COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Meeting Summary

2020 CIG Community Workshop: Advancing Our Understanding of Earth Dynamics in CIG IV

MEETING SUMMARY

The 2020 CIG Community Workshop: Advancing Our Understanding of Earth Dynamics in CIG IV was held over 3 days from 13-15 October 2020. The workshop brought together the geophysics community to address the science that drives computational geophysics and the development of state-of-the-art software. Building the capacity for leadership level computation and promoting the use of cutting-edge algorithms throughout the CIG community demands a broad vision that includes community education, resource development, and increasing and supporting computational expertise to make computing more approachable and accessible. Outcomes from this workshop will inform the development of the CIG IV proposal in 2021.

To promote discussions and give rise to ideas from the community on a broad range of science and infrastructure issues, the agenda included summary science and infrastructure presentations (invited), idea talks (contributed), and a panel whose members pre-recorded presentations to be viewed prior to the start of the workshop. Breakout sessions gave participants the opportunity to discuss presentations and voice their own ideas. Poster talks were included as optional either before or after the 4 ½ hr plenary sessions. See Appendix A.

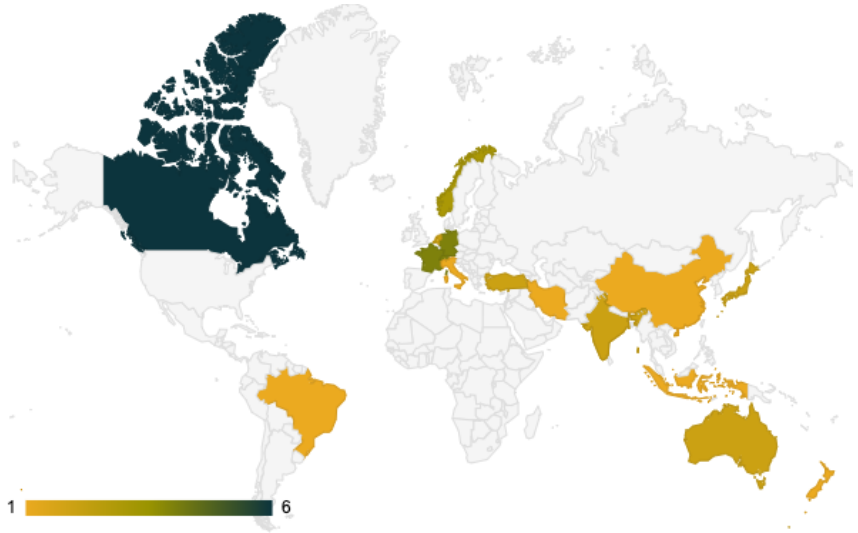

Figure 1. International participation for the workshop came from 17 countries not counting the U.S.

Presented below are the demographics of the participants who registered with Zoom. We are unable to determine the number of unique participants as Zoom reporting was only available for the first 2 days of the workshop. For the first 2 days, there were 110 unique participants out of a total of 141 registrants (See Appendix B).

Of the 141 registrants, 39 (28%) were from outside the United States (Figure 1).

Registrants primarily identified as white (Figure 2) and male (Figure 3) which is reflective of the larger earth sciences community in which 85% of the Ph.D.s awarded at U.S. Institutions in 2016 were awarded to non-Hispanic whites and 74% to males.[1] In general amongst the registrants, the CIG community is less white (66%) and less male (63%) (note that graduate students who have not completed their degree are included in our numbers. Figure 4 shows the career demographics) but there is substantial progress that still needs to be made if we are to become representative of U.S. population. **Lack of diversity was seen as both a key issue and opportunity for our community.** Speakers stressed the importance of mentoring and early engagement for retention in STEM. **This promoted discussions of how to improve geodynamics teaching and pipeline encompassing reaching out to undergrads and making our software more accessible.**

