice Gabriel (2023), University of California San Diego, LMU Munich
- Brad Aagaard (2024), US Geological Survey
- Bruce Buffett (2022), University of California, Berkeley
- Carolina Lithgow-Bertelloni, University of California, Los Angeles
- *Ex officio*, Juliane Dannberg (2022), University of Florida
- *Ex officio,* Lorraine Hwang, 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. See Responsibilities of the SSC.

The SSC consists of 8 elected members including a chairperson and 2 *ex officio* members - the CIG Director and the Chair 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,* Juliane Dannberg (2022), University of Florida
- *Vice Chair,* Ebru Bozdag (2023), Colorado School of Mines
- Sylvain Barbot (2023), University of Southern California
- Peter Driscoll (2024), Carnegie Institution
- Scott King (2022), Virginia Tech
- Harriet Lau (2024), University of California, Berkeley
- Dave May (2024), University of California, San Diego
- John Naliboff (2023), New Mexico Tech
- *Ex officio,* Claire Currie (2022), University of Alberta
- *Ex officio,* Lorraine Hwang, Director CIG

2.4 Working Groups

Working groups (WG) provide the EC and SSC with domain expertise. WG's, formed by the EC, provide input on science drivers, technical challenges and resources necessary for research in their domain. Working groups provide advice to the SSC and EC and form goals and actions for the upcoming year. New this year is the Seismic Cycles Working Group. See Roles and Responsibilities.

CIG's nine working groups represent the main scientific domains and special interests in the CIG community:

Computational Science

This working group informally advises CIG leadership and the other working groups on best practices and identifies opportunities for new partnerships and activities within CIG.

Seismology

The main priority for the Seismology Working Group is the continued advancement in capabilities for high performance computing and to broaden its code and user base.

Dynamo

The long-term goal of the Dynamo Working Group is to produce a series of ever more efficient, massively parallelized, well-documented community dynamo models for broad usage by the dynamo community. With these HPC models, the goal is to significantly decrease the fluid viscosity in such dynamo models by at least two orders of magnitude. This will enable transformative studies of fully developed turbulent dynamo action as it occurs in the Earth's core.

Education Working Group

The Education Working Group is interested in developing open-source materials for teaching geophysics using computation with an emphasis on computational geophysics. Their goal is to develop modules that could be used in a classroom or self-learning setting targeted at undergraduate through early graduate training.

Long-Term Tectonics

The Long-Term Tectonics Working Group's primary goal is to converge towards a community-initiated and maintained 2D and 3D lithospheric deformation computational code (or codes) with flexibility, modularity, and the ability to model a range of geologic processes.

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.

Mantle Convection

The Mantle Convection Working Group activity focuses on developing, supporting and maintaining ASPECT, CitcomS, and CitcomCU.

Seismic Cycles

The goal of the Seismic Cycles Working Group is to organize the community in developing open source computational models to better understand the dynamics of earthquake sequences, swarms, and aseismic slip.

Short-Term Crustal Dynamics

The Short-Term Crustal Dynamics Working Group 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.

CIG Staff along with 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 clearinghouse for best practices in computational solid-Earth Science including benchmarking, regression testing and education/training that are consistent across disciplines.

Appendix B provides a list of working groups and the 66 working group members who are 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 and Physical Sciences 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 Earth and Planetary Sciences Department. MSB houses CIG servers. CIG compute nodes are pooled with others in the Division of Math and Physical Sciences making up to 2048 CPUs available to affiliated CIG developers. CIG has access to high-speed networking and state-of-the art scientific visualization facilities through the DataLab. Due to the global pandemic, CIG Staff transitioned to working remotely in March 2020 in accordance with University of California Davis guidelines through Summer 2021. Campus reopened in Fall 2021 with COVID protocols in place. The pandemic has given us the opportunity to reimagine Headquarters as we prepare for the next phase of CIG.

CIG Headquarters is led by the CIG Director. CIG is supported by a team of research scientists and IT professionals. Support for research staff members may come from other projects. System administration support is received from pooled campus resources. Web support is received from the HUBzero team. Administrative support is received from the Earth and Planetary Sciences Department as well as undergraduate students who also help with special project, routine updates, and code development. 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) leading strategic planning for CIG's mission and goals and acting as the primary representative of CIG to the scientific community, (b) devising a fair and effective process for implementation of CIG's activities based on proposals or work plans such as those submitted to the Executive Committee by the Science Steering Committee, and overseeing CIG's activities, (c) 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, (d) ensuring that funds are properly allocated to various CIG activities, and (e) overseeing the preparation of technical reports.

CIG's team of computational and research science professionals maintains expertise in geodynamics, software development, computing, and numerical methods. They work closely with the Working Groups and sub awardees under direction of the Director and as guided by scientific objectives formulated by the geodynamics community. CIG's staff helps to maintain the infrastructure for the community including: the repository, build and test system, website, email, backend servers, HPC allocations, and related systems and services. The development and technical teams provide software services to the community in the form of programming, documentation, training, and support.

CIG Staff are:

- *Director,* Dr. Lorraine Hwang
- *Technical Lead,* Dr. Rene Gassmoeller (University of Florida)
- *Research Scientist*, Dr. Hiroaki Matsui
- *Postdoctoral Fellow*, Dr. Kali Allison
- *Postdoctoral Fellow*, Dr. Ryan Orvedahl

- *Postdoctoral Fellow*, Dr. Menno Fraters
- *Graduate Student*: Dylan Vassey
- *Junior Specialists*, Chris Mills
- *Laboratory Assistant*: Mack Gregory
- *Student Assistant(s*): Denise Kwong

2.6 The Planning Process

Concepts and ideas 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 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.

In practice, new CIG activities are developed iteratively; CIG typically works closely with community members, 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 are aligned with CIG's mission and goals.

CIG is engaged in several multi-year development projects, including state-of-the-art codes for mantle convection, lithospheric dynamics, dynamo, short-term crustal dynamics, seismic cycles, and seismology. The working groups may provide feedback to each project that are part of an overall work plans which may include software development plans, benchmarks, tutorials, and a schedule for working meetings appropriate to each project.

Computational Models for Seismic Cycles

The Seismic Cycles Working Group has initiated a multi-year effort towards developing open-source computational models to explore sequences of earthquakes and aseismic slip. This topic has overlapping interests with other community including SCEC SEAS and SZ4D Faulting and Earthquake Cycles. Membership on the working groups overlap and we anticipate coordinating with these communities in the future.

Planning efforts have been initiated with a special webinar series featuring the latest research on topics such as: physics-based foreshock and aftershock modeling, arrest and initiation of rupture: insight from structural and frictional heterogeneities, adding more physics into the friction law, implications about the seismic cycle; modeling of slow-slip and tremors, fluid injection and the seismic cycle, fluids and poroelasticity; and foreshocks, aftershocks, and roughness (see section 3.3 Knowledge Transfer and Capacity Building). The webinar series will be followed by a virtual workshop in Fall 2022 focusing on computational methods. The resulting white paper will lay out a multi-year strategic plan to guide development and advisory teams.

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.

The team continues to participate in early use of the latest petascale computing system, led by and deployed at, the Texas Advanced Computing Center (TACC). The award has been used to benchmark the performance of existing CIG software and further its scalability using new numerical methods in preparation for wider community use.[1]

See Section 4 for accomplishments using Frontera.

2.8 Communications

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

geodynamics.org

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

- Provide access and visibility to CIG software including most recent releases and documentation;
- Provide committees and working groups a centralized site for organization of community activities;
- Announce CIG events, including workshops and meetings and to support functions such as workshop registration and virtual posters;
- Disseminate and archive CIG documents including annual reports, strategic plans, by-laws, policies, manuals, tutorials etc.;
- Educate the community on software and computational methods;
- Highlight research being accomplished by scientists using CIG codes and collaborative projects;
- Provide easy access to citation and attribution information for software packages,
- Disseminate news of activities of interest and promote discussion, and
- Promote discussion through its forums.

This year, we completed the transition to a new website hosted by HUBzero® at SDSC.[2],[3] HUBzero® is a platform for creating dynamic web sites for scientific research and educational

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[1] Clevenger, T. C. and Heister, T., Comparison Between Algebraic and Matrix-free Geometric Multigrid for a Stokes Problem on Adaptive Meshes with Variable Viscosity, *Numerical Linear Algebra with Applications*, e2375, DOI:10.1002/nla.2375, 2020.

[2] Hubzero.org. HUBzero began as an NSF sponsored project.

[3] The old website can still be accessed at archive.geodynamics.org

activities. HUBzero® is the underlying platform that runs more than 60 science gateways both hosted and in open-source installations. The HUBzero® middleware interfaces with Globus, CondorHT, PBS, SGE, and other job management systems; so, in addition to SDSC local computing facilities, hubs can send demanding computational tasks off to XSEDE, Open Science Grid, DiaGrid, local clusters, and other national Grid resources such as BOINC.

The move to HUBzero® leverages development across scientific communities and provides access to web development experts positioning the community for future growth and to provide additional computational services.

Forum

All mailing lists have now been moved to the CIG forum. The forum allows easier searching and tagging of discussion threads as well as many modern features such that users can customize how they follow categories and issues, and trusted users can moderate their communities. Any member of the public may register to participate in the forum. Forum categories 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.

As of December 31, 2021, the forum has grown to 622 registered members, up from 525 at the end of 2020. Over half (55%/345) of members have contributed to discussions. New users and contributors have slowed since the forum's inception with the number of overall visits remaining dropping slightly reflective of a slow period of activity for the organization (Figure 1).

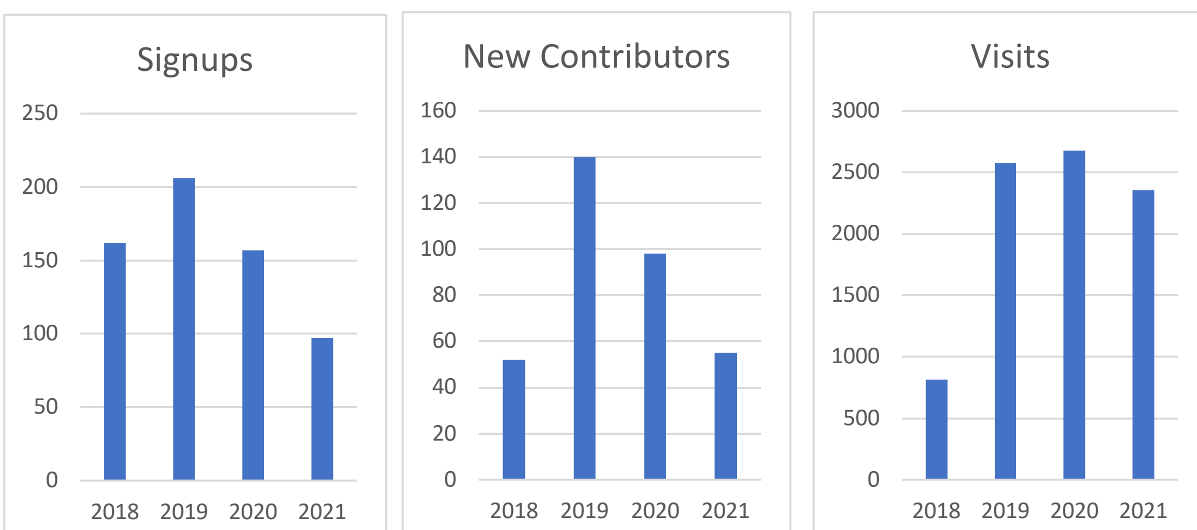

Figure 1. CIG Forum activity since inception (community.geodynamics.org). Shown by month are the (left) number of new users, (center) new contributors, and (right) visits to the forum.

The domain-specific categories for groups that have released codes are used frequently for community support. Any register user 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. Any registered user 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.

ASPECT and PyLith continue to be the most active subject matter categories (Figure 2). However, some of our communities prefer to use github for similar functions, e.g., SPECFEM and hence, forum traffic does not reflect the community's activities.

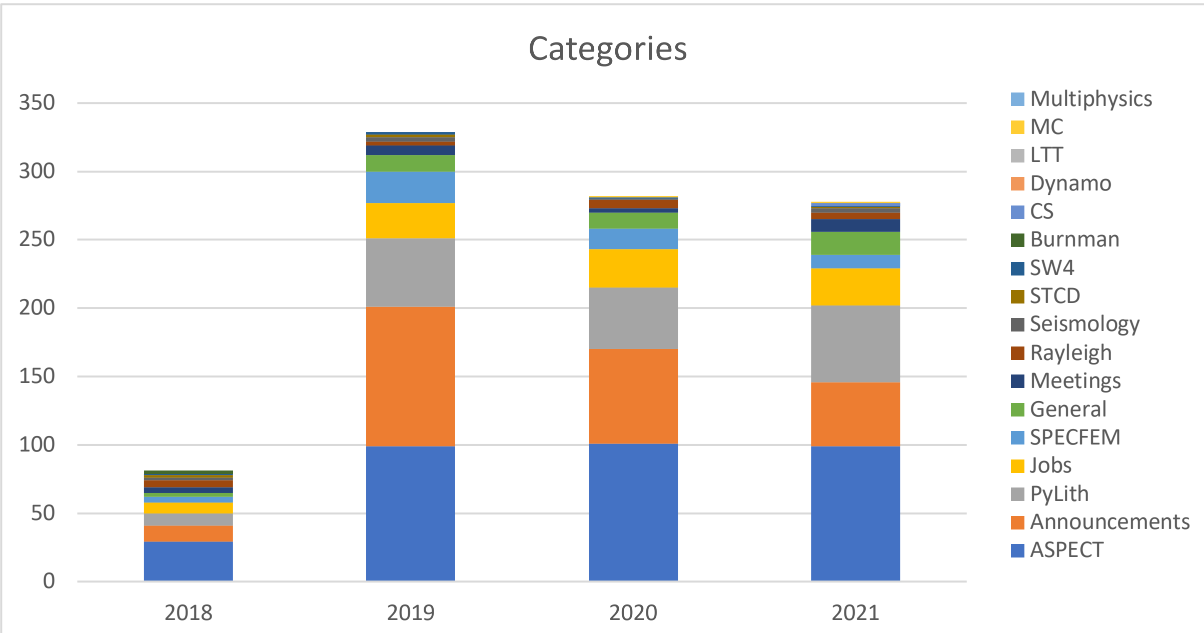

Figure 2. Number of messages posted to the forum by category. Legend is reversed ranked ordered with the users of the ASPECT forum posting the most messages.

