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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. We held regular users' meetings and workshops for community supported software projects ASPECT, PyLith, Rayleigh, and SPECFEM. Outreach activities included virtual and in person workshops: the ASPECT User workshop; ASPECT, Rayleigh, and PyLith Hackathons, and the SPECFEM Developers Meeting. Hackathons continue to be a productive vehicle in completing and initiating projects and collaborations. We had significant international participation in both virtual and in person events. Our webinar series continued along a broad range of topics on melts, deep Earth structure, and proposal writing and research software. The Seismic Cycles Working Group sponsored a near weekly webinar series with 16 speakers on topics in fault mechanics – laboratory experiments and numerical models, important to earthquakes cycle modeling. The CIG Distinguished Speaker program continues its focus in bringing CIG-supported science to colleges and universities that serve underrepresented groups in the geosciences. Virtual visits this year help to expand our international reach.

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 and increasing its numerical efficiency through implementation of interfaces to microstructure evolution and landscape evolution models (ASPECT), new numerical approaches (PyLith), compositional convection and higher order discretization (Rayleigh). This year SPECFEM launched a new website bringing its codebase under one organization. Our plans for the coming year include continuing to support the infrastructure for development of codes across the scientific domains represented by geodynamics, including welcoming new codes and releasing 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 utilizing, managing and renewing CIG's allocation on ACCESS and Frontera, to continue optimizing 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.

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1 CIG Overview

The Computational Infrastructure for Geodynamics (CIG) provides the infrastructure for computation and research in geodynamics. CIG achieves this by enabling the development and dissemination of 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 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, 2022, through July 31, 2023, unless otherwise noted. Activities span both NSF-1550196 & 2149126.

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. 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 the needs of established and emerging communities and other open-source codes, support common infrastructure, and sustain and grow the geodynamics 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 89 member institutions including 11 MSIs and 21 international affiliates. Of these, five (5) are inactive as member representatives have moved to new institutions. See <u>Appendix A</u>.

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 codirectors, 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 <u>Responsibilities of the EC</u>.

The EC has eight (8) members, of which five (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 three (3) *ex officio* members are the two (2) codirectors, and the Chair of the Science Steering Committee.

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

- Chair, Alice Gabriel (2023), UC San Diego and University of Munich
- Vice Chair, Brad Aagaard (2024), US Geological Survey
- Louis Moresi (2025), Australian National University
- Marc Speigelman (2025), Columbia University
- Phaedra Upton (2024), GNS New Zealand
- Ex officio, Ebru Bozdag (2023), Colorado School of Mines
- Ex officio, Bruce Buffet, UC Berkeley, Co-Director of CIG
- Ex officio, Lorraine Hwang, UC Davis, Co-Director of 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 codirectors to assess how tasks are interrelated and related to the broader needs of the community. To make this process as productive as possible, the codirectors 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 <u>Responsibilities of the SSC</u>.

The SSC consists of eight (8) elected members including a chairperson and three (3) *ex officio* members - the two (2) codirectors and the Chair of the Executive Committee. The committee includes expertise in both the geosciences and computational sciences and provides guidance within all the sub-disciplines of computational geodynamics. New this year is a seat reserved for an early career research (one year term).

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

- Chair, Ebru Bozdag (2023), Colorado School of Mines
- Vice-Chair, Dave May (2024), UC San Diego
- Sylvain Barbot, (2023) University of Southern California
- Peter Driscoll, (2024), Carnegie Institution
- Adam Holt (2025), University of Miami
- Harriet Lau (2024), UC Berkeley
- Elvira Mulyukova (2025), Northwestern University
- Early Career, Emmanual Njinju (2023), UC Davis
- Ex officio, Alice Gabriel (2023), UC San Diego and University of Munich
- Ex officio, Bruce Buffet, UC Berkeley, coDirector of CIG
- Ex officio, Lorraine Hwang, UC Davis, coDirector of CIG

Governance this year approved new policies for collaboration with the community and meeting best practices.

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. See <u>Roles and Responsibilities</u>.

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 (EWG) works to promote access to educational materials for geodynamics. The EWG advances the infrastructure and content needed to develop a computationally skilled workforce and increase discovery of the discipline. This is achieved through integrating computation with domain science in upper division and graduate level learning.

Long-Term Tectonics

The Long-Term Tectonics Working Group's primary goal is to converge towards a communityinitiated 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 opensource 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, the SSC and EC work together to identify overlapping needs in both scientific and computational functionality from the different domains, 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, software testing and education/training that are consistent across disciplines.

<u>Appendix B</u> provides a list of working groups. Members of working groups actively engaged with the CIG community are also listed.

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 within the Department of Earth and Planetary Sciences. The HPC

Core Facility manages mass storage and CIG compute nodes which 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.

CIG transitioned from a single director to two (2) codirectors in February 2023. CIG Headquarters is led by the project PI who is a codirector and serves as Director of Operations. CIG is supported by a team of research scientists and IT professionals. Support for research staff members may come from other projects. Web support and development is through HUBzero[®]. 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 of Operations (DO) is the Chief Executive Officer of the organization and Principal Investigator on the CIG Cooperative Agreement. She consults with the second codirector on programs and budgets but bears ultimate responsibility. The codirectors' responsibilities include: (a) leading strategic planning for CIG's mission and goals and acting as the primary representative of CIG to the scientific community, and (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. The DOs responsibilities include: (a) 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, (b) ensuring that funds are properly allocated to various CIG activities, and (c) 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 DO 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 (subawardees) provide software services to the community in the form of programming, documentation, training, and support.

CIG Staff are:

- Director/Co-Director, Dr. Lorraine Hwang
- Co-Director, Dr. Bruce Buffet (University of California Berkeley)
- Technical Lead, Dr. Rene Gassmoeller (University of Florida)
- Research Scientist, Dr. Hiroaki Matsui
- Project Scientist, Dr. Mohamed Gouiza
- Postdoctoral Fellow, Dr. Kali Allison
- Graduate Student: Dylan Vassey
- Junior Specialists, Chris Mills

• Student Assistant: 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 codirectors 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 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 plan which may include software development plans, benchmarks, tutorials, and a schedule for working meetings appropriate to each project.

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 algorithmic improvements to improve both the performance and scalability in preparation for wider community use.

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 hosted by HUBzero[®] at SDSC and 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 their documentation;

- provide access to compute resources for execution of computational notebooks and community codes;
- 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, bylaws, 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 through its forums.

Forum

The CIG forum serves the function of a mailing list for the community. The forum allows easier searching and tagging of discussion threads as well as many modern features so 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, 2022, the forum has grown to 870 users. Almost half (46%/404) of its members have contributed to discussions. New users, contributors, and visits have increased since last year reflective of renewed activity and continual growth of the organization (Figure 1).

The domain-specific categories for groups that have released codes are used frequently for community support. Any registered user may post a question or request 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 less than 7 hrs. CIG staff monitor the lists and 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 issues or discussions for similar functions, e.g., SPECFEM, and hence, forum traffic does not reflect the community's activities.

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.

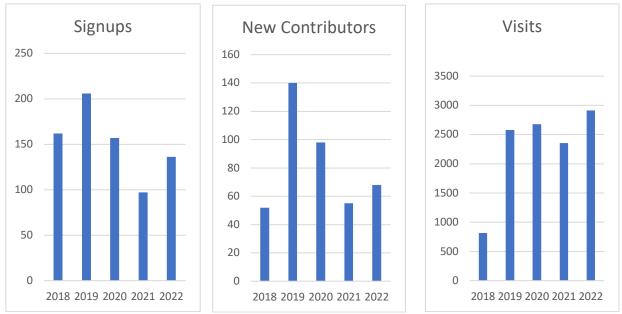


Figure 1. CIG Forum activity since inception (community.geodynamics.org). Shown by month are the (left) number of new users, (center) new contributors, and (right) visits to the forum.

The meeting was held virtually on November 29, 2022, with discussions on how the community can collaborate with the organization and how CIG can continue to support its community.

CIG Quarterly Newsletter

Launched in August 2012, the CIG Quarterly <u>Newsletter</u> 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, CI, 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 <u>webinars</u>, described below, are used for more in-depth communication about software projects, research applications, best practices, and governance matters.