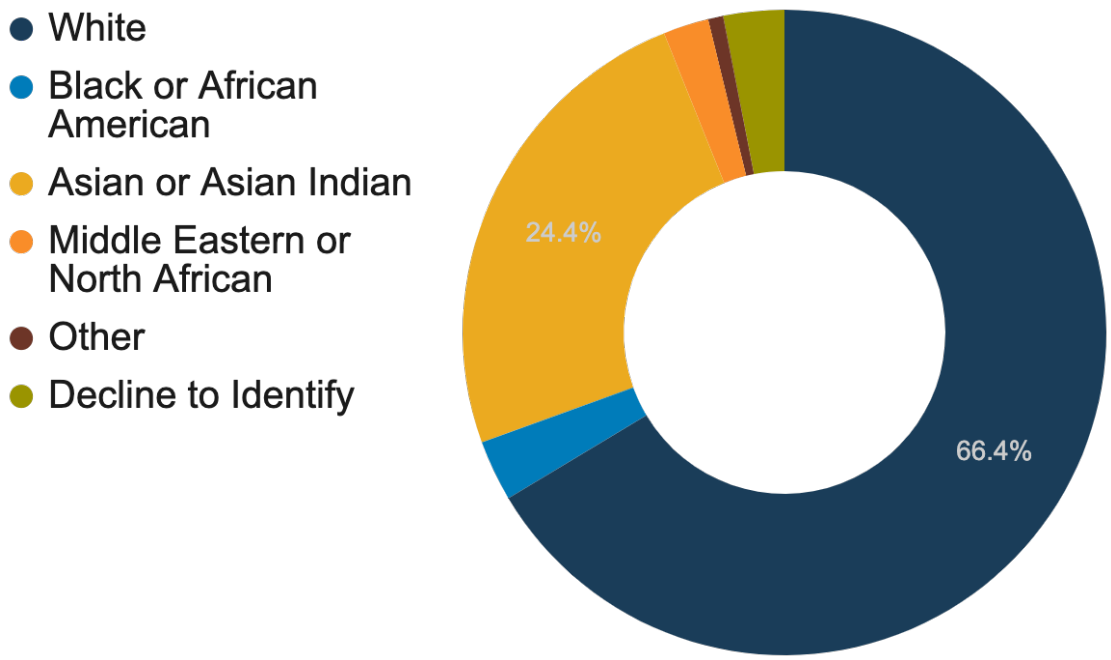

Figure 2. Participant responses when ask to self-identify their race or ethnicity.

[1] https://www.nature.com/articles/s41561-018-0116-6

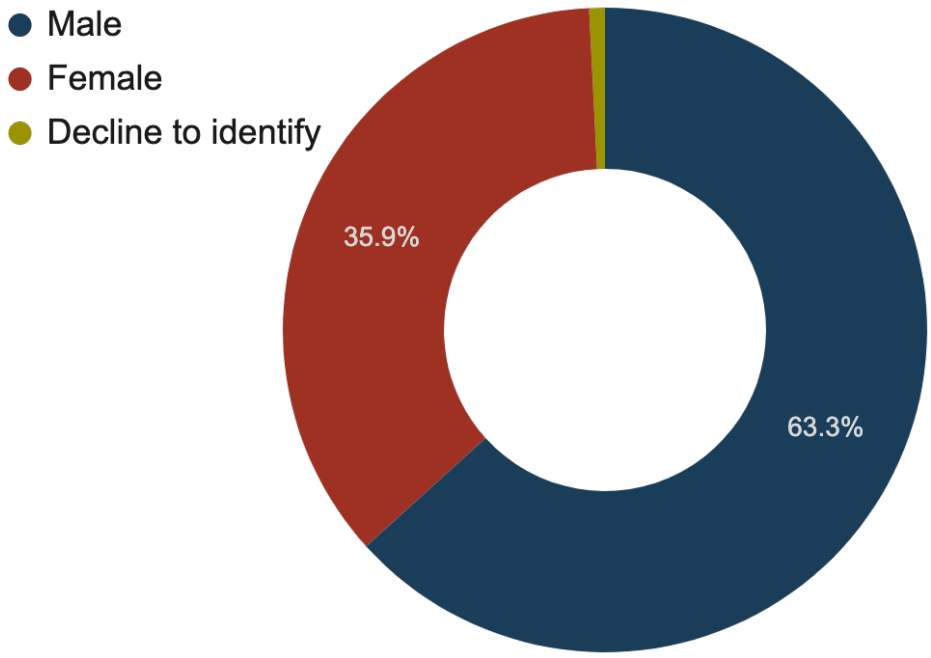

Figure 3. Participant responses when ask to self-identify their gender.

