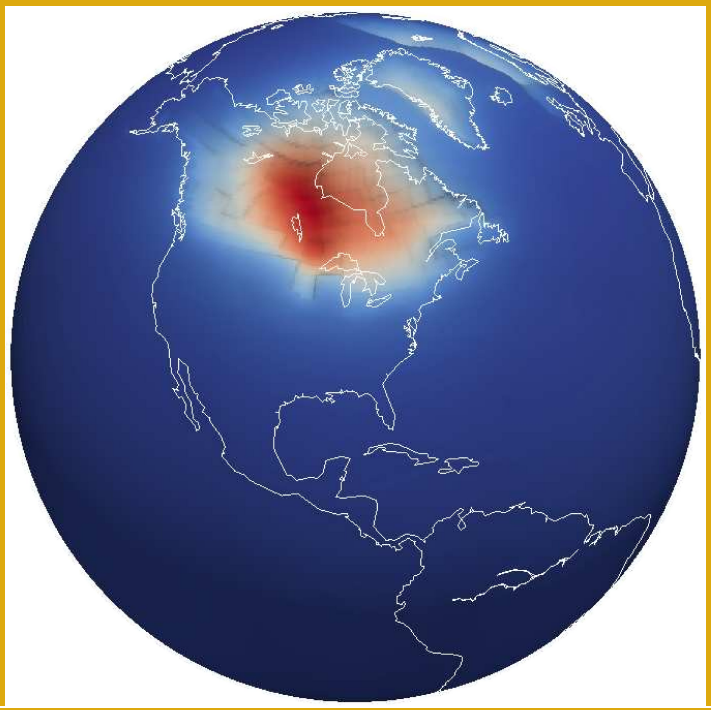

VOLUME 3 ISSUE 1

CIG NEWS ELEMENTS

COMPUTATIONAL INFRASTRUCTURE FOR GEODYNAMICS

IN THIS ISSUE

Research Highlight - Computational Methods

Spectral-element Method Coupled with an Infinite-element Approach

The complete set of governing equations for global dynamic and quasistatic problems – such as post-seismic and post-glacial rebound, tidal loading, and long-period seismology– involves a coupling between the conservation laws of continuum mechanics and Poisson/Laplace's equation. For dynamic problems, such as seismic wave propagation and the free oscillations of the Earth, it is possible to decouple Poisson's equation using an explicit time marching scheme so that it can be solved independently. For quasistatic problems, such as glacial isostatic adjustment and tidal loading, inertia is neglected, requiring an implicit time marching scheme. In the latter case, Poisson's equation cannot be decoupled. Although an explicit time scheme with an independent Poisson's solver is generally fast, such an approach is limited by conditional stability, such that a very large number of time steps is often necessary. On the other hand, an implicit time scheme coupled with Poisson's equation is generally slow but unconditionally stable. In both cases, the unbounded and large-scale nature of the problem poses numerical challenges, particularly for 3D Earth models. Most of the existing methods use spherical harmonics to solve the unbounded Poisson/Laplace's equation. Such methods are often limited to spherically-symmetric models or have to rely on iterative procedures. In view of these challenges, we develop a parallel software package based on the spectral-element method combined with a mapped infinite-element approach. While the spectral-element method is used within the Earth model, the infinite-element approach is employed in the outer region. In the infinite element approach, a so-called infinite-element layer is used to mimic all of space. The outermost edges of an element in the infinite-element layer are mapped to infinity in order to reproduce the behavior of gravitational potential outside the domain of interest, such that the potential decays to zero at infinity. Gauss-Lobatto-Legendre (GLL) quadrature is used for numerical integration in spectral elements. Since GLL quadrature cannot be used in infinite elements due to a singularity, we use Gauss-Radau quadrature instead. Spectral and infinite elements share identical quadrature points on infinite- element boundaries, thereby providing a natural coupling of the infinite-element method with the spectral-element method (see figure next page). We use a generalized Maxwell rheology for viscoelastic deformation and accommodate topography and ellipticity. Both explicit and implicit time schemes are implemented in order to address a range of problems, including long-period seismology, glacial rebound (featured picture), tidal loading, etc.