Annual CIG Business Meeting

The CIG Annual Business meeting is open to the entire geodynamics community, including scientists from non-member institutions. 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 typically held in conjunction with the AGU Fall meeting in December, when many members of the community are gathered in one place. With continuing uncertainty due to COVID-19, the meeting was held virtually on November 18, 2021.

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 on the forum.

GitHub

CIG software is developed using GitHub (see github.com/geodynamics) to support version control, community contributions, and CIG best practices for scientific software development. The platform provides continuous transparency about software development directions and offers a mechanism for contributors to introduce new topics and possible development directions for discussion. CIG provides tutorials and guidance for its software projects to leverage the potential of GitHub as the de-facto standard of software development for open-source projects.

Webinars

Since 2012, CIG's webinars are described below and are used for more in-depth communication about software projects, research applications, best practices, and governance matters.

2.9 Metrics for Success

Activities to fulfill CIG's mission fall into three broad categories: software, people, and research impacts. We use a variety of metrics to monitor activity in each of these areas throughout this annual report. These metrics do not encompass the impacts and improvements in computational capabilities in geodynamics that result from CIG's activities. Those are covered in the later sections of this report.

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 the number of:

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

People

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

- governance participants,
- forum membership,
- workshop participants,
- webinar and online tutorial participants,
- YouTube views,
- education products developed,

- website traffic,
- users of CIG HPC allocations, and
- engagement with other communities.

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 and impact of:

- publications (abstracts, theses, papers) and readership,
- acknowledgements and citations of CIG codes in publications and reports,
- proposals by researchers that draw on or use CIG resources,
- partnerships with other organizations,
- diversity of funding sources,
- invited presentations, and
- special sessions of national meetings organized around CIG resources or codes.

3 Facility Status

CIG's primary focus is the creation, training, and distribution of open-source software via its website geodynamics.org. CIG is now regularly cited in the data management plan of scientists writing proposals to NSF, with PIs citing CIG's software donation policies. CIG's own data management plan focuses on:

- preservation, availability, and credit for 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 improve 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. All software is maintained with full version control and complete revision history in a Git open-source repository. Where deployed, Doxygen routinely updates documentation as extracted from the source files. The build and test framework uses GitHub actions and Azure pipelines Build status is reflected on each software page.

Facility statistics below cover the periods January 1 – December 31, 2021.

3.1 CIG Code Repository

CIG encourages members to donate codes that have scientific value for the geoscience 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 communities.

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:

https://geodynamics.org/software/software-contribute

CIG's support categories reflect code development activity and from where primary support is received:

Developed	Actively adding features to support improved science or performance by CIG (D_CIG) or by community contributors (D_CONTRIB).
Supported	Actively supported, maintained, and upgraded by CIG (S_CIG) or by community contributors (S_CONTRIB).
Archived	No development activity; not supported. No commitment to updates. (A)

Developed Codes have been validated, passed benchmarks established by the appropriate community, and are leading edge codes in geodynamics. Developed codes may either be donated or developed by CIG or other communities. These codes are under active development with a software development plan and are actively supported by CIG or the community through maintenance, technical assistance, training, and documentation.

Supported Codes are mature codes that meet community standards but are no longer undergoing active development. Codes have been benchmarked and documented with examples and references such that they remain useful research tools. Supported codes include codes donated to CIG from members of our community. Minor changes such as bug fixes and binary upgrades are supported.

Archived Codes are included in the CIG GitHub code repository. This allows bug reports to be submitted and accessible to the community although little or no resources are applied for further development, maintenance, or support.

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 lists current repository holdings including software version, total lines of code, % change in number of lines of code from the previous year, number of commits in the repository, number of lifetime developers, and current level of support.

Table 1. Repository Statistics

	Version	Lines of Code	% Chang	Commit s	# Develope	Support Level
Short-Term Crustal Dynamics						
Pylith	3.0.1[*]	443,198	-	-	9	D_CIG
Relax	1.0.7	1,419,923	0%	7	10	D_CONTRIB
VirtualQuake	3.1.1	49,222	-	-	17	D_CONTRIB
SELEN	2.9.13	17,346	-20%	11	5	S_CONTRIB
LithoMop	0.7.2	495,786	-	-	5	A
Long-Term						
Gale	1.6.1/2.0	6,680,841	-	-	62	A
Plasti	1.0.0	10,967	-	-	1	A
SNAC	1.2.0	549,498	-	-	3	A
Mantle Convection						
ASPECT[+]	2.4.0[*]	2,353,815	10%	1080	95	D_CIG
CitcomCU	1.03	70,288	-	-	5	D_CONTRIB
CitcomS	3.3.1	239,696	-	-	21	D_CONTRIB
ConMan	3.0.0	577,882	0%	2	12	S_CONTRIB
Ellipsis3d	1.0.2	51,602	-	-	2	A
HC	1.0.1	491,827	0%	5	7	A
Seismology						
AxiSEM	1.3	109,361	-1%	16	13	D_CONTRIB
Burnman	1.0.1[*]	113,146	14%	275	19	D_CONTRIB
Mineos	1.0.2	331,364	-	-	7	A
Flexwin	1.0.1	95,412	-	-	8	A
Seismic CPML		37,820	-	-	6	S_CONTRIB
Specfem3D		11,215,254	1%	144	58	D_CIG
Specfem3D Globe	7.0.0	2,141,321	-	-	54	D_CIG
Specfem3D Geotech	1.1	2,038,521	-	-	4	D_CONTRIB
Specfem2D		1,871,169	-	-	33	D_CONTRIB
Specfem1D		5,371	-	-	10	S_CONTRIB
SW4	2.01	267,625	-	-	19	D_CONTRIB

Dynamo						
Rayleigh	1.1.0*	79,936	10%	299	28	D_CIG
Calypso	1.2.0	215,012	-	-	-	D_CIG
MAG	1.0.2	134,906	-	-	5	A
Computational Science						
Cigma	1.0.0	356,371	-	-	7	A
Exchanger	1.0.1	5,654	-	-	7	A
Nemesis	1.1.1	788	0%	2	2	S_CONTRIB
Pythia	0.8.1.20	43,705	21%	108	4	S_CONTRIB

*new release
+also being used for long-term tectonics

Statistics are as reported by gitstats[4] which does not discriminate between line types e.g., comments versus code. CIG codes span 6 scientific domains and most use multiple programming languages. The majority of the executable code in the library use shell and scripting languages, C, C++, and Fortran77/90, or Python. Codes that have substantial active development, e.g., addition of new features (net increase) or code re-writing and cleanup (net decrease) are predominantly those that are actively supported by CIG staff (including postdocs), subawardees, or are cooperative efforts with other agencies and research groups.

The CIG Git repositories logged 1947 software commits during 2021. Over the repository lifetime, nearly 545 developers have contributed to code development.

In 2022 CIG held its second Software Developers meeting to discuss current community development practices and common areas of infrastructure improvement (see 3.4). CIG continues to participate in the larger scientific community in working towards establishing FAIR principles for research software, best practices for software repositories, and best practices for credit for software including software citation.

3.2 High Performance Computing

CIG continues to provide opportunities to train scientists on HPC by maintaining allocations of HPC resources on XSEDE community machines. In 2021, CIG has been awarded:

- 50,000 SUs; 2,048 GB (Ranch) on Stampede2
- 1,377,206 Core-hours; 2,048 GB on Expanse
- 15,000 GPU Hours; 2,048 GB (Ocean) on PSC Bridges

Allocation expires September 30, 2022.

[4] https://github.com/hoxu/gitstats (version 55c5c28, 2.25.1)

In 2021, CIG successfully applied for a Frontera Pathways allocation of 182,400 node hours. The allocation is being used by the ASPECT community to improve solvers and parallel I/O as well as to test and optimize features needed for large-scale runs. Development in Calypso continues to improve the parallelization between the simulation and parallel volume rendering module which allows real time visualization. Allocation expires September 20, 2022.

3.3 Knowledge Transfer and Capacity Building

CIG builds and sustains its community through both virtual and in-person events. The Director, Staff, 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, and webinars.

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. Special workshops for community planning reach across government agencies including national labs, other NSF branches, and the U.S. Geological Survey. CIG-sponsored workshops are typically held biannually for each domain. Joint workshops and tutorial sessions 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, Cooperative Institute for Dynamic Earth Research (CIDER), Canadian Geophysical Union (CGU), Earth-Life Science Institute (ELSI), Quantitative Estimation of Earth's Seismic Sources and Structure (QUEST), and Ada Lovelace Workshops (EGU). CIG partners with these and other organizations to expand its impact on the geodynamics community.

Table 2. August 2021 - July 2022 Workshops and Tutorials

Date	Title	Participants
January 19-20, 2022	ASPECT User Workshop	51
February 28, 2022 **March 1, 2022**	CIG Developers Workshop	46
May 15-24, 2022	ASPECT Hackathon	12(5)
June 30, 2022	Crustal Deformation Modeling Workshop	68

Upcoming workshops and training are posted online and advertised through CIG email lists and forum and those of our partner organizations. Due to the global pandemic, we continued to hold early 2022 workshops virtually (Table 2). We returned in person workshops in May 2022 implementing COVID policies that included mandatory vaccinations and onsite testing. Due to the increase in COVID activity in the region, the 2022 Crustal Deformation Modeling also required mask wearing. Food was limited and no eating was allowed in the workshop room. We plan to offer a mix of both in person and virtual workshops in the future.

All events build upon CIG's experience using technology to collaborate with our communities worldwide - PyLith has been offering virtual tutorials since 2015 and our very first entirely virtual workshop was held by the ASPECT community in January 2020 followed by the first virtual hack. By offering our workshops virtually, we have been able to further our reach to new communities including meeting the international demand from emerging economies for access to training on state-of-the-art modeling software.

Workshop details can be found on our website: https://geodynamics.org/events

2022 ASPECT User Workshop

The third virtual ASPECT User Workshop took place January 19-20, 2022. 52 people attended the 2-day event (Fig. 3). In keeping with best practices for inclusivity, participants were lead through the process of renaming their git branch from *master* to *main*. The community contributed keynote talks on new ASPECT features, numerical methods, and current research on rifting, melt generation, topography, and slab sinking rates. The meeting included discussion time as well as opportunities for users to obtain technical help and help with model set-up from others in the community.

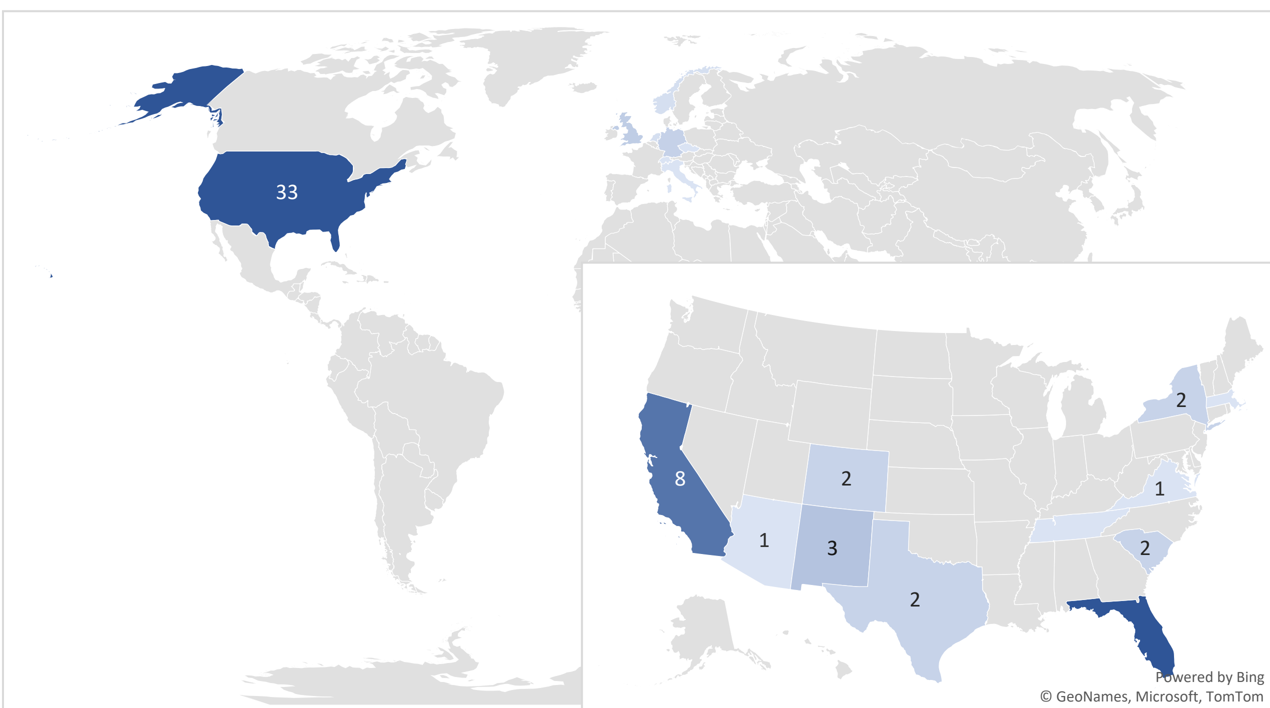

Figure 3. A total of 82 participants from 8 countries attended the event. Approximately 44% identified as female and 44% were early career researchers (graduate students and postdoctoral fellows).

2022 CIG Developers Workshop

The CIG held its second Developers Workshop February 28, and March 1 Developers Workshop February 28 and March 1, 2022. The workshop followed the same general themes as in 2021:

- Expanding the CIG software developer community;
- Making CIG software more accessible to new users;
- Identifying and leveraging common infrastructure; and
- Leveraging collective wisdom to make CIG software better and easier to develop and maintain.

