CIG Workshop: Opportunities and Challenges in Computational Geophysics

Welcome and Overview

Marc Spiegelman (Columbia/LDEO) Chair CIG Executive Committee





Workshop Objectives

- Discuss Opportunities and Challenges in Computational Geophysics
 - Current and Future Computational Geoscience Directions: Successes & Failures
 - Innovations & Opportunities for Community Software Development
 - Education & Training of the Computational Geoscience Community
- Identify critical scientific and computational problems/issues that can be enabled by a community organization such as CIG





Workshop Objectives

- Provide specific recommendations to the CIG-II Proposal Writing committee
 - What science would you like to see enabled by CIG?
 - What computation/software engineering is required to accomplish this?
 - What Community Organizational structures are most effective for accomplishing these goals.
- The PWC meets on Wednesday. This workshop is a critical opportunity for shaping the future of CIG and computational geosciences.





CIG is...

- The Computational Infrastructure for Geodynamics
 - NSF cooperative agreement, funded Sept 2004
 - 1st-SSC elected June 2005
- A *Community driven* organization to leverage advanced scientific computation for the benefit of the solid-Earth geoscience community.
- A *partnership* between Earth Sciences and computational Sciences
- Enables science for a wide range of problems
 - Seismology
 - Mantle convection
 - Magma Dynamics
 - Crustal and Earthquake Dynamics
 - Geodynamo
 - Computational Science
- A structure for developing, supporting and disseminating advanced computational tools for both developers and end-users





CIG Long term vision

From the original Proposal (Feb 2004)

With a high level of community participation, CIG would leverage the state-of-the-art in scientific computing into a suite of *opensource* tools and codes that serve the greater geodynamics community from model developers to end-users of models.

The emphasis would be on developing toolkits and modular codes that ease the development of models and foster the interchange of ideas and algorithms.





Example of a potential scientific goal



An Workflow for exploring the observable seismic consequences of mantle geodynamics





Example of possible (original) CIG implementation



Hiearchical software stack for composing coupled models from common infrastructure and superstructure.





Fundamental Challenge

- How to implement long-range vision
- While meeting the immediate computational and scientific needs of individual sub-disciplines





The Reality

CIG developed/supported a range of software projects in response to specific community needs that explored various approaches and libraries from hardening existing codes to developing new codes from advanced libraries/super-structure.







More experimental Codes

- Exploration for multi-scale/multi-physics coupling
- Magma Dynamics: MADDs (stG, FEniCS/ PETSc, Comsol, deal.ii)
- Mantle Convection: RHEA, Peta-scale AMR for convection (OCI Peta-Apps)
- Geodynamics AMR Suite: (deal.ii)
- + Contributed codes





Points

- When we started: lots of good ideas, but limited experience in developing complex codes for a diverse community.
- After 4 years we've developed considerable experience in a range of problems and approaches.
- Now is the time (and this is the workshop) to reassess the goals, and approaches of CIG and design the next generation of computational tools for Solid Earth Science





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CIG-II Proposal Writing Committee

Bruce Buffett (UC Berkeley), Chair

Brad Aagaard (USGS) Wolfgang Bangerth (TAMU) Thorsten Becker (USC) Mike Gurnis (Caltech) Peter van Keken (U. of Michigan) Louise Kellogg (UC Davis), ex officio, SSC Chair Alan Levander (Rice) Marc Spiegelman (Columbia), ex-officio, EC Chair





Timeline for CIG-II

- Sept. 1, 2008 Final Year of CIG starts
- Dec. 16, 2008 Announce Proposal Writing Committee (PWC) at Business Meeting
- Collect information for Self-study
- March 30-31 CIG Opportunities & Challenges Workshop, Pasadena
- April 1 PWC meets face to face
- May 15-30, Draft CIG-II proposal posted for public comment
- July 9 CIG-Geoinformatics proposal submitted to NSF
- Sept. 1, 2009, CIG Transition begins
 - CIG Carry forward
 - OCI-PetaApps Award
 - Small Supplemental from NSF Geoinformatics
- Jan 1, 2010 CIG-II Begins