Gharti, H.N, J. Austermann, D. Komatitsch, H. Lau, J.X. Mitrovica, D. Peter, J. Tromp, Z. Xie, S. Zampini Efficient numerical solution of global dynamic and quasistatic problems using a spectral-element method coupled with an infinite-element approach, *AGU Fall Meeting 2013*.

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ANNOUCEMENTS

Next Webinar: Thursday February 13

CIG CGU Abstract Deadline:

CGU	February 14
CIG	March 14

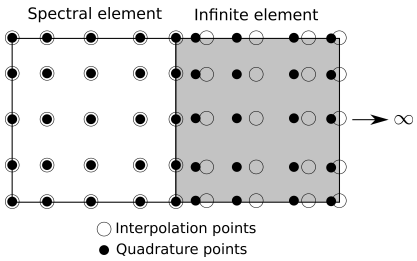
Code Corner

NEW RELEASES

- deal.II 8.1 2013-12-08

ALLOCATIONS

Stampede	*none available*
Yellowstone	*500,000*



Coupling between spectral element and infinite element

NEW RELEASE

deal.II

Version 8.1 of deal.II, the object-oriented finite element library awarded the J. H. Wilkinson Prize for Numerical Software, has been released. It is available for free under an Open Source license from the deal.II homepage at: http://www.dealii.org/
This version is primarily a maintenance release but still has a number of note worthy new features:

- Three new tutorial programs on elastoplastic contact problems (step-42), hybridizable dicontinuous Galerkin methods (step-51), and a simple example of using adaptive mesh refinement for time dependent problems (step-26)
- Significantly better support for shared memory multicore parallelism
- Dozens of new features and bug fixes

For more information see:
http://arxiv.org/abs/1312.2266v4

Wolfgang Bangerth, Timo Heister, Guido Kanschat, and many other contributors.

SPECFEM3D Benchmarks New GPU

The open source code SPECFEM3D, representing an application from Earth Science, is one of several leading scientific applications chosen by NVIDIA to benchmark their latest generation of GPU accelerators. Other applications used to perform the benchmark include from Physics-Chroma, Molecular Dynamics-AMBER, and Material Science-QMCPACK. Congratulations to SPECFEM3D for a being key application to test GPU performance.

More information can be found at:
http://www.nvidia.com/object/gpu-test-drive.html?2

See the Technical Brief for more details:
http://www.nvidia.com/docs/IO/122874/K20-and-K20X-application-performance-technical-brief.pdf

Recognizing Software Contributions

Wolfgang Bangerth and Timo Heister in their SIAM News article, *Quo Vadis, Scientific Software?* discuss the need for recognizing contributions to software development. Software and their underlying libraries are at the core of many scientific modeling codes. Maintainence and contributions to their continual development by the community are vital to advancing science. Those who possess the rare skills to write resusable software must be rewarded and professionally recognized. As a community, we can elevate the contributions to software development by acknowledging open-source projects, elevating the role of software development on both grant proposals and hiring, crediting those who have contributed significantly to a project, and publishing the code in which scientific results are based. See the full article at:
https://www.siam.org/news/news.php?id=2131

Code Donations

Two codes are in the early stages of donation to the CIG open source repository:

BurnMan, developed by Sanne Cottaar, Timo Heister, Ian Rose, Cayman Unterborn, BurnMan, is an open-source mineral physics toolbox to determine elastic properties for specified compositions in the lower mantle by solving an Equation of State (EoS). The toolbox, written in Python, can be used to evaluate seismic velocities of new mineral physics data or geodynamic models, and as the forward model in inversions for mantle composition. The user can define the composition from a list of minerals provided for the lower mantle or easily include their own. BurnMan provides choices in methodology, both for the EoS and for the multi-phase averaging scheme. The results can be visually or quantitatively compared to observed seismic models. Example user scripts show how to go through these steps.

