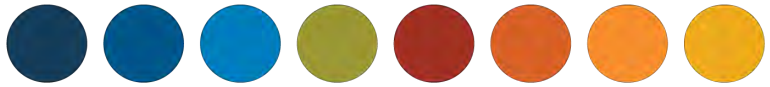
dynamo

mantle convection

long term tectonics

seismology

short term crustal dynamics



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melt and volatiles

education

computational science

2021 CIG Annual Business Meeting
November 18, 2021

Agenda
PST

13:00 **Welcome**

What's new at CIG Headquarters *Lorraine Hwang, Director, UC Davis*

13:10 **Reports on Past Activities**

- **SMOREs Program** *John Naliboff, New Mexico Tech*

Past and Future Perspectives on Software

- **PyLith** *Brad Aagaard, USGS*
- **SPECFEM** *Jeroen Tromp, Princeton University*
- **Rayleigh** *Nick Featherstone, SWRI*
- **ASPECT** *Wolfgang Bangerth, CSU Fort Collins*

13:35 **CIG IV** *Bruce Buffett, coDirector CIG IV, UC Berkeley*

13:50 **Breakout Discussions**

Topic 1. JEDI and Belonging

Topic 2. Engaging Our Community

14:10 **Report Back**

14:20 **Summary Plenary Conversation**

Topic 3. Supporting Earth System Science and Convergent Research

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CIG Staff

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Director

Lorraine Hwang

Technical Lead

Rene Gassmoeller

Research Scientist

Hiroaki Matsui

Postdoctoral Fellows

Kali Allison

Ryan Orvedahl

Junior Specialist

Chris Mills

Elections

Thanks to

- Min Chen
- Katie Cooper
- Louis Moresi
- Krista Soderlund
- Cian Wilson

Nominating Committee

- Jackie Austermann
- Max Rudolph
- Carl Tape

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Executive Committee

Claire Currie, *Chair*

Brad Aagaard*
Bruce Buffett
Alice Gabriel
Carolina Lithgow-Bertelloni*

Science Steering Committee

Julianne Dannberg, *Chair*

Sylvain Barbot
Ebru Bozdag*
Peter Driscoll*
Scott King
Harriet Lau*
Dave May*
John Naliboff

** New Member*

Leadership

EC

SSC

Roles and Responsibilities

- EC

  The Executive Committee (EC) of CIG oversees the administrative affairs of the organization receiving input from the community and committees of the organization.

- SSC

  The Science Steering Committee of CIG oversees software and cyberinfrastructure related activities of the organization receiving input from the community and committees of the organization.

  About > Governance

- WG

  Why Working Groups?
  Working Group Expectations
  Working Group Incentives

  Working Groups

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Working Groups

Why Working Groups?

- Providing input to leadership about community needs
- Organizing community benchmarking exercise
- Organizing workshops and trainings
- Identifying and providing direction in solving computational problems
- Identifying the need for new codes
- Providing mentorship
- Serving as a test bed for new ideas
- Building/seeding a community for new codes

NEW WORKING GROUPS

Software Developer Workshop

Brad Aagaard & Rene Gassmoeller

Seismic Cycles

Sylvain Barbot

Contact leads
or
lorraine@geodynamics.org

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What's New 2022

Events

January 19-20:	ASPECT User Meeting *virtual*
February:	Software Developers Meeting
May 15-24:	ASPECT Hackathon *Wyoming*
June 13-17:	Crustal Deformation Workshop *Colorado*
Tbd	Rayleigh Hackathon

Distinguished Speakers

Climate, Tectonics, and Planetary Life - Adrian Lenardic, Rice University

The Structure of Oceanic Plates using machine Learning on Seafloor Vibrations - Tolulope Olugboji, University of Rochester

University of Idaho *joint with* Washington State University, University of Washington, Universidad Nacional de Colombia *virtual*, Florida International, University of New Mexico, McGill University *joint with* University of Quebec at Montreal *virtual*

2022 SMOREs *recruiting for mentors*

Webinars

2nd Thursday of the month @2P PT

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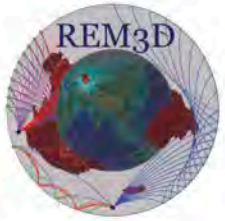
Community Toolboxes