Gold Standard Codes

Documented, supported, open-source codes (multi-platform, regression tested, VC)

- Mantle Convection: CitcomS
- Computational Seismology: SpecFEM family/ Computational Seismology portal
- Short Term Tectonics: Pylith
- Long Term Tectonics: GALE
- Geodynamo: MAG





Current CIG Staff Pasadena (Dec 2008)

- Director Mike Gurnis
- Chief Software Architect Michael Aivazis
- Administrator Ariel Shoresh
- Software Developers
 - Walter Landry
 - Lief Strand
 - Luis Almendariz
 - Eh Tan
 - Sue Kienz Documentation/Webmaster
- Additional Development support
 - Matt Knepely (ANL Subcontract)
 - VPAC Subcontract
 - Texas A&M subcontract (deal.ii)





Current CIG Committees (Dec 2008)

Science Steering Committee

- Louise Kellogg UC Davis Chair
- Wolfgang Bangerth , Texas A&M
- Bruce Buffett, U Chicago
- Andy Freed, Purdue
- Omar Ghattas, UT Austin
- Luc Lavier, UT Austin
- Laurent Montesi, U Maryland
- Jeroen Tromp, Princeton
- Marc Spiegelman, Columbia University, (Ex officio)
- Executive Committee
 - Marc Spiegelman, Columbia Chair
 - Bill Applebe, VPAC
 - Alan Levander (Rice)
 - Carolina Lithgow-Bertelloni (UCL)
 - Peter Olson (JHU)
 - Michael Aivazis (Ex Officio)
 - Michael Gurnis (Ex Officio)
 - Louise Kellogg (Ex Officio)





Current CIG Committees (Dec 2008)

- CIG-II Proposal Writing Committee
 - Bruce Buffett UC Berkeley (chair)
 - Brad Aagaard USGS
 - Wolfgang Bangerth Texas A&M
 - Thorsten Becker USC
 - Louise Kellogg UC Davis (ex-officio SSC chair)
 - Michael Gurnis Caltech
 - Alan Levander Rice University
 - Marc Spiegelman, Columbia University (ex-officio EC chair)
 - Peter van Keken Univ. Michigan







Working Groups (and reps)

- Seismology (Jeroen Tromp)
- Mantle Convection (Shijie Zhong)
- Magma Dynamics (Laurent Montesi)
- Short term Tectonics (Brad Aagaard)
- Long term Tectonics (Mousumi Roy)
- Computational Science (Omar Ghattas)





Seismology (Jeroen Tromp)

- Standalone Codes:
 - SEM: new releases of SPECFEM3D_GLOBE and SPECFEM3D (formerly_BASIN) ??? Downloads. Finalist Gordon Bell Prize for performance SC08
 - Mode codes: Mineos?
- Seismology Science Portal (Strand, Tan)
 - https://crust.geodynamics.org/portals/seismo/
 - Runs both SEM and mode codes
 - Allows upload of users 3-D model
 - Working on integration with geodynamic models (e.g. CitcomS)







- CIG Workshops/Meetings: none 2008
- Future developments
 - SPECFEM_SESAME (GOCAD/CUBIT/METIS Meshing/partitioning + SEM solver) release Summer 2009





Mantle Convection (Shijie Zhong)

• Available Codes at CIG:

- CitcomS: Latest release version 3.0.3 in September, 2008
- CitcomCU: Latest release version 1.0.2 in May, 2007.
- Ellipsis3d: Latest release version 1.0.2 in April, 2007.
- ConMan (Scott King): Latest release in September, 2008.

CIG Workshops/Meetings:

- Mantle/lithospheric dynamics workshop at UC-Davis in July, 2008 (thanks to Billen, Becker, King, & van Wijk).
- Participated in Math/Geo workshop at Santa Fe in September, 2008.





