COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Community-driven organization advancing Earth science by providing the infrastructure for the development and dissemination of software for geophysics and related fields.

2022 CIG Annual Business Meeting

29 November 2023 ◆ 10A-noon PT ◆ *zoom*

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Agenda
PST

10:00 State of CIG

Election Results
Next Year's Activities
CIG IV
How to Collaborate with CIG
Jamboard: What are the collaboration needs of the community?
NSF - Q&A

10:35 What's New

Website - New Features
Working Groups
Software Perspectives
Q&A?

11:45 Discussion

Topic 0: Should CIG have a permanent seat for an early career member on the SSC?

Topic 1: What are the collaboration needs of the community?

Topic 2: How can CIG help meet community collaboration needs?

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State of CIG

CIG III

End of activity cycle January 31, 2023

Award closeout July 31, 2023

CIG IV - *Proposed*

Start date February 1, 2023

End date January 31, 2028

recommendation moving forward

CIG Staff 2022

Director

Lorraine Hwang

Technical Lead

Rene Gassmoeller

Research Scientist

Hiroaki Matsui

Postdoctoral Fellows

Kali Allison

Menno Fraters

Ryan Orvedahl

Graduate Student

Dylan Vassey

Junior Specialist

Chris Mills

Lab Assistant

Mack Gregory

Student Assistant

Denise Kwong

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Elections

Thanks to
Outgoing members:
EC: Bruce Buffet, Claire Currie, & Carolina Lithgow-Betertelloni
SSC: Juliane Dannberg, Scott King, & John Naliboff
Nominating Committee
Max Rudolph, Anne Glerum, Joyce Shi Sim

Executive Committee

Alice Gabriel, *Chair*

Brad Aagaard
Louis Moresi*
Marc Spiegelman*
Phaedra Upton* *2 year*

Science Steering Committee

Ebru Bodag, *Chair*

Sylvain Barbot
Adam Holt*
Dave May
Peter Driscoll
Harriet Lau
Elvira Mulyukova*
Emmanuel Njinju* *1 year*

***Proposal:* SSC Early Career Representative**

- By election
- 1 year renewable
- Early career define as < 4 years from terminal degree
- Total number of seats to remain at 8

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What's New 2023

Working Groups - NEW

- Education
- Software

Events

- Hackathons - ASPECT, Rayleigh, PyLith (June), and JOSS(?)
- Meetings - ASPECT Users, Software Developers,

Distinguished Speakers

Juliane Dannberg, University of Florida

Subducted Slabs, Mantle Plumes, and the Plate Tectonic Cycle
@University of California Riverside, University of Hawaii Manoa, & University of Ottawa

Mathieu Morlighem, Dartmouth College

Can we (yet) predict how fast Greenland is going to melt?
@ Virginia Tech, Appalachian State University, & South Dakota Mines and Technology

Webinars

January 12	Soza Talavera, Utrecht / UCSD
February 9	Tobias Keller, ETH
March 9	Effective Strategies for Writing Proposal Work Plans for Research Software. Chase Million, Million Concepts
April 13	Adina Pusok, Oxford University
May 11	tbd. SZ4D

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IV

Cornerstones

Modeling software

Computational workflows

Training

Community

Modeling software: Providing powerful software to solve computational models, motivated by important science questions, and built on best practices in open source software and scientific computing

Computational workflows: supporting workflows that facilitate the set-up, execution, analysis, and exchange of complex computational models

Training: Enabling a well-educated, well-trained, and diverse 21st century workforce that can effectively use and extend computational models for reproducible discovery and reuse, and that can fully exploit high-performance computing resources

Community: Building and sustaining a diverse and sustainable community of disciplinary and interdisciplinary researchers working together on challenging geoscience and software problems.

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CIG IV

Contributions wanted

Modeling software

- Containerization
- JOSS partnership

Computational workflows

- Identify pilot project(s)

Education & Training

- Python for geodynamics
- Notebooks

Community

- Outreach *CIDER, hackathons, workshops, webinars etc., 2025 CIG ALL community mtg?*
- Access *BJEDI*

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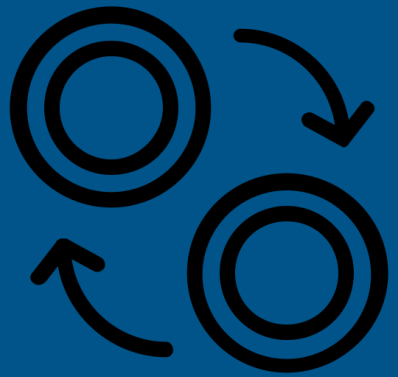
Collaborating



https://geodynamics.org/aboutus/contact/collaborating

WHO we are and WHAT we do

Computational Infrastructure for Geodynamics (CIG)

Community-driven organization advancing Earth science by developing and disseminating software for geophysics and related fields.

provides the infrastructure for the development and dissemination of software

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How We Support Projects

SOFTWARE

- Best practices, GitHub template, & guidance

DISSEMINATION

- Landing pages, Zenodo community

OUTREACH & BROADER IMPACT

- Newsletter, webinar, YouTube, & notebook support

EDUCATION & SOFTWARE TRAINING

- Software training best practices, workshops, & HUBzero platform

ACCESS

- hpc for benchmarking and small runs

How We Support Projects

SOFTWARE DEVELOPMENT

- collaboration with community
- Interests: interoperability and reusability of software components

EXTENDED SUPPORT

- Include us in your next proposal if you need extended support for: software development, software engineering, tutorial development, event support or ???

FAQs

Q. Does CIG's mission include developing software methods/components for my project?

No, CIG does not develop software components for specific projects as part of its core mission. This is a common misconception during proposal reviews. Your proposal should clearly state that CIG supports infrastructure and communities, not software development. Software development by CIG for specific projects must be funded by proposals that include support for CIG; see Extended Support for more information.

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How To Collaborate

Jamboard

https://tinyurl.com/22CIGjam1

Question

What are the collaboration needs of the community?

Instructions

- Add stickies
- Vote for other's ideas by adding a +1 to a sticky
- Rearrange grouping like ideas

Ending Discussion

- Review and summarize stickies
- How can CIG help meet community collaboration needs?

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NSF opportunities for enabling software & cyberinfrastructure in the Earth Sciences

Raleigh L. Martin, *Program Director*
NSF Division of Earth Sciences

November 29, 2022
CIG Business Meeting

Motivation: Growing importance of open, accessible, and reproducible science at NSF

- **OSTP Memo**: *Ensuring Free, Immediate, and Equitable Access to Federally Funded Research* (Aug. 25, 2022)
- **FAIROS RCNs** (NSF 22-553)
  - New NSF program supporting Research Coordination Networks (RCNs) that advance FAIR principles (findable, accessible, interoperable, reusable) and open science (OS) practices
- **Reproducibility & Replicability DCL** (NSF 23-018)

** Public Access Listen and Learn Session for NSF Stakeholders
November 30, 2022, 2 PM EST via Zoom **
https://nsf.zoomgov.com/webinar/register/WN_nKHJhfI4RJGWQnEXqFiaLQ

NSF 23-018

Dear Colleague Letter: Reproducibility and Replicability in Science

October 25, 2022

Dear Colleagues:

A 2019 consensus study report published by the National Academies of Sciences, Engineering, and Medicine (NASEM) discussed the meaning of the terms replicability and reproducibility and identified approaches for researchers, academic institutions, journals, and funders to improve reproducibility and replicability in science [1]. In July 2021, at NSF's request, NASEM convened an expert meeting focused on National Science Foundation (NSF) policies and investments to make reproducible and replicable science easier for scientific communities to understand and execute and to embed reproducibility and replicability within the fundamental scientific method.

Through this Dear Colleague Letter (DCL), NSF reaffirms its commitment to advancing reproducibility and replicability in science. NSF is particularly interested in proposals addressing one or more of the following topics:

1. **Advancing the science of reproducibility and replicability.** Understanding current practices around reproducibility and replicability, including ways to measure reproducibility and replicability, what reproduction and replication means in practice, the right degree of replicability to target, quantitative measures of progress to understand the effectiveness of interventions to improve reproducibility and replicability, and exploration of reasons why studies may fail to replicate.
2. **Research infrastructure for reproducibility and replicability.** Developing and facilitating adoption of cyberinfrastructure tools and/or research methods that enable use of reproducible and replicable practices across one or more science and engineering communities.
3. **Educational efforts to build a scientific culture that supports reproducibility and replicability.** Enabling training in science and engineering communities to identify and encourage best practices for reproducibility and replicability, providing community-building and institutional support, and supporting broad public outreach about rigor, reproducibility, and replicability in science.

Investigators who wish to submit proposals on any of these topics, or others related to advancing reproducibility and replicability in research, are encouraged to reach out to programs and program officers to discuss the fit of their ideas to existing funding opportunities. Definitions of the terms replicability and reproducibility may be found in Reference [1].

Directorate for Geosciences (GEO) opportunities

GEO-wide:

- **EarthCube** supports efforts to promote discovery, integration, and interoperability of data and cyber resources for the geosciences. Though there is currently no EarthCube funding competition, EarthCube awardees remain active (www.earthcube.org)
- **NSF FY23 budget request** seeks support for GEO cyberinfrastructure (CI) incubator; details TBD

Division of Earth Sciences (EAR):

- The **Geoinformatics (GI) program** (NSF 21-583) supports widely-used cyberinfrastructure services (including software) relevant to Earth Scientists. Projects must be motivated by EAR science needs and provide broad value to EAR science communities.
- Proposals to **EAR Disciplinary Programs** may include some development of scientific software within the context of advancing core science research objectives (check with Cognizant POs prior to submission).