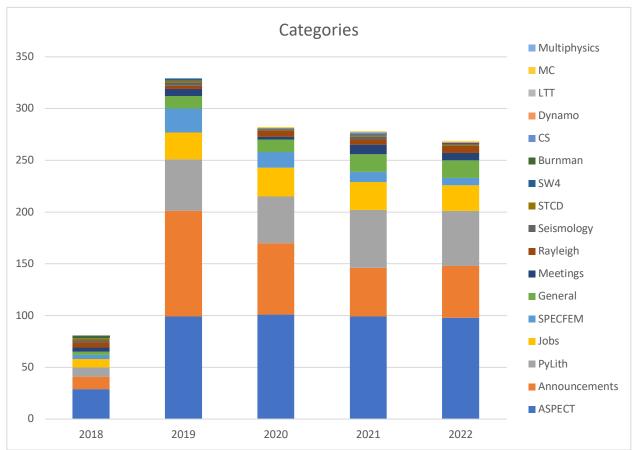


Figure 2. Number of messages posted to the forum by category. Legend is reversed ranked ordered with the users of the ASPECT forum posting the most messages.

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 community codes are released under OSI approved licenses. Sponsored projects are open to all to join and contribute. 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 improving its software engineering practice and maintains a robust repository to facilitate the sharing of validated open-source software. 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 period January 1 – December 31, 2022.

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 the 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. These 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 allocated 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.

	Version	Lines of Code	% Change	Commits	# Developers	Support Level
Short-Term Crustal	Dynamics					
Pylith	3.0.3*	363,752	-45%	470	15	D_CIG
Relax	1.0.7	1,419,923	-	-	10	D_CONTRIB
VirtualQuake	3.1.1	49,112	0%	1	18	D_CONTRIB
SELEN	2.9.13	17,391	3%	4	6	S_CONTRIB
LithoMop	0.7.2	495,786	-	-	5	А
Long-Term						
Gale	1.6.1/2.0	6,680,841	-	-	62	А
Plasti	1.0.0	10,967	-	-	1	А
SNAC	1.2.0	549,498	-	-	3	А
Mantle Convection						
ASPECT ⁺	2.4.0	2,839,356	17%	1469	103	D_CIG
CitcomCU	1.03	70,288	-	-	5	D_CONTRIB
CitcomS	3.3.1	266,520	0%	5	23	D_CONTRIB
ConMan	3.0.0	577,882	-	-	12	S_CONTRIB
Ellipsis3d	1.0.2	51,602	-	-	2	А
HC	1.0.15	493,480	0%	10	7	А
Seismology						
AxiSEM	1.3	109,462	0%	6	14	D_CONTRIB
Burnman	$1.1.0^{*}$	242,713	53%	121	19	D_CONTRIB

Table 1. Repository Statistics

	Version	Lines of Code	% Change	Commits	# Developers	Support Level
Mineos	1.0.2	331,364	-	-	7	А
Flexwin	1.0.1	95,412	-	-	8	А
Seismic CPML		37,820	-	-	6	S_CONTRIB
Specfem3D	4.0.0*	11,215,254	-	-	58	D_CIG
Specfem3D Globe	8.0.0*	2,141,321	-	-	54	D_CIG
Specfem3D Geotech	1.1	2,038,521	-	-	4	D_CONTRIB
Specfem2D	8.0.0*	2,810,599	9%	70	45	D_CONTRIB
Specfem1D		5,371	-	-	10	S_CONTRIB
SW4	3.0*	4,639,674	94%	90	32	D_CONTRIB
Dynamo						
Rayleigh	1.1.0	85,948	7%	288	31	D_CIG
Calypso	1.2.0	215,012	-	-	7	D_CIG
MAG	1.0.2	134,906	-	-	5	А
Computational Scie	nce					
Cigma	1.0.0	356,371	-	-	7	А
Exchanger	1.0.1	5,654	-	-	7	А
Nemesis	1.1.0	788	-	-	2	S_CONTRIB
Pythia	1.0.0*	45,012	20%	20	4	S_CONTRIB

*new release

⁺also being used for long-term tectonics

Statistics are as reported by gitstats¹ which does not discriminate between line types, e.g., comments versus code. CIG codes span six scientific domains and most use multiple programming languages. The majority of the executable code in the library uses 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.

¹ <u>https://github.com/hoxu/gitstats</u> (version 55c5c28, 2.25.1)

Tool statistics are now also available online for each software resource under the Tool Stats tab on its software landing page.

The CIG Git repositories logged 2554 software commits during 2022. Over the repository lifetime, nearly 592 developers have contributed to code development.

CIG's <u>community</u> on Zenodo is a resource for both long term preservation of software and discoverability. Table 2 shows statistics as of July 31, 2023, for actively developed CIG community code for the most *current version/all versions*. Users are also able to download packages from Zenodo.

	# versions	Views	Downloads	Data volume	Unique views	Unique downloads
ASPECT	11	280/2481	11/497	883.9MB/13.6GB	233/2049	11/396
PyLith	11	78/3109	4/598	54.5MB/10.9GB	71/2461	4/386
Rayleigh	6	115/915	6/58	15.69MB/308.4MB	103/677	6/53
SPECFEM2D	1	54/54	37/37	7.2GB/7.2GB	47	47
SPECFEM3D_Cartesian	1	33/33	8/8	2.8GB/2.8GB	32/32	7/7
SPECFEM3D_GLOBE	1	22/22	0/0	0/0	20/20	0/0
SW4	3	499/1261	66/123	928.5MB/1.6GB	461/1148	54/102

Table 2. Zenodo Statistics

3.2 Software Hosting

CIG is utilizing the HUBzero[®] platform to host notebooks and containers. Software launchable from our website supports training, education, and first-time users. Along with general use containers for Jupyter notebooks, the community has contributed Jupyter notebooks for BurnMan and Earth science education (see the AVNI project). Also available is a Debian development environment and an ASPECT virtual desktop.

Software hosting is central in the ongoing development of training materials as well as future educational materials. Model set-ups illustrating geophysical concepts will be developed within notebooks that can be integrated into an educator's curricula. Many of these examples are currently available as cookbooks from ASPECT.

3.3 High Performance Computing

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

- 85,890 SUs; 10,000 GB (Ranch) on Stampede2
- 2,215,314 Core-hours; 2,048 GB on Expanse

Allocation expires September 30, 2023.

In 2022, CIG successfully applied for a Frontera Pathways allocation of 150.696 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, 2023.

Renewal requests for 2023-2024 have been submitted to both ACCESS and Frontera.

3.4 Education & Training

CIG is increasing its efforts to promote the development of a computationally skilled workforce and the discovery of geoscientific disciplines focusing on geophysics and geodynamics. Efforts have been initiated to develop educational resources for use in upper division and graduated level learning. The goals are to:

- identify innovative ways to integrate computing skills, methods and tools in teaching by developing learning resources that integrate computational and domain learning outcomes;
- 2) increase the pipeline of undergraduate and graduate researchers by identifying training needs and funding sources; and
- 3) promote geosciences through the development of outreach content based on computation modeling.

CIG's Education Working Group is actively identifying existing material to leverage in these efforts and creating an online directory of publicly available resources.

CIG in partnership with its code community continues to develop and update training materials. A long-term goal is the conversion of these resources to computational notebooks. Current work is focused on developing the foundational libraries for ASPECT that will assist parameter manipulation and modeling output analysis within the notebook environment.

3.5 Knowledge Transfer and Capacity Building

CIG builds and sustains its community through both virtual and in-person events. The Co-Directors, 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), Ada Lovelace Workshops (EGU), Community Surface Dynamics Modeling System (CSDMS), and Subduction Zone 4D Modeling Collaboratory for Subduction (SZ4D MCS RCN). CIG partners with these and other organizations to expand its impact on the geodynamics community.

Upcoming workshops and training are posted online and advertised through CIG email lists and forum and those of our partner organizations.

In 2022-2023, we continued holding a mix of virtual and in person events (Table 3). 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. Figure 3 shows the combined demographics for the events listed in Table 3 except for the Ada Lovelace Workshop.