Mantle Convection (Shijie Zhong)

Community Driven Activities

Codes

- Release of CitcomS 3.0.3 in September, 2008.
- Donation of ConMan in September, 2008 (thanks to King).
- Continuous development of the 1-D code (HC) led by Becker, Steinberger and others.
- Thermodynamics code by Lithgow-Bertelloni and Stixrude.
- Benchmarking
 - Extensive benchmark of incompressible CitcomS (Zhong et al., G^3, 2008).
 - Cartesian 2-D/3-D compressible convection (King, and other 5 groups, a poster at this AGU).
 - Benchmark of compressible CitcomS (Tan et al., in preparation).

New/Future Developments: AMR

- Code Rhea: massively parallel (~100 K processors) AMR in 3D Cartesian and Spherical geometry (Ghattas' group at UT-Austin with help/collaboration from Tan, Gurnis, and Zhong) (see a poster by Stadler, Burstedde, and a few others at this AGU).
- Deal.ii based parallel AMR codes (Bangerth at UT A&M).

March 30-31. 2009



Mantle Convection (Shijie Zhong)

Evolution of mantle plumes from Rhea on ~100 K processors



Magma Dynamics (Laurent Montési)

- Activities:
 - MADDs Magma Dynamics Demonstration Suite
 - Series of Benchmark problems for coupled magma dynamics/Stokes www.geodynamics.org/cig/workinggroups/magma/workarea/benchmark/McKenzieIntroBenchmarks.pdf
 - Code Implementations:
 - Stg-MADDs: VPAC StGermain code base -- Stokes, Solitary Waves, Ridge (XX Release: Dec 2009 -- major refactoring of VPAC software)
 - Comsol: (Montési) 3-D Stokes, constant porosity/Ridge
 - MADDs-Dolfin: (Spiegelman) Stokes, Solitary Waves FEniCS (FFC/ DOLFIN) + PETSc
 - PETSc FV: (Spiegelman)
 - Deal.ii: (Bangerth) Stokes, Magma Waves
 - Issues: proper integration with Mantle Convection/General multi-physics solvers
- CIG Workshops/Meetings:
 - Participated in Math/Geo workshop at Santa Fe in September, 2008.







Magma Dynamics (Laurent Montési)

MD Goals

- Multiphysics coupling
 - Mantle convection
 - Brittle field / diking
 - Computational thermodynamics (e.g. MELTS)



Deal.ii step 22 adaptively refined mid-ocean ridge Stokes problem (Bangerth, 2008)



Short term tectonics (Brad Aagaard)

Working group activities

- PyLith (Brad Aagaard, Charles Williams, Matthew Knepley)
 - Parallel, 2-D and 3-D finite-element code for modeling crustal
 - deformation associated with earthquake faulting and elastic and/ or
 - viscoelastic rheologies
 - 3 new feature releases plus 1 bugfix release in last 12 months
 - Version 1.3.1 released on Nov 25th
 - Expect 5+ new feature releases in next 2-3 years
- Cataloging of semi-analytic codes (Rob Mellors)
 - Collect codes useful for utility calculations and benchmarking
- Benchmarking crustal deformation codes
 - Working with CIG (Luis Armendariz) to develop infrastructure for benchmarking codes (PyLith, GeoFEST, COMSOL)





Short term tectonics (Brad Aagaard) Workshops:

Numerical Modeling of crustal deformation workshops

- June 23-27, 2008, Colorado School of Mines
 - 7th annual workshop
 - Sponsored by CIG, SCEC, NSF, NASA
 - 60 participants
 - Mixture of science talks and tutorials
- June 22-26, 2009, Colorado School of Mines
 - Seeking funding from same sponsors
 - Expect similar number of attendees
 - Emphasis on application of codes to research problems
 - Suggestions for science talks welcome!





PyLith Example: Charles Williams et al.