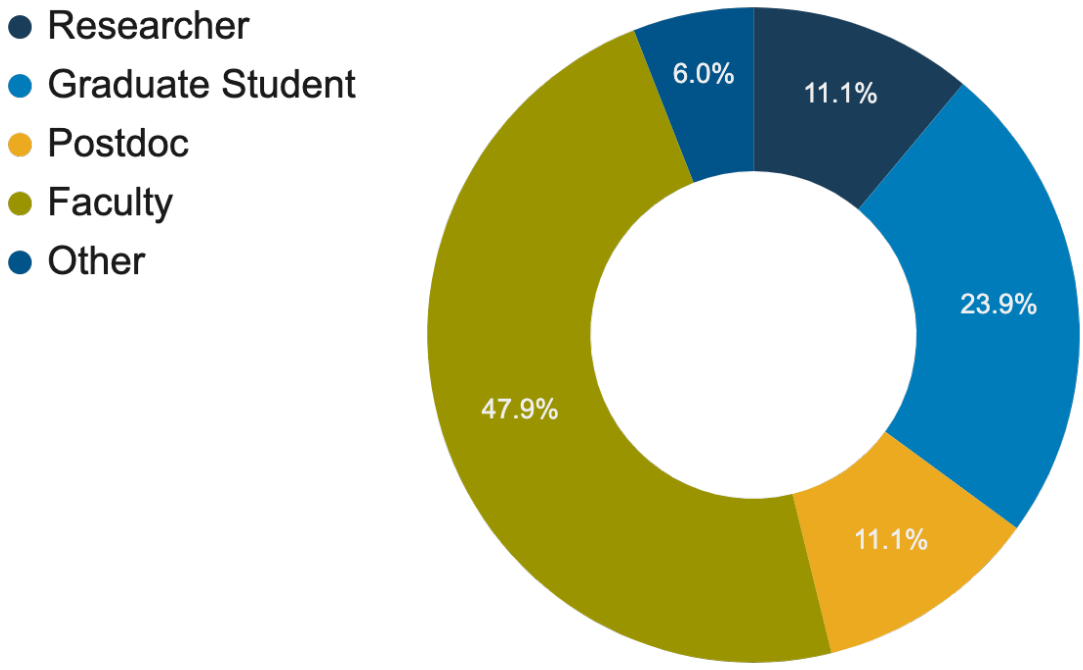

Figure 4. Participant responses when ask to self-identify their career status.

Registrants indicated primary interests across multiple domains (on average 2.6) that CIG traditionally identifies with (Figure 5). **This both confirms the cross-cutting nature of our science and led to discussions within Breakout Sessions that Working Groups should be more focused on processes and not on a layered Earth.**

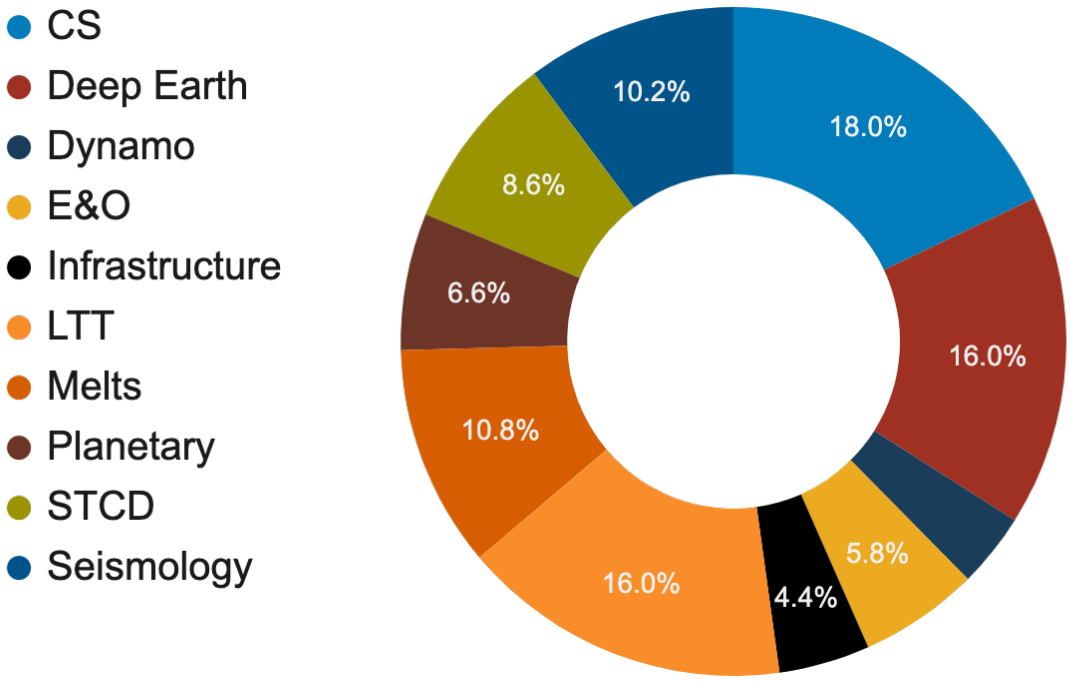

Figure 5. Participant responses when ask to self-identify their primary areas of interests. Participants were allowed to choose more than one.