Visit the NSF Booth (#1313 in the Exhibit Hall)
at the 2022 AGU Fall Meeting

Office of Advanced Cyberinfrastructure (OAC) opportunities

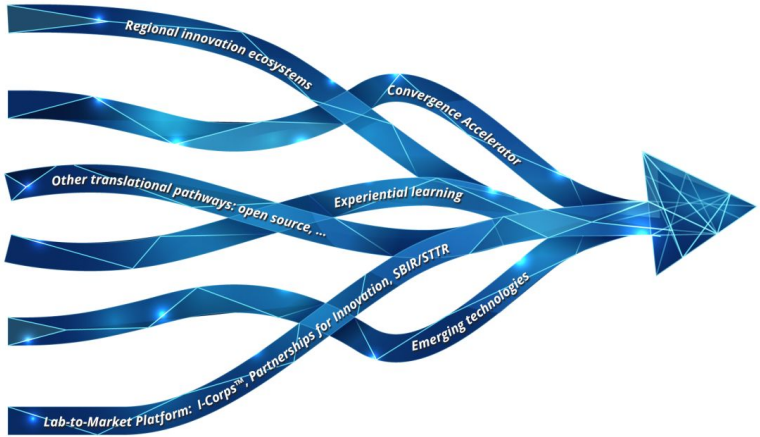
- **Cyberinfrastructure for Sustained Scientific Innovation (CSSI)** (NSF 22-632): Support for robust, reliable, and sustainable data and software cyberinfrastructure (*Deadline:* December 16, 2022)
- **CyberTraining (NSF 23-520):** Supports efforts toward broad adoption of CI tools, methods, and resources; and integration of CI literacy into curriculum / instructional materials (*Deadline:* Feb. 23, 2023)
- **SCIPE (NSF 23-521):** "Strengthening the Cyberinfrastructure Professionals (CIP) Ecosystem" (*Deadline:* Feb. 23, 2023)
- *OAC CI Resource Ecosystem:*
  - **ACCESS**: Coordinates allocations for advanced computing, visualization, and data resources for researchers and educators (follow-on to XSEDE) (https://access-ci.org)
  - **CloudBank:** Enabling access to commercial cloud service resources
  - **Partnership to Advance Throughput Computing (PATh):** Pilot support for high-throughput computing (HTC) resources (see NSF 22-051)

More information here: https://www.nsf.gov/geo/geo-ci

Technology, Innovation, and Partnerships (TIP) opportunities

TIP is NSF's newest directorate. Supports use-inspired research, accelerating development of key technologies, and expanding the STEM workforce

- **Convergence Accelerator:** phased funding model to accelerate solutions toward societal impact (RFI for topics => Workshops => topic selection for project cohorts)
  - *2022 workshop examples:* Ethical Design of AI, Computing Solutions for Climate-Driven Extreme Events
  - *Past cohort examples:* Open Knowledge Networks, AI-driven Innovation via Data & Model Sharing
- **Pathways to Enable Open-Source Ecosystems (POSE)** (NSF 22-552)
  - Supports efforts toward harnessing open-source development approaches for new technology solutions to problems of national and societal importance
  - Applicable to a wide range of "open-source" development (including software and other products)



Q&A (10 min)

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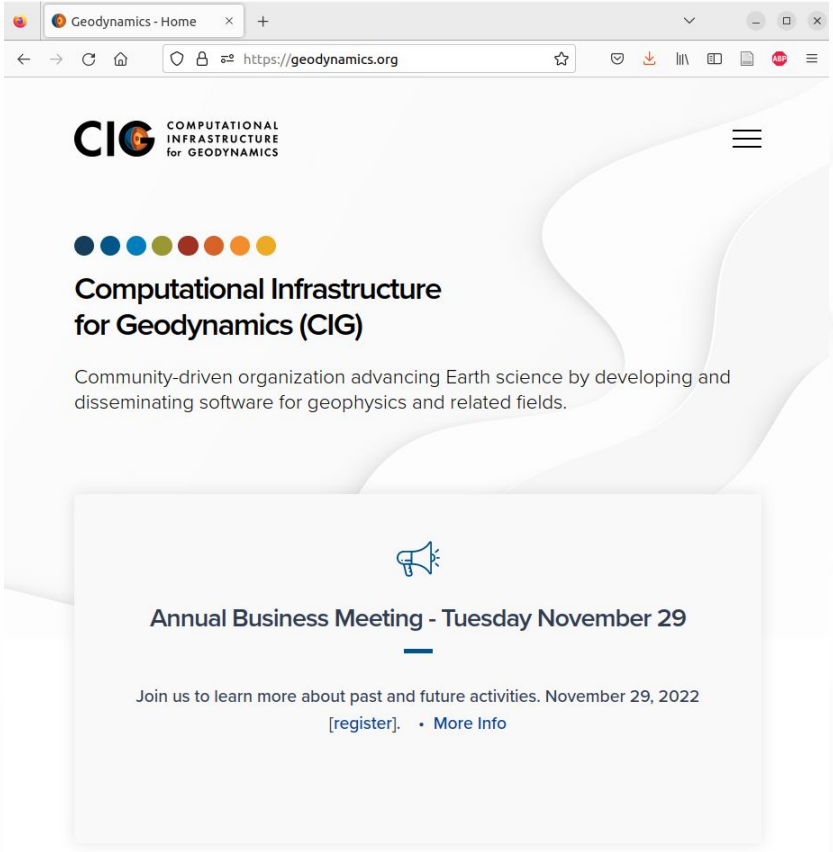
CIG's new home online



- Modern design
- Mobile friendly
- Working groups
- Datasets and wikis
- Education materials
- Executable tools (beta)

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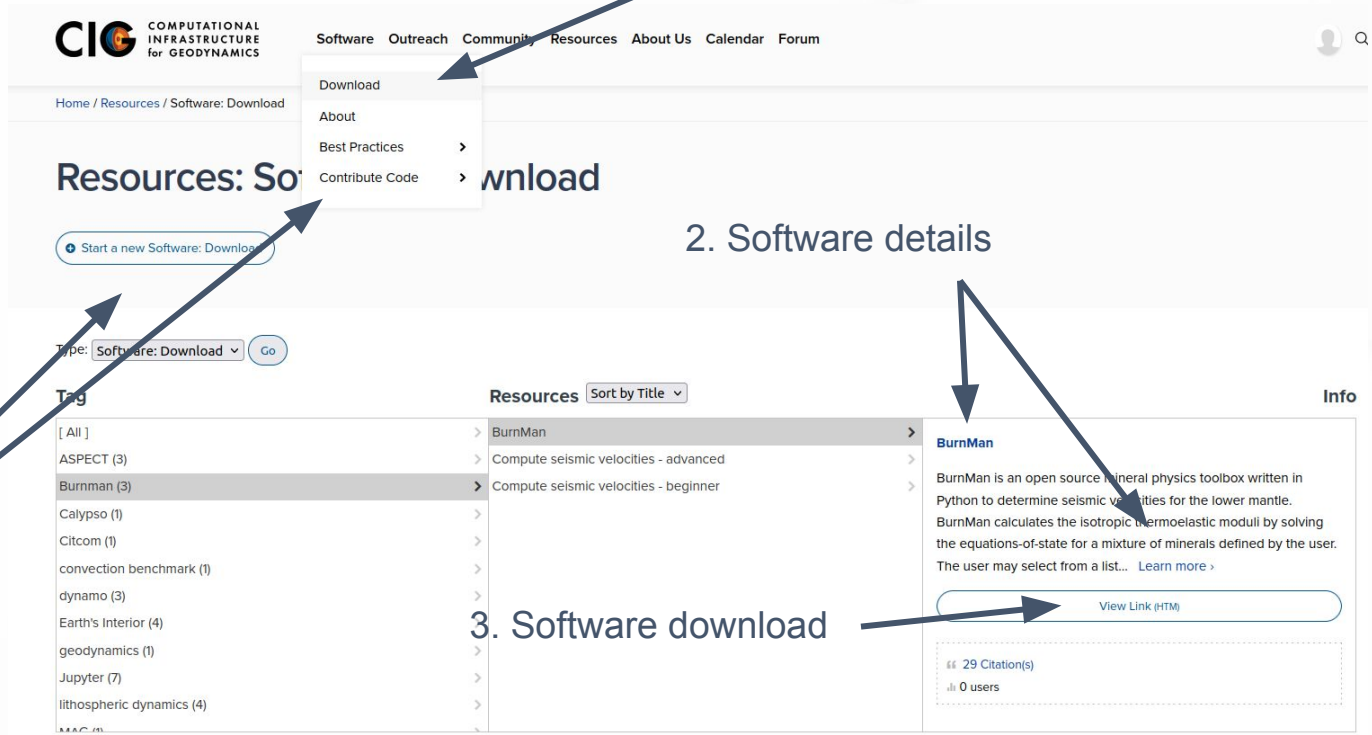
Software download

1. CIG supported software



2. Software details

3. Software download

4. Start new project

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Software details

1. Download software

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Software Outreach Community Resources About Us Calendar Forum

Home / Resources / Software: Download / SPECFEM3D Cartesian / Supporting Docs

SPECFEM3D Cartesian

Edit

View Link (HTM)

Additional materials available (5)

license GPL 3

124 Citation(s)

0 users

By Dimitri Komatitsch (primary-developer)[1], Jean-Pierre Vilotte (primary-developer)[2], Jeroen Tromp (primary-developer)[3], SPECFEM Development Team

1. CNRS, France 2. Institut de Physique du Globe 3. Princeton University, USA

2. Citations in CIG's database

About | Users | Developer | Supporting Docs | Previous versions | Citations | How to cite | Related

(HTM) Repository (download latest release)