Date	Title		Participants
August 27-	Ada Lovelace Workshop		13
September 2, 2022			
September 11-17, 2022	Rayleigh Hackathon		13
October 17-19, 2022	Seismic Cycle Workshop		128
October 27-28, 2022	SPECFEM in-person workshop for developers and users		46
January 31-	ASPECT User Workshop		83
February 1, 2023			
June 12-16, 2023	Rayleigh Hackathon		13
June 12-17, 2023	PyLith Hackathon		18
July 6-15, 2023	ASPECT Hackathon		22
		Total	337

Table 3. August 2022 - July 2023 Workshops and Tutorials

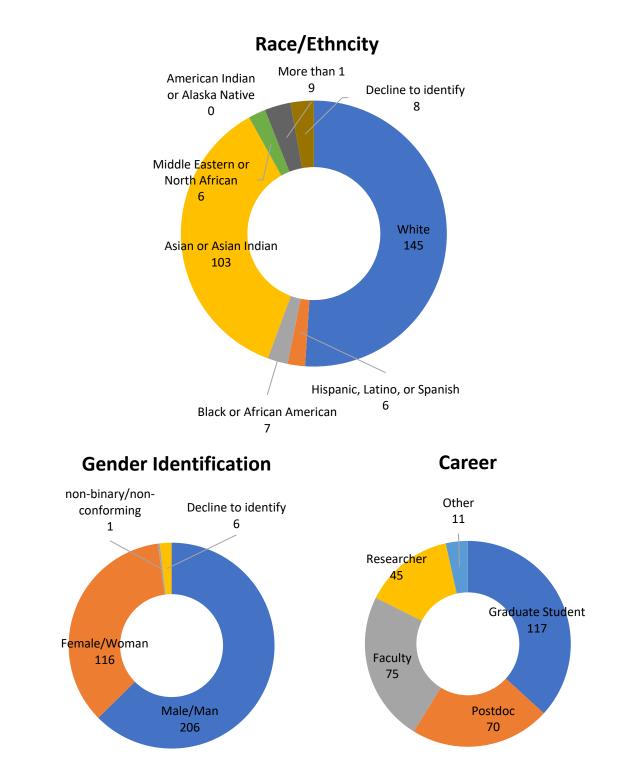


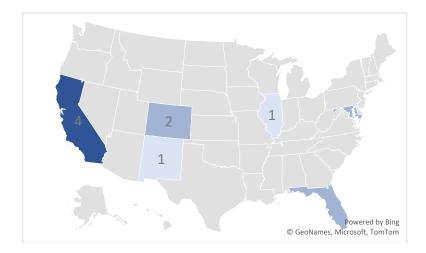
Figure 3. Combined demographics for events listed in Table 3 except for the Ada Lovelace Workshop in which no demographic data was requested. Participants self-identified a. race/ethnicity, gender identification, and career stage.

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

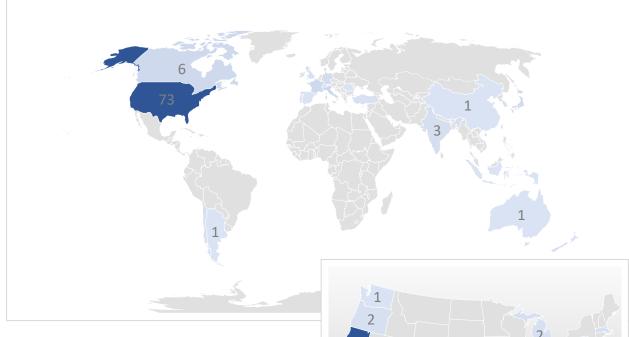
Maps shown below for each event show participation by numbers and geographic distribution.

2022 Rayleigh Hackathon

The 2022 Rayleigh Hackathon was held in person from September 11-17, 2022, in Breckenridge, Colorado. 13 people attended the event. A major focus was modernizing and restructuring of the documentation to make the documentation more useful and coherent, laying out a structure for future content. Improvements were made in the visualization routines and python analysis routines providing a better memory mapping framework. The inclusion of an arbitrary number of active and passive scalar fields in the model was generalized allowing the simulation of more than one field. Progress was also made on data conversion routines for the data from the INCITE project towards making these data available public for reuse and exploring alternative formulation of the Chebyshev polynomials.



2022 Seismic Cycles Workshop



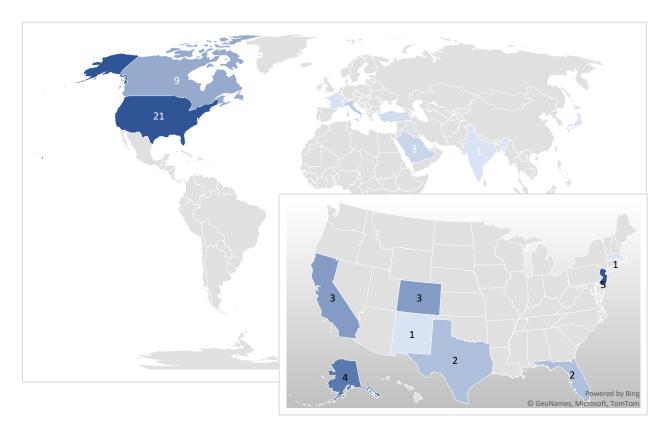
The Seismic Cycle Modeling Online Symposium October 17-19, 2022, brought together online a multidisciplinary group of researchers to discuss the many challenges associated with understanding and modeling the complexity of seismic processes in the oceanic and continental lithospheres. A total of 128 international participants attended at least one



of the three (3) days of the event. Recordings (21) of the event have a cumulative 494 views on YouTube. The program included a recorded pre-workshop presentation reviewing the theory and methods used in seismic cycle modeling. Presentations and discussion included topics on fault friction, fluids, and viscoelastic flow; structural complexity of fault zones; and off-fault deformation and the spectrum of fault slip. Discussions highlighted the complexity of the problems of interest and the broad spectrum of physics to be addressed. The community expressed an interest in module code or codes that are interoperable and use good engineering practices. A post workshop survey indicated that developers of several codes that are publicly available are interested in publishing and/or becoming part of the CIG community.

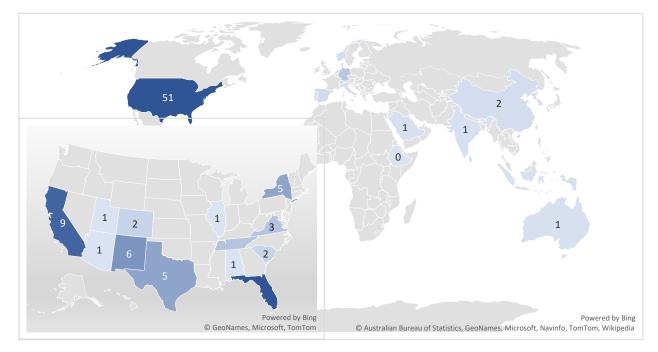
2022 SPECFEM In-person Workshop for Users and Developers

46 users and developers of the SPECFEM codes met October 27-28, 2022, in Toronto, Canada. This workshop was held prior to the SSA Seismic Tomography Conference to organize the community and discuss development plans for the SPECFEM family of codes. This first of its kind workshop brought together the international development community to discuss development directions and needs and gave participants an opportunity to share tools. The workshop launched a new SPECFEM website (specfem.org) and repository (https://github.com/SPECFEM). The community now uses GitHub discussions for communications and has established monthly community meetings. This workshop received funding from the University of Toronto.



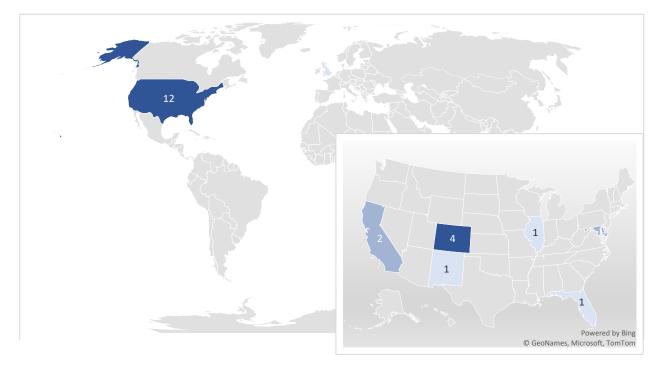
2023 ASPECT User Workshop

The fourth virtual ASPECT User Workshop took place January 31-February 1, 2023. 83 people attended the 2-day event. The workshop included an update to the user community on development of ASPECT, contributed keynote talks on slab dynamics, dynamics at plate boundaries, coupling to surface processes – landscape evolution and ore formation, and viscoelastic deformation and glacial mass. 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.