The multidisciplinary nature of our science combined with the nature of our organization - infrastructure, leads us to ask the fundamental question - **what is the infrastructure necessary to prepare our community for leading edge science?**

CIG as a catalyst for future bleeding-edge research should support development of code that facilitates other (especially NSF-funded) computational research. Hence, this workshop revealed the need to **create connections to communities** e.g. RCNs such as SZ4D that are science driven and to explore intersectionality to other earth science infrastructure organizations e.g. CSDMS & IRIS.

In addressing infrastructure, other key themes and actions:

- Creating a more responsive governance, documenting and, where needed, developing policies; and engaging a large number of enthusiastic early career scientists.

        - Working Groups (WGs) are the link between CIG leadership and the broader CIG community.
            - **Action.** Define an open process for formation and membership of WGs as well as tenure.
            - **Action.** Define the scope of activities supported as well as accountability for execution
            - **Action:** Form WGs around processes and/or activities; de-emphasize a layered Earth approach.
- Continually improving our Best Practices including best practices in growing and sustaining communities.
    - **Action.** Clarify how to contribute to projects
- Redefining what it means to be CIG community software taking advantage of the modern software ecosystem and learning from each other (cross pollination between groups)
    - **Action.** Create opportunities through workshops or committees for community members to interact.
- Building computational modeling and software skills in geodynamics
    - **Action.** Asynchronous learning materials in the form of online tutorials and guides targeting new users.
    - **Action.** Integrating geodynamic specific training & education with software training.
- Increasing diversity in the geosciences.
    - **Action.** Create pathways to reach out to underrepresented groups.
- Increasing accessibility to software making it easier to deploy and use through better user interfaces and access to HPC.
- Data
    - Standardization of models and interfaces
    - Flexible and parallel visualization platforms.
    - Incorporation of observational data into simulations

See Appendix C for key points as summarized by each Breakout Groups.

The above is not by any means an exhaustive list of items discussed. CIG is will continue to incorporate the information discussed during this Workshop and preceding activities in planning for CIG IV.

More workshop information can be found at:
https://geodynamics.org/cig/events/calendar/2020-community-workshop/

Individual links to talks are found in Appendix A. The full meeting playlist can be found on YouTube:
https://www.youtube.com/playlist?list=PLdy04DoEepEyoYhDqJ2Cjgy01eS0-CnTf

Appendix A. Agenda

Prerecorded Talks

Please view prior to the beginning of the workshop to learn more about these communities and their activities.

- **Meeting Welcome**. Lorraine Hwang, *Director, UC Davis* [**YouTube**]*;* Scott King, *Chair SSC, Virginia Tech* [YouTube]
- **CIG Retrospective**. Lorraine Hwang, *Director, UC Davis* [**YouTube**]
- **NSF Opportunities for Geoinformatics.** Eva Zanzerkia, *Program Director, NSF* [**YouTube**]
- **NAS - A Vision for NSF Earth Sciences 2020-2030: Earth in Time**. Carolina Lithgow-Bertelloni, *UC Los Angeles* [**YouTube**]
- **The SZ4D Initiative: Planning a Decadal Effort to Understand Processes that Underlie Subduction Zone Hazards**. Harold Tobin, *University of Washington* [**YouTube**]
- **An Update on the Proposed IRIS-UNAVCO Merger.** Rick Aster, *Colorado State University;* Becks Bendick*, UNAVCO;* Lucy Flesch, *Purdue University;* Bob Woodward, *IRIS* [**YouTube**]
- **Overview of the Community Surface Dynamics Modeling System (CSDMS)**. Greg Tucker, E*xecutive Director, CU Boulder* [**YouTube**]

Session 1: Deep Earth Dynamics and the Dynamo

DAY 1 - TUESDAY OCTOBER 13

08:00		**WELCOME**
08:10		**PLENARY 1A**
	20min	**How to model a living planet?** John Hernlund, *Earth-Life Science Institute, Tokyo Institute of Technology* [**pdf**] [**YouTube**]
	20min	**Computational advances and challenges in planetary dynamo modelling.** Julien Aubert and Thomas Gastine, *Institut de Physique du Globe de Paris* [**pdf**] [**YouTube**]
	10min	Discussion
09:00	30min	**PANEL Q&A** *please submit questions by October 12 to* ***events@geodynamics.org***