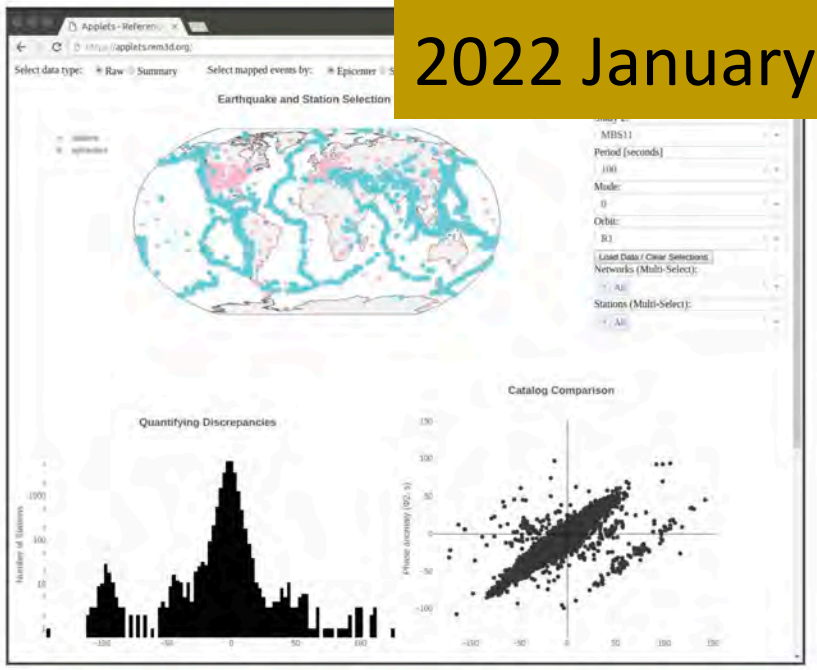
AVNI

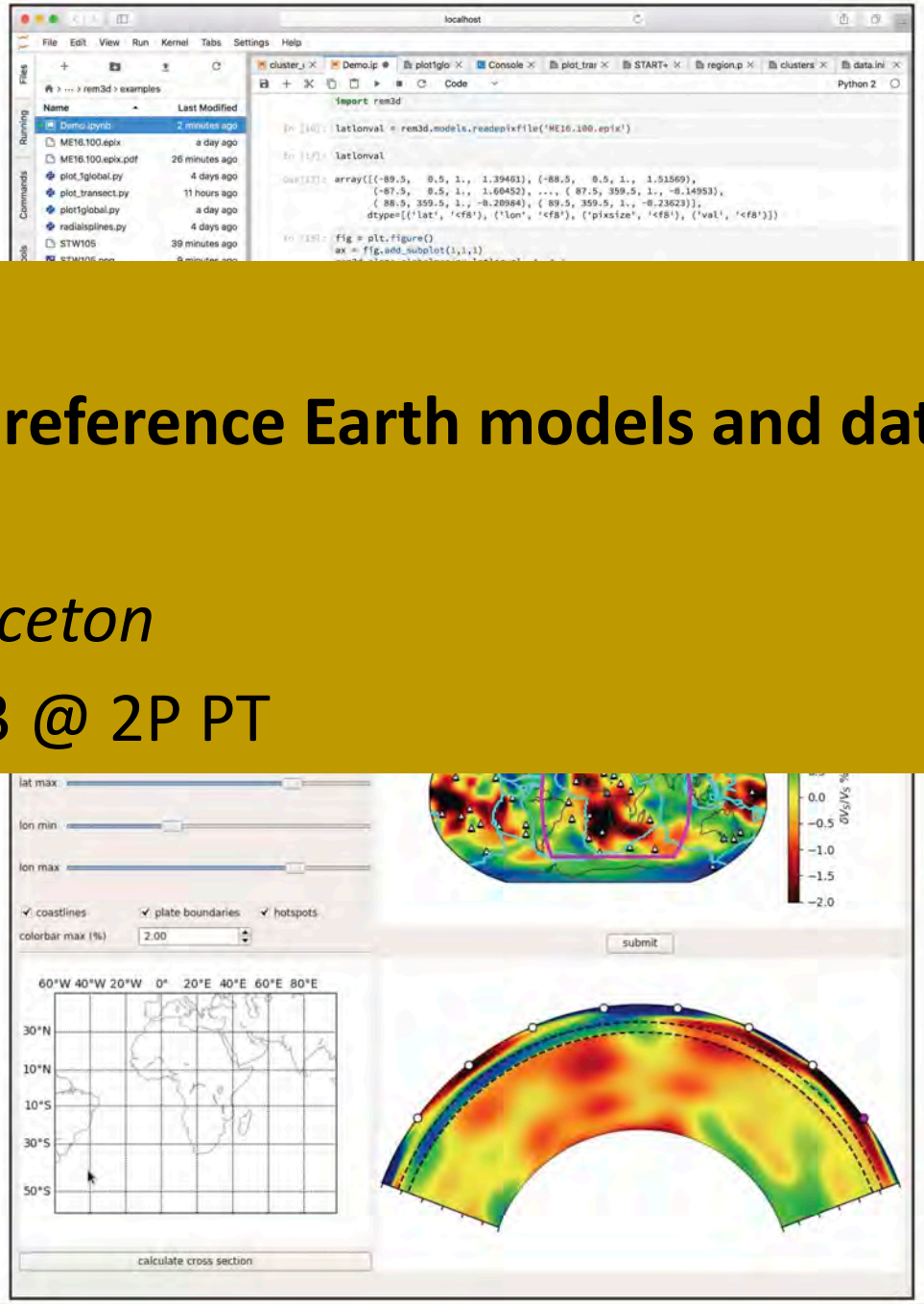
Analysis and **V**isualization toolkit for pla**N**etary **I**nferences



About

REM3D is a Python library for analyzing and interpre
has modules in MATLAB, C and Fortran as well.





Next Webinar

Introduction to reference Earth models and datasets using AVNI

Raj Moulik, Princeton

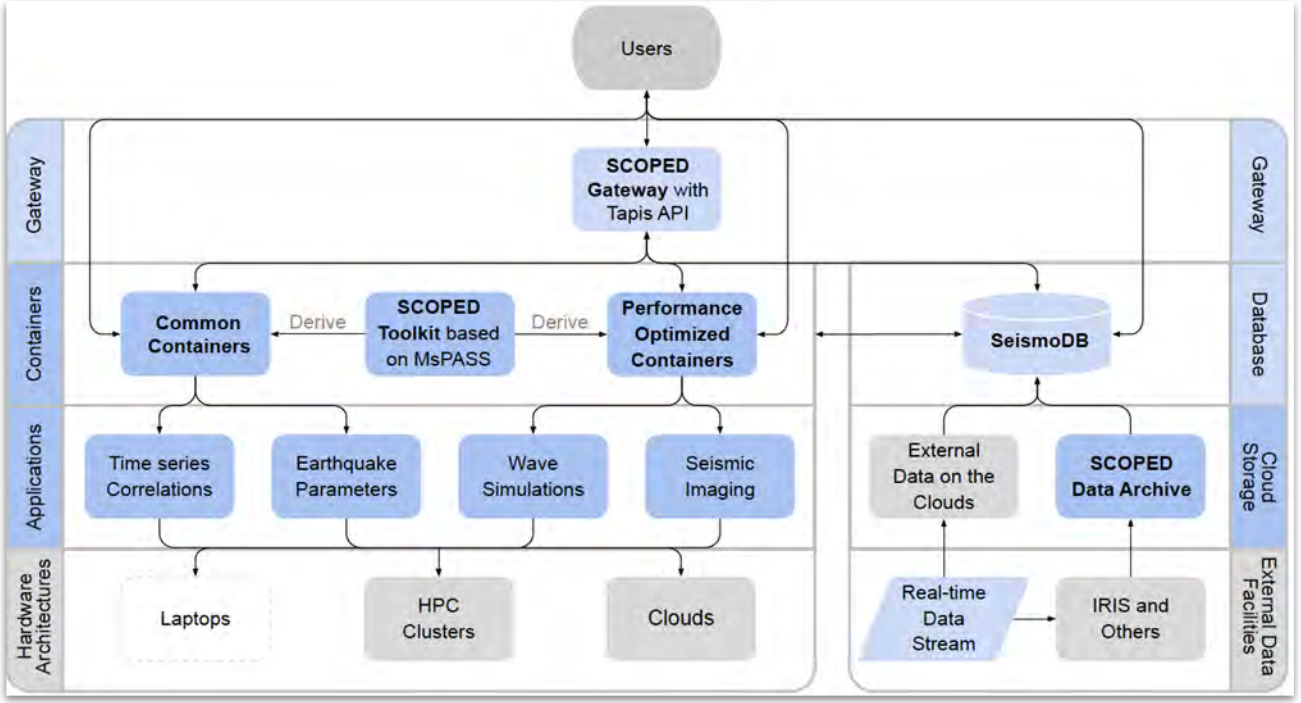
2022 January 13 @ 2P PT

urce Codes

CIG

NSF Cyberinfrastructure for Sustained Scientific Innovation Frameworks Project:

Seismic COmputational Platform for Empowering Discovery (SCOPED)