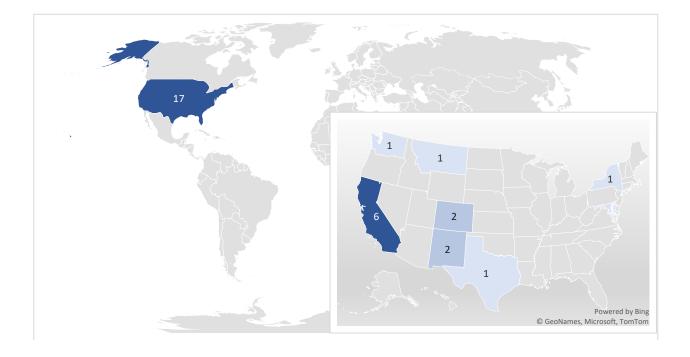
2023 Rayleigh Hackathon

The 2023 Rayleigh Hackathon was held in person on June 12-16, 2023, in Golden, Colorado. 13 people attended the event. Source code improvements completed included the reimplementation of a radial finite-difference scheme and coupled boundary conditions for multiscalar field mode. Projects initiated included the implementation of the pseudo-incompressible approximation and dynamic (in time) boundary conditions. In addition, participants contributed to improving code containerization and new tutorial notebooks.



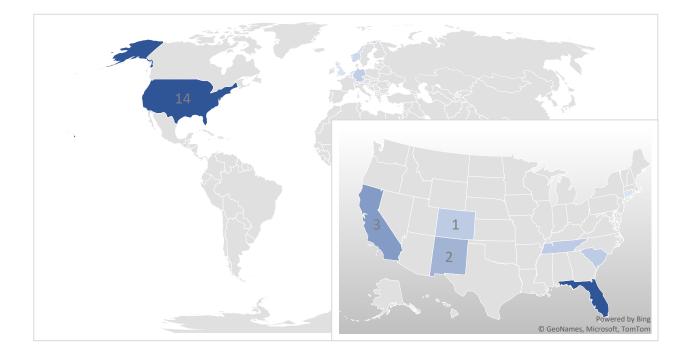
2023 PyLith Hackathon

The 2023 PyLith Hackathon was held in person from June 12-17, 2023, in Golden, Colorado. 18 people attended the event. Participants worked in teams on several ongoing development projects of interest to the community. The hack was centered around five projects: (1) spontaneous rupture using fault friction, (2) extending poroelasticity and adding new tests and examples, (3) developing 2D and 3D examples involving strike-slip faults, (4) integrating PyLith with the cascading adaptive transitional metropolis in parallel (CATMIP) Bayesian inversion framework for inverting for static fault slip, and (5) adding self-gravitation using the current multiphysics formulation in PyLith. Participants learned how to navigate the PyLith code base, how various features are implemented, how to make changes to the code, write examples, and implement tests. The core PyLith development team (Brad Aagaard, USGS; Matt Knepley, University of Buffalo; and Charles Williams, GNS) benefitted from discussions with the other participants about the technical aspects of the various projects as well as general discussions about PyLith design. The in-person format and 6-day duration allowed the groups to make significant progress. Participants appreciated the project-based organization of the hackathon and recommended that future hackathons include online meetings of the various projects before the in-person gathering to self-organize and prepare. Sarah Minson (USGS) provided technical advice on the use of the CATMIP Bayesian inversion framework.



2023 ASPECT Hackathon

The 2023 ASPECT Hackathon was held on July 6-15, 2023, in Lincoln City, Oregon. A total of 22 participants joined this hybrid event. Virtual participants (2) participated via Zoom, and Slack to participate in this 10-day coding event. This year's event focused on the improvement of installation and documentation, the addition of many example cases and benchmarks, and the integration of new features, in particular, to extend ASPECT for new applications. ASPECT's offline manual was removed in favor of an online hosted documentation system, and ASPECT's installation procedure was adapted to simplify shipping and distribution of binary packages, for example, in order to host ASPECT online executable tools on the CIG website. Notable new feature additions were merged including the modeling of crystal-preferred orientation of minerals in mantle flow. This development effort has been ongoing with CIG support for several years and will open up many new applications at the forefront of the field. In addition, significant progress has been made in coupling ASPECT to surface evolution models like FastScape, which when finalized, will open up another new field of applications for ASPECT.



Future Workshops

CIG plans to organize the following community workshops in 2023-2024 (Table 4).

Date	Title
August 10, 2023	Part I. Crafting Quality Research Software and Navigating Publication in Software Journals
September 9, 2023	Part II. Crafting Quality Research Software and Navigating Publication in Software Journals
January 2024	ASPECT User Workshop
February 2023	CIG Developers Workshop
Spring 2023	Challenges for Geodynamic Model Interoperability
April 2023	SPECEM Developer's Meeting
June 10-14, 2024	Crustal Deformation Workshop

Table 4. 2023-2024 Workshops and Tutorials



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 5).

Date	Presenters	Title	
January 12	Sujania Talavera-Soza Utrecht / UCSD	Global 3D model of mantle attenuation using seismic normal modes.	
February 9	Tobias Keller ETH Zürich	Genesis of the El Laco magnetite- apatite deposits by extrusion of iron- rich melt: a modelling perspective.	
March 9	Chase Million Million Concepts	Effective Strategies for Writing Proposal Work Plans for Research Software.	
April 17	Adina Pusok Oxford University	Making the Ocean Floor: Two-phase dynamics of mantle melting and formation of oceanic lithosphere.	

Table 5. 2023 Webinar Schedule

In 2023, the Seismic Cycles Working Group organized a follow-on to their 2022 webinar series focused on rock and fault mechanics (Table 6). The weekly webinars delivered to the community the latest research in advanced topics related to the importance of lithology, texture, and temperature on fault mechanics, the role of fluids in fault zones, and new observations on dynamic ruptures, foreshocks, and aftershocks in the laboratory. Isolating these effects in the laboratory and in the field will help the formulation of new constitutive laws for fault friction and the behavior of the surrounding rocks, allowing more realistic models. Its YouTube Playlist has over one thousand views.

Table 6. 2023 Seismic Cycles Webinar Schedule

Date	Title & Presenters
February 17	Tamara Jeppson, USGS. Complexities in Fault Healing: Evolution of the properties of shear fractures at hydrothermal conditions
February 24	Sharan Shreedharan, Utah State University. Frictional mechanics of shallow slow slip phenomena: An integrated perspective from experiments, numerical modeling and geophysical observations
March 3	Will Steinhardt, UC Santa Cruz. Physical Fault Models: Using Rubber Earthquakes to Understand Seismological Stress Drops and Earthquake Nucleation
March 10	John Bedford, University of Liverpool. <i>Fault strength evolution during the seismic cycle: Insights from the laboratory</i>
March 17	Monica Barbery, Brown University. <i>Exploring flash heating coupled</i> with mm-scale contact evolution in granite
March 24	Hanaya Okuda, University of Tokyo. Hydrothermal friction experiments on simulated basaltic fault gouge and implications for megathrust earthquakes
March 31	Christine McCarthy, Lamont Doherty Earth Observatory of Columbia University
April 7	Vito Rubino, Ecole Central de Nantes. <i>What can we learn about friction evolution and rupture behavior from laboratory experiments?</i>
April 21	Nicola Tisato, University of Texas at Austin. <i>Capturing co-seismic fault deformation and pseudotachylyte formation to unveil earthquake physics</i>
May 5	Lifeng Wang, State Key Laboratory of Earthquake Dynamics, China Earthquake Administration. <i>The role of fault asperity in the</i> generation of laboratory earthquakes.
May 12	Paul Selvadurai, ETH. Unravelling complex deformation and localization of brittle failure in triaxial tests on crystalline rock
May 19	Caroline Seyler, University of Southern California. <i>Measuring healing and failure in experiments on clay-bearing fault gouges</i>
May 26	Matej Pec, Massachusetts Institute of Technology. What does a Brittle-to-Ductile Transition Sound Like?
June 2	Karen Daniels, North Carolina State University. Looking inside granular materials
June 9	Marie Violay & Frederica Paglialunga, EPFL. <i>Mechanical behavior of lubricated faults during earthquake nucleation and propagation</i>

YouTube

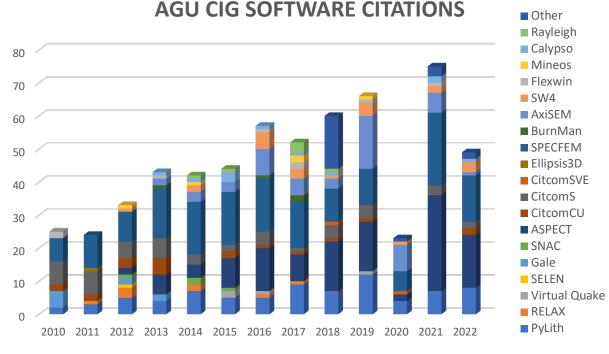
As of December 31, 2022, CIG's YouTube channel, CIG Geodynamics, hosts 307 videos of simulations contributed by the community, and recordings of past webinars and tutorials. The

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 1203 subscribers (up from 1070 in 2020) and approximately 96k 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 totaled 50 (Figure 4).