- Rick Aster, *Colorado State University*
- Carolina Lithgow-Bertelloni, *UC Los Angeles*
- Harold Tobin, U*niversity of Washington*
- Eva Zanzerkia, *Program Director, NSF*

- Greg Tucker*, Executive Director, University of Colorado Boulder*

09:30	15min	**BREAK**
09:45		**IDEA TALKS 1** **1. Infrastructure and how it might help CIG with Diversity, Equity, and Inclusion.** Scott King, *Virginia Tech* **2. Building communities around scientific software.** Wolfgang Bangerth, *Colorado State University* **3. Increasing diversity in the Geodynamics Community through Research Undergraduate Experiences (REUs)**. John Naliboff, *New Mexico Tech*, Lorraine Hwang, *UC Davis*; Dave Stegman, *UC San Diego* [**pdf**] **4. Extending CIG's Influence on Spreading Best Software Practices.** Rene Gassmoeller, *University of Florida* [**pdf**] **5. Extroverted geodynamics: enabling code usage by a wider user base.** Laurent Montesi, *University of Maryland*
10:10	60min	**BREAKOUT 1**
11:10	30min	**REPORT BACK**
11:40		**PLENARY 1B**
	20min	**Broadening diversity and inclusiveness in a quantitative, computational world.** Sharon Mosher, *University of Texas Austin* [**pdf**] [**YouTube**]
	20min	Juan E. Gilbert, *University of Florida* [**YouTube**]
12:20		**Open discussion on Diversity, Equity, and Inclusion** **ADJOURN**
1:00 P	60min	*Poster 1 Q&A will begin 15 min after the meeting adjourns* [**figshare**] [**schedule**]

Session 2: Short Term Crustal Deformation and Melts and Volatiles

DAY 2 - WEDNESDAY OCTOBER 14

07:05	40min	*Poster 2 Q&A will end 15 min prior to the start of the plenary session* [**figshare**][**schedule**]
08:00		**KEYNOTE: CIG IV**
08:15		**PLENARY 2A**
	20min	**Advances and Challenges in Understanding Fault loading, Inter seismic - and Post seismic Deformation.** Ylona van Dinther, *Utrecht University* [**YouTube**]

	20min	**Modeling earthquake source processes: From tectonics to dynamic rupture.** Nadia Lapusta, *Caltech* [**pdf**] [**YouTube**]
	20min	**Modeling fluid migration in subduction zones: Community perspectives from a MCS RCN workshop.** Ikuko Wada, *University of Minnesota* [**pdf**] [**YouTube**]
	10min	Discussion
09:25	15min	**BREAK**
09:40		**PLENARY 2B**
	20min	**Generating and using thermodynamic models with the ENKI platform.** Mark Ghiorso, *OFM Research* [**pdf**] [**YouTube**]
	20min	**The Molecular Sciences Software Institute,** Daniel Crawford, *MolSSI, Virginia Tech* [**pdf**] [**YouTube**]
10:20	10min	**BREAK**
10:30	60min	**BREAKOUT 2**
11:30	30min	**REPORT BACK**
12:00	30min	**Discussion: Visions, Ideas, and Strategies for the CIG of the future**
12:30		**ADJOURN**

Session 3: Long Term Tectonics and Seismology

DAY 3 - THURSDAY OCTOBER 15

08:00		**WELCOME**
08:05		**PLENARY 3A**
	20min	**Challenges and opportunities in long-term tectonic modeling,** Laurent Montesi, *University of Maryland* [**pdf**] [**YouTube**]
	20min	**Deep Earth Seismology: Discoveries, Questions, and Challenges,** Ved Lekic, *University of Maryland* **[pdf]** [**YouTube**]
	10min	Discussion
08:55	15min	**BREAK**
09:10		**PLENARY 3B**
	20min	**Using supercomputers to unravel multi-physics and multi-scale earthquake and tsunami dynamics: targeting exascale high-performance computing,** Alice Gabriel, *University of Munich* [**YouTube**]
	20min	**Machine Learning for Fluid Dynamics**, Steve Brunton, *University of Washington* [**pdf**] [**YouTube**]
09:50	15min	**BREAK**
10:05	25min	**IDEA TALKS 3**