(HTM) Online Documentation

(BIB, 27.76 KB) HowToCiteSPECFEM3DCartesian.bib

(GZ, 94.49 MB) SPECFEM3D_Cartesian_V2.0.2.tar.gz

(PDF, 15.06 MB) manual_SPECFEM3D_Cartesian3.0.pdf

3. How to cite

Seismology

4. Documentation

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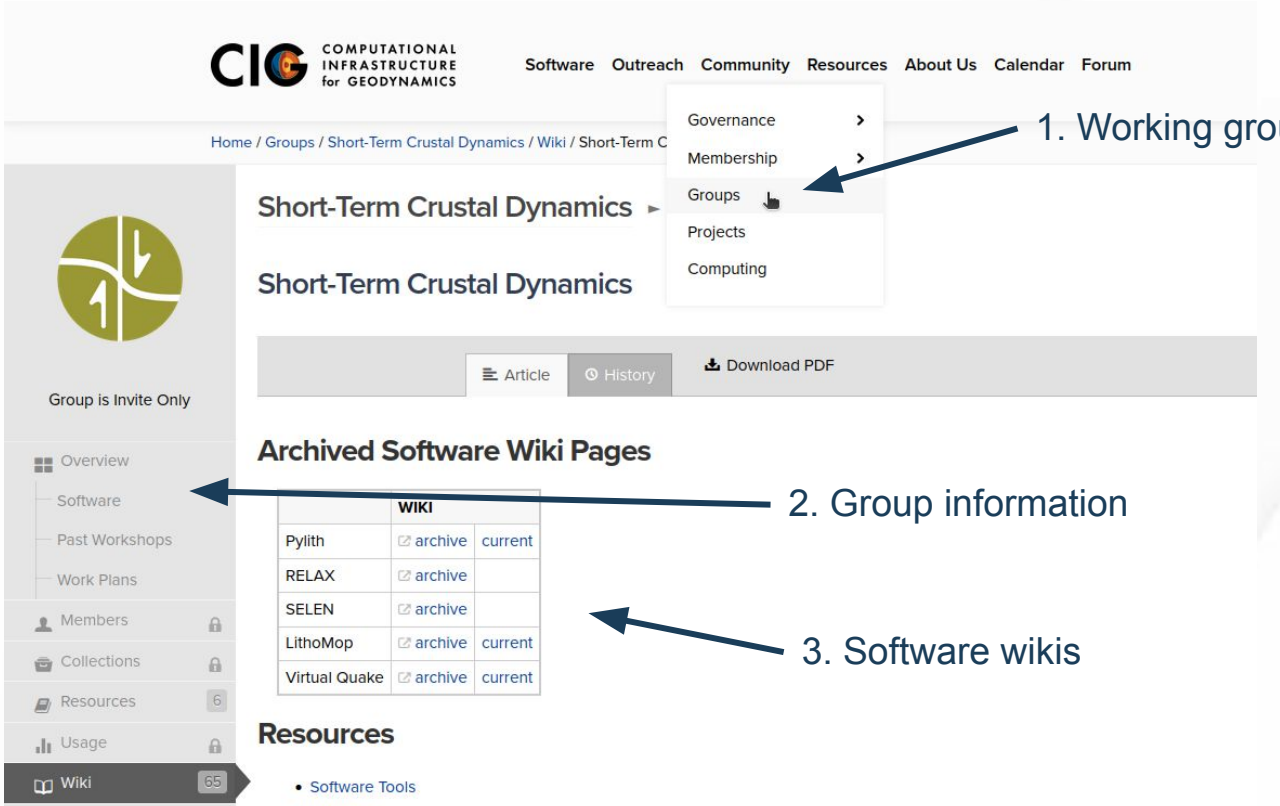
Working groups



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Hosting datasets

- **Small datasets can be hosted on geodynamics.org**
- **Talk to us if you have large datasets that are important for your community**
- **Example for large dataset: incite.geodynamics.org**

INCITE DATA

Navigation

Contents:

Citation and Acknowledgement
Jovian Atmosphere (mheimpel)
Geodynamo (ryadav)
Data conversion program

Quick search

Go

Frontiers in Planetary and Stellar Magnetism Through High Performance Computing

Overview

The data found here was generated as part of the *Frontiers in Planetary and Stellar Magnetism Through High Performance Computing* project as part of the Geodynamo Working Group of the Computational Infrastructure for Geodynamics (CIG). Computational time on *Mira* and support was provided through the DOE INCITE project. More information about this project can be found on the project page .

Data

- **Linked in "Dynamo" working group**

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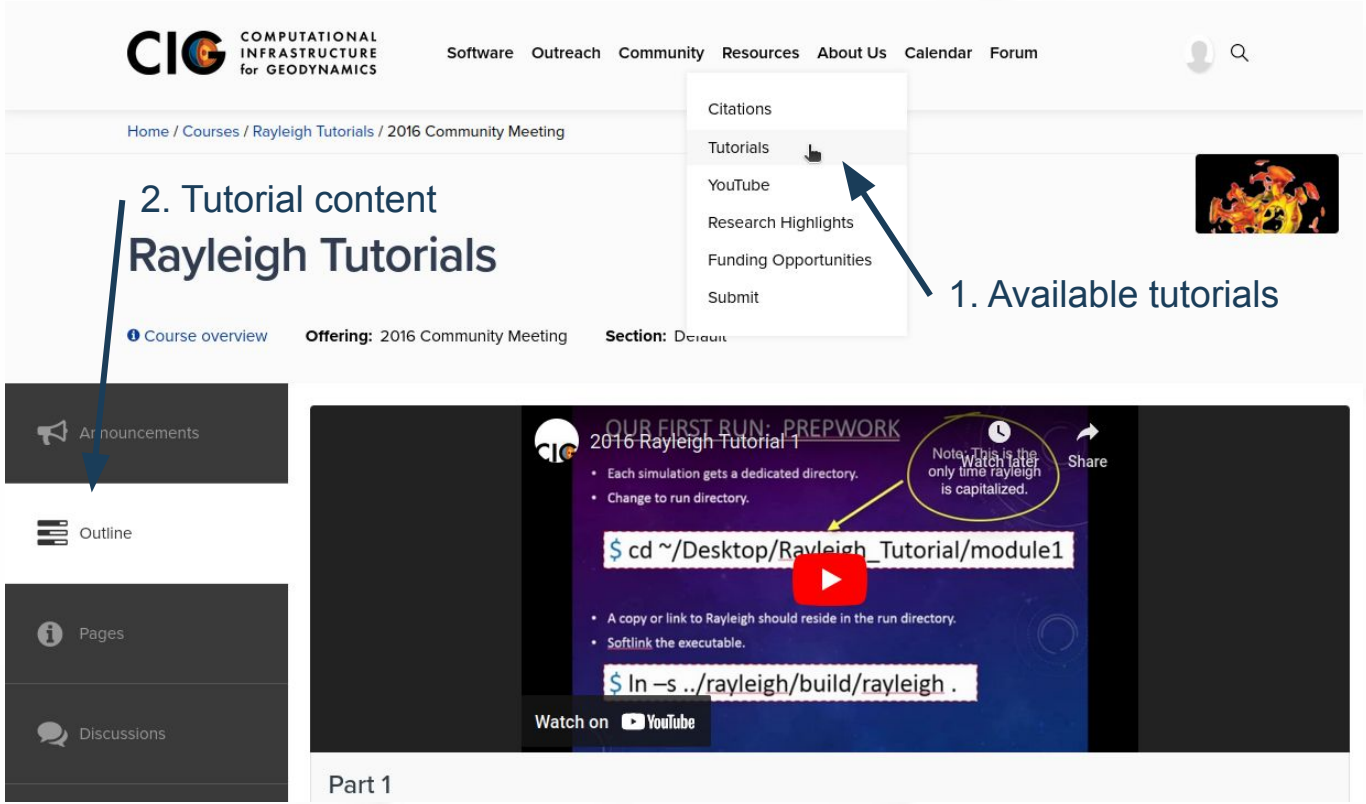
Educational material



Old tutorials recorded (static), future content can be interactive

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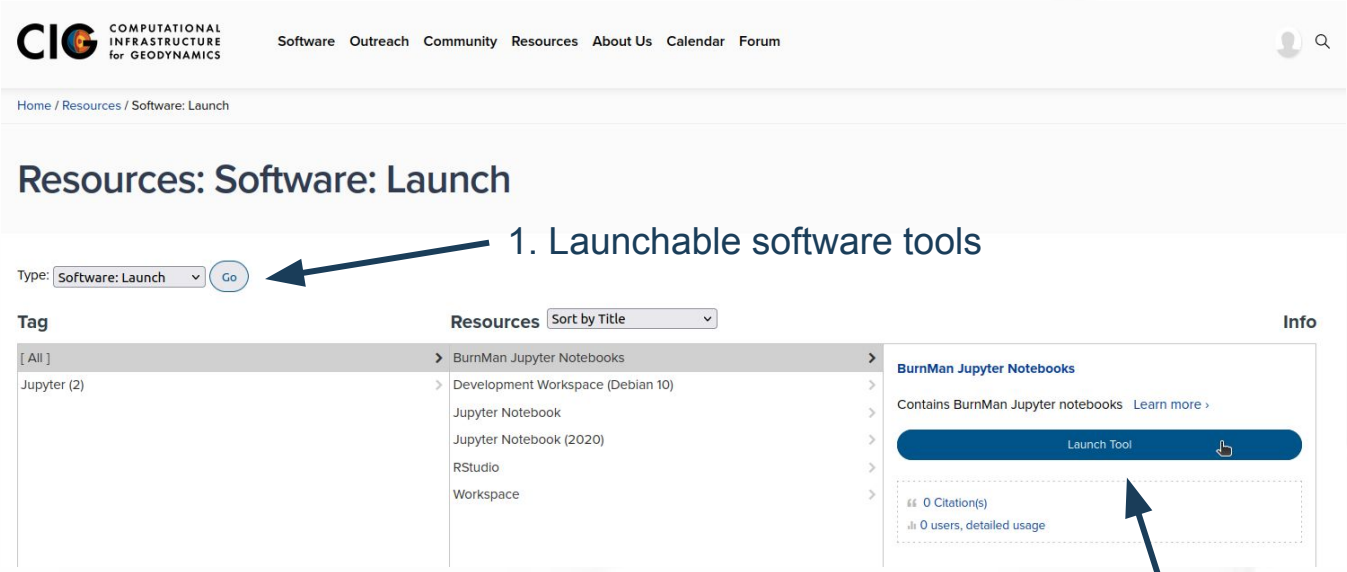
Executable tools (beta)



1. Launchable software tools

2. Launch tool

FAQ

- Currently in beta, actively adding new tools
- Requires geodynamics.org account
- Executed on shared Hubzero hardware
- Intended for education, software tutorials
- Contact us to contribute or report problems

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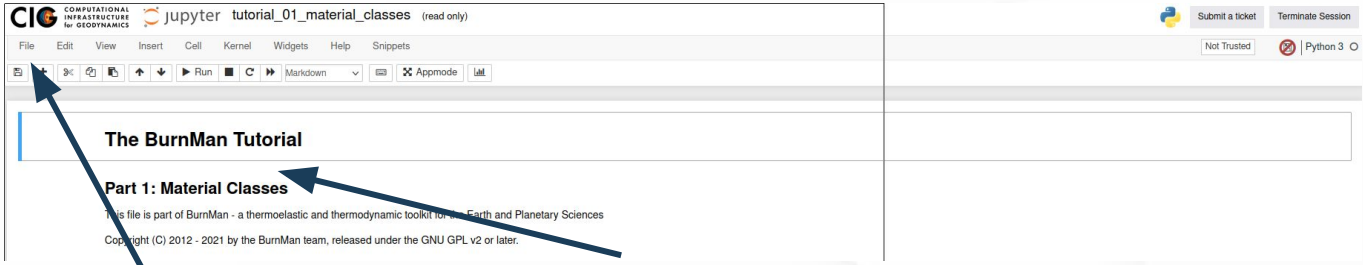
Executable tools (beta) - Python tools