AXISEM, donated by Tarje Nissan-Meyer, is a parallel spectral-element method to solve 3D global acousto-elastic wave propagation. The background model is spherically symmetric (e.g., PREM, IASP91) and meshed automatically for a given dominant seismic period. This allows the computational domain to be collapsed to 2D while the third azimuthal dimension is solved analytically. This 1D-model, 2D-domain, 3D-waves approach leads to unprecedented resolutions for global wave propagation (e.g. up to 1Hz) on moderate computer clusters or workstations. The Fortran90/MPI code is used by a number of international groups, and will be made publicly available soon.
Contact Tarje Nissen-Meyer if you're interested in using this method:
tarjen@ethz.ch

Geodynamo Awarded 1.5M Core Hours @ANL

CIG researchers were recently awarded 1.5 million core-hours for code development and testing on the Vesta system at the Argonne Leadership Computing Facility. The allocation will be used by Dr. Nick Featherstone and Dr. Hiroaki Matsui to develop the Rayleigh and Calypso geodynamo codes. Each of these codes already scales to thousands of cores. Development on Vesta will aim to improve scalability to allow runs on hundreds of thousands of cores, allowing ground breaking studies in magnetohydrodynamics related to planetary core evolution.

XSEDE

No SUs are currently available through CIG's allocation on XSEDE. The entire allocation of 880,000 SUs has been used by CIG developers and others in the geodynamics community for benchmarking and test runs. CIG has requested a supplemental allocation of 1.5M SUs. If you are interested in using XSEDE resources for small scale development or testing of codes, please check the website for availability.

Interested in obtaining your own allocation for research? You may apply for a start-up allocation at anytime or a regular allocation on a quarterly basis. Don't know how to get started? See our website or contact Eric Heien. Eric is UC Davis's XSEDE Campus Champion and can help you with your allocation requests. emheien@ucdavis.edu

Governance

LETTER FROM THE DIRECTOR

Dear Colleagues:

This is an exciting time for CIG, as we are embarking on an extensive strategic planning process, in preparation for writing a renewal proposal next year. In January, the EC and SSC held a retreat to gather information and outline our process. As I write this, we have just wrapped up the first CIG-EarthScope Institute for Lithospheric Modeling, which brought together researchers from the CIG and EarthScope communities for extended discussions of the current state of the art and future directions in modeling and data assimilation. We will be gathering similar input on various topics throughout the summer; stay tuned.

In addition to this collaborative event with EarthScope, CIG is partnering with other organizations to offer workshops, tutorials, and conferences. In May, we will join the Canadian Geophysical Union to hold CIG's Mantle and Lithospheric Dynamics workshop in Banff, featuring talks, posters, and tutorials. In July, CIG staff will support tutorials in computational geodynamics at the CIDER program at the Kavli Institute for Theoretical Dynamics (KITP) in Santa Barbara. In August, we will offer tutorials on the geodynamo code, Calypso, and the AMR mantle convection code, Aspect, at the ELSI SEDI Summer School in Tokyo, Japan. In the coming months, CIG webinars feature a wide range of topics in geodynamics, computational science, and data management. I look forward to seeing many of you at one or more of these events.

Best wishes,

Louise Kellogg

CIG Elections

Congratulations to new Executive Committee Members David Bercovici, Bruce Buffet, and Claire Currie. Scott King has been elected the new EC Chair, and Bruce Buffet, Vice Chair. Brad Aagaard has been elected as the Science Steering Committee Chair and joins Tim Ahern as newly elected members. Thanks to outgoing members Gary Glatzmaier, Mousumi Roy, Matt Knepley, Marc Speigelman, Peter van Keken, and Nadia Lapusta for their service.

New Institutional Member

Welcome to Arizona State University and Allen McNamara as our newest Institutional Member and Member Representative.

WORKING GROUP UPDATES

Annual Work Plans

Annual Working Group Plans are under development. Please contact Working Group Leads to contribute and for more information.

Mantle Convection

Citcom. The Citcom User's Group met on January 22, 2014. Participants discussed the development priority list and the spherical benchmark for Citcom and ASPECT. PETSc will be incorporated into the code and the Python dependencies will be removed from CitcomS. The group hopes to have the initial benchmarking ready for the CIG joint meeting with CGU in Banff in May. See the CItcomS wiki page for more information: http://wiki.geodynamics.org/software:citcoms:start

ASPECT. The ASPECT group is developing tutorials this year for the joint CIG-CGU meeting in May and other workshops this summer. Subscribe to the CIG mailing list for the latest information cig-mc@geodynamics.org

Geodynamo

CIG Staff will begin performance benchmarking contributed geodynamo codes on Stampede soon in anticipation of a benchmarking workshop in early Fall 2014.