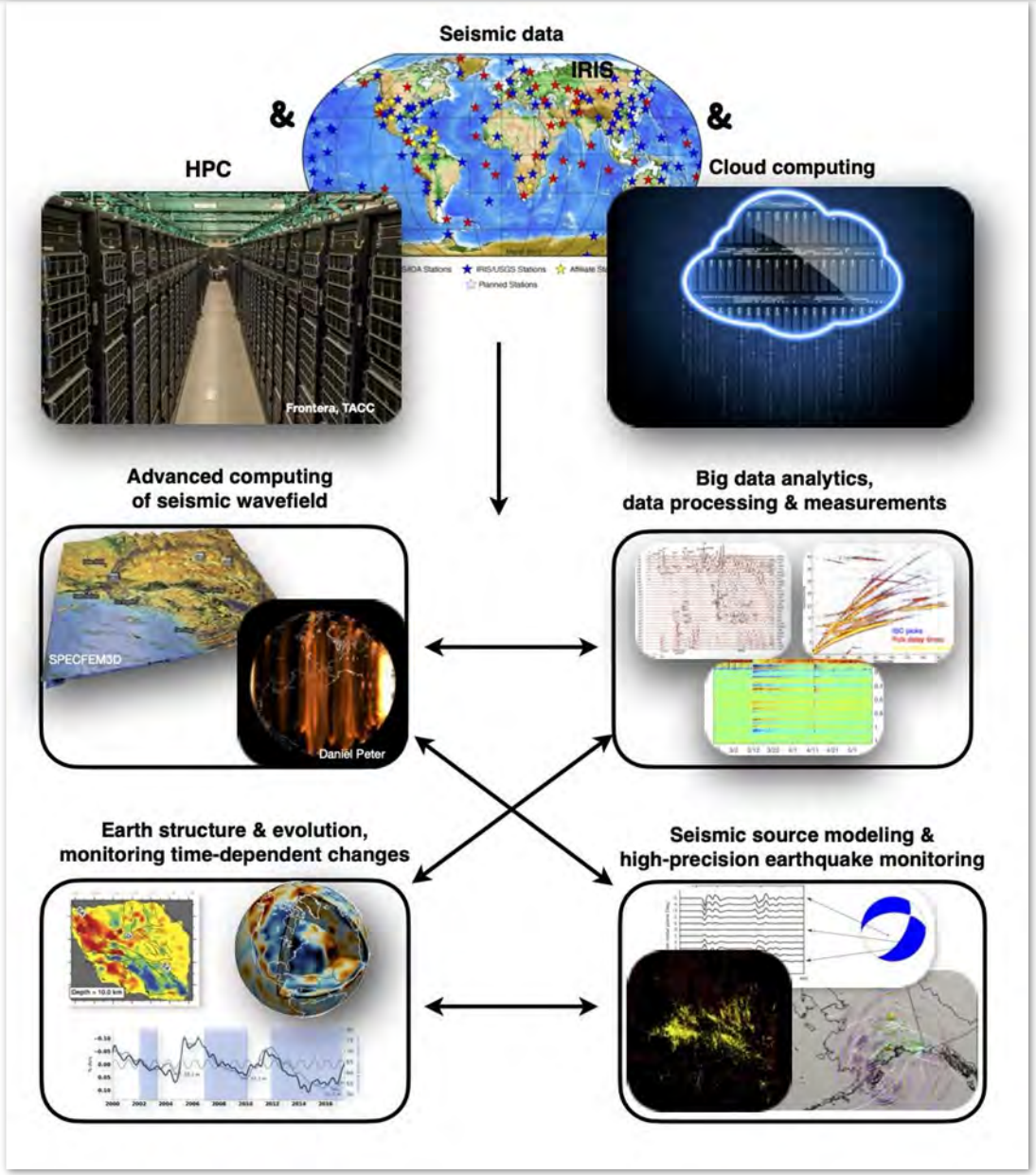
Carl Tape, University of Alaska (ctape@alaska.edu)

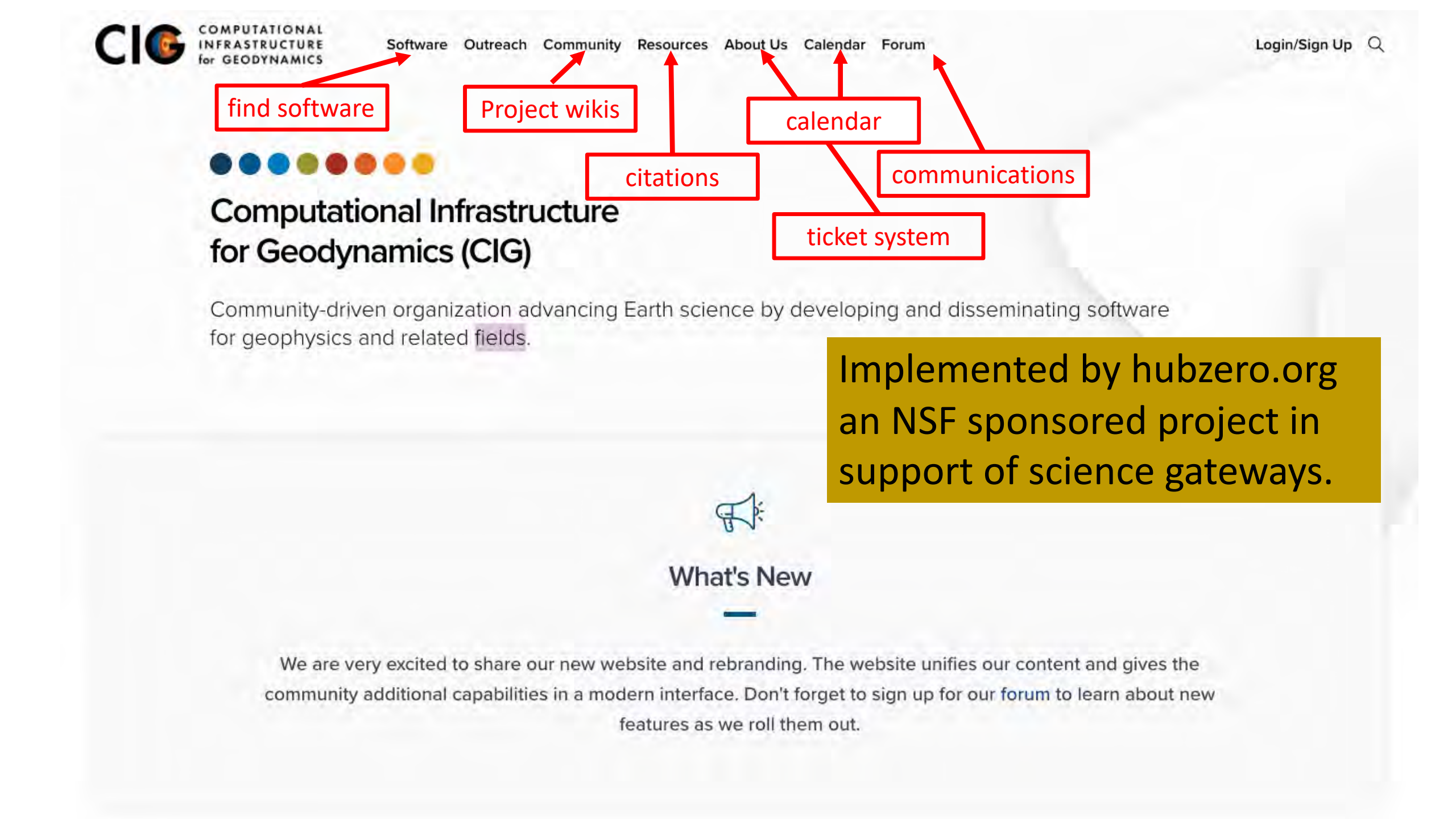
Ebru Bozdağ, Colorado School of Mines (bozdag@mines.edu)

Marine Denolle, University of Washington (mdenolle@uw.edu)

Felix Waldhauser, Columbia University (felixw@ldeo.columbia.edu)

Ian Wang, Texas Advanced Computing Center (University of Texas) (iwang@tacc.utexas.edu)

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Software
Outreach
Community
Resources
About Us
Calendar
Forum
Login/Sign Up
find software
Project wikis
citations
calendar
communications
ticket system
Computational Infrastructure for Geodynamics (CIG)
Community-driven organization advancing Earth science by developing and disseminating software for geophysics and related fields.
Implemented by hubzero.org an NSF sponsored project in support of science gateways.
What's New
We are very excited to share our new website and rebranding. The website unifies our content and gives the community additional capabilities in a modern interface. Don't forget to sign up for our forum to learn about new features as we roll them out.

