

Computational Science Issues

Many geodynamics projects (in magma migration as well as in other areas, within and outside CIG) are initially 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.

Computational Science Issues

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

Computational Science Solutions

Changing this situation requires changing the way we produce software and educating the players in the field. *CIG is there to address 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

Computational Science 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 October 16/17 in Austin, TX.

Computational Science Solutions

Existing, large, and well-tested software libraries provide tools that are worth man-years and 100,000s lines of code of development:

- Large array of linear system handling and solvers: sequential and parallel, direct and iterative (e.g. PETSc, Trilinos)
- Different discretizations: adaptive, low and high order, mixed, continuous and discontinuous, special finite elements for flow or electromagnetic problems (deal.II, getfem, oofem, geofem, ...)
- Support for many different in- and output formats
- Large number of tools typically needed for simulations

Some of these libraries will be represented at the CIG workshop.