Velocity field for plate drived motions and eqs on 55 faults Elastic, Homogeneous properties Elastic, SCEC CVM-H propertie



Maxwell, SCEC CVM-H







Long term tectonics (Mousumi Roy)

- Codes:
 - GALE v 1.3.0: PIC, Visco-Plastic Arbitrary Lagrangian/Eulerian
 - Inflow/Outflow BC's implemented
 - Pressure oscillations are solved
 - Assignment of BC's at nodes is implemented
 - Simple surface processes are implemented
 - Conducted GEOMOD2008 Benchmarks
 - SNAC (StGermaiN Analysis of Continua) 1.0.0, an updated Lagrangian explicit finite difference code for modeling a finitely deforming elasto-visco-plastic solid in 3D, released under the GNU General Public License.





Long term tectonics (Mousumi Roy)

Future objectives:

- Couple GALE, CITCOM, and PYLITH
- Implement AMR (use DEAL II?)
- Joint LTT/MM WG workshop?
- Develop user community dialog (a GALE-specific wiki to discuss/post solutions?)
- Develop example using {z,P,T} dependence of physical properties in GALE
- Solicit user-developed post-processing routines (e.g., analysis of P-T-t paths)





Long term tectonics (Mousumi Roy)

Applications:

3-D Faulting and Magmatism at Mid-Ocean Ridges Garrett Ito (SOEST, University of Hawaii, Honolulu HI) Mark D. Behn (Woods Hole Oceanographic Institution, Woods Hole MA)





2008 Activities

- Improvements in common infrastructure software
 - SVN software repository, bug-tracking database (*Roundup*)
 - Automated regression testing: CIG-Regresstor, Buildbot
 - *Sieve*: parallel manipulation of FE meshes
 - Cigma: facilitates benchmarking by automating comparisons of fields from different meshes
- Codes:
 - Geodynamics AMR suite in *deal.II* C++ library for adaptive FE PDE solution
 - Developed by Wolfgang Bangerth (Texas A&M)
 - Adaptive sequential Stokes solver complete and publicly available (step-22 of the *deal.ll* tutorial)
 - Adaptive sequential Boussinesq solver complete and publicly available from our subversion server (step-31); will be part of next release
 - Parallel Boussinesq solver under development (step-32)
 - Adaptive elasticity solver available (step-16)
 - Initial version of one formulation of magma flow
 - *Rhea*: parallel AMR mantle convection code
 - Developed under NSF PetaApps project (Biros, Ghattas, Gurnis, Zhong PIs; Burstedde, Stadler, Tan, Wilcox research scientists)
 - Based on *p4est/mangll/octor* parallel AMR multi-octree and discretization libraries

March 30-31, 2009

- Supports mesh coarsening/refinement on O(10⁴) cores
- Workshops
 - NSF/CIG Workshop on Mathematical and Computational Issues in the Solid Earth Geosciences, Santa Fe, NM, Sept. 15-17, 2008 Workshop







deal.II adaptive Stokes example



CIG Opportunities Workshop March 30-31, 2009







Examples of adaptivity in Rhea







Computational Science (Omar Ghattas) Planned 2009 Activities

- Common software infrastructure
 - Expand regression testing
 - Expand *Sieve* software suite
 - Expand Cigma benchmarking code
 - Science gateway for benchmarking
- *deal.ll* AMR suite
 - Release of parallel Boussinesq solver
 - Completion of magma migration solver
 - Adaptive solvers for more complicated magma migration models and thermochemical convection
- *Rhea* mantle convection code
 - Spectral element/discontinuous Galerkin discretization
 - Improved solvers (fully implicit Newton-Krylov solver; improved AMG preconditioning)
 - Adjoint capabilities (for adaptivity and for sensitivity analysis)
 - Scalability of AMR to 10⁵ cores





Future Issues:

- Themes emerging from the workshop and CIG 5year strategic plan:
 - Advanced solvers and preconditioners for multiscale multiphysics problems
 - Advanced (high-order, DG) and adaptive discretizations for multiscale, multiphysics
 - Adjoint methods for error estimation and sensitivity analysis
 - Inversion/data assimilation algorithms
 - Uncertainty quantification
 - Earth structure model frameworks
 - Parallel performance and scalability of all of the above
 - from local multicore clusters to TeraGrid petascale systems
- Community input needed and invited!





