NSF Site Visit to the Computational Infrastructure for Geodynamics

Computational Science Issues within CIG

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Computational Infrastructure for Geodynamics

National Science Foundation
WHERE DISCOVERIES BEGIN

Outline

- Present state of Scientific Computing in geodynamics
- Solutions
- CIG workshop on Scientific Computing
- Current CIG work
- Long term plans
- Hurdles

Present State

Many geodynamics projects (within and outside CIG) are successful but run into the same problems:

- Need for complicated meshes
- Discretizations often simplistic
- Poor solver performance limits size of problems
- Limited parallel scalability (parallel solvers, input, output, visualization)

These are exactly the same issues that other applied sciences also face and that CIG is there to address.

Present State

Underlying problem is the traditional approach to software writing:

- One or a few people ("hero programmers") write an application code from scratch
- Manpower and experience is too limited to address basic problems properly; rather code is band-aided every time a problem comes up
- Programmers are application scientists, not software specialists; code not very extensible
- Projects suffocate in their complexity or die when initiators lose interest

Solutions

Changing this situation requires changing the way we produce software and educating the players in the field. ***CIG and NSF are addressing these points.***

Software generation issues:

- We need a good number of people who have an interest in the software itself, not only in the results
- We need funding for these people
- Open Sourcing our projects, opening up development
- More rigorous software engineering practices
- Encourage reuse and sharing of code, abstraction

Solutions

Educating players and the mentality of the field:

- No, it is not ok to write a code from scratch!
- Make existence and availability of codes public
- Foster exchange of ideas, methods, codes between application scientists, mathematicians, and computational scientists
- Promote use of software frameworks
- Promote use of more sophisticated solvers, discretizations, data formats

CIG will address this through a workshop in Oct/Nov.

Workshop on Scientific Computing

A CIG workshop to promote these ideas will be held in Austin, TX in Oct/Nov 2006, organized by Omar Ghattas (UTexas) and Wolfgang Bangerth (Texas A&M).

Goals are to bring together:

- People in geodynamics who find themselves limited by the usual problems
- Mathematicians with methods of interest to CIG
- Computational Scientists with experience in software design and general-purpose software libraries

Workshop on Scientific Computing

Planned topics:

- Meshing
- Linear and nonlinear solvers, preconditioners
- (Higher-order) discretizations and automatic code generation for these topics
- Portable and widely available data formats
- Parallel data storage and visualization
- Packaging, distribution, documentation, etc of large-scale software

Current CIG Work

Present and ongoing work within CIG:

- Collect sources of existing projects
- Document codes, develop benchmarks and testcases
- Make these codes available to the public
- Offer interested parties to participate

- Integration into general "top-level" software frameworks, e.g. Pyre, to facilitate coupling and steering codes

Long Term Plans

- More projects, better documentation
- Work with present authors, funding agencies, universities to promote the idea of Open Source
- Promote the use of general-purpose libraries to potential authors in the field
- Unify the structure of codes in CIG to make them easier to learn

- Integration into general "foundational" software frameworks, e.g. PETSc, deal.II, etc to share more common code and more sophisticated algorithms

Hurdles

- Need to change **the culture** of a field, including
  - application scientists (need to accept our codes)
  - advisors (need to make their students reuse codes)
  - funding agencies and reviewers (need to discourage parallel developments and encourage building on what others have done; accept the value of software development independently of science results)

- Need to overcome "impedance mismatch" between geodynamicists and mathematicians