1. Executable Jupyter notebook

2. "File" -> "Open" to see list of available notebooks

```
In [9]: from burnman.tools.chemistry import formula_to_string
        print(f'{fo_SLB.name} (SLB2011)')
        print(f'Formula: {formula_to_string(fo_SLB.formula)}')
        print(f'Gibbs: {fo_SLB.gibbs:.3e} J/mol')
        print(f'S: {fo_SLB.molar_entropy:.3e} J/K/mol')
        print(f'V_p: {fo_SLB.v_p:.3e} m/s')

        Forsterite (SLB2011)
        Formula: Mg2SiO4
        Gibbs: -2.148e+06 J/mol
        S: 2.747e+02 J/K/mol
        V_p: 8.308e+03 m/s
```

3. Interactive execution

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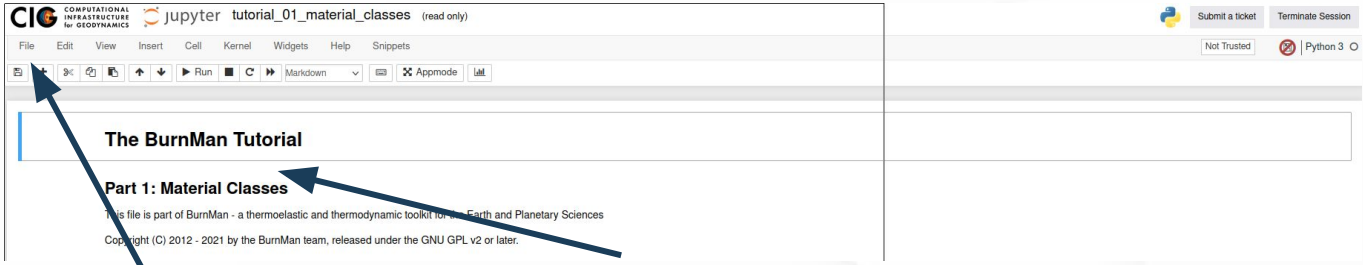
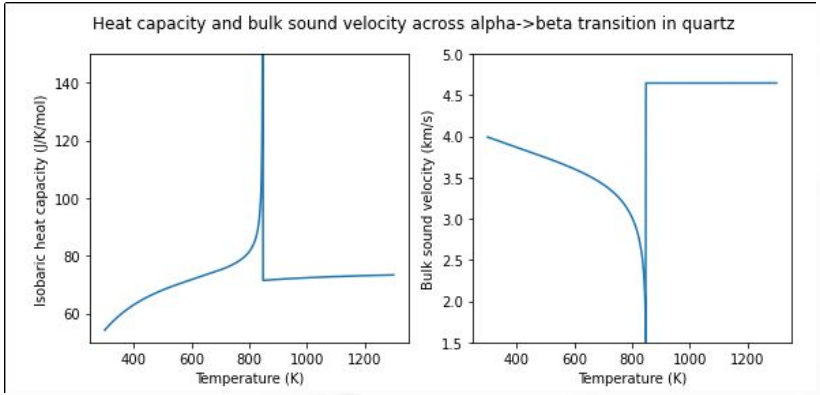
Executable tools (beta) - Python tools



1. Executable Jupyter notebook

2. "File" -> "Open" to see list of available notebooks



4. Interactive plots

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Executable tools (beta) - Binary tools

Running aspect from the notebook

A run will provide the output files that we are then reading later.

1. Execute binary in shell

In [ ]:
```
# Download an ASPECT parameter file
!wget -O convection-box.prm \
  https://raw.githubusercontent.com/geodynamics/aspect/main/cookbooks/convection-box/convection-box.prm

# Set paths to input and output
input_file = "convection-box.prm"
output_dir = "output-convection-box/"
```

In [46]:
```
# Run ASPECT model
!aspect convection-box.prm
```

```
-----------------------------------------------------------------------------
-- This is ASPECT, the Advanced Solver for Problems in Earth's ConvecTion.
--     . version 2.5.0-pre
--     . using deal.II 9.4.0
--     .       with 32 bit indices and vectorization level 1 (128 bits)
--     . using Trilinos 12.18.1
--     . using p4est 2.3.2
--     . running in OPTIMIZED mode
--     . running with 1 MPI process
----------------------------------------

----------------------------------------
-- For information on how to cite ASPECT
--   https://aspect.geodynamics.org/citi
----------------------------------------
Number of active cells: 256 (on 5 levels
Number of degrees of freedom: 3,556 (2,1

*** Timestep 0:  t=0 seconds, dt=0 secon
```

2. Output of model run.

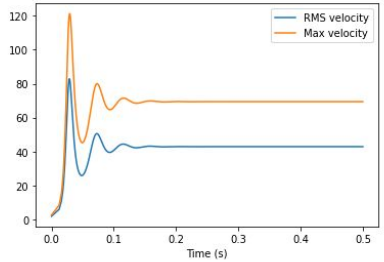
3. Postprocessing in Python or other tools.

In [45]:
```
# or using the pyplot functions (allows more flexibility)

fig, ax = plt.subplots()

ax.plot(data["Time (seconds)"], data["RMS velocity (m/s)"], label="RMS velocity")
ax.plot(data["Time (seconds)"], data["Max. velocity (m/s)"], label="Max velocity")
ax.legend()
ax.set_xlabel("Time (s)")
```

Out[45]: Text(0.5, 0, 'Time (s)')



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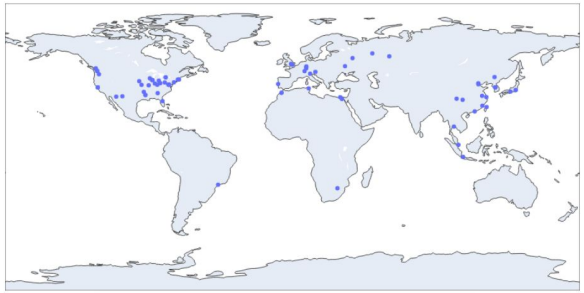
Put your questions into chat!

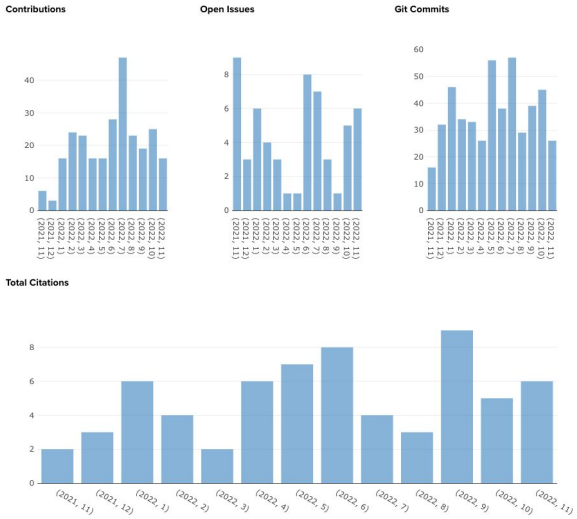
Teaser for 2023
(Github repo stats):

Downloads by Region



Total Downloads	75
Total Contributions	262
Total Commits	477
Total Citations	65

Git Repo



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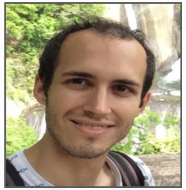
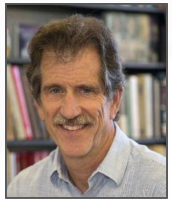
Seismic Cycles Working Group

Seismic Cycles Working Group:

- Kali Allison (UCD),
- Sylvain Barbot (USC, chair),
- Alice Gabriel (UCSD),
- Lorraine Hwang (UCD),
- Dave May (UCSD),
- Pierre Romanet (NIED),
- Paul Segall (Stanford),
- Luca Dal Zilio (ETH)






Purpose:

Build a community of modelers and developers focused on the specific challenges of modeling seismic cycles. Help develop and publish well documented, open-source software for seismic cycle modeling based on a variety of numerical methods that inter-operate.

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Seismic Cycles Working Group

Timeline:

- May-July 2022: weekly online seminar series. YouTube playlist: https://www.youtube.com/playlist?list=PLdy04DoEepEwTtFOR7MkQX1VlpMDOXLE9 (100-200 views per seminar)
- October 17-19, 2022: Online symposium (https://geodynamics.org/events/details/276) 21 speakers (9 women). 128 participants (65% men).
- December 2022: Whitepaper and strategic plan for community engagement and code development plan.
- 2023: Implementation of strategic plan and engaging community in the development and publication of software (developers keep full ownership/authorship)
  - Special volume in Journal of Open Source Software (tentative),
  - Developer workshop(s)

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Seismic Cycles Working Group

Numerical techniques for seismic cycle modeling

- Working group summary: https://www.youtube.com/watch?v=ttSRx2PKJlI&t=159s (337 views)
- For each scientific goal its numerical approach:
  - Boundary element method: quasi-dynamic, fully dynamic, spectral- or time-domain approach
  - Volume-based method: finite difference, continuous and discontinuous Galerkin finite-element method
  - Hybrid methods: integral method with surface and volume elements, domain decomposition
- More theoretical development is needed: curved surface elements, non-uniform slip surface elements, higher-order surface elements.
- Seismic cycle modeling is not a mature field.

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Software Perspectives

- GDMATE *Dylan / John*
- World Builder *Menno Fraters*
- ASPECT *Menno Fraters et al.*
- PyLith *Brad Aagaard*
- Rayleigh *Nick Featherstone*
- SPECFEM *Carl Tape*

Instructions

Reports should cover

Events

Development progress - features, releases, software engineering improvements

Development plans/how to find

8 min each!

GDMATE

Dylan Vasey, UC Davis and John Naliboff, NMT

- **G**eo**D**ynamic **M**odeling **A**nalysis **T**oolkit and **E**ducation
- A Python repository that aids in development, analysis, and education surrounding geodynamic modeling
- Motivating challenges?
  - Duplication of software and effort
  - Best programming practices often ignored
  - Evolving Python ecosystem and packages
    - Overlapping functionality, optimization options, dependencies
  - Barriers to beginning community software development

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

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GDMATE

Dylan Vasey, UC Davis and John Naliboff, NMT

- **Preface ~** This repository is in its infancy and is a proof-of-concept
  - github.com/gdmate/gdmate
- **Key Features**
  - Highly modular code structure with simple, discrete functions
    - Easy to add new code and expand repository to include new topics
    - Optimization
  - Online documentation and Jupyter Notebooks to demonstrate functionality
  - Automated testing of all proposed code changes
  - Clear guidelines for community contributions
  - Installable Python package

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GDMATE

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File Edit View Run Kernel Tabs Settings Help

Launcher | visualization.ipynb

Download GitHub Binder Markdown Python 3 (ipykernel)

Filter files by name

/

Name	Last Modified
build	5 days ago
docs	5 days ago
gdmate	5 days ago
gdmate.eg...	5 days ago
notebooks	2 minutes ago
tests	5 days ago
apt.txt	5 days ago
license.txt	5 days ago
meta.yaml	5 days ago
README....	5 days ago
setup.py	5 days ago

Visualization Examples

[1]:
```
import gdmate as gd

import matplotlib.pyplot as plt
import numpy as np
import pyvista as pv
```

Start Xvfb if on headless machine

Pyvista plotting will require Xvfb if running headless (e.g., on Binder). If you are using a local machine, you do not need to run this, but on Binder and other headless environments you will.