SMOREs
pilot

Summer **M**odeling **R**esearch **E**xperience**s** (SMOREs)

2021 Pilot Program Overview and Future Plans

John Naliboff, NMT

Acknowledgements

- **Dave Stegman (UCSD)**

Organization and advice from prior REU activities

- **CIG SSC Members - Sylvain Barbot, Krista Soderlund, Cian Wilson**

Review of applications

- **Participants: Mentors and Students**

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Overview

Challenges and Motivation

- Members of the geodynamics community come from a broad range of communities, many of which are the least diverse in STEM
- Too few undergraduates with proper numerical and computational backgrounds

Solution

- Provide funded training and research opportunities for undergraduates
- Specifically target underrepresented groups in advertising

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Participants

Students* (out of 35 applicants)

- Elena Ehrlich (North Carolina State)
- Keneni Godana (University of Illinois at Chicago)
- Dante Hickey (Reed College)
- Hiva Mohammadzadeh (Pierce College *now at* UC Berkeley)
- Brittany Okonkwo (UC Santa Barbara)

Mentors

- Magali Billen (UC Davis)
- Katie Cooper (Eastern Washington)
- Eric Mittelstaedt (University of Idaho)
- John Naliboff (New Mexico Tech)
- Max Rudolph (UC Davis)
- Shi Joyce Shim (Georgia Tech)
- Suzanne Smrekar (NASA - JPL)
- Dave Stegman (UC San Diego)
- Laura Waters (New Mexico Tech)
- Jolante Van Wijk (New Mexico Tech)

Team approach in assigning mentor pairs.

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Structure
virtual

- **2 weeks virtual tutorials**
  - Basics of python
  - Geodynamic Processes
  - Geodynamic Modeling
- **6-8 week research projects**
- **Meet weekly:**
  - Project updates, tips for grad school applications, …

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Capstone Presentations at October 2021 CIG Webinar!

Outlook & Path Forward

2022 SMOREs ?

- New program leader and mentors.
- Extend to more areas of the geodynamics community
- Begin with CIG-organized training sessions available to all members of the community

•2023 and Beyond (In a Perfect World)

- NSF REU program supports a large number of students distributed across the community
- Program begins with ~ two weeks of tutorials hosted at CIG headquarters:
  - Week 1: Basic computational methods in geodynamics
  - Week 2: Choice of domain-specific tutorials (earthquake cycle, mantle convection)

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WANTED: Mentors for 2022

Contact John Naliboff or Lorraine Hwang

Software
Perspectives

Past and Future Perspectives

- PyLith - *Brad Aagaard*
- SPECFEM - *Jeroen Tromp*
- Rayleigh - *Nick Featherstone*
- ASPECT - *Wolfgang Bangerth*

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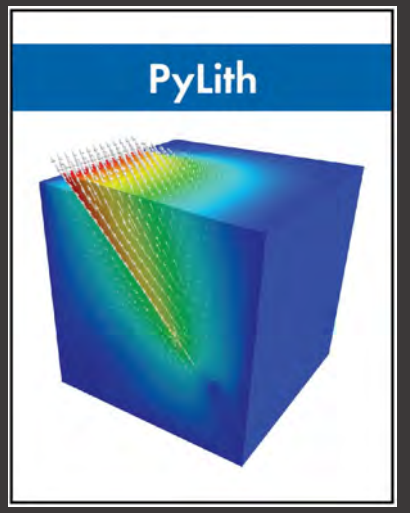

PyLith

Brad Aagaard, Matthew Knepley, Charles Williams

USGS

GNS SCIENCE TE PŪ AO

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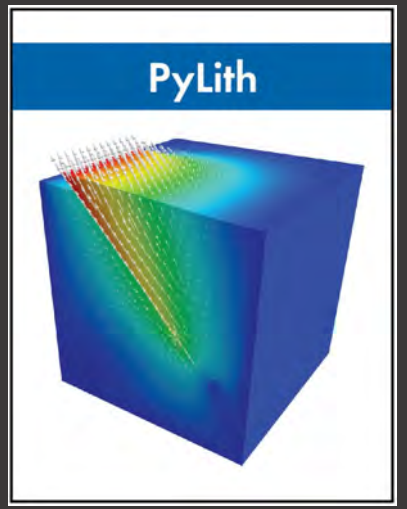
PyLith 2007–2021: By the numbers



7 Science workshops
12 Tutorials
2 Hackathons
32 Releases
8700 Commits
10,000 Downloads

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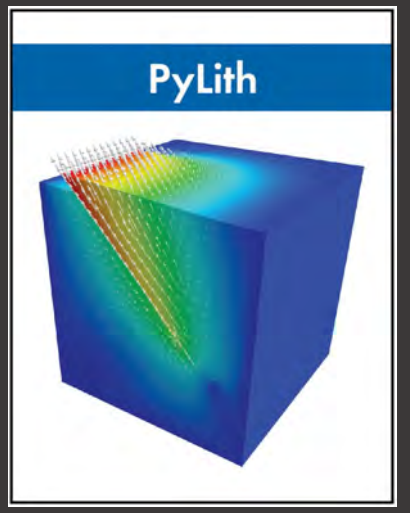
PyLith 2007–2021: A retrospective



A better user experience

- Binaries for Linux and macOS
- Installer for building from source
- User manual with lots of examples
- Informative error messages
- Docker container for development

Better code

- More extensive use of PETSc (discretization, data structures, solvers)
- Improved modularity
- Multiple levels of testing (unit tests, MMS tests, full-scale tests)
- Better development workflow (Git branches with pull requests)

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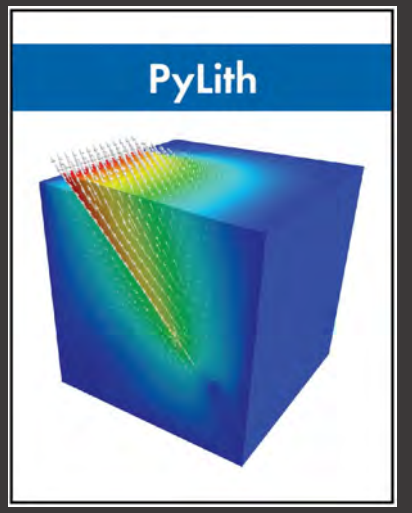
PyLith 2022 and beyond



An even better user experience

- Online documentation
- Jupyter-based examples
- More research-level examples
- Open-source meshing options
- Containers for clusters