Summary

- CIG provides documented/supported codes for a broad range of solid earth geoscience communities
- Much current development is in support of specific communities
- However, many problems share common components & scientific needs supported by new developments (e.g. AMR, Variable viscosity Stokes)
- Question? How to continue supporting core constituencies, while implementing new technology, to develop the next generation of multi-purpose, interoperable codes.





Rhea scaling



Advection-diffusion scalings on 65K cores on TACC Ranger. Overhead of AMR has become insignificant.





2008 Accomplishments

- Improvements in common infrastructure software
 - SVN software repository, bug-tracking database (*Roundup*)
 - Automated regression testing: *CIG-Regresstor*, *Buildbot*
 - Sieve: parallel manipulation of FE meshes
 - Cigma: facilitates benchmarking by automating comparisons of fields from different meshes
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c deal.II adaptive Stokes example

2008 Accomplishments, cont'd

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 - Developed under NSF PetaApps project (Biros, Ghattas, Gurnis, Zhong PIs; Burstedde, Stadler, Tan, Wilcox research scientists)
 - Based on *p4est/mangll/octor* parallel AMR multioctree and discretization libraries
 - Supports mesh coarsening/refinement on O(10⁴) cores
- NSF/CIG Workshop on Mathematical and Computational Issues in the Solid Earth Geosciences, Santa Fe, NM, Sept 15-17, 2008
 - Focus on math. and comp. issues in mantle convection, magma dynamics, and crustal dynamics & earthquake cycle
 - Assess and define challenges for linear and nonlinear solvers, multiscale/multiphysics methods, AMR, inverse problems and uncertainty quantification of frontier solid earth geoscience problems
 - Foster new collaborations among solid earth geophysicists and computer/computational scientists and mathematicians to address these problems







CIG Opportunities Workshop March 30-31, 2009



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 - Adjoint capabilities (for adaptivity and for sensitivity analysis)
 - Scalability of AMR to 10⁵ cores







Long Term Tectonics Working Group

WG Members: Dennis Harry, Co-Lead, Mousumi Roy, Co-Lead, Thorsten Becker, Todd Ehlers, Noah Fay, Ritske Huismans, Carolina Lithgow-Bertelloni, Dietmar Muller, Patrice Rey, Jolante van Wijke





Achievements

- Gale
 - Inflow/Outflow BC's implemented
 - Pressure oscillations are solved
 - Assignment of BC's at nodes is implemented
 - Simple surface processes are implemented
 - Conducted GEOMOD2008 Benchmarks





Current Projects (Short-Term Goals)

• GALE

- Collect geological examples from user community
- Minor cleanup of documentation need user feedback
- Analyze slow(?) Uzawa convergence
- Parallelize surface processes (erosion) calculation
- Sync GALE with UNDERWORLD and establish formal protocol for regular syncs
- Implement flow-through BC's
- Implement deformed tower boundary

Future Plans (Long Term Goals)

- Couple GALE, CITCOM, and PYLITH
- Implement AMR (use DEAL II?)
- Joint LTT/MM WG workshop?
- Develop user community dialog (a GALE-specific wiki to discuss/post solutions?)
- Develop example using {z,P,T} dependence of physical properties in GALE
- Solicit user-developed post-processing routines (e.g., analysis of P-T-t paths)







Long term vision

From the 2007 Strategic Plan

create a set of computational tools and data structures that

- Can be commonly applied within the geodynamics community.
- Promote more interaction between different geodynamic subdisciplines.
- Enable the development of models of Earth evolution that intimately couple lithosphere, convecting mantle and core
- Provide the capability to eventually simulate, and *understand*, the planet as a whole.