1. The Need for Coupling of Tectonic and Surface Processes in CIG-IV. Phaedra Upton, *GNS Science*

2. Towards a Computational Geodynamics Visualization and Data Analysis Framework. John Naliboff, *New Mexico Tech;* Sascha Brune, *GFZ Potsdam;* Thilo Wrona, *GFZ Potsdam;* Guillaume Duclaux, *Université Côte d'Azur;* Chris Havlin, U*. Illinois*; and Dave May, *UC San Diego* [**pdf**]

3. A community plan towards reproducible simulations of complex lithospheric dynamics. *CIG Long-Term Tectonics Working Group* [**pdf**]

4. Best Practices: Guidelines, Resources, and Education. Brad Aagaard, *USGS* [**pdf**]

10:30 60min **BREAKOUT 3**
11:30 30min **REPORT BACK**
12:00 30min **Summary Discussion - CIG of the Future**
12:30 **ADJOURN**

Appendix B. Participants

Total Registered (Zoom): 141

Brad	Aagaard	USGS
Yongki Andita	Aiman	University of Vienna
Kali	Allison	University of Maryland
Paula	Antoshechkina	Caltech
Richard	Aster	Colorado State University
Julien	Aubert	Institut de Physique du globe de Paris
Jon	Aurnou	UCLA
Jacqueline	Austermann	Columbia University
Wolfgang	Bangerth	Colorado State University
Xiyuan	Bao	University of California, Los Angeles
Thorsten	Becker	UT Austin
Mark	Behn	Boston College
Magali	Billen	UC Davis
Ömer	Bodur	Istanbul Technical University
Matthew	Bogumil	University of California, Los Angeles
Ebru	Bozdag	Colorado School of Mines
Sascha	Brune	German Research Centre for Geosciences (GFZ Potsdam)
Steven	Brunton	University of Washington
Bruce	Buffett	UC Berkeley
Susanne	Buiter	RWTH Aachen University
Roland	Burgmann	UC Berkeley
Recep	Cakir	Washington Geological Survey
Roberta	Carluccio	The University of Melbourne
William	Chen	University of Minnesota
Eunseo	Choi	The University of Memphis
Kiran	Chotalia	University of Florida
Clinton	Conrad	University of Oslo
Cathy	Constable	UC San Diego, Scripps Institution of Oceanography
Michele	Cooke	University of Massachusetts Amherst

Katie	Cooper	WSU
Vernon	Cormier	University of Connecticut
Daniel	Crawford	Virginia Tech/Molecular Sciences Software Institute
Claire	Currie	University of Alberta
Juliane	Dannberg	University of Florida
Xuesong	Ding	UCLA
Saruul	Dorjpalam	Ohsaki Research Institute
Reza	Dousti	Institute for Advanced Studies in Basic Sciences (IASBS)
Peter	Driscoll	Carnegie Science
Thomas	Duvernay	Australian National University
Cynthia	Ebinger	Tulane University
Aboubaker	Farah	Hassan II University of Casablanca
Megan	Flanagan	EditSprings
Lucy	Flesch	Purdue University
Alice	Gabriel	LMU Munich
James	Gallagher	OPeNDAP
Rene	Gassmoeller	University of Florida
Christopher	Gerbi	University of Maine
Mark	Ghiorso	OFM Research
Juan	Gilbert	University of Florida
Carlos	Gomez	Southern Illinois University
Aakash	Gupta	University of Alaska Fairbanks
Dennis	Harry	Colorado State University
Elizabeth	Hearn	independent research geophysicist
Timo	Heister	Clemson University
John	Hernlund	Earth-Life Science Institute
Gabrielle	Hobson	
Mark	Hoggard	Harvard University
Adam	Holt	University of Miami
Lorraine	Hwang	UC Davis
Mohammad	Ismaiel	DST Inspire Faculty
Garrett	Ito	University of Hawaii
Yaqi	Jie	Michigan State University
Joshua	Jones	Virginia Tech