[2]:
```
pv.start_xvfb()
```

Plot a 2D grid as an image on a Matplotlib axes

The function `pyvista_vis.pv_plot_2d` takes a 2D Pyvista mesh and plots it using the bounds specified and colors it by the appropriate field. The code block below creates a sample Pyvista mesh of 9 cells (16 points), assigns each cell a value of 0-8, and the plots the 4 cells in the lower left on a Matplotlib axes with colors determined by the assigned value of the cell

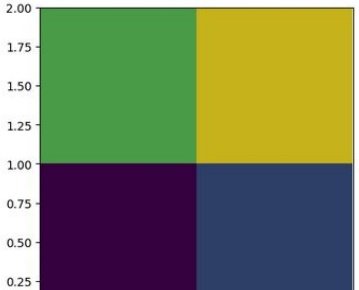
[3]:
```
# Create unstructured grid mesh of 4x4 points and 3x3 cells
mesh = pv.UniformGrid(dims=(4, 4, 1)).cast_to_unstructured_grid()

# Assign scalar value of 0-8 to each of the nine cells
mesh['sample_field'] = np.arange(9)

# Set up Matplotlib figure/axes
fig,ax = plt.subplots(1)

# Plot the mesh on the axes and color by the scalar values
ax = gd.pyvista_vis.pv_plot_2d(mesh,'sample_field',bounds=[0,2,0,2],ax=ax)
```

```
/srv/conda/envs/notebook/lib/python3.7/site-packages/pyvista/core/grid.py:511: PyVistaDeprecationWarning: `dims` argument is deprecated. Please use `dimensions`.
  '`dims` argument is deprecated. Please use `dimensions`.', PyVistaDeprecationWarning
```



GDMATE

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Development Plans

- Winter-Spring 2023: Add existing software to repository
  - Multiple 2D/3D visualization tools
  - Automated feature extraction (faults)
  - Thermochronology
  - Compilation of published material properties and equations
  - Educational material
  - Additional contributions people would like to make!

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Development Plans *continued*

- Summer 2023: Initial release and presentation to the community
  - Solicit new software contributions
  - Assess whether this is a fruitful path forward (if yes, see below)
- Summer 2023
  - Begin planning for long-term development and funding
    - CIG Working Group?
    - CSSI or Geoinformatics proposal submission?
    - Annual Hackathons?

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GDMATE

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Assessment: Is GDMATE (or general concept) a good idea?

1. Are the underlying functionality and workflows easy to use?
2. Can functionality and workflows easily be used for inputs derived from different codes?
3. Is the package designed in a way that enables straightforward development for new applications?
4. Is use and development suitable for both novice and advanced users?
5. Is large amounts of funding required for the package to be successful in both the short- and long-term?
6. Can the package be readily used for educational purposes during CIG tutorials and classroom exercises?

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World Builder

Menno Fraters, UC Davis

1. Why the GWB?
2. How does the GWB help?
3. What can it do?
4. GWB improvements and the CIG integration project
5. Goals
6. Results
7. Future plans

World Builder

Menno Fraters, UC Davis

1. Why the GWB?

1. Making complex synthetic models is hard.
2. They are hard to reproduce.
3. They are often hard to share between codes.

World Builder

Menno Fraters, UC Davis

2. How does the GWB help?

1. Human readable input file
2. Code, language and platform independent
3. Good documentation
4. Readable and extensible code
5. Strict version numbering

World Builder

Menno Fraters, UC Davis

Geodynamic World Builder

2. What can it do?

```
{
  "version":"0.3",
  "coordinate system":{"model":"cartesian"},
  "features":
  [
    {"model":"mantle layer", "name":"upper mantle", "min depth":100e3, "max depth":660e3,
       "coordinates":[[0,0],[0,1000e3],[2000e3,1000e3],[2000e3,0]],
       "composition models":[{"model":"uniform", "compositions":[4]}]},

    {"model":"oceanic plate", "name":"Overriding plate", "max depth":100e3,
       "coordinates":[[0,0],[0,1000e3],[1500e3,1000e3],[1600e3,250e3],[1500e3,0]],
       "temperature models":[{"model":"plate model", "max depth":100e3, "spreading velocity":0.01,
                              "ridge coordinates":[[400e3,-1],[-100e3,2000e3]]}],
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       "composition models":[{"model":"uniform", "compositions":[3], "max depth":50e3},
                             {"model":"uniform", "compositions":[1], "min depth":50e3}]},

    {"model":"subducting plate", "name":"Slab",
       "coordinates":[[1500e3,1000e3],[1600e3,350e3],[1500e3,0]],
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       "segments":[{"length":300e3, "thickness":[100e3], "angle":[0,60],
                    "composition models":[
                       {"model":"uniform", "compositions":[3], "max distance slab top":50e3},
                       {"model":"uniform", "compositions":[2], "min distance slab top":50e3}]},
                   {"length":500e3, "thickness":[100e3], "angle":[60,20]}],
       "temperature models":[{"model":"plate model", "density":3300, "plate velocity":0.02 }],
       "composition models":[{"model":"uniform", "compositions":[2], "max distance slab top":100e3}]}
  ]
}
```

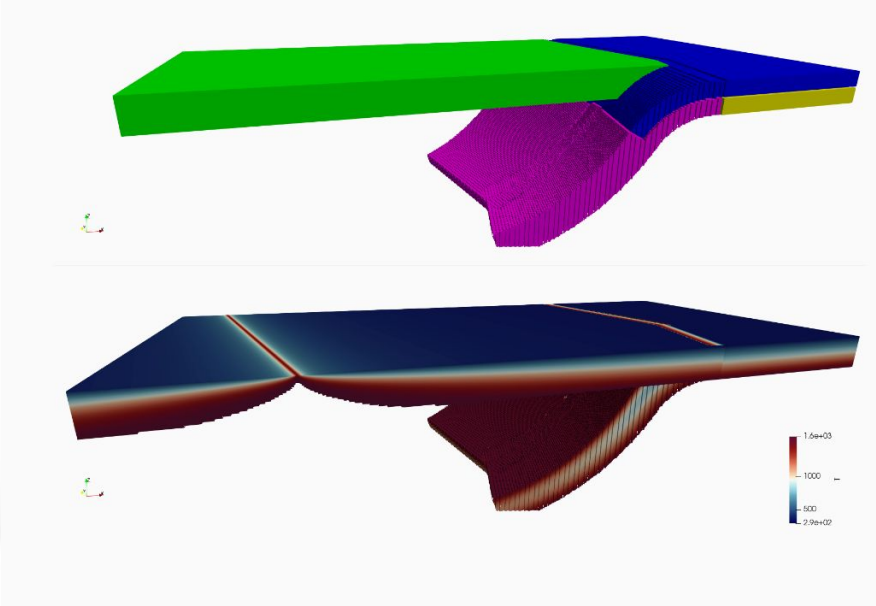

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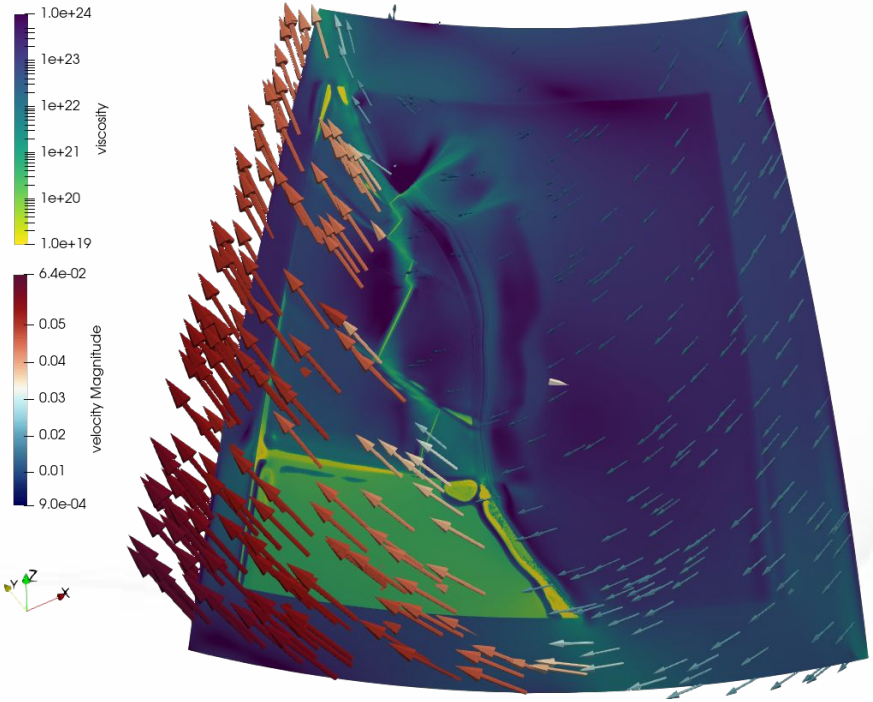
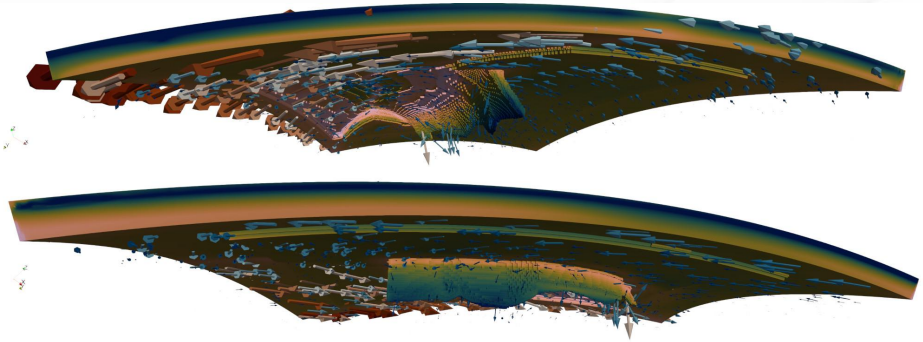
World Builder

Menno Fraters, UC Davis

2. What can it do?



Setup made by GWB, run with ASPECT and visualized in Paraview.



