

Computational Science Roundtable Discussion

October 18, 2006

Discussion Topics

- Update/edit lists of challenges and tools
- Could/should we build CIG codes from common components?
- Implementation test “cases”
 - Finding efficient solver/preconditions for problem X
 - Workflow tools

Cross-Cutting Computational Issues

Challenges & Wish Lists versus Tools

Categories:

- General
 - Model construction
- Software
 - User interface
 - Discretization schemes
 - Solvers/preconditioners
 - Constitutive models

Model Construction

Challenges & Wish Lists

- Complex, nonplanar geometry
- Complex discretization criteria
- Recipes for constructing models

Tools

- Meshers
(e.g., LaGriT, CUBIT, CMU??)
- Workflow managers
(e.g., Vistrails)
- Adaptivity
(e.g., deal.ii)
- Spatial databases
(e.g., SCEC CVM, USGS Bay Area VM)

User Interface

Challenges & Wish Lists

- Modularity
- Usability
- Record keeping

Tools

- Simulation frameworks (e.g., Pyre)
- Workflow managers (e.g., Vistrails)

Discretization Schemes

Challenges & Wish Lists

- Runtime selection of basis fns & quadrature
- Parallel manipulation of FE topology
- Adaptive mesh refinement

Tools

- Generic FE topology (e.g., Sieve, deal.ii)
- Generic basis & quadrature (e.g., FIAT, deal.ii)
- Adaptivity (e.g., deal.ii, Sierra, Sundance, Abani's research code)
- Weak Form Integrators (e.g., FFC, Sundance)

Solvers/Preconditioners

Challenges & Wish Lists

- Ability to handle many solvers/preconditioners
- Tools to identify efficient solvers/preconditioners
- Efficient solvers/preconditioners for problem X

Tools

- Solver/preconditioner suites (e.g., PETSc, trilinos)
- Preconditioners (e.g., Hypre, SuperLU)

Constitutive Models

Challenges & Wish Lists

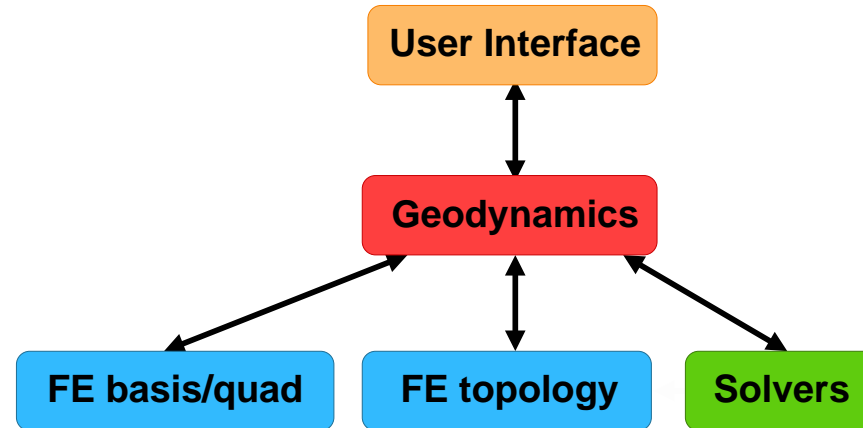
- Ability to handle many constitutive models
- Interface with empirical models
- Communicate with developers of empirical models

Tools

- Constitutive library (e.g., Underworld)

Long-Term Development Strategy

Architecture of a CIG Simulation Code



- Could we build CIG codes from common components? Yes
- Should we build CIG codes from common components?