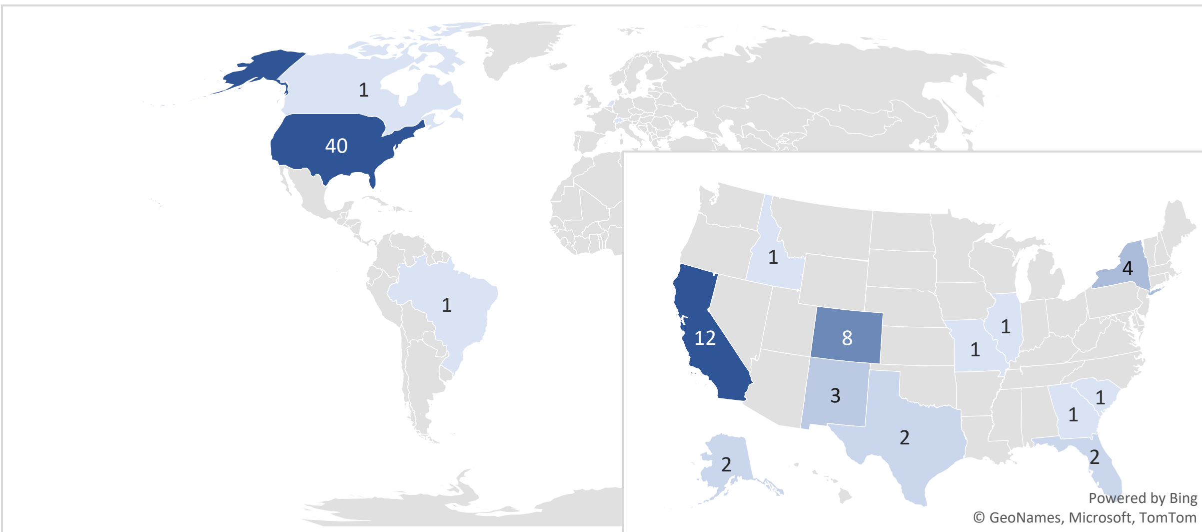

Figure 4. A total of 46 participants from 7 countries attended the event. Approximately 17% (8) identified as female and 28% (13) were early career researchers (graduate students and postdoctoral fellows).

The 46 workshop participants (Fig. 4) represented developers of CIG community codes, those interested in contributing to the community codes, and researchers interested in improving their own codes. The workshop was held online and consisted of six discussion sessions with short presentations introducing each set of topics.

The workshop focused on the following specific topics and recommendations:

- Alignment of CIG Best Practices with Journal of Open Source Software (JOSS) review criteria as a pathway to publishing a peer-reviewed paper associated with open source software;
- Updates to CIG Best Practices for documentation and testing to encourage more dynamic and interactive html documentation and the use of continuous integration testing tools such as GitHub Actions and Azure Pipelines;
- Using libraries to leverage accelerator architectures, Kokkos as an example;

- Building containers for high-performance computing systems, e.g., Shifter, Singularity, Charliecloud, and Sarus, is not easy and is still undergoing significant development;
- Using the hIPPYlib library for Bayesian inference; and
- Introduction to SCOPED (Seismic COmputational Platform for Empowering Discovery) project for Improving accessibility and portability of seismic inversion software.

Workshop Report [pdf].

2022 ASPECT Hackathon

The 2021 ASPECT Hackathon was held from May 15-24, 2022 in Cody, Wyoming. A total of 17 participants joined this hybrid event (Fig. 5). Virtual participants (5) participated via Zoom, and Slack to participate in this 8-day coding event. This year's event focused on the development of foundational features and the core of ASPECT and less on supporting individual models and simulations as in the past. Consequently, we welcomed a smaller number of new participants (3). A major focus of the workshop was the conversion of the current manual to display via readthedocs.io (see https://aspect-documentation.readthedocs.io/en/latest/), making progress on outstanding projects, and adding cookbooks.

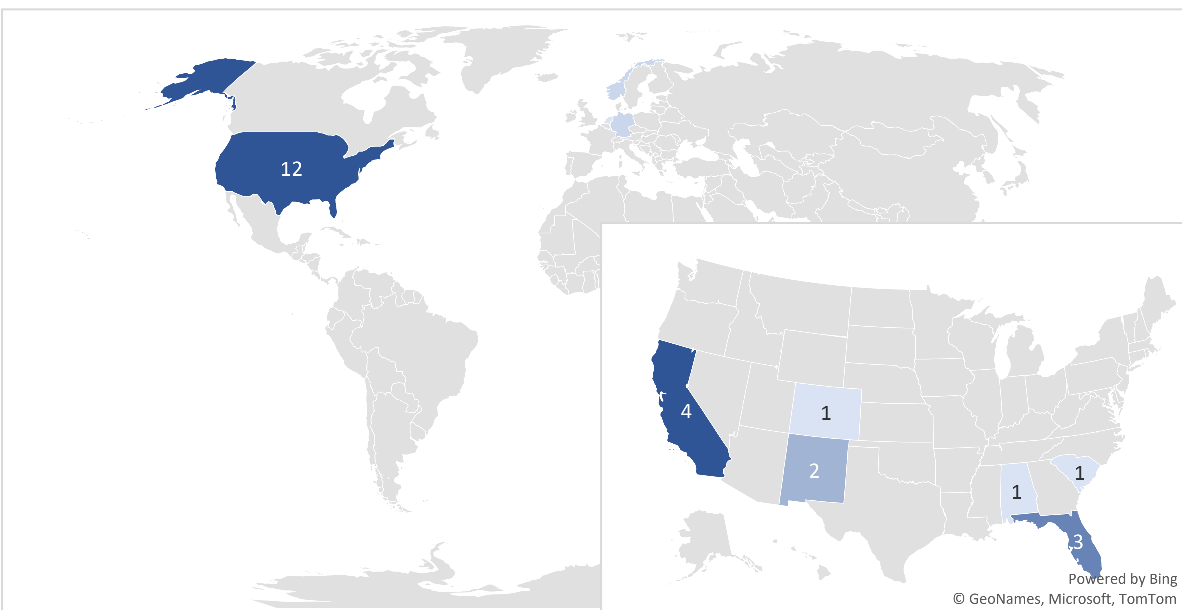

Figure 5. A total of 16 participants contributed towards the development of ASPECT during the hackathon with 44% (7) identifying as female.

The 2022 hackathon was more productive than the one in the previous year – a welcome quantitative confirmation of our long-held belief that holding hackathons in person is preferable to virtual versions. Compared to the nine hackathons we have held over the years, this hackathon ranks in the top half in terms of productivity. As in previous years, somewhere around one quarter to one third of the ASPECT development happens during hackathon weeks.

Workshop Report [pdf]

2022 Crustal Deformation Modeling Workshop

The 2022 Crustal Deformation Modeling Workshop was held from June 20-24, 2022 in Golden, Colorado. The workshop was co-sponsored with SCEC who provided travel support for some participants. While we accepted 70 participants, a total of 63 participants attended due to COVID and COVID relate impacts. As in previous years, the majority of participants were early career (Fig. 6).

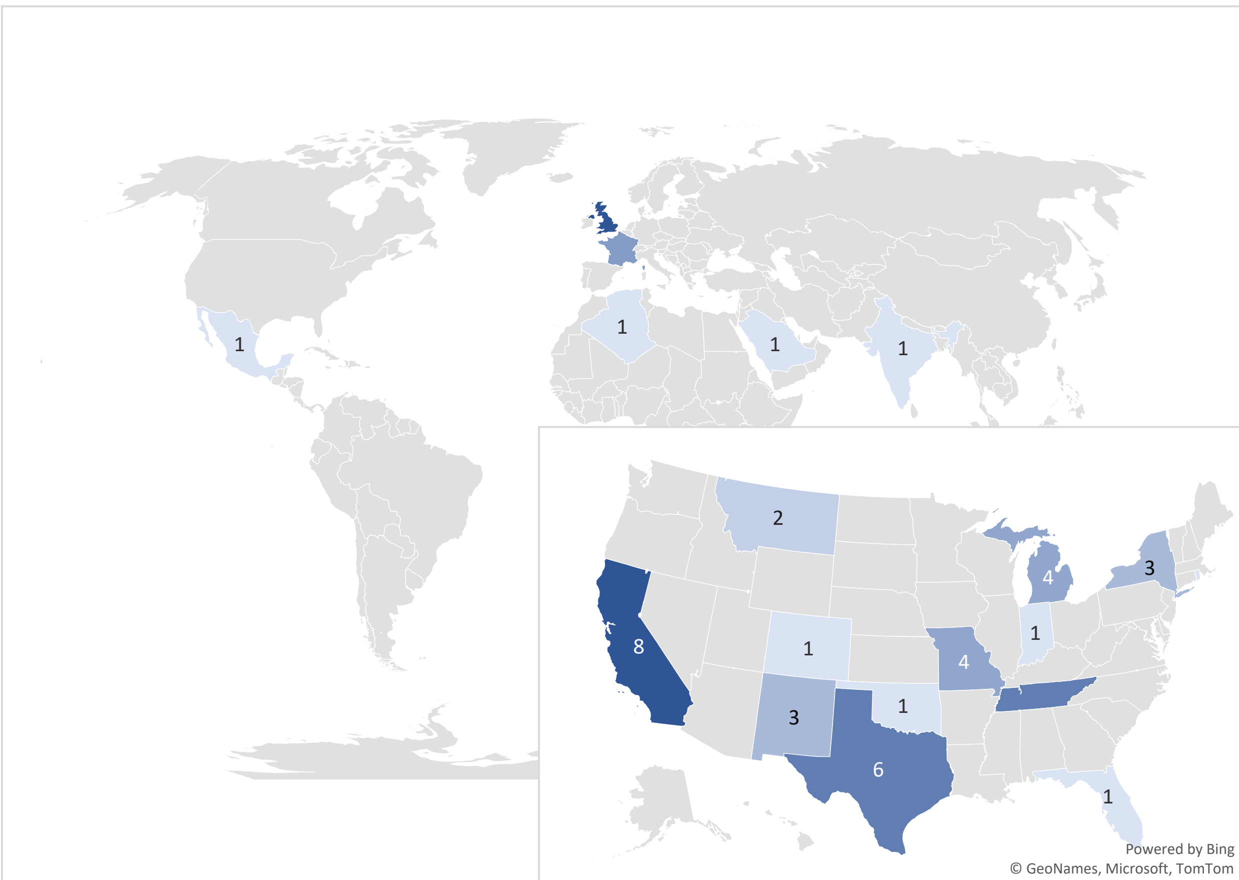

Figure 6. A total of 63 participants from 8 countries attended the event. Approximately 32% (20) identified as Woman, 75% (47) as early career researchers (graduate students and postdoctoral fellows); 41% (26) identified as White; 40% (25)) as Asia or Asian Indian, 10% (6) Hispanic, Latino, or Spanish; 3% (2) Middle Eastern or North African, and 3% (2) Prefer not to respond.

The workshop featured PyLith tutorials, posters, and presentations. Tutorials showcases new features in v3.0.0 and introduced a new set of online resources. Invited speakers presented on seismic cycles; inverting for fault slip; faulting, fluids, and surface loading; and crustal mechanics on planetary bodies.

Workshop Report [pdf]

Future Workshops

CIG plans to organize the following community workshops in the remainder of 2022 (Table 3). Events through January will complete activity for this award.

Table 3. 2022-2023 Workshops and Tutorials

Date	Title
September 12-16, 2022	Rayleigh Hackathon
October 26-28, 2022	SPECFEM Developer's Workshop
Fall	Seismic Cycles Workshop
January 2023	ASPECT User Workshop
February 2023	CIG Developers Workshop
Spring	ASPECT Hackathon
Summer	PyLith Hackathon

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. The one-hour webinars are recorded for later viewing on the CIG YouTube channel and linked to CIG website (Table 4).

In addition, as part of the planning process, the Seismic Cycles Working Group organized a webinar series (Table 5). The webinars explored a wide range of physics and phenomena associated with seismic cycles and to deliver to the community the latest research.

Table 4. 2021- 2022 Webinar Schedule

Date	Presenters	Title
October 14	Elena Ehrlich Keneni Godana Dante Hickey Hiva Mohammazadeh	SMOREs Showcase
January 13	Raj Moulik, Princeton University	Introduction to reference Earth models and datasets using AVNI
February 17	Takumi Kera, Tohoku University	Energy transfer among flow and magnetic fields with different equatorial symmetry during the dipole reversal in a geodynamo simulation
March 10	Ryan Orvedahl, UC Davis	Dynamo Simulations of Planetary Cores
April 14	Kali Allison, UC Davis	Interaction Between Earthquakes and Interseismic Deformation
May 12	Robert Walker, University of Buffalo	Poroelastic Implementation in PyLith

Table 5. 2022 Seismic Cycles Webinar Schedule

Date	Title & Presenters
May 6	**Physics-based foreshock and aftershock modeling** 1. Mainshock and aftershock sequence simulations in a nonplanar fault network So Ozawa, *University of Tokyo* 2. Rupture styles and recurrence patterns in seismic cycles linked to physical properties of the fault zone Shiying Nie, *University of Southern California*
May 13	**Arrest and initiation of rupture: insight from structural and frictional heterogeneities** 1. Many ways to slip: aseismic fault creep and its transition to dynamic rupture Sohom Ray, *IIT Roorkee* 2. Theoretical insights on the arrest of earthquake rupture Pablo Ampuero, *University of Géoazur*
May 20	**Adding more physics into the friction law, what are the implications about the seismic cycle?** 1. Implementation of quasistatic viscoelasticity and poroelasticity using memory variables into dynamic earthquake sequence

	simulation with SBIEM Hiroyuki Noda, *Kyoto University* 2. Fault-size dependent fracture energy, seismogenesis, and cascading rupture on multi-scale fault networks Dmitry Garagash, *Dalhousie University*
June 3	**Modeling of slow-slip and tremors.** 1. Cycles of slow slip events on non-planar subduction faults and their implications on megathrust earthquakes Duo Li, *Ludwig-Maximilians-Universität München* 2. Modeling spontaneous and triggered slow-slip events at the Hikurangi subduction plate interface Bunishiro Shibazaki, *Building Research Institute* 3. Numerical modeling of deep long- and short-term SSEs in the Nankai and Hyuganada region Takanori Matsuzawa, *National Research Institute for Earth Science and Disaster Resilience*
June 17	**Fluids and heterogeneities** 1. Earthquake cycle simulations with creep compaction and dilatancy. Yuyun Yang, *Harbin Engineering University* 2. Seismic cycles and earthquake statistics on heterogeneous faults. Camilla Cattania, *Massachusetts Institute of Technology*
July 1	**Foreshocks, aftershocks, and roughness** Yuval Tal, *Ben-Gurion University of the Negev* 2. Modeling shallow slow slip events along the Hikurangi margin: Insights into their segmentation and the effect of pore-pressure cycling Andrea Perez-Silva, *Victoria University of Wellington*
July 8	**Fluid injection and the seismic cycle?** 1. A spectral boundary-integral method for faults and fractures in a poroelastic solid: Simulations of a rate-and-state fault with dilatancy, compaction, and fluid injection. Elias R. Heimisson, *ETH Zürich* 2. Fluids in earthquake cycle models. Pierre Dublanchet, *MINES ParisTech*

YouTube

CIG's YouTube channel, CIG Geodynamics, hosts 291 videos of simulations contributed by the community, and recordings of past webinars and tutorials. The channel links to playlists of other community members (such as recorded lectures). Viewers can also access webinar videos through geodynamics.org. Visitors are directed to the site mainly as a referral through YouTube, or google searches. Visitors come from an international community with the top viewers from North America, Europe, India, Asia, and South America. The page has 1070 subscribers (up from

701 in 2020) and over 88.2k lifetime views (since 2008). The most popular videos are CIG webinars and tutorials.