World Builder *Menno Fraters, UC Davis*

3. GWB improvements and the CIG integration project

1. Funded to:
   a. Make improvements to the GWB
   b. Bring the GWB into the CIG community

World Builder

Menno Fraters, UC Davis

4. Goals

1. New Sphinx based documentation.
2. Make GWB fully self contained.
3. More efficient interfaces.
4. A lot of new useful features like variable plate thickness, better slabs and dataset integration (slab2).

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World Builder *Menno Fraters, UC Davis*

5. Results

1. Goals mostly achieved (sphinx, interfaces, plate thicknesses, etc.).
2. Porting of documentation still in progress.
3. Slab2 integration still in progress.
4. When done, will publish a JOSS paper with CIG.

World Builder *Menno Fraters, UC Davis*

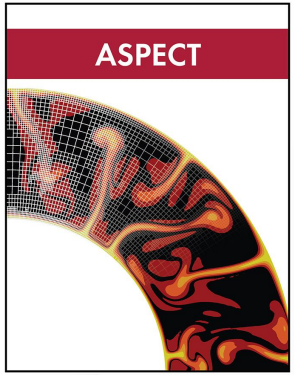
6. Future plans:

Will mostly likely focus on:

1. New interfaces to geodynamic models
2. New features and plugins for features

But will be based on community requests.

ASPECT *- Menno Fraters, UC Davis*



1. What is ASPECT and what is it becoming?
2. 2022 ASPECT Events
3. Contributions and contributors
4. Main new features in last release.
5. Main new features since last release
6. Name change after next release! Or is it?

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

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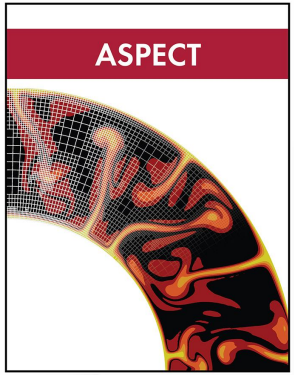
ASPECT *- Menno Fraters, UC Davis*



1. What is ASPECT and what is it becoming?
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ASPECT - Advanced Solver for Problems in Earth's ConvecTion

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

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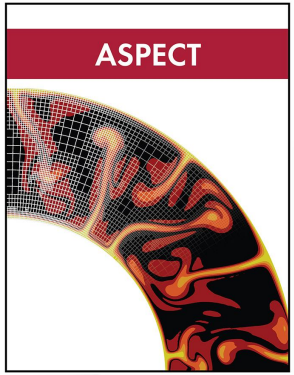
ASPECT *- Menno Fraters, UC Davis*



2022 Activities

1. bi-weekly meetings
2. 2022 ASPECT user meeting (Jan 19 - 20, 2022)
3. 2022 Hackathon (May 15 - 24, 2022)

Plan (tentative dates):

ASPECT user meeting: Jan 31 - Feb 1, 2023

ASPECT hackathon: TBA (2023)

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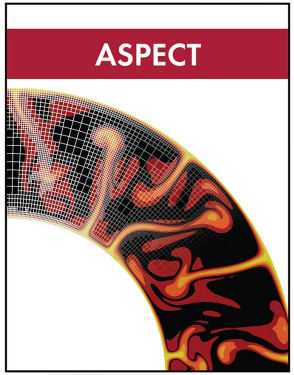
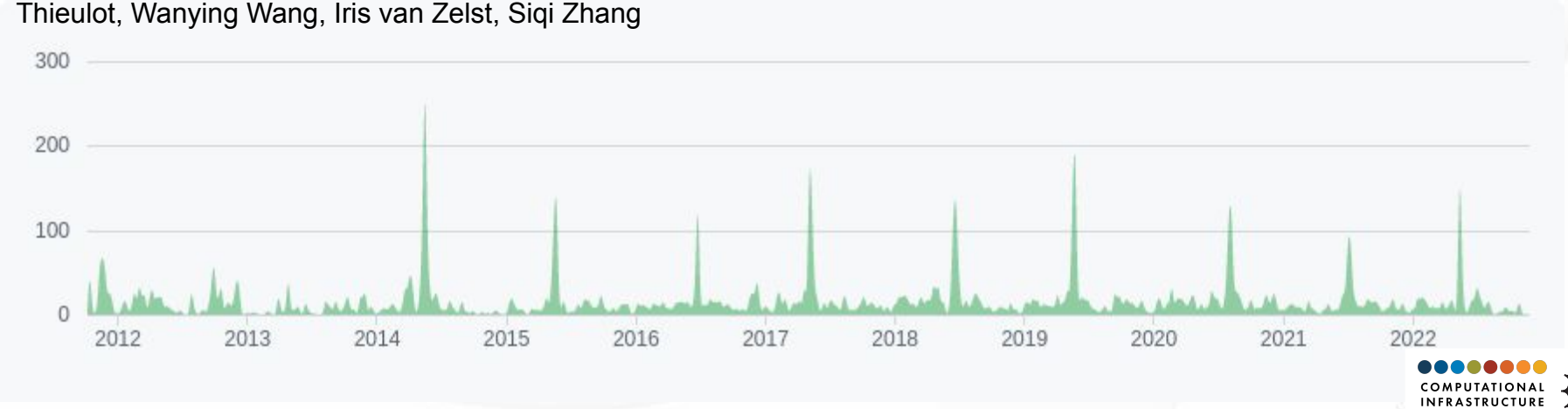
ASPECT - *Menno Fraters, UC Davis*



Contributions and contributors

By Wolfgang Bangerth, Juliane Dannberg, Menno Fraters, Rene Gassmöller, Anne Glerum, Timo Heister, Bob Myhill, John Naliboff

With contributions by: Jacqueline Austermann, Magali Billen, Markus Bürg, Thomas Clevenger, Samuel Cox, William Durkin, Grant Euen, Thomas Geenen, Ryan Grove, Eric Heien, Ludovic Jeanniot, Louise Kellogg, Scott King, Martin Kronbichler, Marine Lasbleis, Haoyuan Li, Shangxin Liu, Hannah Mark, Elvira Mulyukova, Bart Niday, Jonathan Perry-Houts, Elbridge Gerry Puckett, Tahiry Rajaonarison, Fred Richards, Jonathan Robey, Ian Rose, Max Rudolph, Stephanie Sparks, D. Sarah Stamps, Cedric Thieulot, Wanying Wang, Iris van Zelst, Siqi Zhang



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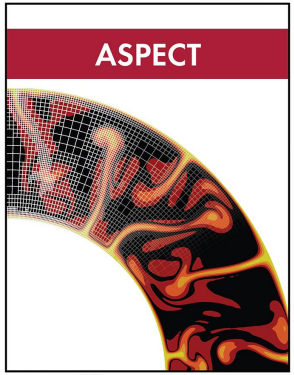
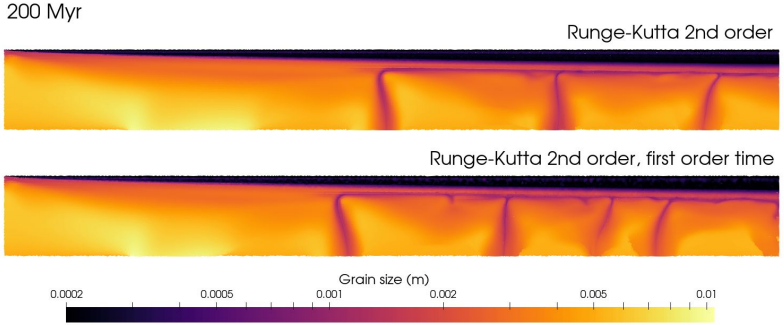


Main new features in last release:

1. Matrix-free GMG Stokes solver for Newton, Elasticity, Free Surface (Jiaqi Zhang and Timo Heister)
2. Compositional fields can now be advected by Darcy's law (Daniel Douglas)
3. Major improvements on particles (performance and accuracy) (Rene Gassmoeller, Mack Gregory, Gerry Puckett)
4. Allowing material models to read in one or more Perple_X or HeFESTo table files (Bob Myhill)
5. Many more new features and bug fixes (Many authors)



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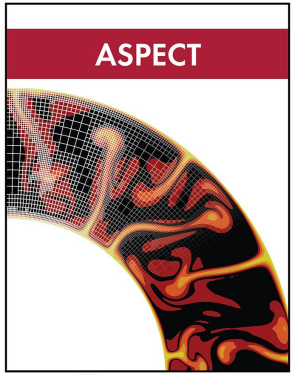
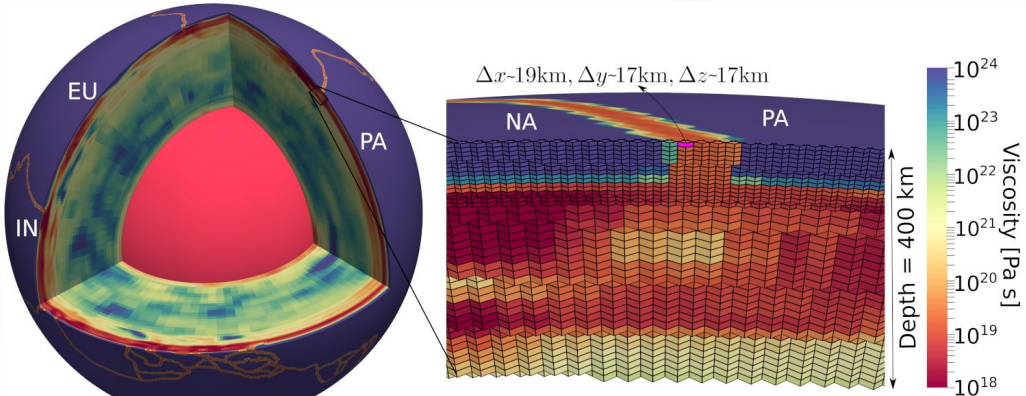


Main new features since last release:

1. More matrix-free GMG Stokes solver improvements (Jiaqi Zhang and Timo Heister)
2. New sphinx based documentation (Chris Mills and many others)
3. Basic CPO tracking functionality (Menno Fraters)
4. Material model that computes density and viscosity based on seismic tomography and additionally includes weak plates boundaries (Aruhsi Saxena)