Pros

- Leverage limited resources
- Less code to maintain
- Improvements propagate

Cons

- One size fits all?
- Requires much more coordination

Adaptive Mesh Refinement

Intermediate-term goals

- PyLith
 - Poor man's adaptive mesh refinement: Post-simulation error analysis and refinement intermediate goals
- Bangerth/Lavier Plasticity code
 - Applicable to laboratory rock physics, long-term tectonics, short-term tectonics (fault evolution)
 - Not CIG Software -- currently in Bangerth's svn repository
 - Rich man's adaptive mesh refinement: Code integrated with deal.ii

Short-, Intermediate-, and Long-Term Goals of CIG

	Short-Term Goals	Intermediate-Term Goals	Long-Term Goals
Short-Term Tectonics	PyLith 0.8, a parallel version of code with visco-elasticity functions, due by June 26, 2006 Workshop. Goal is to have 20-30 users after workshop in June.	PyLith 1.0, which incorporates static and dynamic functions. Target date 1/01/07.	Adaptive Mesh Refinement using PyLith. Future goals would be to allow code to couple with other geophysical codes. Also Adaptive Spherical geometry.
Computational Seismology	Have 1D mode code supplied by Ritzwoller and given Pyre wrap, with mode catalog and mode summation. Also, a fully Pyrized and normal version of the Global and Basin SPECFEM code will be ready by the next workshop (Oct. 2006). The stand-alone (and hopefully Pyre version) will have full documentation.	Highest priority for two packages: a 1D package for Cartesian reflectivity, and a finite difference 3D wave propagation (?) code. Goal will be more specifically defined after SPICE meeting.	On demand/on request seismology. Community is currently working on a rudimentary web interface. Another goal is for coordination of model databases.
Computational Science	When community meets for workshop in Oct. 2006, specific intermediate and long-term goals will be discussed.	To be defined at workshop.	Work on integration of computer sciences and geophysics into single framework.

Short-, Intermediate-, and Long-Term Goals of CIG (cont'd)

	Short-Term Goals	Intermediate-Term Goals	Long-Term Goals
Long-Term Tectonics	<p>GALE beta to be released for some users, with additional functionality, August 2006.</p> <p>Outreach to community via a two-day code tutorial, Fall 2006.</p>	<p>Code with 3D Spherical Elasticity, either via GALE or SNAC (available April 2007). This code would tie into Short-Term Tectonics via reducing time-steps in 2D computations -- beneficial to both communities.</p> <p>Host workshop in conjunction with a pre-meeting at EARTHSCOPE in Spring 2007.</p>	<p>Develop new code with mesh refinement, Adaptive Mesh Refinement.</p>
Magma Migration	<p>When community meets for workshop in August 2006, specific intermediate and long-term goals will be discussed.</p>	<p>To be defined at workshop.</p>	<p>TBD at workshop but possibly including integration of magma dynamics in global mantle convection, development of a regional plate-boundary modeling toolkit for ridges, arcs, and plumes, integration of fluid flow in lithospheric deformation.</p>

Short-, Intermediate-, and Long-Term Goals of CIG (cont'd)

	Short-Term Goals	Intermediate-Term Goals	Long-Term Goals
Geodynamo	Benchmark and adapt two serial geodynamo codes, MAG and MoSST; development of user interfaces. Preliminary community building discussions will be held during SEDI in July 2006.	Community building workshop in 2007, to utilize and train users on the two serial codes, possibly partnering with other organizations. Test user interfaces and web portal. Addition of parallel code in web portal.	New dynamo code using common components with Mantle Convection codes including common Earth structure framework and grid and adaptivity.
Mantle Convection	Deliver beta version of compressible spherical code (CitComCS 3.0) by Dec. 2006. Basic visualization package by Dec. 2006. 1D code (HC 1.0) version Dec. 2006.	CitcomCS 3.N with possible additions (self consistent thermodynamics) designed by community).	New code with adaptivity, and Adaptive Mesh Refinement.

Cross-Disciplinary Goals - Infrastructure

Mostly Completed	Long-Term
Web site (implemented Plone)	
Automatic Builds (implemented Buildbot)	On demand/on request computing using web interface
Benchmarking	Benchmarking (<i>BM.py</i>)
Regression testing (developed <i>CIG-Regresstor</i>)	
Launcher package (developed <i>Addendum.py</i>)	
Software repository (implemented SVN)	

Cross-Disciplinary Goals - Scientific Computing

Mostly Completed	Long-Term
Sieve code	AMR
PETSc/Pyre framework for codes.	Early parallel mesh generator (TK of Texas) to be altered to become solution adaptive, and therefore provide possible AMR that can be scaled to billions of elements and thousands of processors.
HDF5 -- output of codes in similar format for ease in benchmarking and for future visualizations.	Continue use of PETSc and Pyre to develop software frameworks.