See Appendix C.



Appendix C.

Figure 4. 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 2022-2023 CIG Distinguished Speakers completed 5 visits (Table 7) 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 7. CIG Distinguished Speakers and Host Institutions

2021-2022	
Subducted Slabs, Mantle Plumes, and the Plate Tectonic Cycle	March 7: University of California Riverside March 10: University of Hawaii Manoa
Julianne Dannberg, University of Florida	March 30: University of Ottawa <i>virtual</i> March 11: Appalachian State University
Can we (yet) predict how fast Greenland is going to melt?	March 17: Virginia Tech
Mathieu Morlighem, Dartmouth College	April 14: Dakota Mines & Technology

The two 2023-2024 CIG Distinguished Speakers are:

- Harriet Lau, Brown University. Evolving Solid Earth Dynamics as a Trigger for the Mid Pleistocene Transition
- Miki Nakajima, University of Rochester. Origin of Moons in the Solar System and Beyond

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 23 user-developers who have made 1473 commits to the repository in 2022 as well as to the broader user community. Many of these commits have added major new features to the code and were incorporated into the latest release of the software in July 2023, ASPECT 2.5.0.

Significant accomplishments of the past year

ASPECT 2.5.0 was released on July 31, 2023. It included many changes (see <u>https://aspect.geodynamics.org/doc/doxygen/changes between 2 84 80 and 2 85 80.html</u> for details) including:

• ASPECT now includes version 0.5.0 of the Geodynamic World Builder.

- ASPECT's manual has been converted from LaTeX to Markdown to be hosted as a website at https://aspect-documentation.readthedocs.io
- ASPECT now requires deal.II 9.4 or newer.
- ASPECT now supports a DebugRelease build type that creates a debug build and a release build of ASPECT at the same time.
- ASPECT now has a CMake option ASPECT_INSTALL_EXAMPLES that allows building and installing all cookbooks and benchmarks. ASPECT now additionally installs the data/ directory. Both changes are helpful for installations that are used for teaching and tutorials.
- ASPECT now releases the memory used for storing initial conditions and the Geodynamic World Builder after model initialization unless an owning pointer to these objects is kept. This reduces the memory footprint for models initialized from large data files.
- Various helper functions to distinguish phase transitions for different compositions and compositional fields of different types.
- The 'adiabatic' initial temperature plugin can now use a spatially variable top boundary layer thickness read from a data file or specified as a function in the input file. Additionally, the boundary layer temperature can now also be computed following the plate cooling model instead of the half-space cooling model.
- ASPECT now supports tangential velocity boundary conditions with GMG for more geometries, such as 2D and 3D chunks.
- Phase transitions can now be deactivated outside a given temperature range specified by upper and lower temperature limits for each phase transition. This allows implementing complex phase diagrams with transitions that intersect in pressure-temperature space.
- There is now a post processor that outputs the total volume of the computational domain. This can be helpful for models using mesh deformation.
- Added a particle property 'grain size' that tracks grain size evolution on particles using the 'grain size' material model.

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

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.

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 July 2023.
- Holding bi-weekly online community meetings.
- Delivered tutorials at CIDER and 2023 CSDMS Annual Meeting

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

The Earth's inner core has solidified and grown with the cooling of the Earth in the last one billion years. Dr. Hiroaki Matsui (UCD) has performed dynamo simulations to investigate parameter ranges to sustain the intense magnetic field in the past Earth when the solid inner core was smaller than present day. He has and continues to investigate the dependency of the range of the amplitude needed for convection (Magnetic Reynolds number, Rm) to sustain the dipolar magnetic field and its dependency on the inner core size. The results² show that the lower limit of Rm increases with smaller inner core size, while there is almost no dependency of the upper limit of Rm to sustain the dipolar magnetic field.

Frontera

Calypso obtained good performance by using MPI and OpenMP hybrid parallelization for simulation and visualization modules for parallel volume rendering (PVR) and line integral convolutions (LIC). After the optimization of ordering of the loops, Calypso obtained approximately 30% better performance than the previous version.

Data in Calypso can be visualized during, and post simulation runs. PVR is used for visualization of the scalar component, and Parallel Line Integral Convolution (LIC), newly developed, to visualize vector fields. After implementing domain re-partitioning and sleeve extension modules

² Y. Nishida, H. Matsui, M. Matsushima, A. Kumamoto, and Y. Katoh, (submitted), Investigation of dipolar dominance in geodynamo simulations with different inner core sizes, Geophysical Journal International.

for LIC, good parallel performance for the LIC module for up to 28,672 cores was obtained. However, the elapsed time for the volume rendering and initialization of the simulations rapidly increases with the number of MPI processes. More investigations are warranted to find the best MPI and OpenMP configurations using more than 28,672 cores for the simulation and visualizations.

Project goals for the upcoming year

Investigations continue to under the required parameter ranges to sustain the intense magnetic field in the past Earth when the solid inner core is smaller than that in the present. Investigations planned include:

- Models in a full sphere without the solid inner core to investigate the past geodynamo before the solidification of the inner core.
- Models implementing thermal conduction and simple latent heat models at the inner core boundary (ICB). Recent studies suggest aspherical growth of the inner core and latent heat distribution. Models will investigate the effects of the aspherical latent heat and thermal structure on the ICB. This requires running simulations with varying amplitude of latent heat.

Frontera

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

Calypso has eight (8) active users in four (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.

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

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

Significant accomplishments (August 2022 - Jan 2023)

PyLith v3.0.3 was released in October 2022. This release included additional leveraging of PETSc routines for output and fixed several small bugs related to running in parallel and fault related integrations. Since the bugfix release, PyLith development focused on implementing a more modular approach for computing the terms in the finite-element integrations. The new approach allowed the kernels associated with the governing equations and bulk rheologies to be implemented with about 40% less code that is significantly easier to maintain.

Project goals for the upcoming year

Future implementation of features is guided by several target applications, including earthquake cycle modeling with quasi-static simulation of interseismic deformation and dynamic simulation of coseismic deformation, inversion of geodetic data for slow slip events, fault creep, and long-term fault slip rates and, quasistatic and dynamic modeling of fluids and faulting.

A new release v3.0.4 is planned for September 2023 which will include additional features and bug fixes.

See <u>Development Plans</u> which are part of the PyLith documentation.

Outreach and Broader Impacts

The PyLith development team presented three posters at the 2022 AGU Meeting, updating the community on PyLith development, including poroelasticity and fault friction. The e-Poster format enabled the developers to showcase the online documentation and tutorials.

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, especially features related to faults. PyLith tests using the Method of Manufactured Solutions verify several features that are not yet verified in the PETSc test suite.

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 were facilitated by two (2) hackathons. Development efforts include:

1. Documentation updates: The Rayleigh documentation underwent a substantial update and reorganization during the September hackathon. In addition, the webpage style was updated to reflect a more modern and streamlined look. <u>https://rayleigh-</u>documentation.readthedocs.io/en/latest/

2. Compositional convection: Rayleigh can now solve equation sets describing the evolution of multiple scalar fields, analogous to the temperature field. This major update to the code allows the user to model compositional convection and/or the movement of passive tracer fields. The former can be used to model the separation of iron from light elements in the Earth's liquid outer core, and the subsequent plating of iron onto the solid inner core.

3. Finite-difference discretization in radius: Rayleigh now allows the option to use 4th-order finite differences in the radial direction, in lieu of the standard Chebyshev approach. The radial grid afforded by the Chebyshev approach, which clusters grid points near the boundaries, can be overly constraining in systems where fine resolution is required in the interior region. This new option allows the user to specify the location of radial grid points to suit the problem under consideration. At the moment, a 4th-order scheme is employed, but future versions of the code will allow the user to specify the degree of accuracy employed in the scheme.

4. Model Data. A large number of Rayleigh simulations were generated as part of the INCITE project *Frontiers in Planetary and Stellar Magnetism Through High Performance Computing* supported by the Department of Energy. The data (90 TB) and tools are now available for download. The data consists of two (2) targets, the: 1. Geodynamo and 2. Jovian atmosphere. The parameters and visualization examples for each model are documented in the code manual.

