

## "Numerical techniques for thermo-mechanical-fluid-flow modelling in geosciences"

### Abstract:

3D geodynamic modelling of lithospheric-scale deformation remains a challenge as it requires scalable multigrid algorithms that perform well in the presence of large and abrupt jumps in viscosity. In recent years, we have developed LaMEM (Lithosphere and Mantle Evolution Model), which was originally a finite element code, that can be combined with a marker-and-cell method (to model large strains) and that can be used in an Eulerian, Lagrangian or ALE manner. LaMEM is build on top of the parallel PETSC package (<http://www.mcs.anl.gov/petsc>), which allows us to use a large repertoire of smoothers, iterative solution techniques as well as algebraic multigrid preconditioners such as ML. We can use either Q1P0, stabilized Q1Q1 or Q2P-1 elements (all configurable from the command-line). Recently, we have also added a staggered grid finite difference (FDSTAG) solver, such that we can now tackle the same setup with either a finite element or a finite difference solver.

Here, we discuss the relative performance of the FD versus the FEM method for a few selected benchmark cases. It is demonstrated that the staggered finite difference method is a very competitive method compared to finite element methods in terms of accuracy and in case the jumps of viscosity are not aligned with the element boundaries (as is the case in most geodynamic simulations). Yet, compared to a higher-order finite element, the FD method requires an order of magnitude less memory (and is thus naturally faster).

If one wishes to use iterative or multigrid solvers in combination with 3D geodynamic codes, it is crucial to use stable or stabilized finite elements, as otherwise the number of required solver iterations increase with increasing grid size. Only the stabilized Q1Q1 elements and the Q2P-1 element fulfill this criteria. The Q1Q1 element, however, is not fully incompressible. This is not so much a problem in geodynamic simulations that ignore the free surface, but it becomes crucial if one wishes to study both mantle dynamics and a self-consistent free surface simultaneously in which case the stabilized Q1Q1 can give wrong results (i.e. the mantle compacts).

So if one wishes to use a Finite Element method for such applications one has to use higher order elements (Q2P-1), which are computationally expensive. The staggered FD formulation, however, behaves as a stable finite element, with iterations that are independent on the employed grid resolution. So in a way, the FDSTAG formulation behaves like the 'ideal' low order finite element, because it is stable and uses little memory.

One argument that is often held against the finite difference approach is that it cannot be used to simulate a self-consistent free surface. Many authors that used a finite difference approach have therefore employed a 'sticky-air' layer above the computational domain that has zero density and a low viscosity. So far, however, it was not clear whether this approach indeed yields the correct surface topography. We have therefore recently performed an extensive benchmark in which the sticky air approach was compared with finite element codes that have a self-consistent free surface and the results strongly suggest that it is indeed possible to obtain the correct surface topography with a sticky-air approach, provided that the viscosity and thickness of this 'air' layer are sufficiently large [1]. Moreover, the free surface stabilization technique we proposed some time ago [2] can be generalized for finite differences without loss of accuracy [3], which means that adding a pseudo free surface will not reduce the timestep significantly.

These results thus all highlight that the staggered finite difference method is an extremely competitive method for geodynamic simulation. Yet, a number of questions remain open such as whether it is better to use a coupled velocity-pressure multigrid approach (as is used for example by Paul Tackley and Taras Gerya), or whether a decoupled approach (which we currently employ) is more robust.

In addition, we will show some of the recent progress we have made in adding two-phase flow formulations to visco-elasto-plastic lithospheric dynamics code.

[1] Crameri F., Schmeling H., Golabek G.J., Duretz T., Orendt R., Buitter S., May D.A., Kaus B.J.P., Gerya T.V., Tackley P.J. (2011, submitted). A benchmark comparison of numerical surface topography calculations in geodynamic modelling. *Geophysical Journal International*.

[2] Kaus B.J.P, Mühlhaus H., May D.A. (2010). A stabilization algorithm for geodynamic numerical simulations with a free surface. *Physics of the Earth and Planetary Interiors*. Vol. 181, p. 12-20.

[3] Duretz, T., D. A. May, T. V. Gerya, and P. J. Tackley (2011), Discretization errors and free surface stabilization in the finite difference and marker-in-cell method for applied geodynamics: A numerical study, *Geochem. Geophys. Geosyst.*, 12, Q07004, doi:10.1029/2011GC003567