Workshops

Short-Term Tectonics	June 26-30, 2006 workshop to be held in Golden, CO. Workshop will focus on using available (LaGriT, Cubit) and new codes (PyLith 0.8) as well as community discussion on benchmarks, meshes, and case studies. Presumably would co-sponsor meeting in June 2007.
Magma Migration	August 18-19, 2006, Columbia U. Meeting to discuss current software needs of community in magma dynamics and magma migration.
Computational Seismology	October 31-November 2, 2006, Washington U in St. Louis. Second CIG Computational Seismology workshop as part of "Seismic Imaging Workshop."

Workshops (cont'd)

Computational Sciences	October 16-17, 2006, Austin, TX. Cross-disciplinary workshop bringing together various geophysical and computer science experts to work on common theoretical and mathematical obstacles to scientific coding. Followed by Computational Science Round Table October 18.
Mantle Convection	Summer 2007 workshop to discuss science, current software development, and future plans for new code in adaptivity and AMR.
Geodynamo	Pre-meeting to begin community building in Spring 2007 as part of SEDI program, to be followed up by a full workshop later in 2007.
Long-Term Tectonics	Pre-meeting discussion to be held before EARTHSCOPE in March 2007.

Annual Goals and Milestones

Sept. 1, 2006 - Aug 31, 2007

I. Common Infrastructure

- a) Maintain LAN, servers, desktops, notebook computers
- b) Maintain Plone site (<http://geodynamics.org>)
- c) Maintain repository (SVN)
- d) Maintain and expand regression testing (*CIG Regresstor*)
- e) Expand *Sieve* software suite
- f) Expand benchmark code (*BM.py*)

Annual Goals and Milestones (cont'd)

II. Core Computational Software

- a) Computational Seismology code (normal mode, NM), including Pyrization
- b) Continue migrating NM and *SPECFEM* codes under Pyre into Web Services
- c) Compressible mantle convection code development (*CitcomCS3.0*)
- d) Mantle convection support, HC
- e) Long-term tectonics code development (*Gale 1.0*)
- f) Long-term tectonics code migration into SVN (*SNAC 1.n* donation)

Annual Goals and Milestones (cont'd)

II. Core Computational Software (cont'd)

- g) Short-term tectonics code development (*PyLith 1.0*)
- h) Geodynamo migration into SVN, release, benchmarking MAG/MoSST
- i) Geodynamo pre-/post-processing
- j) Initiate development of magma dynamics software
- k) Move toward incorporating AMR

Annual Goals and Milestones (cont'd)

III. Organizing Community Participation

- a) Annual meeting of EC, November 2006, Columbia University, NYC
- b) Computational Science Workshop, Oct. 16-18, held at Institute for Computational Engineering and Science (ICES), Austin, TX
- c) Computational Science Round Table, Oct. 18, 2006, ICES, Austin, TX
- d) Computational Seismology meeting in association with Imaging workshop at Washington U., St. Louis, Oct. 31-Nov. 2, 2006
- e) Annual Business Meeting, Dec. 12, 2006, at Fall AGU, San Francisco, CA
- f) Annual meeting of SSC, May 2007, Pasadena, CA
- g) Finite-element modeling of fault interactions workshop (co-sponsorship with SCEC, Summer 2007)

CIG Goals -- Added/Revised Based on Workshop Presentations and Round Table Discussion

- Variable viscosity Stokes solver computational benchmark (*intermediate*; Mark Spiegelman)
- Workflow tracking using Vistrail, etc. (*intermediate*; Short-Term Tectonics)
- Common Rheology Module (*intermediate*; CIG-wide)
- Common Code Elements - solvers, meshers, etc. (*long-term*; CIG-wide)
- Training/Outreach to build code-user base (*intermediate*; Short-Term and Long-Term Tectonics, Geodynamo...)