AGU Presence

This year we searched the abstracts for software mentions and solicited community members for relevant abstracts. The number of abstracts recovered from last year to a total of 75 (Figure 7).

See Appendix C.

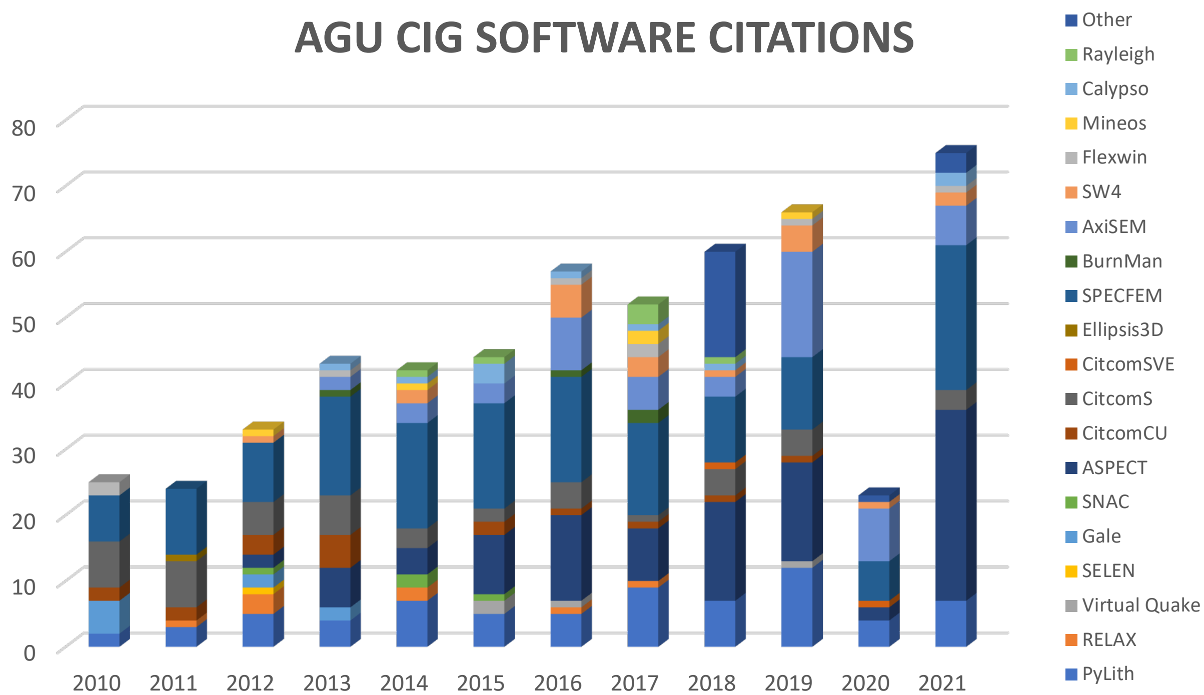

Figure 7. Number of CIG software mentions in an AGU abstract.

Distinguished Speaker Series

The CIG Distinguished Speaker Series continues into its 4th year. The CIG Speakers Series seeks to promote computational modeling in geodynamics and related earth science disciplines. Speakers are drawn from a diverse pool of experts with exceptional capability to communicate the power of computation for understanding the dynamic forces that shape the surface and operate in the interior of our planet. Lectures are aimed at a broad scientific audience suitable for departmental or university colloquia series, and similar venues. Institutions with strong math and computational science departments or with diverse populations that are underrepresented in STEM are encouraged to apply.

The two 2020-2021 CIG Distinguished Speakers completed 5 visits (Table 6) to R1 & R2 institutions as well as HSI or MSIs. The program received positive feedback from both Host

Institutions and Speakers. Speakers had opportunities to interact with both students and faculty in formal and informal settings taking advantage of the opportunity to deliver guest lectures and exchange research ideas and perspectives on career paths in geosciences.

Table 6. CIG Distinguished Speakers and Host Institutions

2021-2022	
Climate, Tectonics, and Planetary Life Adrian Lenardic, Rice University	September 30: University of Idaho *joint with* Washington State University U. Washington Universidad Nacional de Columbia *virtual*
The Structure of Oceanic Plates using Machine Learning on Seafloor Vibrations Tolulope Olugboji, University of Rochester	November 10: Florida International October 22: McGill University *joint with* University of Quebec at Montreal *virtual*

The two 2022-2023 CIG Distinguished Speakers are:

- Juliane Dannberg, University of Florida
- Mathieu Morlighem, Dartmouth College

4 Software Development

4.1 ASPECT

ASPECT is a finite element code to model problems in thermo-chemical convection in both 2D and 3D models and supports large-scale parallel computations. Its primary focus is the simulation of processes in the Earth's mantle, and it is being extended to studies of lithospheric deformation and magma/mantle dynamics.

ASPECT is being developed by a large, collaborative, and inclusive community. Ten (10) Principal Developers maintain the openly accessible repository on GitHub and provide feedback to 31 user-developers who have made 1005 commits to the repository in 2021 as well as to the broader user community. Many of these commits have added major new features to the code and will be incorporated into the next release of the software in July 2022, ASPECT 2.4.0.

Significant accomplishments of the past year

ASPECT 2.4.0 was released on July 23, 2022. It will include many changes (see https://aspect.geodynamics.org/doc/doxygen/changes_current.html for details) including:

- New: The mesh displacements for free surface problems are computed by the GMG solver when the GMG Stokes solver is used.
- Changed: The global limiter for the least squares particle interpolation plugin was replaced by a bounds preserving slope limiter that respects local bounds on each cell.
- New support for Newton Stokes in the GMG solver

- New: GMG solver with support for mesh deformation / free-surface boundaries
- Fixes to particle generators
- New: The "Compositional fields" subsection in ASPECT has a new parameter called "Types of fields" that is used to specify the types of all the "compositional" fields.
- New cookbooks and benchmarks
- Improved: Particle operations have been optimized for speed.
- New: ASPECT now has a ThermodynamicTableLookup equation of state plugin. This plugin allows material models to read in one or more Perple_X or HeFESTo table files, interpolate material properties at desired pressures and temperatures, and use the interpolated properties as material model outputs.
- ASPECT collects and outputs physical units for all fields that are written into VTU files.

In addition, ASPECT has seen many performance improvements, new benchmarks, tests, fixes, and smaller features.

Particles

A new high-order particle interpolation algorithm and limiters for the two high-order accurate particle interpolations have been implemented. The new limiters have led to the high order accurate Quadratic Least Squares (QLS) particle interpolation algorithm becoming the preferred method of particle interpolation in ASPECT, since with this algorithm, a researcher can now track particle properties with high accuracy while maintaining a constant number of particles per cell as the grid is refined, and eliminates the problem of overshooting and undershooting. The limiting algorithm works well on the falling droplet problem shown in Fig. 8 keeping the indicator property within its [0, 1] range, while the particle interpolation without limiting results in values outside this range.

Frontera

Access to Frontera enabled the development of necessary features in the finite element library deal.II that is used by ASPECT and major new developments in ASPECT itself to support fast, scalable computations and more recently scalable IO for checkpointing and graphical output. Previous development work has focused on implementing the matrix-free multigrid solver in ASPECT. Applying it to a Stokes problem with large viscosity contrasts is non-trivial but they were able to show great results on Frontera scaling to 100k MPI ranks and up to 200 billion degrees of freedom (100x larger than possible before). The new solver is 3x faster and uses 10x less memory, which allowed us to increase the total problem size dramatically.[1,5]

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[5] Clevenger, T.C, A Parallel Geometric Multigrid Method for Adaptive Finite Elements PhD thesis, Clemson University, 2019. https://tigerprints.clemson.edu/all_dissertations/2523/

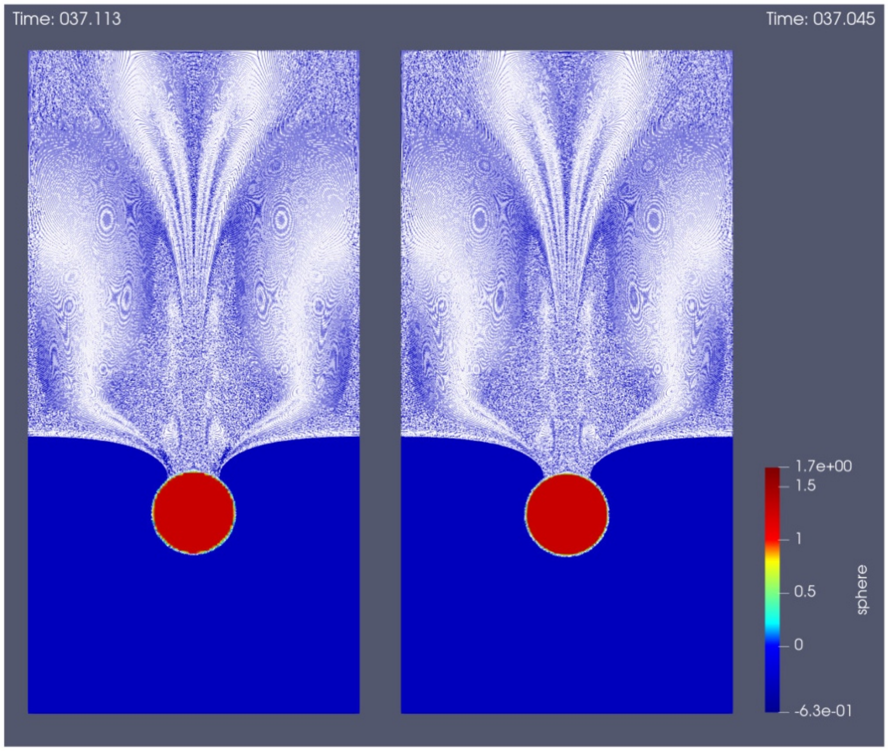


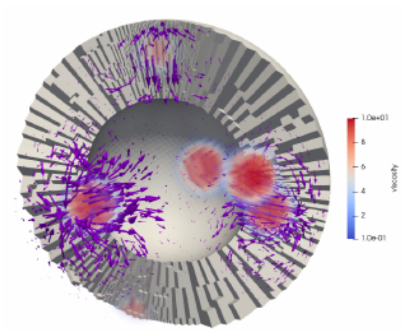
Figure 8. The indicator function sphere_l(**x**) for the droplet on the left is limited and therefore remains in the interval [0, 1], while the indicator function sphere_r(**x**) on the right is not limited which results in large overshoots and undershoots that exceed the range [0, 1] as can be seen in the colorbar.

In the past year, the team refined and improved the linear solver to dramatically speed up and scale up parallel input and output for input data sets, graphical output, and checkpointing. The team:

- Developed a new geometric multigrid strategy using global coarsening for better workload distribution for highly adaptively refined meshes.[6] Medium-sized runs on Frontera are now showing 2-3x better performance (Fig. 9).
- Made the matrix-free solver in ASPECT applicable to many more complicated problems including models with free surface deformation, support for highly nonlinear problems using the Newton solver, and more flexibility regarding boundary conditions.
- Improved IO came more for larger computations. With the help of Frontera staff, ASPECT now supports very large checkpointing and graphical output files by reimplementing MPI I/O support. Early performance tests show an improvement of

[6] Munch, P., Heister, T., Saavedra, L.P., Kronbichler, M. Efficient distributed matrix-free multigrid methods on locally refined meshes for FEM computations. submitted, 2022. https://arxiv.org/abs/2203.12292

about 10x to the old implementations. This required working around Intel MPI large IO bugs and implementing a new low-level MPI IO layer in deal.II.[7,8]



L	#DoFs [1e6]	global coarsening #it	global coarsening solve [s]	global coarsening V-cycle [s]	local smoothing #it	local smoothing solve [s]	local smoothing V-cycle [s]
5	10.0	25	1.38	0.003	25	1.15	0.006
6	20.7	25	1.61	0.006	25	1.84	0.008
7	43.2	25	2.26	0.009	26	2.63	0.013
8	88.0	22	2.39	0.013	27	4.15	0.022
9	178.0	25	4.62	0.020	28	7.87	0.047
10	355.0	26	6.47	0.039	28	13.66	0.109
11	715.7	27	10.65	0.069	27	23.67	0.214
12	1441.4	28	22.17	0.141	29	50.85	0.436
13	2896.7	28	37.38	0.266	26	99.07	0.971
14	5861.9	29	77.94	0.515	26	193.19	2.060

Figure 9. Stokes flow in a spherical shell using global coarsening GMG in ASPECT showing a 2-3x improvement over the old solver ("local smoothing").[7]

These new improvements were utilized in setting up a series of global 3D instantaneous models of mantle convection with a goal of finding a model that could generate the present-day surface velocities. This range of resolutions investigated results in models with approximately one billion degrees of freedom, and a typical output size of 18 GB. In investigating the importance of different model components, 62 models were run. The best-fit model has a directional fit of 92% and can explain 85% of the average speed relative to the observed GPS velocities (Fig. 10).