Even better code

- Multiphysics with easier implementation of equations and constitutive equations
- Improved efficiency, scalability, and optimization

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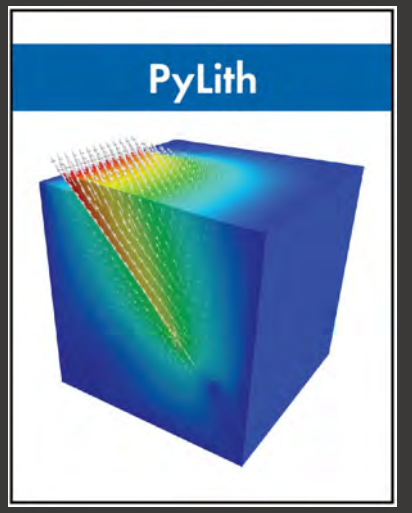
PyLith 2022 and beyond



New capabilities

- Earthquake cycle modeling
  Couple quasistatic and dynamic problems (project solution and state variables)
- Data assimilation using adjoints
- Poroelastic fault rheologies

More developers

- More hackathons to facilitate user contributions
- Leverage postdocs and NSF/USGS internships to expand developers

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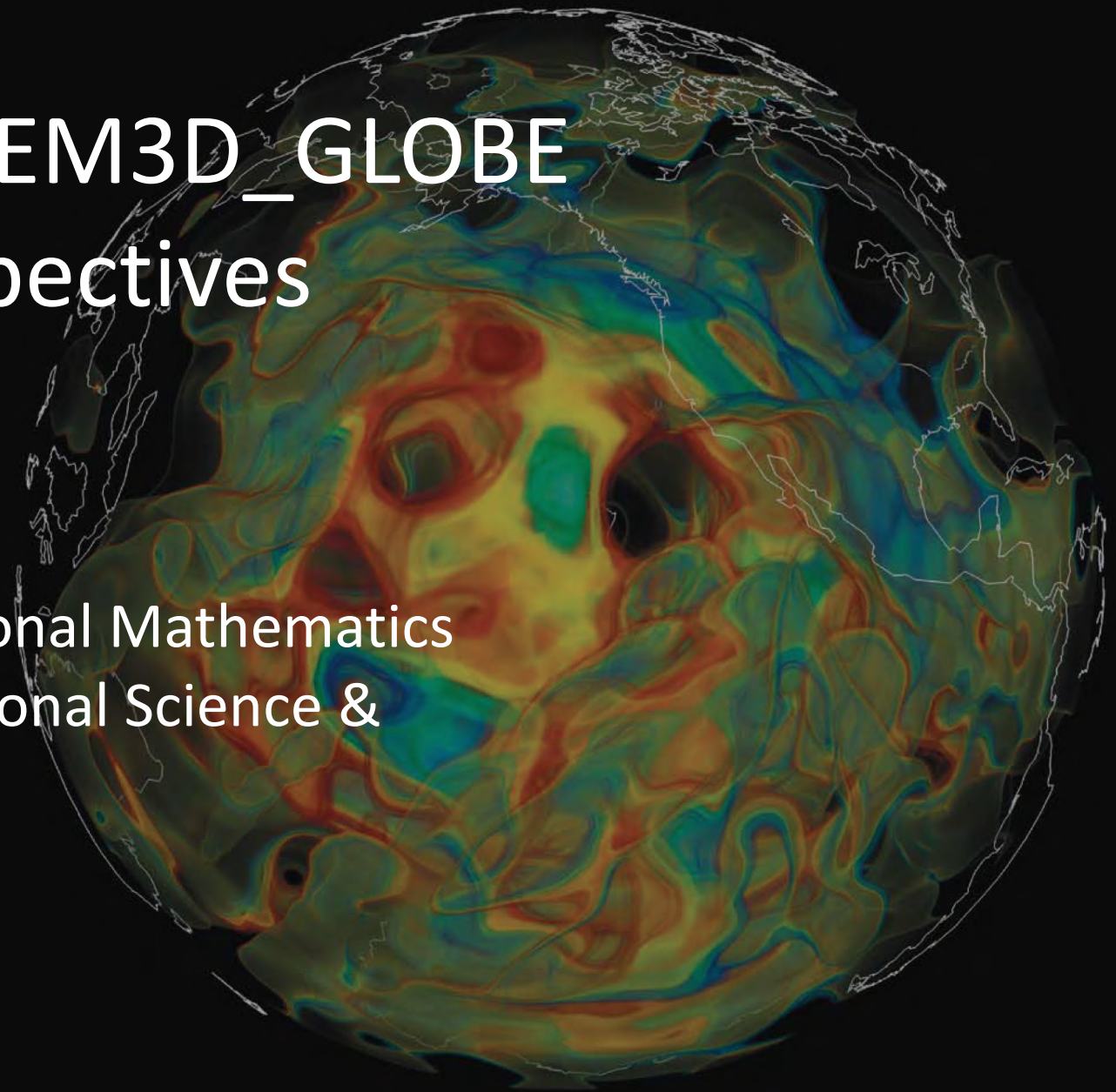
SPECFEM3D & SPECFEM3D_GLOBE
Past and Future Perspectives



Jeroen Tromp

Department of Geosciences

Program in Applied & Computational Mathematics

Princeton Institute for Computational Science & Engineering

SPECFEM3D

Looking back …

- The greatest challenges in academic software development are code stability, portability, and documentation.
- Graduate students and postdocs come and go, and generally have little training in proper software development, testing, documentation, and maintenance.
- It takes significant time, effort, and expertise to install and optimize software on a new computational platform.
- Education and training are very important, and workshops should be offered once or twice a year, ideally as part of another meeting.
- Again, students and postdocs come and go, and it is a challenge to maintain a steady workshop/hackathon program.

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SPECFEM3D

Looking back …

- In addition to the main solvers, such as SPECFEM3D and SPECFEM3D_GLOBE, peripheral software is often just as important.
- For example, the adjoint tomography workflow involves extensive software that is constantly evolving and thus fragile.
- Performing large-scale inversion at supercomputing centers is challenging due to frequent hardware failures.
- Workflow management tools, such as EnTK, can help stabilize HPC workflows.

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SPECFEM3D

Looking forward …

- To reduce the interminable burden of software development and maintenance, we have initiated a collaboration with the Kokkos team at SANDIA/ORNL as part of the DOE Exascale Project.
- Kokkos is a C++ programming model for developing performance portable applications targeting all major HPC platforms.
- We will hire a full-time dedicated Research Software Engineer to be in charge of software development.
- This RSE will be part of a rapidly growing group of currently 15 RSEs on campus.

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SPECFEM3D

Looking forward scientifically…

- Full gravity: coupling conservation of linear momentum with the Poisson/Laplace equation.
- Combination of spectral- and infinite-element methods.
- Co-seismic and post-earthquake deformation and gravity perturbations.
- Frequency-domain full-gravity free oscillation solver.
- Future developments based on this approach will also address problems in post-glacial rebound, sea level variations, dynamic topography, and tidal loading.

