CIG Overview

NSF Workshop on Tectonic Modeling
Breckenridge, Colorado
June, 2005

Overview

- Quick Overview of the Computational Infrastructure for Geodynamics (CIG)
- Why did we come up with CIG initiative?
  - *Want to move forward with more sophisticated methods faster*
  - *With EarthScope, and similar initiatives, the user base for modeling is expanding*
  - *But, the present mode of software development is showing its limitations*
- Some details of CIG
  - *Summary of the CIG vision for a geodynamics tool box*
- What would CIG like to come out of this workshop?
  - *What are the present methods & codes and their strengths & weaknesses*
  - *Starting to establish community Benchmarks*
  - *What new tools does the community need to move forward*

Quick Overview of the Computational Infrastructure for Geodynamics (CIG)

CIG is an NSF Center that provides computational infrastructure for the (solid) earth sciences community with community oversight.

The overall goal is to leverage the current state of the art in scientific computing into a suite of open source toolkits and codes that serve the greater community from model developers to the end-users of models.

Quick Overview of the Computational Infrastructure for Geodynamics (CIG)

A small core (~4-5) of dedicated software engineers and architects guided by scientific objectives driven by the Geodynamics community. This Software Development Team will provide software service to the community in terms of programming, documentation and support.

We will partner with science-neutral activities from the Computer Science/Scientific Computation communities & implement current "best-practices" into community specific toolkits for scientific computation in solid-earth sciences.

Guidance for the programmers will come from Science Steering Committee whose emphasis is to identify & balance common components needed across the disciplines.

Present State of CIG

- Member Institutions (32, plus 4 Foreign Affiliates)
- Funded by NSF GeoInformatics Program within EAR Division
- Managed by Caltech for the community through a five-year cooperative agreement
- Ultimate authority rest with an elected Executive Committee (Mark Richards, Chair)
- Science Steering Committee
  - *Will be in place by mid-June, 2005 -- please participate*
- Resources
  - *3-4 In house software engineers*
  - *Technical writer/web master; Administrative support*
  - *Support Matt Knepley (PETSc), Argonne National Lab*
  - *Some support for other subcontracts for software development*
  - *Support for workshops and for visitors at CIG*

Why did we come up with CIG initiative - 1 ?

- Want to move forward with more challenging problems and these require more sophisticated methods. We would hope to have these methods come on line faster.
  - *Multi-scale*
    - *Clearly important for your problems -- faults, shear zones*
    - *But also important for many forefront areas*
      - *Short term tectonics -- dynamic rupture -- fault-talk*
      - *Global geodynamics -- plate boundaries and large-scale mantle convection*
      - *Melt migration -- large scale flow, localized melting*
      - *Seismology -- very fine-scale structure within the whole earth*
  - *Multi-physics*
    - *Local simulations of microphysics (crystal fabric, thermodynamics, etc.) within a geodynamics context.*
  - *Closer connection with data*
    - *Computational tools that assimilate some data sets and output and predict others*

Why did we come up with CIG initiative - 2?

- The user base for modeling with the “geosciences” is expanding
  - *Simulation as a forth (or a modified third) pillar of science is becoming more widely appreciated*
  - *Many large, integrative projects (such as a field project) has a component of “modeling”*
  - *Wide use of computational models will be needed to pull off the “intellectual challenge” of the EarthScope vision*
- But, the present mode of software development is showing its limitations

The Tradition of Model Development in Earth Science

- Individually written (usually begun as a graduate student)
- Created for a narrow range of applications
- Codes have unique identity, not modular
- Minimal documentation
- No extensive validation
- Unlimited number of versions
- Calculations separated from graphics and analysis
- Long development times (ex: DYNAMO=15 yrs; TERRA=10+ yrs)
- Brief maintenance (especially as developer changes research direction)

What will be CIG Software and in the Tool Box?

Superstructure

?

Geodynamic Specific

?

Infrastructure

?

Library ?

Example: Mantle convection coupled to lithosphere

Superstructure

- Monitor Simulation
- Couple Fluid to Solid
- Visualization

Geodynamic Specific

- Rheology modules
- Assess plate-tectonics

Infrastructure

- Mesher: Solid & Fluid
- Solver: Solid & Fluid

Library: PETSc, BLAS, MPI

Example of Geodynamic Specific & Infrastructure Layers

Geodynamic Specific

- SNARK -- particle based FEM with implicit solver
- SNAC -- Lagragian explicit FEM

Infrastructure

- StGermain: A framework with entry points & plugins for: building meshes, advecting particles, calling solvers, I/O…..