Other Work

Other work performed as part of this award that is not part of the ASPECT release mentioned above:

- Continued work on porting new features to the geometric multigrid solver (now supporting Newton derivatives, elasticity, and free surface mesh deformation)
- Support for large, parallel IO in deal.II to support writing very large graphical output and checkpoint files and reading large checkpoint files and ASCII structured data files. The performance of graphical output has been substantially improved (10x on Frontera).
- deal.II has gained the ability to share large data tables between MPI processes located on the same node, reducing the duplication of such data tables (see also above).

[7] Heister, T., Ingimarson, S., Pengfei Jia, Jiaqi Zhang, Case study: performant, large, unstructured, parallel IO. In preparation. 2022

[8] Arndt, D., Bangerth W., Feder, M., Fehling, M., Heister, T., Heltai, L., Kronbichler, M., Maier, M., Munch, P., Pelteret, J.-P., Sticko, S., Turcksin B., and Wells, D., The deal.II Library, Version 9.4, 2022. To be submitted.

- We have worked on deal.II 9.4.0 (to be released in June) with a very large number of improvements that will affect ASPECT, in particular to the performance of particle schemes.
- As part of CIG's strategy to provide software container images, we have integrated ASPECT's docker image build process into its continuous integration pipeline to automatically build updated container images and provide them to the community.

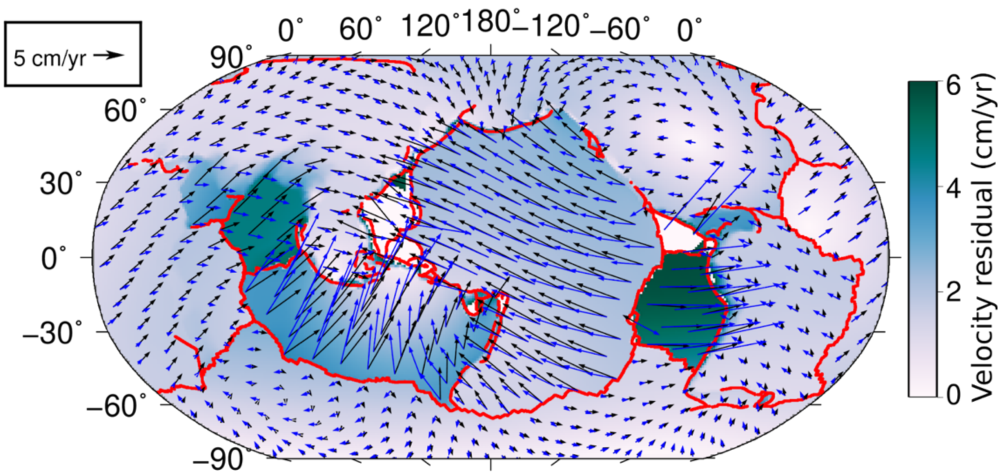


Figure 10. Velocity residual together with the modeled velocity at the surface (blue arrows) and the observed GPS velocities (black arrows) for the best-fit model.[9]

Project goals for the upcoming year

The developers have the following goals for ASPECT's development in the next year:

- Lead hackathons, community meetings, and user meetings
- Improve visualization features in ASPECT especially for large-scale simulations.
- Improve the applicability of the geometric multigrid solver to other models, for example with periodic boundary conditions.
- Provide a basic interface for bulk-surface coupling that allows for solving equations on the surface of the earth.
- Continue improvements on the visco-elastic-plastic (VEP) rheology, including integration and testing with compressible equations of state.
- Extend the documentation of new features that have been added.

[9] Saxena, A., Dannberg, J., and Gassmoeller, Developing global mantle flow models to investigate effects of plate-driving forces on observed surface deformation, European Geophysical Union, 2022

Outreach and Broader Impacts

The community has been active in community building through the following support and outreach activities:

- Organizing the Virtual User Meeting in January 2023.
- Hosting the 2023 ASPECT hackathon in May 2023.
- Holding bi-weekly online community meetings.

4.2 Calypso

Calypso is a three-dimensional magnetohydrodynamics (MHD) model to solve geodynamo problems. It uses a pseudo-spectral method and a finite difference method in the horizontal and radial discretization, respectively. Calypso is parallelized through both MPI and OpenMP. In MPI parallelization, the directions of domain decomposition are changed in the spherical harmonics transform. A parallel volume rendering module has been included in Calypso to enable visualization during the simulation runtime.

Significant accomplishments of the past year

Frontera

The 3-D Line Integral Convolution (LIC) module for visualization of vector fields such as the velocity or magnetic field was implemented in 2021 (Fig. 11).

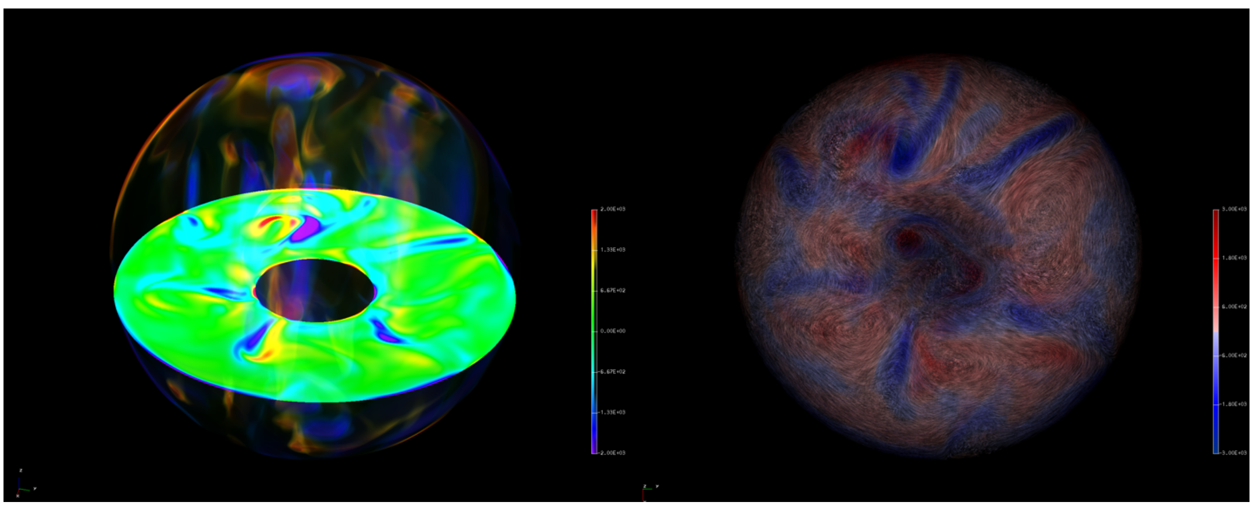


Figure 11. Visualization results by the volume rendering module (left) and by LIC module (right). In the left panel, the z-component of the vorticity $\boldsymbol{\omega}z$ is displayed by the volume rendering and section at z = -0.3. In the right panel, the flow pattern in the southern hemisphere is displayed by LIC colored by the $\boldsymbol{\omega}_z$

Both the simulation and visualizations including the LIC module keeps good scaling up to 28,672 cores. Through optimization of the loop orders in the simulation modules, simulation time decreases approximately 0.7 times as compared to the modules in Ver.1.2. The present optimization of the simulation module will be included in the next release of Calypso Ver. 2.0.

Also investigated was the performance of OpenMP parallelization. In these tests the spatial resolution and total number of nodes, while changing the relative number of OpenMP threads and MPI processes is fixed. The performance for simulation decreases with increasing the number of threads, while the LIC module almost keeps its performance by increasing the number of threads. On the other hand, the performance volume rendering module increases rapidly with increasing the number of threads (i.e., decreasing the number of MPI processes).

Project goals for the upcoming year

The next release, v2.0, is currently in testing. This version will have a large number of updates to use modern Fortran 90 and 2003 features. In v2.0, MPI-IO and data compression modules using zlib are introduced. This significantly reduces the number of data files and hence, data size. The modules developed by Takumi Kera modules to decompose symmetric and anti-symmetric components of fields and forces will also be included. After release of v2.0, the parallel volume rendering (PVR) module will be migrated along with an independent data viewer program for cross section and isosurface data rendering.

To model the effects of turbulence on the large-scale convection and magnetic field generation of the Earth's core, a sub-grid scale model (SGS) model will be developed and investigated. In previous studies, only the characteristics of the SGS terms from resolved, direct simulations were studied. To establish the validity of this approach, it is necessary to perform both large- and small-scale simulations for reference. In addition, fully resolved simulations will be run using nonlinear terms obtained by filtered large-scale fields to investigate which turbulence process is the most important for generating and sustaining the geodynamo.

Outreach and Broader Impacts

Calypso has 8 active users in 4 universities. Several projects are starting:

- Geodynamo modeling for the past Earth. The early Earth had a smaller solid inner core than present.
- Investigation of energy transfer between kinetic and magnetic energies during the geomagnetic dipole reversal.
- Comparison of evolution of the dipole component between dynamo simulation and observed geomagnetic field using stochastic models.
- Effects of aspherical growth of the inner core due to the thermal heterogeneity at the inner core boundary driven by the convection of the outer core.[10]

4.3 PyLith

PyLith is portable, scalable software for simulation of crustal deformation across spatial scales ranging from meters to hundreds of kilometers and temporal scales ranging from milliseconds to thousands of years. Its primary applications are quasi-static and dynamic modeling of

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[10] Matsui, H., Effects of the latent heat at the inner core boundary on the thermal structure at ICB in numerical dynamo simulations, American Geophysical Union Fall Meeting, New Orleans, LA, Dec., 2021.

earthquake faulting. Other applications include modeling crustal deformation from dike intrusions and inflation/deflation of volcano magma chambers.

Significant accomplishments of the past year

We released PyLith v3.0.0 in June 2022 followed by two bugfix releases. This major release includes changes to the underlying finite-element formulation to support a more flexible specification of the governing equations and higher order basis functions. It includes implementations for (1) elasticity for linear isotropic materials and linear Maxwell, generalized Maxwell, and power law viscoelastic models; (2) incompressible elasticity for linear isotropic materials, and (3) poroelasticity for linear isotropic materials. Other new features include support for importing finite-element meshes from Gmsh in addition to Cubit, LaGriT, and simple ASCII files, a modular approach to initial conditions, conversion to Python 3, default solver options based on the governing equations and formulations selected, an updated suite of examples, conversion of the manual from LaTeX to Sphinx and Markedly Structured Text (the documentation is available as html, PDF, and EPUB at https://pylith.readthedocs.io), and testing with the Method of Manufactured Solutions.

We conducted two days of in-person tutorials at the June 20-24, 2022 Crustal Deformation Modeling workshop. We also pre-recorded the tutorials and presentation slides and added them to the PyLith courses available through the CIG website.

Project goals for the upcoming year

Our focus for the coming year will be to complete migrating features from v2 to v3, improve scalability and benchmarking results, add support for earthquake cycle modeling that couples dynamic and quasistatic simulations, and switch to the latest version of the Pyre framework (which we use for managing simulation parameters and launching parallel jobs). We plan to hold another hackathon to accelerate development by facilitating contributions from users and educating them on the software development process.

See Development Plans which are part of the PyLith documentation.

Outreach and Broader Impacts

The June 2022 Crustal Deformation Modeling workshop highlighted a broad range of PyLith uses, including modeling of coseismic and postseismic geodetic data with quasistatic simulations, computing static Green's functions for fault slip in complex geologic structures, modeling surface loads due to water, and modeling deformation of Enceladus (one of Saturn's moons) due to faulting driven by tidal forces. The science talks and discussions also raised awareness of earthquake cycle modeling studies and Southern California Earthquake Center benchmarking efforts of the Sequences of Earthquakes and Aseismic Slip (SEAS) project and how adjoints can be used to improve the computationally efficiency of Bayesian inversions.

PyLith development continues to drive development of the DMPlex finite-element data structures and operations in PETSc. PyLith serves as an important test bed for new DMPlex features. For example, the finite-element integration for interior interfaces (i.e., faults) needed by PyLith required adjusting the DMPlex interface for specifying terms in the integration so that it was much more flexible. As a result, new features are added to DMPlex that facilitates its use in numerical modeling in other scientific disciplines.

4.4 Rayleigh

Rayleigh has been developed under the guidance of the Geodynamo Working group. Its development has been led by working-group member Nick Featherstone. Rayleigh is a 3-D convection code designed for the study of dynamo behavior in spherical shell geometry. It evolves the incompressible and anelastic MHD equations in spherical geometry using a pseudo-spectral approach. Rayleigh employs spherical harmonics in the horizontal direction and Chebyshev polynomials in the radial direction. The code has undergone extensive accuracy testing. It demonstrates excellent parallel performance on national level supercomputers, including the Mira supercomputer at Argonne Leadership Computing Facility. In addition, this project benefits a broader scientific community, with specialists in stellar and planetary convection/dynamos now using the software as well.

Significant accomplishments of the past year

This year's Rayleigh efforts focused on optimization of its Legendre transform algorithm and on the formalization of some aspects of the Rayleigh development and release cycle. The optimization projects were carried out in close collaboration with CIG postdoc Ryan Orvedahl who carried out the bulk of coding and experimentation.

Exploration of SHTns Legendre Transform Library

This year, we continued to explore the utility of the SHTns Legendre transform library. This library has enabled performance improvements in other spherical dynamo software. One of those codes (Magic) seems to perform slightly better than Rayleigh, apparently due to the use of SHTns. To that end, we implemented an option to use SHTns in Rayleigh last year, and this year, we have now extensively performance-tested the library. Through our tests, we found that using this library offered no improvement over Rayleigh's intrinsic Legendre transform algorithms. This finding is consistent with earlier, less-detailed testing carried out by Featherstone a decade ago, and more recent tests carried out by Philippe Marti (author of the QuICC code) about five years ago.

One benefit of this exercise, however, was the discovery that certain loops associated with Rayleigh's transpose (All-to-All) procedures were amenable to additional optimizations. Rayleigh has 4 such routines that are called throughout each timestep, and by optimizing one of those routines, we were able to consistently measure a 5-10% speedup depending on the problem size. This new transpose is now part of the main Rayleigh source code. Our results suggest that continued consideration of data layout and transpose looping may offer additional avenues for modest improvement. This feature may be responsible for the observed performance discrepancies.