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Rayleigh

Rayleigh

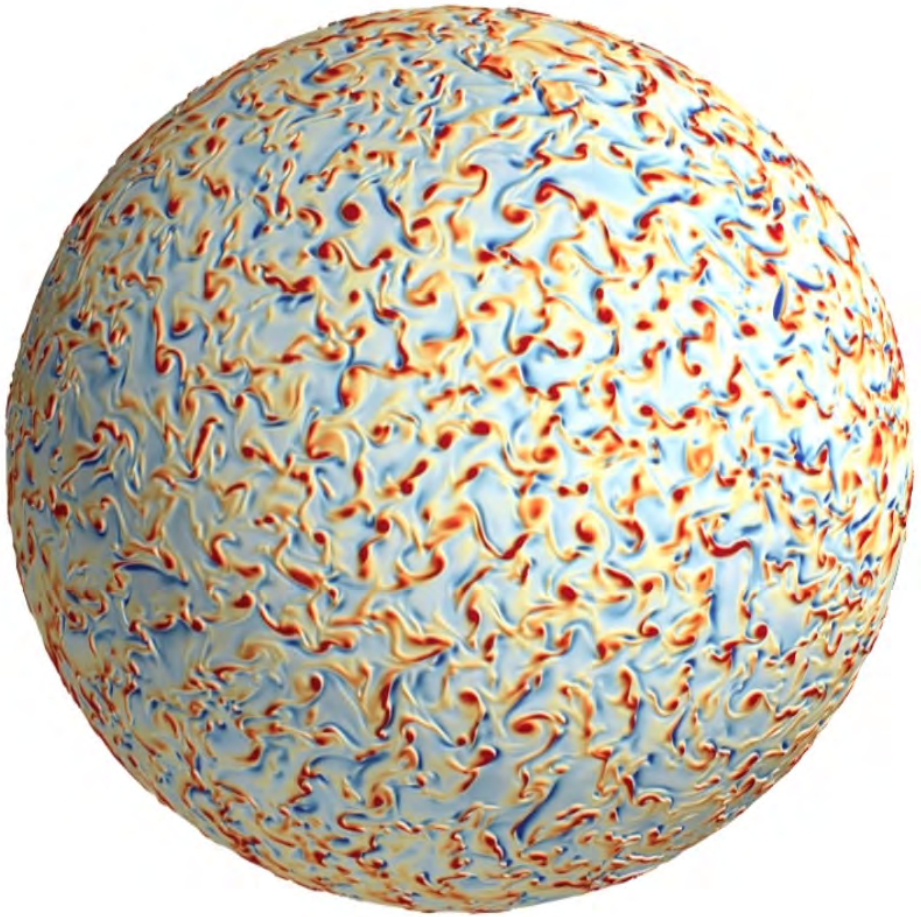
CIG-developed

Geodynamo Software

Nick Featherstone

Southwest Research Institute

SwRI



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Rayleigh CIG III

- Software development fully supported by CIG II and CIG III
- Targeted at the geodynamo:
  - pseudospectral MHD
  - spherical geometry
  - efficient parallelization (2014—2017 INCITE; 500M core hours)
- Releases
  - Initial Beta: 2016
  - Public: 2018
- Broader Impacts
  - Ph.D. theses (currently six)
  - Undergraduate Involvement
    - LASP/HAO REU
    - Calkins & Featherstone groups @ CU Boulder
  - Planetary and Stellar Interiors … *cross-cutting*
  - Solaris NASA MidEx (Phase I selected, Phase II TBD)
- Community Engagement
  - Tutorial workshops: 2016 (UC Davis) and 2018 (CU Boulder)
  - Hackathons: 2018,2019, 2021 (CU Boulder and virtual)

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SwRI

Rayleigh
community

First Rayleigh Hackathon: 2018

Dept. of Applied Mathematics and JILA, University of Colorado Boulder

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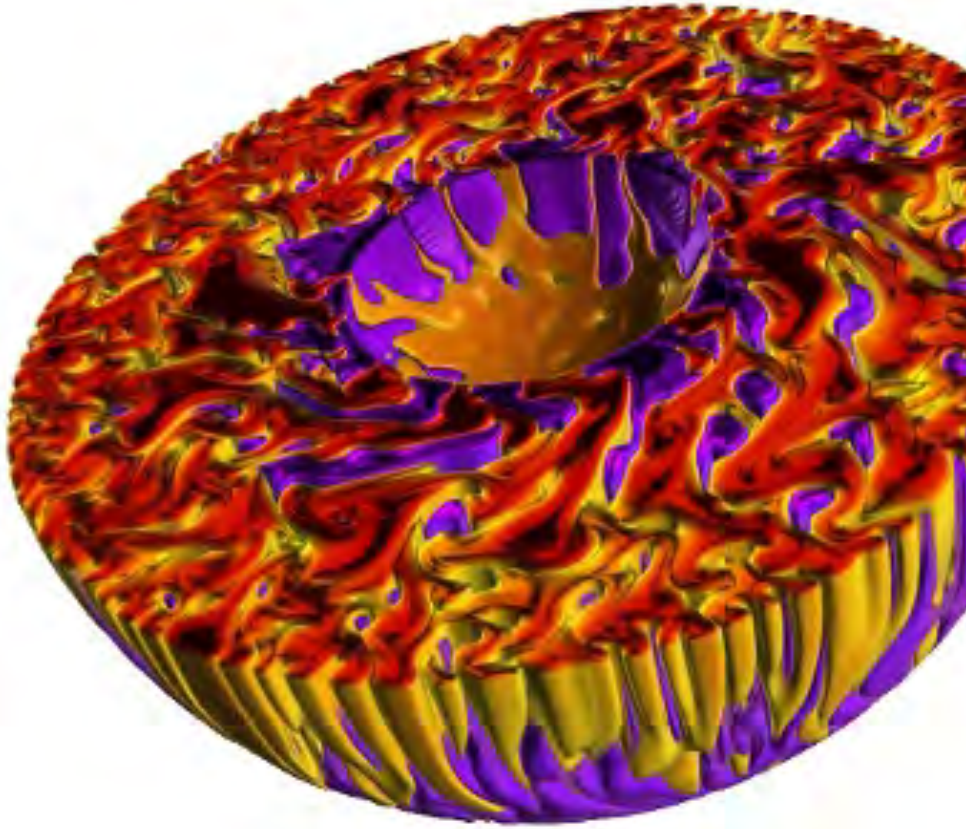
Rayleigh
future

Rayleigh Code: Looking to the Future

- Recently formed core development team -- we now have critical mass!
  - Philipp Edelmann, Rene Gassmoeller, Loren Matilsky, Ryan Orvedahl, Cian Wilson
- Regular release cycle
  - 1.0.0 released November 2021
  - Quarterly releases beginning Marcl
- Community engagement
  - Continued hackathons
  - Monthly user meetings
  - Monthly developer meetings
  - Checkpoint repository
- Long-term development goals
  - GPU-capability (Ryan Orvedahl)
  - Sparse matrix formulations
    - Chebyshev tau w/ quasi-inverse
    - Finite-element in radius
  - Additional physics
    - Centrifugal buoyancy
    - Aspherical boundaries
    - Full compressibility



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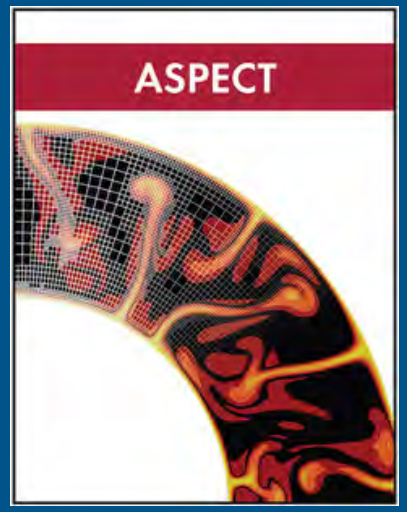
SwRI

ASPECT
Past and future perspectives

Wolfgang Bangerth, for all involved in the project

ASPECT

Hypothesis



My hypothesis:

ASPECT was meant as a mantle convection code.