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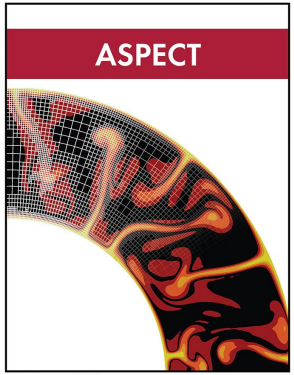

Future Plans

1. NetCDF support for structured data (Timo Heister)
2. D-Rex integration in the CPO code (Menno Fraters)
3. Surface processes (Anne Glerum and Derek Neuharth)
4. Updated to VEP rheology (multiple developers, led by Anne Glerum)
5. More coupling between fluid transport and solid deformation (many)
6. Global coarsening GMG for 2-3x faster adaptive computations (Timo Heister)
7. Name change (T for Tectonics):
   "Advanced Solver for Problems in Earth's Convection and Tectonics"

(see https://github.com/geodynamics/aspect/projects/2)

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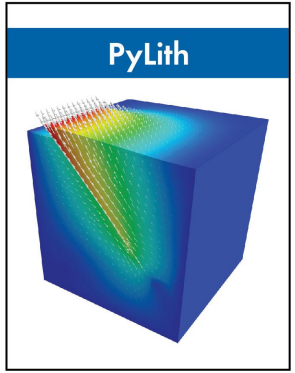
PyLith *Brad Aagaard, USGS*



2022 Activities

- Crustal Deformation Modeling workshop
- PyLith v3 (12 contributors)

2023 Planned Activities

- PyLith Hackathon, June 11-18, 2023
- Additional PyLith releases

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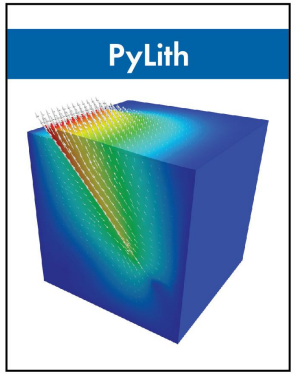
PyLith *Brad Aagaard, USGS*



Crustal Deformation Modeling Workshop

June 20-24, Colorado School of Mines, Golden, CO

Themes

- Earthquake cycle modeling
- Inverting for fault slip
- Faulting, fluids, and surface loading
- Crustal deformation mechanics of Enceladus

2 days of PyLith tutorials + 3 days of science talks and discussions

63 participants from 8 countries

- 75% early career

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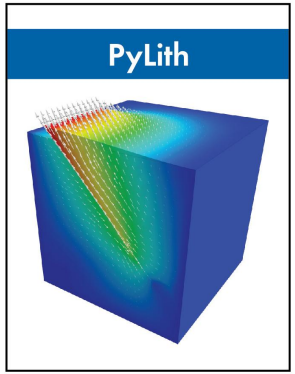
PyLith *Brad Aagaard, USGS*



New Features in PyLith v3

- Multiphysics formulation: elasticity, incompressible elasticity, poroelasticity
- Flexible spatial and temporal discretization via PETSc
- Import finite-element meshes from Gmsh (open-source)
- Default solver settings (preconditioners, tolerances) based on physics
- New example suite
- Documentation converted to Sphinx + MyST: pylith.readthedocs.io
- Converted to Python 3
- Testing with Method of Manufactured Solutions
- Simulation metadata with utility for searching metadata

PyLith v3.0.3 released October 14, 2022

- Source code
- Binary packages for Linux and macOS (x86_64 and arm64)

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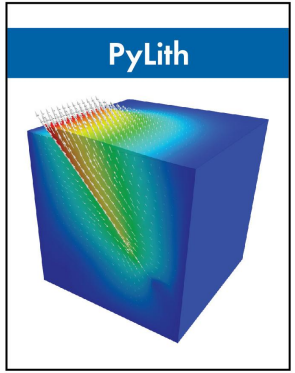
PyLith *Brad Aagaard, USGS*



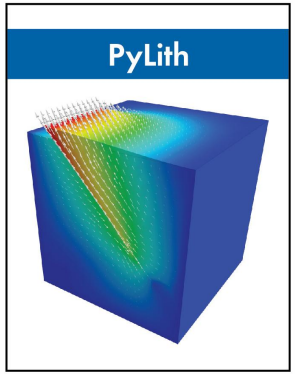
PyLith Development Plan: target applications

- 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
- Quasi-static and dynamic modeling of fluids and faulting

PyLith Manual → Introduction → Development Plan

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS NSF

PyLith *Brad Aagaard, USGS*



PyLith Development Plan: upcoming releases

- **v3.1 (Spring 2023)**
  - Dynamic elasticity with prescribed slip
  - Parallel mesh loading
  - Other small improvements
- **v3.2 (Summer 2023)**
  - Spontaneous rupture
  - Small strain formulation for elasticity
  - Elastoplastic bulk rheology
  - Integration with libCEED (Matt Knepley and Jed Brown)
  - More flexible specification of time-dependent boundary conditions
- **v4 (Spring 2024)**
  - Coupling quasi-static and dynamic problems with compatible meshes
  - Migrate examples to Jupyter notebooks
  - Update to current Pyre simulation framework
  - Adaptive mesh refinement

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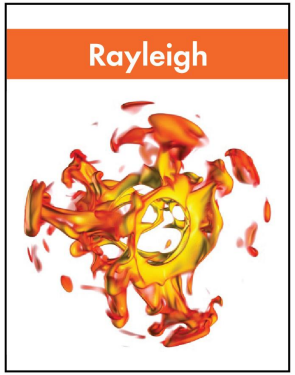
Rayleigh *Nick Featherstone, SWRI*



Development Team

Philipp Edelmann, Nick Featherstone, Rene Gassmoeller, Loren Matilsky
Ryan Orvedahl, Cian Wilson

Events

- 2022 Rayleigh Hackathon
  - September / Breckenridge, CO
  - 11 attendees – in-person!
- 2023 Hackathon in planning stages
- Monthly development team meetings

Developments

- Transpose optimization
- Major documentation overhaul (hackathon activity)
- 1.1 Release
- GPU-capable Legendre Transforms (Ryan Orvedahl)
  - proof-of concept; OpenACC/CUDA

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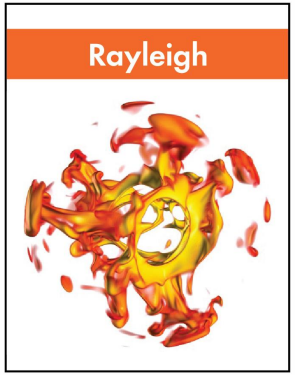
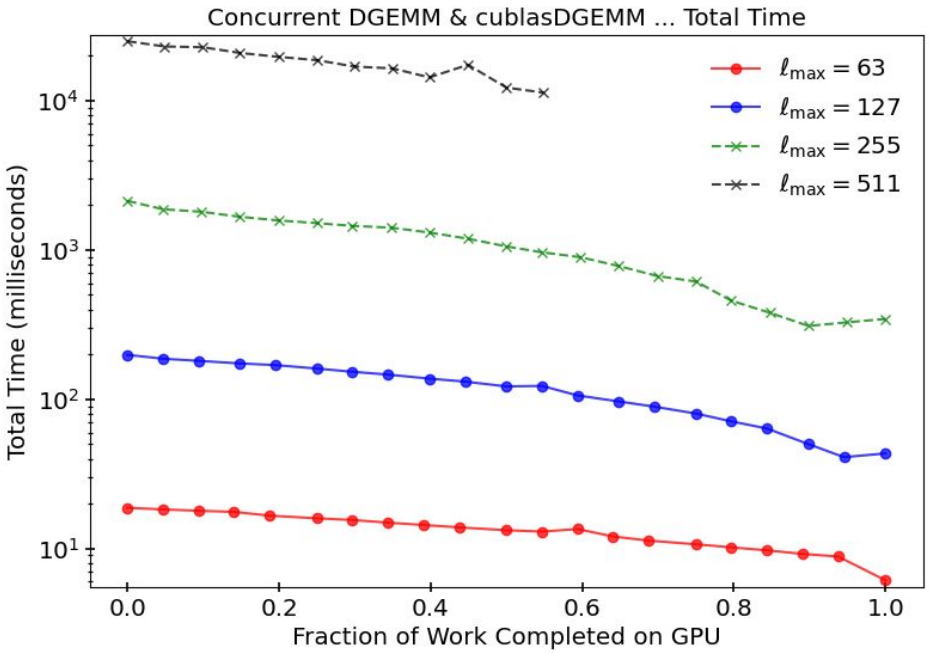
Rayleigh *Nick Featherstone, SWRI*



- GPU-capable Legendre Transforms
  - Multiple, different-sized calls to DGEMM
  - Strategy: split DGEMM calls between CPU and GPU



NASA Pleiades
NVIDIA V100 GPU
Intel Skylake CPU

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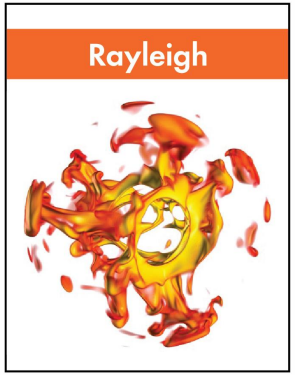
Rayleigh *Nick Featherstone, SWRI*



2023 Development Plans

- GPU-capable Legendre Transforms
  - Integrate into main branch
- GPU-capable Linear Solves
  - Explore potential
- Multiple chemical species
  - Cian Wilson
  - Implementation complete
  - UI in-development
- Finite-differences in radius
  - Philipp Edelmann & Rathish Ratnasingam
- Targeting quarterly release cycle

www.github.com/geodynamics/rayleigh

https://rayleigh-documentation.readthedocs.io/en/latest/

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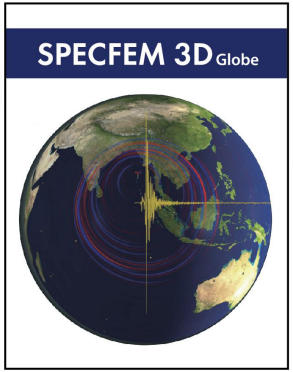
SPECFEM