GPU-enabled Legendre Transforms

GPU-enabled Legendre transforms capability has been a long-term goal of the Rayleigh project as it will enable access to large-scale machines, such as Summit at ORNL. We have designed a new Legendre transform algorithm that operates on the CPU and the GPU simultaneously. This algorithm uses a combination of OpenACC and CUDA directives. During each timestep of Rayleigh, a single MPI rank is responsible for conducting a large number (often a few hundred) of Legendre transforms. Our hybrid algorithm offloads some specified fraction of this work to the GPU, and transforms are then carried out simultaneously on both GPU and CPU.

Initial results are extremely promising. Performance increases until as much as 90% of the work is off loaded to the GPU. The degree of performance gains depends on the problem size, but it is typically 50% or greater.

Our next steps will be to incorporate this standalone algorithm into the main Rayleigh code.

Code Governance

This year, we have also begun to formalize some aspects of the Rayleigh development process. Rayleigh contributors now meet once a month to discuss development goals, code issues, and outstanding pull requests. As part of those discussions, we decided to adopt a quarterly release cycle for Rayleigh. Version 1.0.0 was released in the fall of 2021, and version 1.1.0 was released in April 2022. These releases are posted on Zenodo.

Project goals for the upcoming year

Our primary development aim for the next year is to implement the GPU-Legendre transform into the main Rayleigh code and to then explore similar optimizations for the linear solve. This will likely consume the bulk of Rayleigh development time during the next year.

Several smaller development goals will be pursued as well. One of these is to implement compositional convection, a phenomenon of interest to several users due to its relevance to problems in Earth's core, white dwarf formation, and ice-giant interiors. Adding a solid inner core (currently the inner core is omitted) for geodynamo problems is another goal. Both of these additions were developed in draft form at last year's Rayleigh workshop.

We plan to work on these over the summer of 2022 and at the next hackathon, to be held in September of 2022.

Outreach and Broader Impacts

The equations that Rayleigh evolves in spherical geometry are broadly applicable to both planetary and stellar interiors. This year saw the Rayleigh user base grow both in terms of students and postdocs. Two graduate students at CU started using the code this year to look at Rossby-wave generation in the deep solar interior and to study problems in the geodynamo.

New postdocs are also using the code: Carnegie in working on problems involving compositional convection in the Earth's core; McGill University on topics in stellar and ice-giant convection.

Results stemming from Rayleigh figured heavily in making the science case for the proposed Solaris mission. That proposal for a solar polar explorer made it into phase II, but it was ultimately not selected for programmatic reasons. Nevertheless, Rayleigh results and movies were featured prominently in the NASA site visit of Fall 2021 and the NASA HQ presentation in February 2022.

4.5 SPECFEM

SPECFEM3D_GLOBE simulates global and regional (continental-scale) seismic wave propagation. Effects due to lateral variations in compressional-wave speed, shear-wave speed, density, a 3D crustal model, ellipticity, topography and bathymetry, the oceans, rotation, and self-gravitation are all included.

Significant accomplishments of the past year

Core Spectral-Element and Spectral-Infinite-Element Code Developments

The first major area of research activity involves further development and implementation of the spectral- infinite-element method for problems in planetary geophysics. The resulting package, SPECFEM-X, currently accommodates 1) coseimic and postearthquake deformation with both moment-density tensor and split-node source implementations, 2) coseismic and postearthquake earthquake-induced gravity perturbations, 3) gravity anomalies, and magnetic anomalies, and 4) gravito-elastodynamics (Fiig. 12). The package has been implemented on GPUs using CUDA.

The second major area of research has been the continued development of the spectral-element seismic wave propagation solvers SPECFEM3D and SPECFEM3D_GLOBE for forward and adjoint simulations. We have implemented 'source encoding' for regional and global earthquake full waveform inversion. This approach makes the inversion process independent of the number of sources and receivers.

Peripheral Software Developments

In collaboration with Shantenu Jha at Rutgers University, the Ensemble Tool Kit (EnTK) is being developed and used for workflow management. This workflow management tool stabilizes and expedites seismic imaging and inversion workflows by providing recovery mechanisms for simulation failures. EnTK is used for global full waveform inversion and source inversions performed at Oakridge Leadership Computing Facility and Princeton High-Performance Computing Research Center.

In collaboration with ORNL and the ObsPy group (Lion Krischer), we continue to maintain and develop the Adaptable Seismic Data Format (ASDF). All provenance related to earthquakes, stations, and processing is stored in an HDF5 container to ensure complete reproducibility.

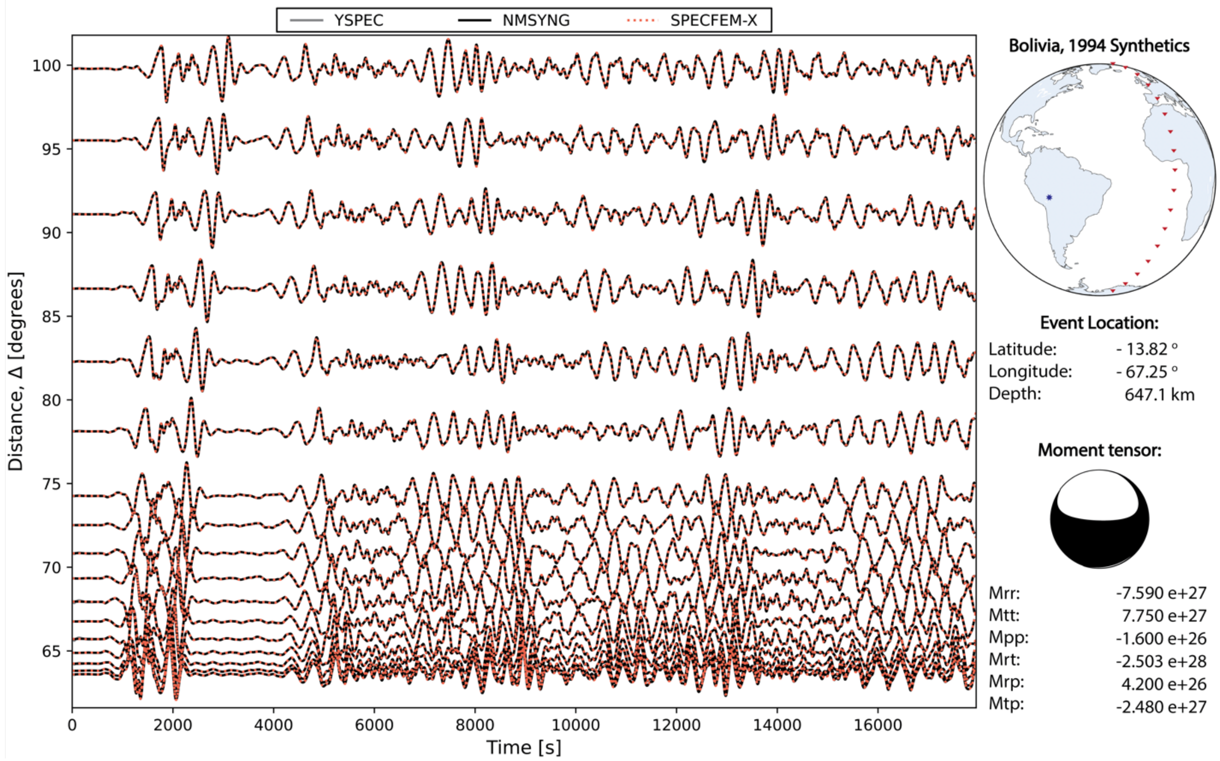

Figure 12. Gravito-elastodynamic simulation of global seismic wave propagation after the deep 1994 Bolivia earthquake. Shown is the perturbation in the time-dependent gravitational potential due to density perturbations induced by the motion. Standard normal-mode synthetics calculated based on the packages YSPEC and NMSYNG are compared with the SIEM solution based on SPECFEM-X. The model is isotropic PREM, and the passband is 50 s – 500 s.

Outreach and Broader Impacts

We are also planning to add routine 3D global Centroid Moment Tensor (CMT) inversions to Princeton's global ShakeMovie website to complement the synthetic seismograms and movies that are currently made routinely available to the community.

We are planning for the first SPECFEM Developer's meeting October 27-28, 2022 in conjunction with the Seismological Society of America's Seismic Tomography Meeting.

4.6 AVNI

AVNI is a geoscience resource designed to identify regions of scientific interest, validate new techniques, plan future instrumentation deployments, and test hypotheses about the Earth's deep interior.

The current phase of AVNI development has been focused on documenting the software and finalizing its release. The overarching goal is to present methods and data formats that will facilitate rapid prototyping of multi-scale models by reconciling and assimilating features ranging from reservoir (~0.1 - 10 km) to global scales (~500 - 5000 km).

Significant accomplishments of the past year

Work has progressed on three complementary aspects: (1) Code repositories comprising modular libraries with model classes and scalable HDF5 formats for archival, (2) API (Application Programming Interface) calls for querying model and data evaluations with fast, benchmarked forward solvers, (3) Web-based applets for visualization and outlier analyses. Both (1) and (2) are utilized by (3) and can be accessed on the client side with Jupyter notebooks and command-line tools. All aspects (1-3) required server and client-side components that involved transferring to a new setup currently hosted at Princeton University.

Documentation, testing, and other best practices have now been included such that AVNI meets CIG standards for software.

Once authentication and hosting services are configured at Princeton, the web portal will be available for user testing and training.

Outreach and Broader Impacts

The first CIG webinar to introduce AVNI was held on January 13, 2022. The recording and descriptions are available online. The webinar had 77 registrants, with representation across all disciplines in the solid Earth geosciences. Feedback was collected from the community on applications for which they would be interested in having notebooks developed.

4.7 World Builder

The Geodynamic World Builder (GWB) or World Builder for short, is an open-source code library that sets-up initial conditions for computational geodynamic models and/or visualize complex 3d tectonic setting, in both Cartesian and spherical geometries. GWB aims to make it easy for users to set up reproducible, complex, geodynamic models. The model is written to a structured, human readable input file which the user builds by arranging tectonic features and attaching different physical properties e.g., temperature.

GWB is written in C++ with wrappers for C, Fortran and Python. It can be linked by different geodynamic codes to create starting models. It also comes with its own tools to query and visualize the model setups. It has been successfully linked to SEPRAN, ELEFANT, and ASPECT. The latest release of the GWB is shipped with every release of ASPECT since ASPECT version 2.1.0. Active users include at research groups at 5 universities. In addition, GWB currently has 11 contributors, 25 forks and 17 stars on GitHub.

Significant accomplishments of the past year

The first release of the GWB was designed for creating regional scale geodynamic models of intermediate complexity. Since then, the types of use of the GWB by users has already by far exceeded its original design scope. To address the needs of the its growing user base improvements have been made to its usability and performance including:

- Improved documentation through reorganization of the manual and conversion to markdown

- Added ability to used data sets such as Slab 2.0
- Added and improved model geometry such as variable plate thickness (Fig. 13) and implementation of faults and subducting slabs (Fig. 14).
- Added new external interfaces for velocity topography, gravity, and mesh generation and efficient model queries.
- Greatly improved the accuracy of complex line features such as subducting slabs and faults (Fig. 14)

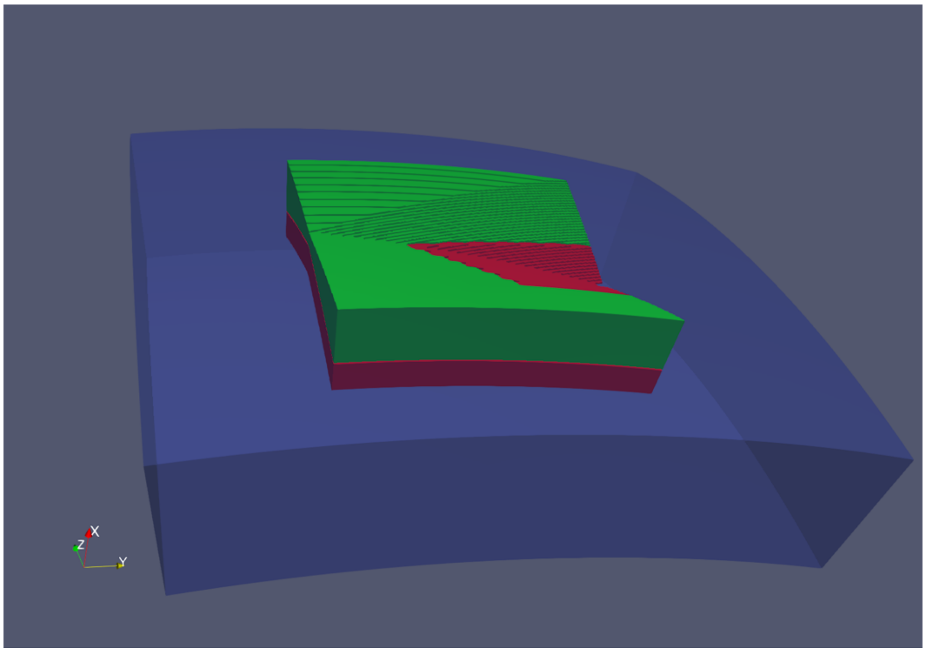

Figure 13. Example of variable thickness in area features.

Outreach and Broader Impacts

In the coming year, GWB will offer a tutorial. In addition, a JOSS paper is in preparation that will serve as a proof of concept for utilizing an alternative path for acceptance into the CIG community.