Library: PETSc, MPI

Example of Geodynamic Specific & Infrastructure Layers

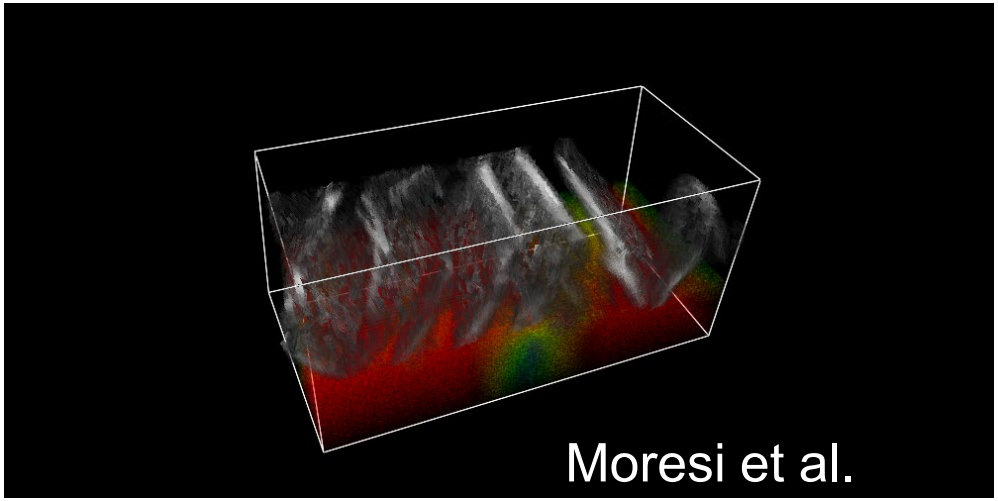
- SNARK -- particle based FEM with implicit solver
- SNAC -- Lagragian explicit FEM

Geodynamic Specific
SNARK: Monash group (Moresi)
SNAC: Caltech/Texas groups (Gurnis, Lavier)

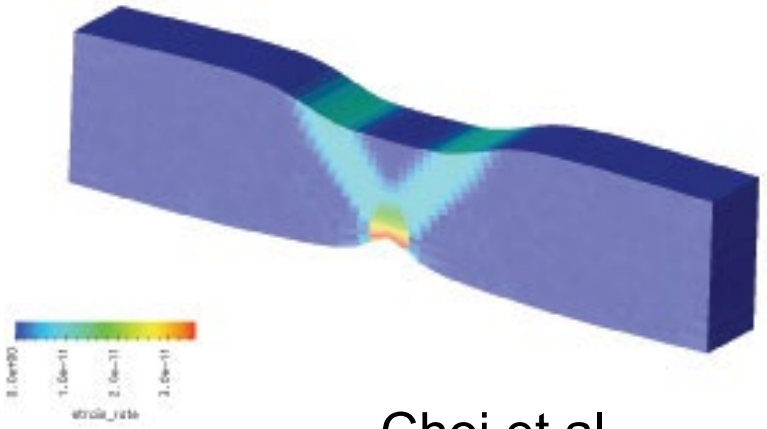
- StGermain: A framework with entry points & plugins for: building meshes, advecting particles, calling solvers, I/O…..

Infrastructure:
Software Engineers at the Victorian Partnership for Advanced Computing (Steve Quenette Team Leader)

SNARK & SNAC



Moresi et al.



Choi et al.

StGermain: A framework with entry points & plugins for: building meshes, advecting particles, calling solvers, I/O…..

Quenette et al.

What CIG-SSC needs from you

- Evaluate the current state of your computational tools
  - *Strength and weakness of methods*
  - *Codes in existence that use these methods and the strength and weakness of the codes*
  - *Availability of these codes (freely available, open source)*
  - *A "draft catalog" of these codes -- (name, several sentences about each one)*
- Start a process of benchmarking
  - *Articulate the parameters of these benchmarks*
  - *How should your benchmarks be presented (data formats, necessary meta data)*
  - *Get "buy-in" from members of the community and then have the results of these BM on the web*
- What software will be needed for your science?
  - *Reengineering/repackaging existing codes?*
  - *New tools and components within a framework?*
  - *Listing the priority of needs would be most helpful*
- A Workshop Report posted on the Web
- Your report will be used by the Science Steering Committee to establish CIG priorities

Workshops Summer 2005

- Fault systems and tectonics (joint with SCEC)
  - *Brad Hager, Carl Gable & Mark Simons*
  - *LANL in July*
- Mantle convection
  - *Shijie Zhong, Adrian Lenardic, Scott King & Marc Parmentier*
  - *Boulder, CO, in June*
- Computational seismology (joint with IRIS)
  - *Jeroen Tromp, Guy Masters, Michael Ritzwoller, Michael Wysession, & Alan Levander*
  - *Stevenson WA just before IRIS meeting*
- Long-term tectonics
  - *Dennis Harry, Sean Willett & Luc Lavier*
  - *Breckenridge, CO in June*