Carl Tape, UAF & Daniel Peter, KAUST



- 2022 was a major year for SPECFEM, in terms of training, community organization, software improvements, and future plans
- **training**: virtual workshop for users in Oct; in-person developers workshop in Nov (Toronto)
- **community organization**: the Toronto workshop led to rapid organization of the SPECFEM community, including www.specfem.org forming during the workshop, repos transferring from the CIG github org to the new SPECFEM github org, all discussions steered to the SPECFEM github (and away from emails, email lists, CIG forum), establishment of Google Scholar page, establishment of monthly zoom discussions
- **software improvements**: acceleration of commits since Oct 2022 focusing on standardization across SPECFEM packages, cosmetic, documentation, and also important bug fixes
- **future plans**: specfem_kokkos (Rohit Kakodkar, Princeton); overhaul wiki page (e.g., development plan); continued coordination with NSF CSSI SCOPED project; establish a master update every 6 months

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2022 SPECFEM virtual workshop for users (October 5–7, 2022)

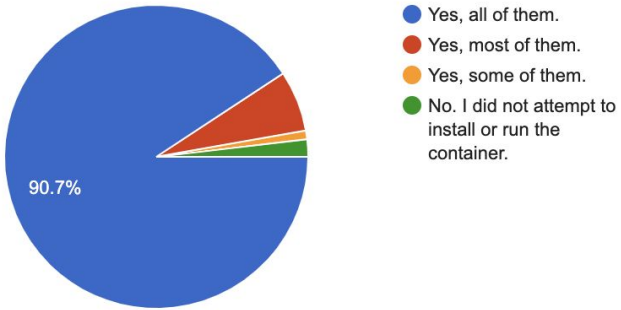
Workshop by the numbers:

- 3 days, 4 hours/day, 10 hosts, 4 invited speakers
- 4 software packages: specfem2d, specfem3d, seisflows, pyatoa
- travel and registration costs: $0
- investment by lead host (Bryant Chow): significant!
- 303: filled out google survey of interest
- 187: Day 1 attendance from *all over the world*
- >130: running Jupyter Notebooks
- 108: survey responses (Day 1)
  - wavefield simulations and simulation-based seismic inversions worked (with MPI) on participants' own laptops on 4 different operating systems.
- >49: "Yes, this is the first kernel I've made." (Day 2)
- 63: full 12-hour participation through Day 3

Did the example instructions work for you?

Copy

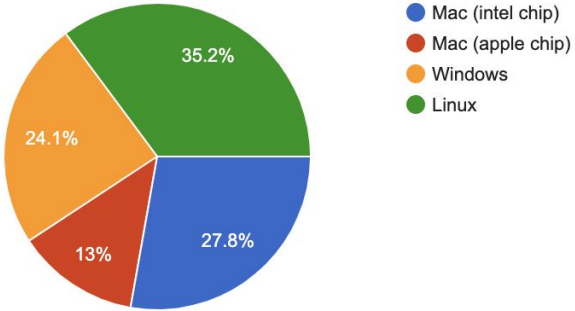
108 responses

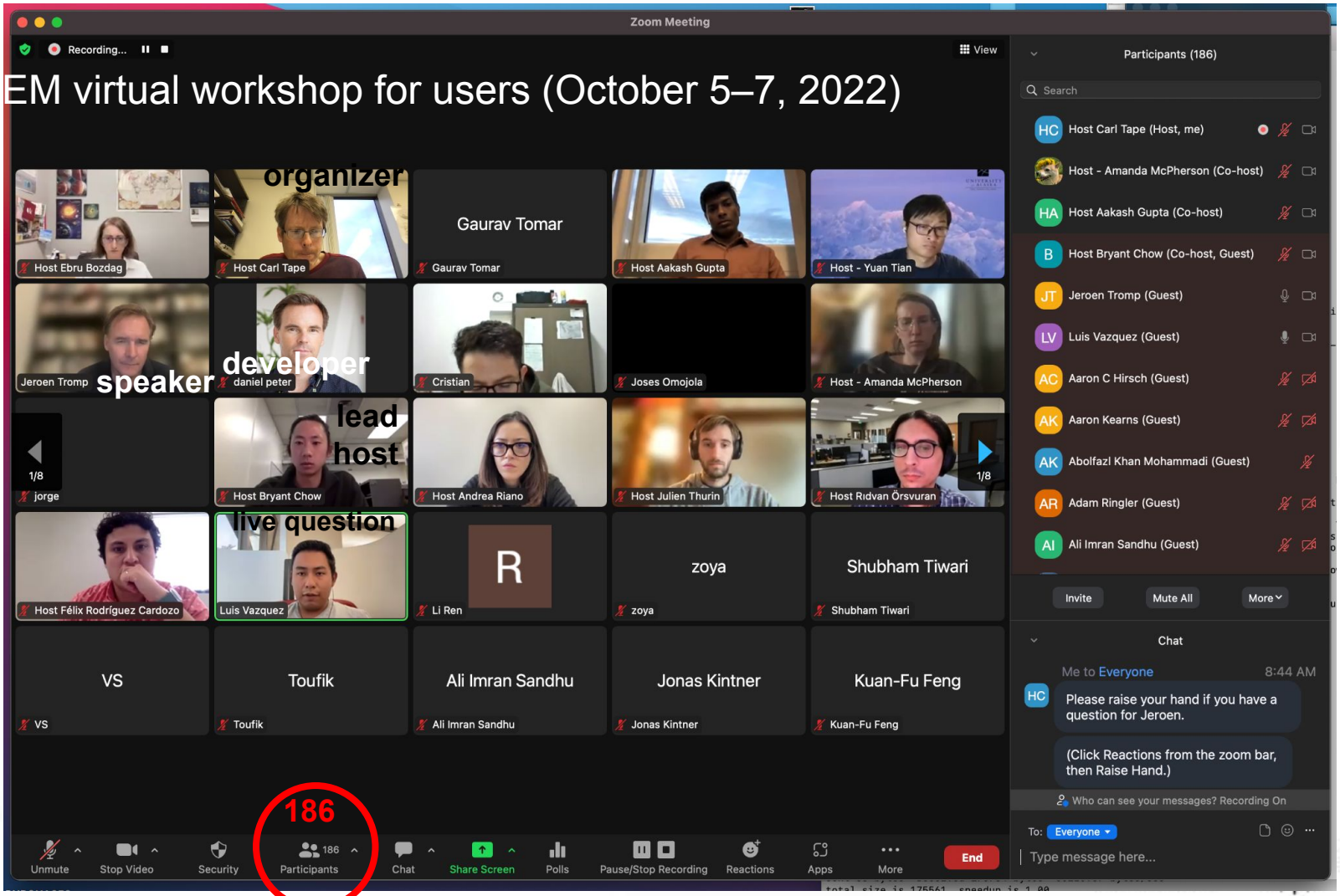


What operating system did you use?

Copy

108 responses




Zoom Meeting
Recording...
View
EM virtual workshop for users (October 5–7, 2022)
organizer
speaker
developer
lead host
live question
Host Ebru Bozdag
Host Carl Tape
Gaurav Tomar
Host Aakash Gupta
Host - Yuan Tian
Jeroen Tromp
daniel peter
Cristian
Joses Omojola
Host - Amanda McPherson
1/8
jorge
Host Bryant Chow
Host Andrea Riano
Host Julien Thurin
Host Rıdvan Örsvuran
1/8
Host Félix Rodríguez Cardozo
Luis Vazquez
Li Ren
zoya
Shubham Tiwari
VS
Toufik
Ali Imran Sandhu
Jonas Kintner
Kuan-Fu Feng
186
Unmute
Stop Video
Security
Participants
Chat
Share Screen
Polls
Pause/Stop Recording
Reactions
Apps
More
End
Participants (186)
Search
Host Carl Tape (Host, me)
Host - Amanda McPherson (Co-host)
Host Aakash Gupta (Co-host)
Host Bryant Chow (Co-host, Guest)
Jeroen Tromp (Guest)
Luis Vazquez (Guest)
Aaron C Hirsch (Guest)
Aaron Kearns (Guest)
Abolfazl Khan Mohammadi (Guest)
Adam Ringler (Guest)
Ali Imran Sandhu (Guest)
Invite
Mute All
More
Chat
Me to Everyone
8:44 AM
Please raise your hand if you have a question for Jeroen.
(Click Reactions from the zoom bar, then Raise Hand.)
Who can see your messages? Recording On
To: Everyone
Type message here...

workshop webpage

contains links to materials:

- docker instructions
- software container
- speaker slides
- videos for all 3 days

2022 SPECFEM virtual workshop for users

(go here for information on the developers workshop in Toronto)

A virtual workshop for learning to use SPECFEM, open-source software for seismic wave propagation and seismic imaging in 2D and 3D. Codes featured include SPECFEM2D, SPECFEM3D, Seisflows, and Pyatoa.

DAY 0 [Tues] October 4, 12:00–13:00 US Eastern time [*verifying software installs only*]

DAY 1 [Wed] October 5, 12:00–16:00 US Eastern time

DAY 2 [Thu] October 6, 12:00–16:00 US Eastern time

DAY 3 [Fri] October 7, 12:00–16:00 US Eastern time

Where: zoom

Agenda: here (includes background reading)

Registration: If interested, please fill out this survey to provide your basic information.

Format: Participants will install and run software on their own machines, then interact with hosts and other participants via zoom.

Requirements: Participants will need access to a computer and have permission to install docker and also the software container for the workshop.

Costs: none

Host: Bryant Chow

Starting point: docker install, download software container

Invited talks: Jeroen Tromp, Daniel Peter, Qinya Liu, Bryant Chow (speaker slides here)

Organizer: Carl Tape (ctape[a]alaska.edu)

Recordings: Day 1, Day 2, Day 3

Participants, please help us by doing the short post-workshop surveys for Day 1, Day 2, and Day 3.

(via Carl Tape webpage)

	Specfem Users Workshop	Specfem Developers Workshop
Dates	October 5–7, 2022	October 27–28, 2022
Venue	zoom	Toronto
Organizers	Bryant Chow, Carl Tape	Qinya Liu, Lorraine Hwang, Carl Tape
Participants (virtual)	187 (Day 1 max)	~12
Participants (in person)	0	~30
Goals	• learning about SEM and the software packages • Running SPECFEM2D and 3D in parallel on user's laptop • performing simple iterative seismic imaging examples (kernels and model updates)	• discussing the scientific needs of the SPECFEM community • establishing practices to strengthen the SPECFEM community of users and developers (members wanted!) • identifying tasks needed at all levels of participation

Discussion

Collaborating with CIG Review/Summary:

What are the collaboration needs of the community?

Question:

https://tinyurl.com/22CIGjam2

How can CIG help meet community collaboration needs?

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thank you
THE
END
Presentation will be posted.
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