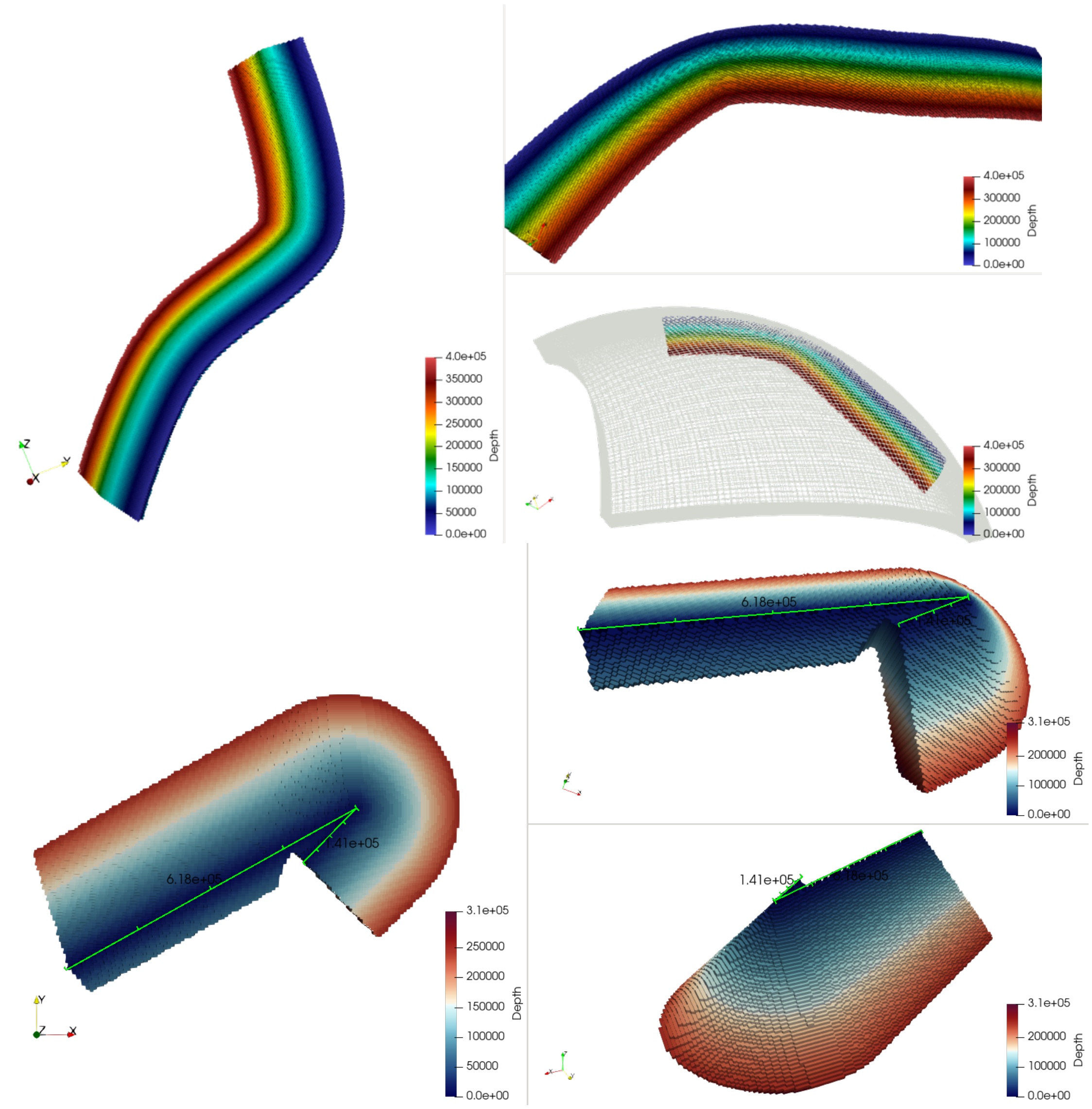

Figure 14. Examples of slabs with complicated geometries. Shown are slabs with sharp angles which main continues (top). This also works well in spherical coordinates (bottom).

5 Software Pipeline

5.1 GDMATE

The GeoDynamic Modeling Analysis Toolkit and Education (GDMATE) software repository aims to meet a diverse range of needs within the computational geodynamics and broader Earth science community. The repository will serve as a stable platform for collating and developing open-source tools that create inputs for geodynamic models, or processes their outputs (e.g., visualization, image processing). The underlying code will be written in software languages accessible to the broader geoscience community such as Python and Julia, while also optimized to readily support processing of massive data sets and use on HPC facilities. An extensive suite of educational modules will demonstrate both advanced applications of the toolkits and the fundamental coding methods required for further development of existing or new applications. A key functionality will be development in a notebook environment and its execution on the CIG HUBzero® platform.

6 Scientific and Broader Impacts

6.1 Publications

Publications included in our database include refereed papers submitted by authors as well as those found using google scholar based on keyword search by author, software package name, or DOI. In 2020, the community published 145 journal articles and theses using CIG codes. See Appendix D.

6.2 Cross Cutting Initiatives

CIG is the sponsor for the CSDMS Geodynamics Focus Research Group (FRG). The Geodynamics FRG's goals are to provide input to the CSDMS effort on how to best represent geodynamic processes and models within CSDMS. The membership and interests of the Geodynamics FRG overlap with CIG's and will provide a connection for future collaborations.

CIG met jointly with the Modeling Collaboratory for Subduction SZ4D, CSDMS, VIKTOR to learn from each other, coordinate community efforts, take stock of best practices, hear about the future plans of all the different efforts, and formulate strategies to collaboratively and synergistically move forward within computational solid earth science, creating new opportunities and filling gaps for enhancing diversity, research, training, and teaching.

CIG is also in discussions with SCEC to further collaborate on software for their communities.

Beyond the Geosciences

CIG participates and contributes to communities outside the geosciences that impact the research it supports including communities in high performance computing and software sustainability through initiatives such as FORCE11, WSSSPE, codemeta, IDEAS_ECP, RDA, US RSE, URSSI, and the Consortium of Scientific Software Registries and Repositories. CIG staff and community members have delivered talks on best practices in software and community building to these and other communities.

CIG has been involved with the development of FAIR for Research Software Principles (FAIR4RS) which was recently published.[11]

CIG Is also helping to organize a software citation workshop in August 2022 that will bring a broad scientific community together to discuss challenges to software citation implementation.

[11] https://zenodo.org/record/6623556#.YrIet-zMLAB

7 CIG III 5-Year Budget

A.&B.	Salaries and Wages	2,434,254
C.	Fringe	1,012,062
D.	Equipment	60,000
E.	Travel	289,900
F.	Participant Support	956,455
G.	Other Direct Costs	2,527,492
H.	Total Direct Costs	7,280,165
I.	Indirect Costs	1,538,829
	Total Costs	$8,818,994

Total 5-year commitment by NSF: $8.82 M
In 2020-22, in kind support for computational time was received from XSEDE and Frontera.

Appendix A: Institutional Membership

U.S. Institutions (69)

Argonne National Laboratory (MSC)
Arizona State University
Boston University
Brown University
California Institute of Technology
California State University, Northridge
Carnegie Institution of Science, DTM
Clemson University
Colorado School of Mines
Colorado State University
Columbia University
Cornell University
Georgia Institute of Technology
Harvard University
Indiana University
Johns Hopkins University
Lawrence Livermore National Laboratory
Los Alamos National Laboratory (ES)
Massachusetts Institute of Technology
Michigan State University
National Center for Atmospheric Research
New Mexico Institute of Mining and Technology
Northwestern University
Oregon State University
Pennsylvania State University
Portland State University
Princeton University
Purdue University
Rensselaer Polytechnic Institute
Rice University
State University of New York at Buffalo
State University of New York at Stony Brook
Texas A&M University
Tulane University
U.S. Geological Survey
University of Alaska, Fairbanks
University of Arizona
University of California, Berkeley
University of California, Davis
University of California, Los Angeles
University of California, San Diego
University of California, Santa Cruz
University of Colorado
University of Connecticut
University of Florida
University of Hawaii
University of Houston
University of Kentucky
University of Louisiana at Lafayette
University of Maine
University of Maryland
University of Memphis
University of Michigan
University of Minnesota
University of Missouri-Columbia
University of Nevada, Reno
University of New Mexico
University of Oklahoma*
University of Oregon
University of Rochester
University of Southern California
University of Texas at Austin
University of Utah
University of Washington
Virginia Polytechnic Institute and State University
Washington State University
Washington University in St. Louis
Woods Hole Oceanographic Institution

International Affiliates (21)

Aachen University
Australian National University
Cardiff University
Durham University
Earth Observatory of Singapore
Geological Survey of Norway (NGU)
GNS Science
Johannes Gutenberg University Mainz
Monash University
Munich University LMU
University of Alberta
University of Bristol, UK
University College London
University of Leeds
University of Melbourne
University of Oslo
University of Science and Technology of China
University of Sydney
University of Toronto
University of Tuebingen, Germany
Victorian Partnership for Advanced Computing

*New members

Appendix B: CIG Working Group Members

Computational Science (8)

- Brad Aagaard, U.S. Geological Survey
- Wolfgang Bangerth, Colorado State University, Fort Collins
- Jed Brown, University of Colorado, Boulder
- Nick Featherstone, Southwest Research Institute
- Timo Heister, Clemson University
- Matthew Knepley, University of Buffalo
- Eldridge G. Puckett, University of California, Davis
- Marc Spiegelman, Columbia University

Dynamo (8)

- *Lead,* Peter Driscoll, Carnegie DTM
- John Aurnou, University of California, Los Angeles
- Bruce Buffett, University of California, Berkeley
- Mike Calkins, University of Colorado, Boulder
- Philip Edelmann, LANL
- Hiroaki Matsui, University of California, Davis
- Maria Weber, Delta State University
- Cian Wilson, Carnegie DTM

Education (10)

- Magali Billen, University of California, Davis
- Katie Cooper, Washington State University
- Sanne Cottar, University of Cambridge
- Lorraine Hwang, University of California, Davis
- John Louie, University of Nevada, Reno
- Louise Moresi, Australian National University
- Gabriele Morra, University of Louisiana
- Federik Simons, Princeton University
- Sarah Stewart, University of California, Davis
- John Vidale, University of Southern California

Long-Term Tectonics (8)

- *Co-Chair,* John Naliboff New Mexico Tech
- *Co-Chair,* Jolante van Wijk, New Mexico Tech
- *Co-Chair,* Cedric Thieulot, Utrecht University
- Mark Behn, Boston College
- Susanne Buiter, GFZ Potsdam
- Claire Currie, University of Alberta

- Lijun Liu, University of Illinois, Urbana-Champaign
- Eric Mittelstaedt, University of Idaho

Magma Migration (8)

- *Lead,* Marc Spiegelman, Columbia University
- Mark Behn, Boston College
- Marc Hesse, University of Texas, Austin
- Garrett Ito, University of Hawaii
- Richard Katz, Oxford University
- Matt Knepley, University of Buffalo
- Ikuko Wada, University of Minnesota
- Cian Wilson, Carnegie DTM

Mantle Convection (8)

- *Lead,* Scott King, Virginia Polytechnic Institute
- *Lead,* Shijie Zhong, University of Colorado, Boulder
- *Lead,* Thorsten Becker, University of Texas, Austin
- Juliane Dannberg, University of Florida
- Timo Heister, Clemson University
- Margarete Jadamec, University of Buffalo
- Mark Richards, University of Washington
- Max Rudolph, University of California, Davis

Seismic Cycles (7)

- *Lead,* Sylvain Barbot, University of Southern California
- Kali Allison, University of California Davis
- Luca Dal Zilio, ETH Zurich
- Alice Gabriel, University of California San Diego, LMU Munich
- Dave May, University of California San Diego
- Pierre Romanet, NIED Japan
- Paul Segall, Stanford University

Seismology (5)

- *Lead,* Carl Tape, University of Alaska at Fairbanks
- Ebru Bozdag, Colorado School of Mines
- Carene Larmat, Los Alamos National Lab
- Arthur Rodgers, Lawrence Livermore National Lab
- Andrew Valentine, Australian National University

Short-Term Crustal Dynamics (4)

- *Lead,* Brad Aagaard, U.S. Geological Survey

- Eric Hetland, University of Michigan
- Eric Lindsey, Earth Observatory Singapore
- Charles Williams, GNS Science

Appendix C: 2021 Fall AGU Presentations

List of presentations by CIG scientists at the 2021 Fall AGU meeting. This list combines of self-reported abstracts with keyword search on software package names.

Monday, December 7

A002-0003 - Improving the Accuracy and Efficiency of Hybrid Finite Element / Particle-In-Cell Methods for Modeling Geologic Processes. *Mack Gregory and Elbridge Gerry Puckett.*
DI13A-04 - Controls on basaltic pile formation in the lower mantle. *Kiran Chotalia, Juliane Dannberg, and Rene Gassmoeller.*
DI13A-07 - The Interplay Between Recycled and Primordial Heterogeneities: Predicting Earth Mantle Dynamics Via Numerical Modeling. *Matteo Desideri, Anna J. P. Gülcher, and Maxim Ballmer.*
DI15B-0014 - Interrogating Core Mantle Boundary Structure Using P2KP Diffracted Phases and High Frequency Synthetic Seismograms. *Stuart Russel, Sanne Cottaar, and Jessica C E Irving.*
DI15B-0015 - A new global dataset of long period S wave travel time and attenuation measurements sensitive to lower mantle. *Stephanie Durand, Eric Debayle, Yanick R Ricard, and Thomas Bodin.*
DI15B-0019 - The Morphology, Evolution and Seismic Visibility of Partial Melt at the Core-Mantle Boundary: Implications for ULVZs. *Juliane Dannberg, Robert Myhill, Rene Gassmoeller, and Sanne Cottaar.*
DI15B-0023 - New body-wave time-delay database towards improving the seismic tomography of the lowermost mantle. *Lei LI, Stéphanie Durand, Yanick R Ricard, and Eric Debayle.*
DI15C-0028 - Seismic Imaging of the Pacific Plate using Amphibious Receiver Function with Tuned Dereverberation Filters. *Ziqi Zhang and Tolulope Olugboji*
EP12D-08 - Plume-induced heat flux anomalies and the associated thinning of the continental lithosphere. *Björn Heyn and Clinton P. Conrad.*
G15C-06 - CitcomSVE: A Publicly Available Software Package for Modeling Earth and Planetary Mantle's Viscoelastic Deformation in Response to Surface and Tidal Loads. *Shijie Zhong, Kaixuan Kang, Geruo A, and Chuan Qin.*
IN14B-05 - Using machine learning to select frequency windows on the normal-mode spectra. *Shiyu Zen, Hsin-Ying Yang, Jeroen Tromp, and Li Zhao.*
S11B-04 - Adjoint Seismic Tomography of the Antarctic Continent Incorporating both Earthquake Waveforms and Green's Functions from Ambient Noise Correlation. *Zhengyang Zhou, Douglas Wiens, and Andrew Jason Lloyd.*
S12B-07 - Accounting for Oceanic Reverberations in MERMAID Waveforms. *Rachel Willis, Ebru Bozdag and Roel Snieder.*
S13B-023D - Numerical Modeling of the Asymmetry of the Seismic Source for Underground Explosions. *Carene S Larmat, Zhou Lei, Yu-Hsuan Lee, and Howard J Patton.*
S14B-05 - An Analysis of Recorded and Simulated SH Wave Reverberations in the Upper Mantle beneath the USArray. *Meichen Liu, Jeroen Ritsema, and Carlos Alberto Moreno Chaves.*