But ASPECT is also a “platform”:

- To do things we didn’t expect
- To learn how to build, learn, educate, teach, do
- To copy

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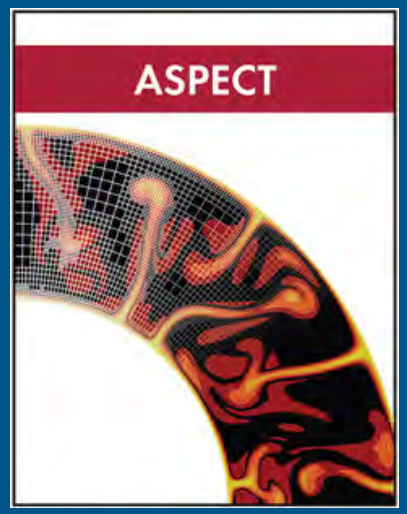
ASPECT
to "do"



ASPECT as a tool to "do"

Originally intended to do "classical mantle convection"

- The design of the software has allowed us and others to do so much more than intended:
  - Crustal dynamics
  - Coupling with surface models
  - Many many more material models, postprocessors, etc.
  - …

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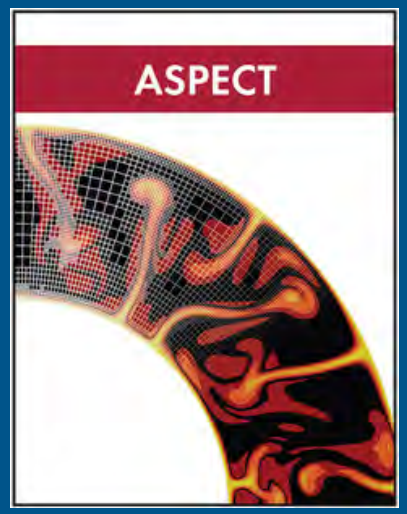
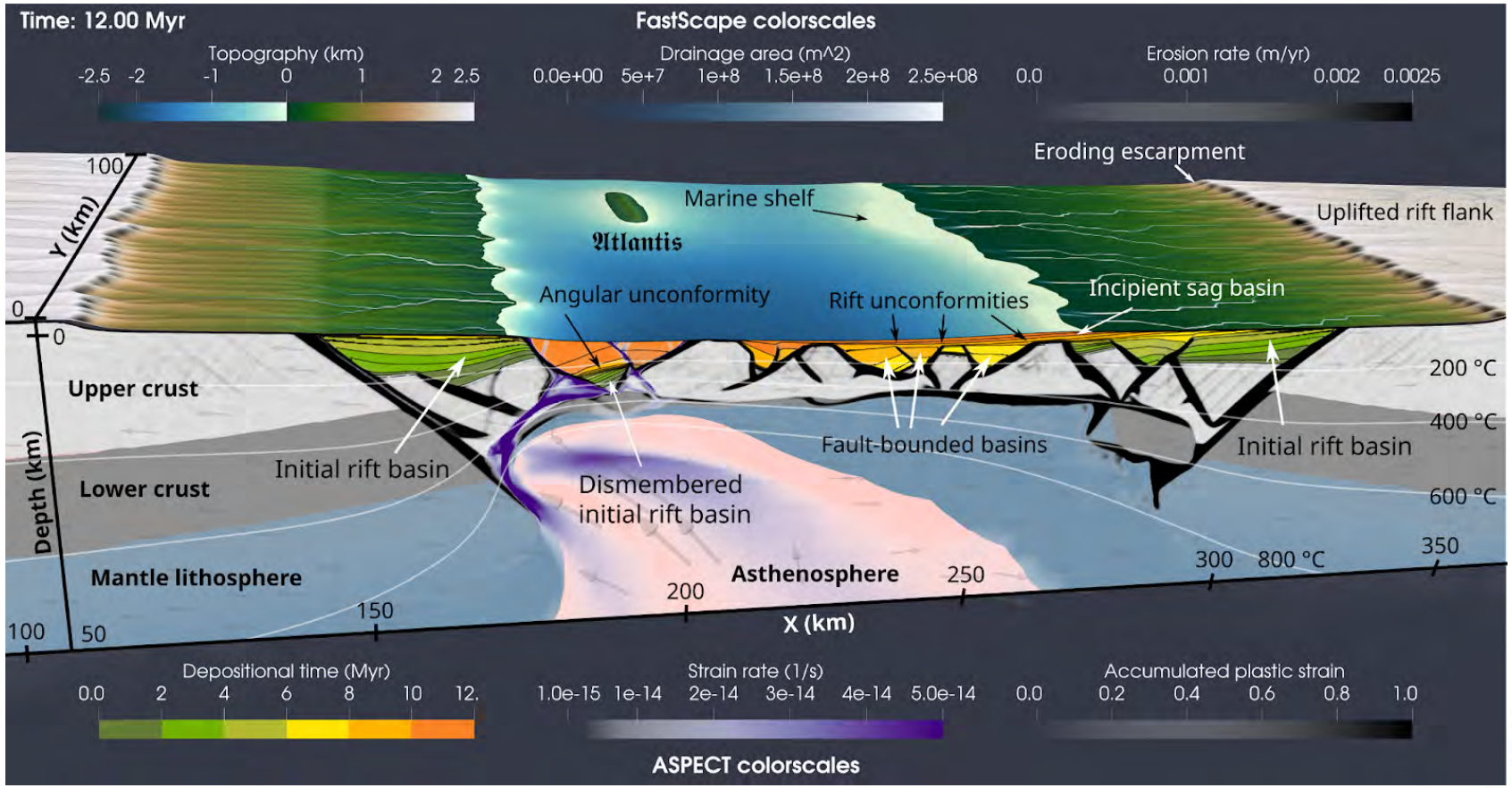
ASPECT as a tool to “do”

ASPECT

to “do”





https://www.youtube.com/watch?v=i6BPkmqI160

Neubarth, Brune, Glerum, Wrona, Braun, Yuan (2021)

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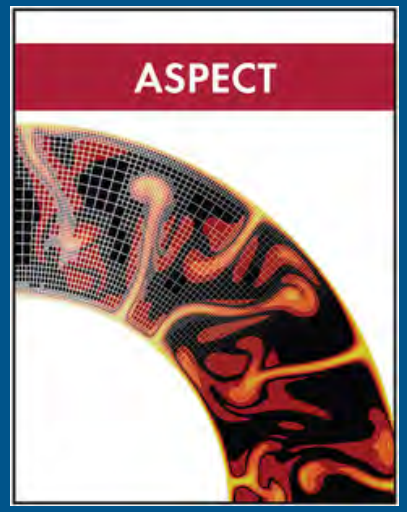
GFZ Helmholtz Centre Potsdam

➢ Modularity and “plug ins” as a serendipitous design!