Scott	King	Virginia Tech
Ágnes	Király	CEED, University of Oslo
Simon	Klemperer	Stanford University
Valere	Lambert	California Institute of Technology
April	Allen Langhans	Syracuse University
Nadia	Lapusta	California Institute of Technology
Carene	Larmat	Los Alamos National Laboratory
Marine	Lasbleis	Université de Nantes, CNRS
Vedran	Lekic	University of Maryland
Carolina	Lithgow-Bertelloni	UCLA
Mingqi	Liu	ETH Zurich
Tianshi	Liu	University of Toronto
Xiaowen	Liu	University of Alberta
John	Louie	Univ. of Nevada, Reno
Hao	Lu	CERI, University of Memphis
Mingda	Lv	Michigan State University
Risa	Madoff	University of North Dakota
Philip	Maechling	USC
Lucan	Mameri	University of Montpellier
Hiroaki	Matsui	University of California, Davis
Amanda	McPherson	University of Alaska Fairbanks Geophysical Institute
Dave	May	UCSD
Lara	Meyer	ETH Zurich
Edie	Miglio	Politecnico di Milano
Tushar	Mittal	MIT
Eric	Mittelstaedt	University of Idaho
Laurent	Montesi	University of Maryland
Gabriele	Morra	UL at Lafayette
Thomas	Morrow	Boston College
Sharon	Mosher	University of Texas at Austin
John	Naliboff	New Mexico Institute of Mining and Technology
Kodi	Neumiller	OPeNDAP
Emmanuel	Njinju	Virginia Tech
Keely	O'Farrell	University of Kentucky

Jean-Arthur	Olive	Ecole Normale Supérieure / CNRS
Anthony	Osei Tutu	University of Arizona
Zhihong	Pan	University of Alberta
Jonathan	Perry-Houts	CIG
David	Quiroga	University of Alberta
Tahiry	Rajaonarison	Virginia Tech
Robin	Reichlin	NSF
Adam	Ringler	USGS
Arthur	Rodgers	Lawrence Livermore National Lab
Poulami	Roy	IISER
Max	Rudolph	UC Davis
Arushi	Saxena	University of Florida
Jana	Schierjott	University of Hawaii
Ebru	Şengül Uluocak	Canakkale University, Dept. of. Geophysics
Rafael	Silva	IAG-USP
Shi Joyce	Sim	Georgia Institute of Technology
Mohamed	Sobh	TU Bergakademie Freiberg
Krista	Soderlund	University of Texas Institute for Geophysics
Marc	Spiegelman	Columbia University
D. Sarah	Stamps	Virginia Tech
Dave	Stegman	Scripps Institution of Oceanography, UCSD
Zhe	Su	
Paul	Tackley	ETH Zurich
Carl	Tape	University of Alaska Fairbanks
Cedric	Thieulot	Utrecht University
Xiaochuan	Tian	Lamont-Doherty Earth Observatory
Meng	Tian	University of Bern
Harold	Tobin	University of Washington
Xiaopeng	Tong	Institute of Geophysics, China Earthquake Administration
Gregory	Tucker	CSDMS / University of Colorado Boulder
Phaedra	Upton	GNS Science
Ylona	van Dinther	Utrecht University
Jolante	van Wijk	New Mexico Tech

Ikuko	Wada	University of Minnesota – Twin Cities
Robert	Walker	University at Buffalo
Maaike	Weerdesteijn	Centre for Earth Evolution and Dynamics (CEED), University of Oslo
Cian	Wilson	Carnegie Institution for Science
Ziyi	Xi	Michigan State University
Liang	Xue	Syracuse University
Clara	Yoon	USGS
Tai-Chieh	Yu	University of Alberta
Eva	Zanzerkia	NSF
Bo	Zhang	California Institute of Technology

Appendix B. Breakout Groups

Key points from Breakout Groups

Day 1.