[S15C-0261](#) - Modeling the Effect of Subsurface Structure on Shear Wave Generation: the Case of the Yucca Flat Basin at the Source Physics Experiment Phase II Site. *Ting Chen, Carene S Larmat, Richard Alfaro-Diaz, Charlotte A Rowe, W. Scott Phillips, Asher May, and Joshua Rubin Abrams.*
[S15D-0273](#) - Removal of Continuous Topographic Scattering in Dense Array Receiver Functions Imaging. *Siyuan Zhang, Zengxi Ge, and Zhen Guo.*
[S15E-0292](#) - Effect of the Coriolis Force on Body Wave Polarization Anomalies Inferred From 3D Wave Simulations. *Neala Creasy, Daniel Andrew Frost, Ebru Bozdag, and Roel Snieder.*
[S15E-0299](#) - Cartesian Meshing Spherical Earth (CMSE): A code package for meshing the earth geometry based on SPECFEM3D_Cartesain. *Guoliang Li, Min Chen, Jiaqi Li, and Ross Maguire.*
[T15C-0181](#) - Numerical Modeling of Lithospheric Drip and Associated Melts at the East African Rift. *Carlos Daniel Gomez.*

Tuesday, December 8

[DI21A-07](#) - Overriding Plate Topography Shaped by Subduction Evolution. *Antoniette Greta Grima, Thorsten W Becker, and Claudio Faccenna.*
[DI25A-0004](#) - Controls on plate tectonic evolution: from Early Earth to present day. *Elodie Kendall, Stephan V. Sobolev, Dr. Sascha Brune, Anne Glerum, and Frederic Gehrke.*
[DI25B-0028](#) - The Segregation of Recycled Basaltic Material Within Mantle Plumes Explains the Detection of the X-Discontinuity Beneath Hotspots: 2D Geodynamic Simulations. *Martina Monaco, Juliane Dannberg, and Rene Gassmoeller.*
[G24A-05](#) - Viscoelastic heterogeneity and San Andreas Fault seismic-cycle deformation: An investigation using PyLith finite-element models and the SCEC Community Rheology Model. *Elizabeth H Hearn.*
[G25B-0357](#) - Power-law Viscoelastic Flow of the Lower Makran Accretionary Prism Following the 2013 Baluchistan Earthquake. *Guo Cheng and William D Barnhart.*
[G25C-0370](#) - Numerical analysis of postseismic displacement of infer the lithospheric strength beneath the East Sea (Sea of Japan). *Hyeon Seob Kim, Nawon Kim, Minsu Kim, and Byung-Dal So.*
[P25E-2199](#) - Can a Seismometer Detect Events from Europa's Silicate Interior? Yes, if ... . *Angela G Marusiak, Mark P Panning, Steve Vance, Simon C Staehler, and Saikiran Tharimen.*
[S21C-04](#) - Cube2sph: a toolkit enabling accurate and efficient continental-scale seismic wave simulation using SPECFEM3D. *Qinya Liu, Tianshi Liu, Bin He, Kai Wang, Yujiang Xie, Catherine Rychert, and Nicholas Harmon.*
[S21C-05](#) - Seismic Imaging of Fault Zone Structure Using 3-D Full Waveform Inversion of Denoised Ambient Noise Cross-correlation (ANC) from 1-D Linear Arrays. *Xiang Li, Hongrui Qiu, and Fenglin Niu.*
[S23B-07](#) - Mantle Q structure from S, SS, SSS and SSSS amplitude measurements. *Min Zhu, Shuyang Sun, Ying Zhou, and Qingju Wu.*
[S25G-0317](#) - Adjoint tomography of the Colima Volcanic Complex using seismic ambient noise. *Eduardo Valero Cano, Armando Espindola-Carmona, and Daniel B Peter.*

T24A-03 - A Reference Dataset of Short-Period Surface Wave Dispersion for Model Update of the African Crust. *Siyu Xue and Tolulope Olugboji*
T25B-0176 - Autoadaptive Bayesian Construction of Short-period Phase Velocity Maps and Uncertainties Across Africa. *Yuri Tamama and Tolulope Olugboji*
T25C-0193 - A time-dependent catalog of episodic tremor and slow slip in Cascadia. *Noel M Bartlow and Charles A Williams Jr.*
T25E-10 - The effect of mantle convection modulated by mantle temperature heterogeneity on rifting propagation. *Min Seok Jang and Byung-Dal So.*

Wednesday, December 9

DI34A-04 - Geodynamic Drivers of the East African Rift System (Invited). *Anne Glerum and Sascha Brune.*
DI34A-06 - ThermoCodegen: New Software for Consistent Integration of Thermodynamics and Geodynamics. *Marc W Spiegelman, Owen Evans, Mark S Ghiorso, Lucy E L Tweed, and Cian R Wilson.*
DI34A-07 - Implementing and benchmarking high-performance particle methods in the geosciences and beyond. *Rene Gassmoeller, Cedric Thieulot, Elbridge Gerry Puckett, Shahab Golshan, and Bruno Blais.*
DI35A-0001 - Dynamics of Upper and Lower Mantle Subduction and its Effects on the Amplitude and Pattern of Mantle Convection. *Erik van der Wiel, Cedric Thieulot, Wim Spakman, and Douwe J J Van Hinsbergen.*
DI35A-0004 - Rheological Memory in Global Plate-like Mantle Convection. *Lukas Fuchs and Thorsten W Becker.*
DI35A-0008 - How phase transitions change convection patterns through the Earth's history: A modeling study. *Ranpeng Li, Juliane Dannberg, Rene Gassmoeller, Carolina R Lithgow-Bertelloni, and Lars P Stixrude.*
DI35D-0051 - Effects of the latent heat at the inner core boundary on the thermal structure at ICB in numerical dynamo simulations. *Hiroaki Matsui*.
DI35D-0070 - The generation mechanism of the equatorially antisymmetric flow associated with dipole reversal in geodynamo simulation. *Takumi Kera, Hiroaki Matsui, Masaki Matsushima, and Yuto Katoh.*
G31A-05 - Solid Earth uplift due to contemporary ice melting above low-viscosity regions of Greenland's upper mantle. *Maaike F. M. Weerdesteijn, Clinton P Conrad, Jesse Reusen, Rebekka Steffen, and John B Naliboff.*
NH33A-08 - The role of topographic amplification in triggering landslides from the 2005 M7.6 Kashmir Earthquake. *Audrey Dunham, Eric Kiser, Jeffrey S Kargel, Umesh K Haritashya, Scott Watson, and Daniel H Shugar.*
S35A-03 - Teleseismic P-waves from secondary microseism events: a systematic comparison between sea-state hindcast and seismic data back-projection. *Ruohan Zhang, Pierre Boué, Univ. Grenoble Alpes, Michel Campillo, and Ma Jianwei.*

T35A-0186 - Modeling the Effects of Initial Continental Rift Structure on the Symmetry and Vergence of Collisional Orogens Formed by Rift Inversion. *Dylan Alexander Vasey, John B Naliboff, and Eric Cowgill.*

Thursday, December 10

DI45A-0006 - Developing Instantaneous Subduction Models to Investigate ThermalShear Instability as a Deep Focus Earthquake Failure Mechanism in the Tonga Subduction Zone. *Rebecca A Fildes, Magali I Billen, and Marcel Thielmann.*

DI45C-0022 - Piercing Point Dependent Seismic Azimuthal Anisotropy Observed in Central China and Its Geodynamic Implications. *Yan Jia, Kelly Hong Liu, Fansheng Kong, Lin Liu, and Stephen S Gao.*

DI45C-0024 - Effects of Crust and 3D Mantle Heterogeneity on Shear Wave Splitting Using 3D Wave Simulations. *Neala Creasy and Ebru Bozdag.*

DI45C-0025 - A ray-theory based imaging approach for constraining upper mantle anisotropy using teleseismic shear wave delays. *Rosalia Lo Bue, Brandon VanderBeek, Francesco Rappisi, and Manuele Faccenda.*

DI45C-0027 - Constraining deep mantle anisotropy with shear wave splitting measurements: Challenges and new measurement strategies. *Jonathan Wolf, Maureen D Long, Kuangdai Leng, and Tarje Nissen-Meyer.*

DI45E-12 - Reproducing Present-Day Plate Motions in High-Resolution Global Mantle Flow Models with Plate Boundaries. *Arushi Saxena, Juliane Dannberg, and Rene Gassmoeller.*

DI45E-13 - Towards an Investigation of the Effects of Dynamic Topography on Vertical Land Motions Along the North American Atlantic Coast. *Karen Williams, D. Sarah Stamps, Jacqueline Austermann, Tahiry Andriantsoa Andriantsoa Rajaonarison, and Emmanuel Atem Njinju.*

H45J-1300 - Poroelasticity and Poroelastic Benchmarking in Pylith. *Robert Lewis Walker II, Matthew Knepley, Brad Aagaard, and Charles A Williams Jr.*

MR43A-07 - On the Implementation and Usability of CPO Evolution in Geodynamic Modelling. *Menno Fraters and Magali Billen*.

P45B-1093 - Extending the open-source code ASPECT to solve the sea level equation on a heterogeneous Earth. *Maaike F. M. Weerdesteijn, Clinton P Conrad, Andrew Hollyday, Jacqueline Austermann, and Rene Gassmoeller.*

S44B-08 - Global Centroid Moment Tensors based on 3D Green's Functions. *Lucas Sawade, Stephen Beller, Wenjie Lei, Goran Ekstrom, and Jeroen Tromp.*

T41A-06 - Understanding the Socorro Magma Body based on an 16+ yr record of geodetic observations. *Mousumi Roy, Ronni Grapenthin, Grant Block, Emily Jo Graves, Mark H Murray, and Andrew Vern Newman.*

T41D-03 - Revisiting the Effects of Shear Zone Strength, Low Temperature Plasticity and Mantle Phase Transitions in 2-D Subduction Dynamics. *Haoyuan Li and Magali I Billen.*

T42A-06 - Investigating Potential Melt Sources for the Magma-Poor Albertine-Rhino Graben of the East African Rift System Using 3D Geodynamic Modeling with ASPECT. *Asenath Kwagalakwe, D. Sarah Stamps, Emmanuel Atem Njinju, and Estella A Atekwana.*

T43D-03 - Control of Upper Crustal Rock Strengths on the Extension and Propagation of Early-Stage Continental Rifting: Insights from Fracture Mechanics. *Solomon Seyum, Cade Quigley, and Folarin Kolawole.*
T44A-01 - The effects of an evolving subduction thermal structure on dehydration and rheology: coupling geodynamic and thermodynamic models with the experimental and rock records. *Cailey Brown Condit, Adam Holt, and Victor Guevara.*
T45B-0210 - A Mass-Conserving Thermal Structure for Slabs in Instantaneous Models of Subduction. *Magali I Billen and Menno Fraters.*
T45B-0232 - Three-dimensionality of Slab Thermal Structure in Dynamic Subduction Models. *Valeria Turino and Adam Holt.*

Friday, December 11

IN52A-06 - The TEMPEST Initiative. *James H Roberts, Alyssa Rhoden, Matthew Walker, Maxwell L Rudolph, Jonathan Kay, Justin Krier, and Malick Gaye.*
P55C-1945 - Seismic Analogs for the Detection of Subsurface Lunar and Martian Void Spaces. *Linden Wike, Nicholas C Schmerr, Ernest Bell, Doyeon Kim, Jacob A Richardson, Kelsey Young, and Patrick Whelley.*
S51B-07 - Three-Dimensional Kinematics and the Crustal Deformation of Tsunami Earthquakes. *Oluwaseun Idowu Fadugba and Diego Melgar.*
S52B-06 - One Year of Sound Recorded by a MERMAID Float in the Pacific: Infrasonic Noise and Hydroacoustic Signals. *Sirawich Pipatprathanporn and Frederik J Simons.*
S55C-0148 - Analysis of Hydroacoustic Signals from the 4 August 2020 Beirut Explosion. *Ross Geoffrey Heyburn and Stuart E.J. Nippress.*
S55E-0189 - Coupled Models in PyLith for Earthquake Cycle Simulations. *Kali L Allison, Brad Aagaard, and Matthew Knepley.*
S55E-0197 - Moment tensor solutions and 3D wavefield simulation in Garhwal Himalayas. *Vipul Silwal and Rinku Mahanta.*
T51B-02 - The Evolution of Fold and Thrust Structures in the North-West Himalayas and their Implications for Seismic Hazard in the Region. *Aisling O'Kane, Alex Copley, Supriyo Mitra, and Samuel Edward Wimpenny.*
T52A-01 - Modeling slab temperature and dehydration evolution over the lifetime of a subduction zone. *Adam Holt and Cailey Brown Condit.*
T55E-0114 - Laterally Heterogeneous Crustal Mechanical Properties Control Early Rift Asymmetry. *Cade Quigley, Solomon Seyum, and Folarin Kolawole.*

Appendix D: Publications

Articles in 2021 using CIG codes either reported by authors or discovered using keyword searches on google scholar.

1. Abreu, R., and S. Durand (2021), Understanding Micropolar Theory in the Earth Sciences II: The Seismic Moment Tensor, Pure and Applied Geophysics, doi:10.1007/s00024-021-02894-w.
2. Albaric, J., D. Kühn, M. Ohrnberger, N. Langet, D. Harris, U. Polom, I. Lecomte, and G. Hillers (2021), Seismic Monitoring of Permafrost in Svalbard, Arctic Norway, Seismological Research Letters, doi:10.1785/0220200470.
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Earthquake From a Balloon Using Its Acoustic Signature, Geophysical Research Letters 48(12), 2021.
12. Butler, R., and S. Tsuboi (2021), Antipodal seismic reflections upon shear wave velocity structures within Earthâ€™s inner core, Physics of the Earth and Planetary Interiors, 106802.
13. Calkins, M. A., R. J. Orvedahl, and N. A. Featherstone (2021), Large-scale balances and asymptotic scaling behaviour in spherical dynamos, Geophysical Journal International 227(2), 1228–1245, doi:10.1093/gji/ggab274.
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Theses

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