ASPECT
education



ASPECT as a tool to learn/teach/educate

A **lot** of work has gone into ASPECT as an educational tool:

- Manual with many cookbooks (now 600+ pages)
- User workshops
- Classroom material
- In-person and virtual workshop teaching materials
- **Hackathons** as a tool to build a developer community and to build a code

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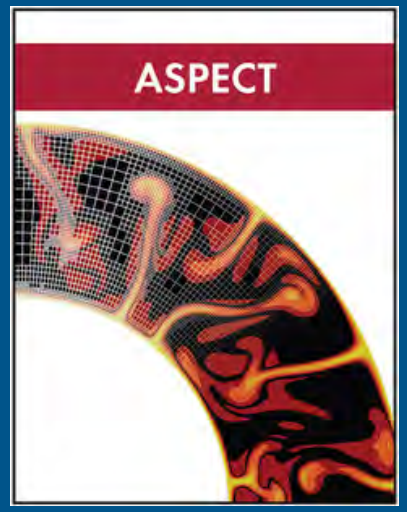
ASPECT
education



ASPECT as a tool to learn/teach/educate

But, our efforts also show:

- How much work it takes to get all of this organized
  (And that little of this would have happened without CIG support.)

- How much education our students actually require in computational science

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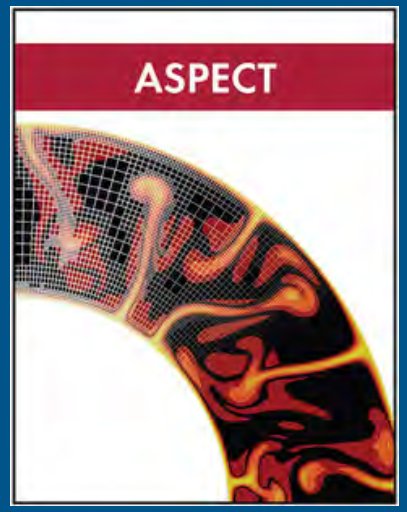
ASPECT
model



ASPECT as a "model"

Many things have gone right over the past 10 years:

- The right people, having fun working on the project
- Stable funding for important work
- Technically sound decisions on software design and documentation creation
- People developing careers on/with ASPECT

ASPECT as a tool to learn lessons on what works, and what can be copied.

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CIG IV Writing Committee

Thanks to …

Wolfgang Bangerth

Sylvain Barbot

Ebru Bozdag

Bruce Buffett (Chair)

Rene Gassmoeller

Lorraine Hwang (Director)

Laurent Montesi

Max Rudolph

Marc Spiegelman

Jolante van Wijk

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Solicitation

Geoinformatics (GI)

Six Essential Elements

1. Modern cyberinfrastructure
2. Engagement
3. Scientific motivation
4. Metrics
5. Sustainability plan
6. Management plan

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Context

Changing Computational Landscape

Examples

Explosion of open-source software

Growth of software repositories (GitHub)

Changing publication standards (FAIR)

Trends in computing (Python, Jupyter Project,…)

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Overview

Cornerstones

Modeling software

Computational workflows

Training

Community

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Modeling Software

Greater emphasis on shared/common infrastructure

New capabilities (subawards, coding events, postdocs)

Installation and distribution of software

Code certification and publication

Emerging computing paradigms

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Computational Workflows

New tools for complex simulations

Hosting models and workflows

Model system interfaces (enable model coupling)

Integrating and exporting data

Common model configurations

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Training

Building on lessons learned

User workshops and training material

Learning modules for computational geoscience

Advanced computing skills (hackathons, …)

User & developer training fellowships

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Community Building

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Broadening participation

Expand developer base (within and beyond CIG)

Outreach (speaker program, undergrad. research experience)

Justice, equity, diversity, and inclusion

Promote multidisciplinary collaborations (CIDER)

Broader scientific engagement

Sustainability

Evolution toward community-driven development

Principal developers support community activities

Sustainability requires a base level of project support

Increasing reliance on widely used libraries

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Management

HQ remains @UC Davis

Transition to coPIs

- division of operations and governance

Technical infrastructure team

- 2 staff + postdocs

Community Manager

- leads education and diversity efforts

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Questions

13:00 **Welcome**

What's new at CIG Headquarters *Lorraine Hwang, Director, UC Davis*

13:10 **Reports on Past Activities**

- **SMOREs Program** *John Naliboff, New Mexico Tech*

Past and Future Perspectives on Software

- **PyLith** *Brad Aagaard, USGS*
- **SPECFEM** *Jeroen Tromp, Princeton University*
- **Rayleigh** *Nick Featherstone, SWRI*
- **ASPECT** *Wolfgang Bangerth, CSU Fort Collins*

13:35 **CIG IV** *Bruce Buffet, coDirector CIG IV, UC Berkeley*

13:50 **Breakout Discussions**

Topic 1. JEDI and Belonging

Topic 2. Engaging Our Community

14:10 **Report Back**

14:20 **Summary Plenary Conversation**

Topic 3. Supporting Earth System Science and Convergent Research

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Breakouts

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Breakouts

(3)

Self-assign

20 min

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Topic 1. JEDI and Belonging

Much work has been done on Justice, Equity, Diversity, and Inclusion and Belonging through and in other organizations. Rather than duplicating efforts, what can CIG uniquely contribute to the movement/efforts?

List of facilitating questions:

- How are we similar to other communities?
- How are we different?
- Are their good examples of JEDI policies that we can build from?
- What are our strengths (and weaknesses) that we can capitalize on?

Outcomes:

Discussions towards defining the focus, charge, and priorities for a CIG BeAJEDI working group.

Topic 2. Engaging our Community

In our mission statement, we state that "CIG is a community driven organization …" How do we maintain a vibrant and diverse community?

List of facilitating questions:

- What motivates members to contribute to and/or become part of our community?
- What are the best ways to "connect" to the community?

Outcomes: Actionable ideas to increase community participation.

Plenary

Supporting Earth System Science and Convergent Research

In addressing challenging societal problems, future research requires input from a diverse group of researchers.

Computation/computational models will play an important role.

What is CIG's role in supporting earth system science and convergent research?

List of facilitating questions:

- How do we define ourselves?
- What are CIG's strengths and weaknesses?
- What is our scope and what is within scope of our mission?
- What are the opportunities for engagement & collaboration?
- What can we do to facilitate conversations across communities?

Outcomes:

Common understanding of how CIG can contribute to new science initiatives. Input in developing a CIG "How to collaborate with us" statement.

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Adjourn

Beaver Moon

Lunar Eclipse

3hr 28 min

1:03A PT peak

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