Project goals for the upcoming year

The development team is in the process of completing documentation on new features which will be included in the September version release.

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

The fall SPECFEM user meeting spurred on several key initiatives for the community. This includes the launching of specfem.org. The new website is now the nexus to find information

on the project and get help with the code. Recurring developers' meetings have also been established led by Carl Tape, University of Alaska Fairbanks and Daniel Peters, KAUST. All versions of the code - SPECFEM2D, SPECFEM3D Cartesian and SPECFEM3D_GLOBE, have had a major versioned release and a regular release schedule is now being planned.

Under the leadership of Jeroen Tromp and Rohit Kakodkar, Princeton University, SPECFEM is working towards a new version that will unify the code base. SPECFEM Kokkos is a C++ implementation of the software suite using the Kokkos programming model. Kokkos, largely developed with national lab support, is a production level solution for writing modern C++ applications in a hardware agnostic way, thus allowing a single source code that can run across all modern architectures.

Outreach and Broader Impacts

The SPECFEM community continues to offer training workshops. This includes the 2022 SPECFEM virtual workshop for users offered by Carl Tape and Bryant Chow, University of Alaska Fairbanks and workshops through the NSF SCOPED project.

A follow-on SPECFEM Developer's meeting and a special session focusing on computational seismology is being planned for and in conjunction with the Seismological Society of America's Seismic Annual Meeting in April 2024.

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 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

The code repository for AVNI is now public: <u>https://github.com/globalseismology</u> and hosting services for the web portal have been configured at Princeton. Its website on globalseismology.og will be continually improved as papers on the project are published (Rapid prototyping, interactive visualization and data validation tools for models of planetary, *manuscript in preparation*)

Interactive research notebooks that introduce AVNI were released and deployed (https://geodynamics.org/tools/solidearth). Anyone with access can execute the code through their web browser without going through the overhead of buying hardware or installing software.

Outreach and broader impacts

The project was presented at 2022 AGU (https://agu.confex.com/agu/fm22/meetingapp.cgi/Paper/1190048).

AVNI software ecosystem was used in an undergraduate course at Princeton that offered a quantitative introduction to Solid Earth system science.

4.7 BurnMan

BurnMan is a Python library for generating thermodynamic and thermoelastic models of planetary interiors. The BurnMan project has seen active and intense development over the past year with the release of two releases (1.1.0 and 1.2.0). New features include among others a more flexible equilibration solver, the implementation of additional and recently published thermodynamic databases, new property models, and a new equation of state fitting function. In addition, the software was published in the Journal of Open Source software as a software publication.

5 Software Pipeline

5.1 GDMATE

The GeoDynamic Modeling Analysis Toolkit and Education (GDMATE) is an in-development software repository in its initial stages that 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 process their outputs (e.g., visualization). The underlying code will be written in software languages accessible to the broader geoscience community such as Python and will also be optimized for processing massive data sets and for use on HPC facilities. An extensive suite of educational modules will demonstrate both advanced applications of the software and the fundamental coding methods required for further development of existing or new applications. A key feature will be development in a Jupyter notebook environment and its execution on the CIG HUBzero[®] platform.

Significant accomplishments over the past year

Over the course of 2022-2023, the framework for GDMATE was developed with the following key accomplishments:

- Consulted with colleagues in the geodynamic community to identify best practices for project development.
- Created open-access GitHub repository (<u>https://github.com/gdmate/gdmate</u>).
- Established the project philosophy, guidelines for usage, and installation instructions, which are included in the project documentation.
- Created the initial codebase structure for deployment as an installable Python package.
- Collated a list of existing software that can be integrated within the project, as well as long-term software and scientific goals.
- Implemented automated testing via pytest and GitHub Actions, integrated source code with Jupyter notebooks to demonstrate code functionality and created online documentation with Sphinx and ReadtheDocs.

Outreach and broader impacts

At this stage, only a limited number of colleagues have provided feedback on the repository, with the initial phase of source code development beginning in Fall 2023. Our goal is to present the initial functionality during a CIG-led workshop in Summer 2024 while also seeking additional funding in Fall 2023 to further expand the codebase.

5.2 World Builder

The Geodynamic World Builder (GWB) is an open-source code library intended to set up initial conditions for computational geodynamic models and/or visualize complex 3d tectonic settings, in both Cartesian and Spherical geometries. The WorldBuilder project has published a major release in the reporting timeframe (0.5.0), which will be the last release before the software leaves its Beta status behind for version 1.0.0. The release included many new features, for example the implementation of a half-space cooling model for oceanic plates, a smooth temperature distribution for subducted plates that ensures mass conservation, a new gravity plugin system, a new smooth fault transition model, and optimizations to use the World Builder in massively parallel environments.

6 Scientific and Broader Impacts

6.1 Publications

Publications included in our database include refereed papers submitted by authors as well as those found through Google Scholar using keyword search by author, software package name, or DOI. In 2022, the community published 141 journal articles and 9 theses using CIG codes. See <u>Appendix D</u>.

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 continues planning efforts with the Modeling Collaboratory for Subduction SZ4D and CSDMS to further modeling needs and code interoperability between the communities. A joint workshop is planned for Spring 2024.

CIG is planning to hold a hands-on workshop in conjunction with the SCEC Annual meeting to further the publication of codes in JOSS. This is a follow-up activity for the Seismic Cycles Working Group in promoting open-source codes for seismic cycle modeling. A special issue of JOSS is in the planning stages.

CIG is supporting a one-day ASPECT tutorial at the IMAGinING RIFTING Workshop, which will be held in Marrakech (Morocco) on October 23-27, 2023.

CIG will also cosponsor a session on SSA to promote the inclusion of more topics in computational seismology.

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 staff and community members also act as reviewers for software journals like the Journal of Open-Source Software, and SoftwareX, and domain journals such as Seismological Research Letters and Geoscience Data Journal. In addition, CIG staff and community members act as maintainers for the underlying computational science libraries (in particular PETSc and deal.II) that are essential dependencies of CIG software.

CIG is leading efforts to set up a Diamond Open Access Journal (DOAJ) focused on publishing research in the fields of geodynamics and geodynamic modeling. A core team of six researchers and faculty members from the US and Europe have organized and put forth an action plan. This community-led initiative, like several other DOAJs that were created in recent years, intends to tackle the unfairness of the classical for-profit publishing. It is part of a growing movement within academia that aspires to a more open science landscape.

7 CIG III 5-Year Budget

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

Total 5-year commitment by NSF: \$8.82 M

In 2020-23, in kind support for computational time was received from XSEDE and Frontera.

Appendix A: Institutional Membership

U.S. Institutions (68)

Argonne National Laboratory (MSC) Arizona State University^M **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^M 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^M University of Arizona^M University of California, Berkeley University of California, Davis^M University of California, Los Angeles University of California, San Diego University of California, Santa Cruz^M University of Colorado University of Connecticut University of Florida University of Hawaii^M University of Houston^M 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^M 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^M 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

[™]Minority Serving Institution

Appendix B: CIG Working Group Members

Research Software (3)

- Brad Aagaard, U.S. Geological Survey
- Rene Gassmoeller, University of Florida
- Lorraine Hwang, University of California Davis

Dynamo<u>(8)</u>

- 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 (8)

- Juliane Dannberg (University of Florida)
- Gabriele Morra (University of Louisiana at Lafayette
- John Naliboff (New Mexico Tech)
- Max Rudolph (University of California Davis)
- Sarah Stamps (Virginia Tech)
- Iris van Zelst (German Aerospace Center, DLR)
- SSC Liaison: Adam Holt (University of Miami)
- CIG Liaison: Moh Gouiza (University of California Davis)

Long-Term Tectonics

Magma Migration

Mantle Convection

Seismic Cycles

- 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

7.1.1 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

7.1.2 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: 2022 Fall AGU Presentations

List of presentations by CIG scientists at the 2022 Fall AGU meeting. This list combines of self-reported abstracts with keyword search on software package names.

Monday, December 12

<u>DI13A-01</u>. Exploring the Cascadia slab structure coupling 3D thermomechanical and CPO modeling. *Menno Fraters, Magali I Billen, John B Naliboff, Lydia Staisch and Janet Tilden Watt.* <u>S12A-01</u>. An overview of global full-waveform inversion workflow. *Andrea Riano Escandon, Ridvan Orsvuran, Armando Espindola-Carmona, Quancheng Huang, Ebru Bozdag, and Daniel B Peter.*

<u>S12A-07</u>. ATLAS3D: Multiscale Model Assimilation & Reconciliation of Heterogeneity in the Earth's Mantle. Raj Moulik, Frederik Simons, and Anant Hariharan.