- Better use [of] governance to communicate and set priorities: two -way street from WG to SSC and back again. Advertise process and solicit feedback.
- Make sure everyone interested is invited to participate, including international
- Build collaborative relationships with other disciplines: paleomag, planetary, geomag, core materials
- Improve dynamo code availability, data repo, tutorials, visualizations
- Should we interact with the Deep Earth Working group?
- Convene workshop to discuss larger interests?
- A group specifically focused on long-term tectonics no longer make sense, as we deal with a wide range of processes over many temporal and spatial scales. What might make more sense is to have a working group for “lithospheric dynamics” that heavily interfaces with a mantle convection and multi-physics (magma/fluid transport, surface processes) working group.
- Instead of “layered” working groups, we could [have] working groups that are “process/work-flow” based. This could be a group focused on outreach, development of GUIs for specific codes, help with installation, etc.
- Increasing diversity. Long-term solutions involve undergraduate education material, but a short-term solution could be a working group that focuses on code installation help and other forms of outreach.
- There should be more connections with workings, perhaps through dual appointments to multiple working groups.
- Does the [governance] Structure meet the community's needs? Not for melts and fluids. New developments are central and require coordination. CIG could help with this coordination and bridge across disciplines.
- Explore alternative funding models: small grants to enhance cross-disciplinary initiatives, maybe through problem-focused hackathon-like, or proof of concept problems?
- What is a computational infrastructure? Reduce burden to developers (Relieve developers from maintenance, user help, certification).
- Focus on interdisciplinary science problems. Link lithosphere with surface and deeper problems, common interfaces, etc.
- Discussed CIG “certification” a bit...asked what is in it for developers...user support and central support infrastructure
- Validation, Verification and Best Practices
- Guidance to limitations of codes (e.g., meshing a discontinuity; numerical dispersion)
- oversight/guidance for pull requests on codes
- Workflows to get a student up and running (also: continuity across different codes)
- Community development
    - Crustal Deformation Modeling Workshops (every other year) with more regular interaction (quarterly online science + user forums/discussions)
    - High level interaction among disciplinary groups (coupling from a bird’s eye view)
- Governance: working group facilitate activities; current developers + other members of community is working pretty well. Would be good to formalize responsibilities and process.
- Lower barriers to entry: suite of codes (would be nice to get entry level codes “CIG certified”)

Day 2

- Next-scale computing: challenges involve multi-scale, multi-physics problems, such as interfacing thermodynamic and geodynamic models
- Extracting quantitative information from complex results
- Model reproducibility - need for standard practices for 3D, spherical earth models, archiving of detailed run setup etc.
- Machine learning - mining results from many 3D models. Archiving and exchanging results?
- Training - need for high-quality training materials for the next generation of geodynamicists. Coordination with XSEDE trainings for HPC?
- Making dynamo codes more user friendly will go a long way toward DEI. Top goal of the committee.
- We need to have a bigger emphasis on integrated education efforts - basic software training, fundamentals of modeling, training on specific-domain topics, best practices and techniques in software design. Also sharing of teaching resources.
- We need to make tools that make complicated software more accessible, and then have training available for when people want to go to more advanced stages.
- There is a huge demand in LTT (and other domains) for computational manpower, resources and software - writing software, maintenance, basic training, help with writing code. With increasing need, some or all domains of CIG are going to be overwhelmed.
- It makes sense to have software engineers and other support staff that can work across domains (CIG, CSDMS) and having to write separate smaller grants is quite burdensome and not efficient. We need to think bigger.
- General consensus (8 people) that multi-physics, crossing disciplinary boundaries is critical for many problems people want to explore in the future.
- But these problems are very challenging
- How CIG can facilitate interactions between different models/fields to go towards a multiphysics framework?
- What's the best mechanism to accomplish this: workshops, codes, code infrastructures?
- Interfacing Scientists rather than models
- Changing the "working group model" being more inclusive/agile.
- How to incorporate new code developments (e.g. ENKI)
- Training vs education question. Particularly important for multi-physics modeling (molssi model)
- CIG - science neutral beginnings - CIG facilitate training for adhering to general code guidelines, best practices
- UQ (didn't discuss, but essential to complex models -- how complex does a model need to be to be useful?)
- let observations guide modeling efforts (pylith, seismo)
- geophysics problems require more than just seismic data (need geodesy)
- dynamic rupture as possible new area for CIG
    - highlight: gravity into wave propagation code for tsunami + seismic waves
- Some information sharing of data sets on structure grids (cheese)
- consider moment tensor code (there are many options)
- Training is still needed so researchers are sharing a common language

Day 3

- CIG could help with model data exchange (define format)
- Explore ML techniques, because of unknown applications at the moment (CIG fellowship?)
- Hero Exascale runs are only useful with full buy-in of community
- We all agree education/training is critical, but there is not going to be a CIG IV without strong scientific goals
- New data analysis and visualization tools have wide support. This is critical for comparisons to nature (validation). Here, we need to be sure to link with external groups.
- Consensus that we should consider combining with other groups (CSDMS)
- ML in seismology: address physics, extract information from large datasets.
- “hero runs” (toward exacscale) and trickle-down effect to broader base of users
- 3D modeling of small-scale heterogeneities: Do we need 3D modeling? What can we learn from it?
- Education and training and (informal) workflows to shorten time to science
- Verification of numerical methods, validation to observed data, reproducibility, UQ, resolution analysis!