Tutorials for Calypso are under development. Subscribe to the CIG mailing list for the latest information: cig-geodyn@geodynamics.org

Short Term Crustal Dynamics

Testing is being completed on Pylith 2.0.0. Look for an announcement soon via the mailing list: cig-short@geodynamics.org

Submitted by B. Aagaard.

Long Term Tectonics

The Working Group organized the first CIG-EarthScope Institute for Lithospheric Modeling workshop. Over 45 participants from a broad range of backgrounds including users and developers met at the EarthScope National Office in Tempe, Arizona February 3-4 to identify needs for lithosphere-scale modeling. The workshop report will be posted to the website when completed.

EVENTS

Webinar Schedule

CIG webinars draw from a pool of experts from mathematicians, to computer scientists, and to geoscientists, among others to bring together a cross-cutting community of faculty, students and researchers to both inform and disseminate knowledge on the tools and methodologies employed to further the study of problems in geodynamics.

The one hour webinars will be held the 2nd Thursday of each month October through April (no webinar in December due to AGU) at 2pm PT unless otherwise noted. Webinars will be recorded for later viewing. Reminders and details are sent through the cig-all mailing list.

February 13 - *Exascale Visualization: Why Things Will Change For You*, Hank Childs
March 13 – Mackenzie Smith
April 10 - Aspect Team
May 8 – Lead: Jon Aurnou. *CIG's Community Dynamo Code Development Project*

Next Webinar

Thursday, February 14, 2013 @ 2 pm PT

Exascale Visualization: Why Things Will Change For You
Hank Childs
Assistant Professor, University of Oregon
Exascale computing is on the horizon, and may appear as soon as 2019. So what does this mean for visualization? Plenty. Exascale machines will place severe constraints on I/O, power, data movement, and architecture. The massive data sets produced by these machines will likely require a variety of techniques to be visualized, such as in situ processing, multi-resolution processing, and/or data reduction, all while running on an accelerator. In this webinar, Hank will describe the exascale landscape and discuss why and how visualization will look different.
Submitted by Hank Childs.

For details on all CIG webinars see: http://www.geodynamics.org/cig/community/Webinar

Upcoming Meetings

May 4-8, 2014. CIG Mantle and Lithospheric Dynamics Workshop, Joint with the Canadian Geophysical Union 2014, Banff, Alberta.

Attendees will have the opportunity to participate in both the CGU and CIG meetings. CGU abstract deadline is February 14. Abstract deadline for CIG sessions on mantle convection, lithospheric dynamics and computational methods is March 14.

All registration will be through CGU: http://www.cgu-ugc.ca/meetings/index.htm

We strongly recommend becoming a member of CGU to take advantage of the best meeting rates. Accommodations are limited so reserve early.

Visit our website for complete session information, application for travel support, and logistics.

June 23-27, 2014. Crustal Deformation Modeling Workshop, Stanford, California.

This year's biannual Crustal Deformation workshop co-sponsored by SCEC will be hosted by Stanford Unviversity. Participation is limited to 60 attendees. Visit our website for more information and to application for attendence.

For more information on CIG hosted events, please go to geodynamics.org

References

Recently Published

Sekhar, P.; and S.D. King, 3D Spherical Models of Martian mantle convection constrained by melting history, Earth and Planetary Science Letters, **388**, p. 27-37, 2014. DOI: 10.1016/j.epsl.2013.11.047

Please send us your recent publications as well as research highlights so we may continue to keep the geosciences community informed of all the current research being conducted in geodynamics with CIG codes.

Submit to: geodynamics.org/cig/community/documents/reference

Past and present EC and SSC members recently met in Santa Fe, New Mexico to begin the strategic planning process for the renewal of CIG. Contribute your ideas at upcoming CIG workshops or through the Working Groups. Left to right: Lorraine Hwang, Roger Buck, Gary Glatzmaier, Roy Savoian, Jed Brown, Wolfgang Bangerth, Jolante Van Wijk, Time Ahern, Brad Aagaard, Claire Currie, Mousumi Roy, Scott King, Louise Kellogg, and Bruce Buffett

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Computational Infrastructure for Geodynamics (CIG) is a membership-governed organization that reports and promotes Earth science by developing and maintaining software for computational geophysics and related fields.

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NSF