<u>S12A-12</u>. Towards "box tomography" of ultra-low velocity zones at the earth's core-mantle boundary. *Chao Lyu, Hengyi Su, Carl Martin, Yder Masson and Barbara Romanowicz.*

<u>S12A-13</u>. Waveform Modeling of Seismic Records from MERMAID (the Ultimate Emerging Hardware). *Sirawich Pipatprathanporn* and *Frederik J Simons*.

<u>S12E-0186</u>. Amplification of Torsional Ground Motion in 2-D Heterogeneous Elastic Medium. *Varun Singla and Ivan Lokmer.*

<u>S12F-0197</u>. Poroelastic Faulting in Pylith. *Robert Lewis Walker II, Matthew Knepley, Brad Aagaard, Charles A Williams Jr and Shengduo Liu.*

<u>S12F-0203A</u>. Numerical Experiment in Small-Angle Scattering: From X-Ray to Seismology. *Solymar Ayala Cortez, Aaron A Velasco and Steven H Harder.*

<u>S15B-05</u>. Adjoint-State Surface Wave Tomography: Incorporation of Surface Topography and Application in Hawaii. Ping Tong, Shijie Hao and Jing Chen.

<u>T11A-01</u>. A comparison of free-surface numerical simulations of rifting based on ASPECT. *Min Seok Jang, Byung-Dal So and Young-Gyun Kim.*

<u>T12C-0111</u>. Straight from the Source: Towards Simulation of Dike Injection Governed by Melt Supply in Long-Term Tectonic Models. *Daniel King and Eric L Mittelstaedt.*

<u>T12E-0127</u>. Effects of Elastic Heterogeneity on Finite Source Inversion: Comparison with Okada Model. *Minsu Kim and Byung-Dal So.*

<u>T15A-04</u>. Investigating Melt Generation Beneath the Northern Western Branch of the East African Rift System Using 3D Geodynamic Modeling with ASPECT. *Asenath Kwagalakwe, D. Sarah Stamps, Emmanuel Atem Njinju, Estella A Atekwana and John Mary Kiberu.*

<u>T15E-01613D</u>. Modeling of Dynamics in the Hikurangi-Kermadec Subduction System. *Daniel Douglas, John B Naliboff, Menno Fraters, Donna Eberhart-Phillips, Susan M Ellis and Juliane Dannberg*.

Tuesday, December 13

<u>DI22B-0001</u>.Three-dimensional Reference Earth Model Project: Data, Techniques, Models & Tools. *Pritwiraj Moulik* and the 3D Reference Earth Model (REM3D) Consortium.

<u>DI23A-07</u>. Lithospheric Thermal Models from Seismic Fields. *Amanda Leaman, Anthony R Lowry, Derek Schut and Patrick Ball.*

<u>DI32B-0013</u>. Magnetic Raynolds number range to sustain dipolar magnetic field in geodynamo simulations with different inner core sizes. *Hiroaki Matsui, Yuki Nishida, Masaki Matsushima, Atsushi Kumamoto and Yuto Katoh.*

P22E-2118. BALLOON BORNE VENUS SEISMOLOGY : TOWARDS A PRELIMINARY NOISE MODEL.
 David Mimoun, Raphael F. Garcia, Solène Gérier, Pierre Raynal, Ervan Kassarian, Marie Lou
 Davezac, Daniel C Bowman, Siddharth Krishnamoorthy, Albert Hertzog and James A Cutta.
 P22E-2119. Infrasound from large earthquakes: numerical modeling and analysis of
 stratospheric records. Solène Gérier, Raphael F. Garcia, Pierre Raynal, Albert Hertzog and Roland
 Martin.

<u>P26B-06</u>. Modeling earthquake-generated infrasound wavefields on Venus. *John Wilding, Leo Martire, Siddharth Krishnamoorthy, James A Cutts, Leah Sabbeth and Jennifer M Jackson.*

<u>S22D-0197</u>. Simulation of Strong Ground Motion Data from the 18 March 2020 M_w 5.7 Magna, Utah, Earthquake to Evaluate the Wasatch Front Community Velocity Model (WFCVM). *Sean Hutchings, Keith D. Koper and Arben Pitarka*⁻

<u>S25A-02</u>. Implementing Earthquake Cycle Simulations in PyLith. *Kali L Allison, Brad Aagaard and Matthew Knepley.*

<u>S25A-03</u>. New Features in PyLith Version 3 Including Multiphysics Capabilities and Higher Order Discretizations. *Brad Aagaard, Matthew Knepley and Charles A Williams Jr.*

<u>T22A-05</u>. Isolating the Thermal Effects of Continental Collision using Dynamic Subduction Models. *Valeria Turino and Adam Holt.*

<u>T22D-0128</u>. Effect of crustal flow on bivergent metamorphic core complex exhumation and detachment faulting in western Anatolia. *Omer Bodur, Oguz Gogus, Dr. Sascha Brune, Ebru Sengul Uluocak, Anne Glerum and Hasan Sözbilir, Dokuz.*

<u>T25D-0154</u>. Influence of Farallon Slab Loading on the Intraplate Stress Field of Eastern North America: Implications for Intraplate Seismicity. *Erin Hightower, Michael Gurnis, and Wei Mao.*

Wednesday, December 14

<u>DI32B-0008</u>. The Depth Dependence of Seismic Scattering in the Inner Core. *Ravi Wickramathilake and Vernon F Cormier.*

<u>DI32C-0020</u>. Modeling Mechanisms for Trench Parallel Flow in the Cocos-Nazca Subduction System. *Bailey Valint and Margarete Ann Jadamec.*

<u>DI32C-0028</u>. Three-Dimensional Dynamics of Asthenospheric Flow and Plate Motion in the Boso Triple Junction. *Jane Halfhill and Margarete Ann Jadamec.*

<u>DI32C-0029</u>. Numerically Modelling Along-strike Rheologic Variations in 3D Subduction Zones. Derek J Neuharth, Whitney M Behr and Adam Holt.

<u>DI35A-07</u>. Influence of depth-dependent thermal conductivity on numerical dynamos, and implications for geodynamo evolution. *Peter Driscoll, Cian Wilson, and Kai Luo.*

<u>P35F-1925</u>. Synthetic Modeling of Multi-Offset GPR and Seismic Data for Void and Buried Rock Detection on the Moon. *John Coonan, Linden Wike, Doyeon Kim, Rebecca R Ghent, Sarah Kruse, Vedran Lekic, Jacob A Richardson and Nicholas C Schmerr.*

<u>S35C-03</u>. Toward a Green function database for Global 3-D centroid moment tensor inversions. *Lucas Sawade, Liang Ding, Meredith Nettles, Goran Ekstrom, Qinya Liu and Jeroen Tromp.*

<u>T32E-0205</u>. Role of the Andean structure in the Post-Seismic Deformation Following the 2014 Mw 8.1 Iquique Earthquake in Chile: New insights from a Finite Element Model Constrained by GNSS and InSAR Data. Juliette Cresseaux, Anne Socquet, Mathilde Radiguet, Marie-Pierre Doin, David Marsan, Mathilde Marchandon, Flora Huiban, Rémi Molaro-Maqua, Marcos Moreno and Gaëlle Deschamps-Huygen.

Thursday, December 15

<u>DI45A-0012</u>. Effects of Core-Mantle Boundary Topography in Lower Mantle Dynamics. *Alina Valop and Scott D King.*

<u>DI45A-0015</u>. Phase transitions impact variations in layering of convection throughout Earth's history: Insights from a new entropy method. *Ranpeng Li, Juliane Dannberg, Rene Gassmoeller, Carolina R Lithgow-Bertelloni and Lars P Stixrude.*

<u>DI45C-0041</u>. Changing Patterns in Core-Mantle Boundary Heat Flux Throughout the Past Billion Years of Earth's History. *Frederick S Lacombe, Juliane Dannberg, Rene Gassmoeller, Courtney Jean Sprain and Daniele Thallner.*

<u>S41C-04</u>. Investigation of complex seismic wave propagation in sedimentary basins via 3-D waveform modeling. *Yuan Tian, Carl Tape, and Bryant Chow.*

<u>S42A-01</u>. Do Strain-rate Variations Determine Where Deep Earthquakes Occur in Subducting Slabs? *Rebecca Fildes* and Magali Billen.

