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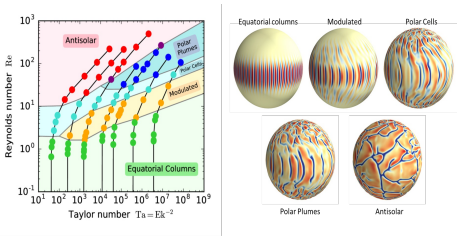

Research Highlight

Reusable & Open Source Data from the Rayleigh Simulation Library

Rayleigh is a CIG-developed code, targeted at the geodynamo, that solves the magnetohydrodynamic (MHD) equations in a rotating 3-D spherical shell under the Boussinesq and anelastic approximations. The code is pseudo-spectral in nature, meaning that all state variables are represented by a basis function expansion throughout large portions of the calculation. In Rayleigh, this expansion is carried out using spherical harmonics on spherical surfaces and Chebyshev polynomials in radius. Derivatives are calculated to very high accuracy using the properties of these basis functions. This high-accuracy, a major advantage of a pseudo-spectral approach, comes with a price, however. As the fluid system is evolved in time, Rayleigh transitions repeatedly between the spectral, basis-function configuration, where derivatives are calculated, and the physical-space configuration, where basis-functions have been summed and where nonlinear terms are calculated.

This repeated cycling between data configurations can incur significant communications overhead. Rayleigh's unique parallel design substantially mitigates this issue, enabling the efficient use of large-scale supercomputing resources, such as TACC's Stampede 2 ... continued.

contributed by
Ryan Orvedahl, UC Davis and Nick Featherstone, SWRI

CIG IV Update

Dear Community,

The Proposal Writing Committee has been meeting weekly for the past several months to prepare for the next stage of CIG. Much of our initial discussion has focused on the vision of CIG moving forward. A familiar experience to everyone is the rapid pace of change in the computational landscape over the past few years. This is especially true when we reflect on the changes since the inception of CIG in 2005. Explosive growth of open-source software and tools, such as the Python ecosystem and JupyterLab, as well as increasing availability of FAIR data have transformed the way researchers interact with data and models. None of these things were part of the discussion when CIG was first proposed. We see opportunities to expand role the of CIG, ensuring that it continues to drive scientific discovery.

A traditional focus of CIG has been the development of modeling software for the geodynamics community. While this goal continues to be important in our plans, the availability of sophisticated modeling software is not enough. We also need to build a community of researchers to use these tools effectively. An additional motivation for our expanded vision of CIG is the growing complexity of model setup and analysis. Increasingly these activities include the challenging task of integrating model software. Present efforts are largely uncoordinated with little opportunity to share or extend successful approaches. It is time to extend the original aspirations of CIG to include the entire computational workflow.

Our vision for the coming years is focused on developing sustainable software tools and software workflows, while building sustainable communities of users and developers. In executing this vision we propose to build the necessary community infrastructure on the following four cornerstones: (1) **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; (2) **Computational workflows**: supporting workflows that facilitate the set-up, execution, analysis, and exchange of complex computational models; (3) **Training**: Enabling a well-educated and well-trained 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; and (4) **Community**: Building and sustaining a diverse and sustainable community of disciplinary and interdisciplinary researchers working together on challenging geoscience and software problems.

We welcome your input and engagement to make a strong case for continued support to the National Science Foundation.

Sincerely on behalf of the Writing Committee,
Bruce Buffett, *Chair*

News

CIG Community XSEDE Resources

CIG was recently awarded compute resources on the following XSEDE resources:

- Stampede2: 50,000 SUs
- Expanse: 1,377,206 Core-hours
- Expanse: 15,000 GPU Hours

Allocation usage is open to the community for use in benchmarking and small runs in preparation of your own allocation request. Code scaling for CIG community codes on XSEDE are available on our website [scaling]. Please contact us if you would like access to the CIG allocation and/or help applying for your own allocation: help@geodynamics.org

Allocations expire March 31, 2022.

Speaker Series

We are excited to introduce the 2021-2022 CIG 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*

Learn more information about their talks and careers in the geosciences [more info].

Apply to Host a Speaker

The CIG Speaker Series seeks to promote computational modeling in geodynamics and related Earth science disciplines. The series aims to bring computational geodynamics speakers to institutions that may not otherwise have access to speakers with expertise in computational science or computational geophysics. By doing so, we aim to connect speakers and CIG with audiences from a variety of STEM domains, and to broaden participation in CIG and to work toward building a more diverse community within computational geodynamics. Institutions interested in hosting a Speaker in 2021-2022 should **apply by June 1.**

See the website for more information.

CIG Postdoctoral Fellows

CIG welcomes to our team Postdoctoral Fellows Ryan Orvedahl and Kali Alllison. Ryan is implementing new approaches to improve the performance of Rayleigh and improving workflows for sharing data with a broader community. Beginning June 1, Kali will be adding new functionality to PyLith for earthquake cycle modeling to explore the interaction between a strike-slip fault and its ductile root over a timescale of thousands of years.

CIG will be accepting Postdoctoral Fellowship applications through June 30, 2021. [more info]

Awards and Honors

Congratulations to Alice Gabriel who is the 2021 recipient of SSA's Charles F. Richter Early-Career award. Alice has been honored for her innovative research in earthquake rupture dynamics and tsunami genesis, among other topics, using physics-based models and high-performance computing. [more info]

Governance

New Member

Welcome to our newest International Affiliate, University of Cambridge and Member Representative John Rudge.

Events

Software Developers Meeting

Many thanks to lead organizer Brad Aagaard and the committee of Jed Brown, Katie Cooper, Rene Gassmoeller, Lorraine Hwang, and Marc Spiegelman for convening our very first developers workshop. The CIG Developers Workshop resulted in a number of recommendations that we think will help expand the CIG developer community, make software more accessible to new users, and increase developer productivity through use of common infrastructure and best practices for software development. This includes building a broad user base with sufficient support through documentation, tutorials, user forums, hackathons, scientific workshops, and mentoring to maintain a healthy suite of software developers and maintainers. Communities also need to offer opportunities, like this workshop, for developer teams to interact with each other to exchange ideas, identify common infrastructure, and interact with users to discuss modeling workflows and development priorities. [report]

2020-2021 Workshops

- **2021 May 24-28.** Rayleigh Hackathon. Virtual. [info]
- **2021 June 7-10, 14-16.** PyLith Hackathon. Virtual. [info]
- **2021 June 21-August 20.** Summer Modeling Research Experiences in Geodynamics. Virtual, multiple locations. [info]
- **2021 July 6-16.** ASPECT Hackathon. Virtual. [info]

Remember to join our forum to receive announcements for these and other 2021 events.