<u>S42B-02</u>. Topography Effect on Seismic Waveform Tomography: A Quantitative Study. *Kaiyue Zheng, Yi Wang, and Li Zhao.*

<u>S46A-023D</u>. High-Frequency Ground Motion Simulations of the M_w6.0, 24 August 2016 Amatrice, Italy Earthquake; validations against observations and ground motion models. *Aybige Akinci, Arben Pitarka, Pietro Artale Harris, Pasquale De Gori and Mauro Buttinelli.* <u>T42C-0139</u>. Numerical Modeling of Transient Crustal Deformation in the Korean Peninsula after the 2011 Tohoku Earthquake. *Eunseo Choi, Ryann Lam, Khadija Nadimi and Seok Goo Song.* <u>T43A-03</u>. An Updated Episodic Tremor and Slip Catalog for Cascadia. *Noel M Bartlow and Charles A Williams Jr.*

<u>T43B-06</u>. Role of surface processes in controlling the evolution of rifting in Ethiopia. *Ameha Muluneh, Dr. Sascha Brune, Giacomo Corti and Derek Keir.*

<u>T45A-25</u>. Magmatic fluids and upper mantle earthquakes in cratonic rifts: Examples from East Africa. *Eduardo Arzabala, Cynthia J Ebinger, Aude Lavayssière, Connor Drooff and Derek Keir.* <u>T45D-0149</u>. Fault zone evolution along complex plate boundaries: A case study from the Eastern California shear zone. *George Pharris, John B Naliboff and Veronica Prush.*

Friday, December 16

<u>DI53A-03</u>. Do Mantle Plumes Merge? Joseph Lewis-Merrill, Wan Ki Lo, Kavya Agarwa and Carolina R Lithgow-Bertelloni.

<u>DI53A-04</u>. Higher-order Accurate Particle Methods Improve Models of Transient Geodynamic Processes: Benchmarks and Applications. *Rene Gassmoeller, Juliane Dannberg, Elbridge Gerry Puckett, Mack Gregory, Cedric Thieulot and Wolfgang Bangerth.*

<u>S52E-0093</u>. Where do Underground Explosion Wavefields Fully Transition to Purely Elastic? *Carene S Larmat, Zhou Lei, Bryan Euser and Howard J Patton.*

<u>S52E-0096</u>.Numerical Modelling of a Meteorite Impact Seismic Source Using the Stress Glut Theory. *Marouchka Froment, Philippe Henri Lognonné, Carene S Larmat, Zhou Lei, Esteban Rougier and Taichi Kawamura.*

Appendix D: Publications

Articles in 2022 using CIG codes either reported by authors or discovered using keyword and DOI searches on google scholar.

2022 Publications

- 1. Abrahamson, Norman, Camilo Pninlla-Ramos, Payman Tehrani, Michael Perez, Alex Krimotat, (2022), "Modeling of Vertical Component Ground Motion for Soil-Structure-Interaction Analyses", *Transactions*, SMIRT-26: July 10-15, 2022.
- Abreu, R., Peter, D., Thomas, C., (2022), "Reduction of wind-turbine-generated seismic noise with structural measures", *Wind Energy Science*, 7, 3: pg: 1227-1239, (DOI: 10.5194/wes-7-1227-2022).
- Adourian, S., Lyu, C., Masson, Y., Munch, F., Romanowicz, B., (2022), "Combining different 3-D global and regional seismic wave propagation solvers towards box tomography in the deep Earth", *Geophysical Journal International*, 232, 2: pg: 1340-1356, 10, (DOI: 10.1093/gji/ggac394).
- 4. Altoé, Isabella Lorrainy, (2022), "Thermo-Compositional Structure of the North and South American Cratonic Lithosphere", pg: 169, Imperial College London, Department of Earth Science and Engineering, April.
- 5. Altoe, Isabella, Goes, Saskia, Assumpção, Marcelo, (2022), "Thermo-compositional structure of the South American Platform lithosphere: Evidence of stability, modification and erosion", *Geochemistry, Geophysics, Geosystems*, 23, 11: pg: e2022GC010516, (DOI: 10.1029/2022GC010516).
- Andric, T., (2022), "Providing priors to Bayesian array optimization for the Sardinian candidate site of the Einstein Telescope", IL NUOVO CIMENTO, 45, 183: (DOI: 10.1393/ncc/i2022-22183-7).
- Artale Harris, P., Scognamiglio, L., Magnoni, F., Casarotti, E., Tinti, E., (2022), "Centroid Moment Tensor Catalog With 3D Lithospheric Wave Speed Model: The 2016–2017 Central Apennines Sequence", *Journal of Geophysical Research: Solid Earth*, 127, 4: pg: e2021JB023068, (DOI: 10.1029/2021JB023068).
- Ba, Zhenning, Wu, Mengtao, Liang, Jianwen, Zhao, Jingxuan, Lee, Vincent W., (2022), "A two-step approach combining FK with SE for simulating ground motion due to point dislocation sources", *Soil Dynamics and Earthquake Engineering*, 157: pg: 107224, (DOI: 10.1016/j.soildyn.2022.107224).
- 9. Bahadori, Alireza, Holt, William E., Austermann, Jacqueline, Campbell, Lajhon, Rasbury, E. Troy, Davis, Daniel M., Calvelage, Christopher M., Flesch, Lucy M., (2022), "The role of

gravitational body forces in the development of metamorphic core complexes", *Nature Communications*, 13, 1: pg: 5646, Sep, (DOI: 10.1038/s41467-022-33361-2).

- Bahadori, Alireza, Holt, William E., Feng, Ran, Austermann, Jacqueline, Loughney, Katharine M., Salles, Tristan, Moresi, Louis, Beucher, Romain, Lu, Neng, Flesch, Lucy M., Calvelage, Christopher M., Rasbury, E. Troy, Davis, Daniel M., Potochnik, Andre R., Ward, W. Bruce, Hatton, Kevin, Haq, Saad S. B., Smiley, Tara M., Wooton, Kathleen M., Badgley, Catherine, (2022), "Coupled influence of tectonics, climate, and surface processes on landscape evolution in southwestern North America", *Nature Communications*, 13, 1: pg: 4437, Aug, (DOI: 10.1038/s41467-022-31903-2).
- 11. Baron, Julie, Primofiore, Ilaria, Klin, Peter, Vessia, Giovanna, Laurenzano, Giovanna, (2022), "Investigation of topographic site effects using 3D waveform modelling: amplification, polarization and torsional motions in the case study of Arquata del Tronto (Italy)", *Bulletin of Earthquake Engineering*, 20, 2: pg: 677-710, Jan, (DOI: 10.1007/s10518-021-01270-2).
- Beghein, C., Li, J., Weidner, E., Maguire, R., Wookey, J., Lekić, V., Lognonné, P., Banerdt, W., (2022), "Crustal Anisotropy in the Martian Lowlands From Surface Waves", *Geophysical Research Letters*, 49, 24: pg: e2022GL101508, (DOI: 10.1029/2022GL101508).
- Bening, Maulidia A., Sahara, David P., Triyoso, Wahyu, Kusumawati, Dian, (2022), "Modeling the Impact of the Viscoelastic Layer Thickness and the Frictional Strength to the Lithosphere Deformation in a Strike-Slip Fault: Insight to the Seismicity Pattern along the Great Sumatran Fault", *GeoHazards*, 3, 4: pg: 452-464, (DOI: 10.3390/geohazards3040023).
- 14. Bhakta, Tuhin, Bob Paap, Vincent Vandeweijer, (2022), "Monitoring of CO2 plume movement using time-lapse distributed acoustic sensing (DAS) data", *Second International Meeting for Applied Geoscience & Energy*, August.
- Bishop, Jordan W., Fee, David, Modrak, Ryan, Tape, Carl, Kim, Keehoon, (2022), "Spectral Element Modeling of Acoustic to Seismic Coupling over Topography", *Journal of Geophysical Research: Solid Earth*, 127, 1: pg: e2021JB023142, (DOI: 10.1029/2021JB023142).
- Blanco-Martín, Laura, Jahangir, Emad, Rinaldi, Antonio P., Rutqvist, Jonny, (2022), "Evaluation of possible reactivation of undetected faults during CO2 injection", *International Journal of Greenhouse Gas Control*, 121: pg: 103794, (DOI: 10.1016/j.ijggc.2022.103794).
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