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Lagrangian numerical techniques for modelling multicomponent flow in the presence of large viscosity contrasts: Markers-in-bulk versus Markers-in-chain

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Many problems in geodynamic applications may be described as viscous flow of chemically heterogeneous materials. Examples include subduction of compositionally stratified lithospheric plates, folding of rheologically layered rocks, and thermochemical convection of the Earth's mantle. The associated time scales are significantly shorter than that of chemical diffusion, which justifies the commonly featured phenomena in geodynamic flow models termed contact discontinuities. These are spatially sharp interfaces separating regions of different material properties.

Numerical modelling of advection of fields with sharp interfaces is challenging. Typical errors include numerical diffusion, which arises due to the repeated action of numerical interpolation.

Mathematically, a material field can be represented by discrete indicator functions, whose values are interpreted as logical statements (e.g. whether or not the location is occupied by a given material). Interpolation of a discrete function boils down to determining where in the intermediate node-positions one material ends, and the other begins. The numerical diffusion error thus manifests itself as an erroneous location of the material-interface.

Lagrangian advection-schemes are known to be less prone to numerical diffusion errors, compared to their Eulerian counterparts. The tracer-ratio method, where Lagrangian markers are used to discretize the bulk of materials filling the entire domain, is a popular example of such methods. The Stokes equation in this case is solved on a separate, static grid, and in order to do it – material properties must be interpolated from the markers to the grid. This involves the difficulty related to interpolation of discrete fields. The material distribution, and thus material-properties like viscosity and density, seen by the grid is polluted by the interpolation error, which enters the solution of the momentum equation.

Errors due to the uncertainty of interface-location can be avoided when using interface tracking methods for advection. Marker-chain method is one such approach, where rather than discretizing the volume of each material, only their interface is discretized by a connected set of markers. Together with the boundary of the domain, the marker-chain constitutes closed polygon-boundaries which enclose the regions spanned by each material. Communicating material properties to the static grid can be done by determining which polygon each grid-node (or integration point) falls into, eliminating the need for interpolation. In our chosen implementation, an efficient parallelized algorithm for the point-in-polygon location is used, so this part of the code takes up only a small fraction of the CPU-time spent on each time step, and allows for spatial resolution of the compositional field beyond that which is practical with markers-in-bulk methods.

An additional advantage of using marker-chains for material advection is that it offers a possibility to use some of its markers, or even edges, to generate a FEM grid. One can tailor a grid for obtaining a Stokes solution with optimal accuracy, while controlling the quality and size of its elements. Where geometry of the interface allows – element-edges may be aligned with it, which is known to significantly improve the quality of Stokes solution, compared to when the interface cuts through the elements (Moresi et al., 1996; Deubelbeiss and Kaus, 2008). In more geometrically complex interface-regions, the grid may simply be refined to reduce the error.

As materials get deformed in the course of a simulation, the interface may get stretched and entangled. Addition of new markers along the chain may be required in order to properly resolve the increasingly complicated geometry. Conversely, some markers may be removed from regions where they get clustered. Such resampling of the interface requires additional computational effort (although small compared to other parts of the code), and introduces an error in the interface-location (similar to numerical diffusion). Our implementation of this procedure, which utilizes an auxiliary high-resolution structured grid, allows a high degree of control on the magnitude of this error, although cannot eliminate it completely.

We will present our chosen numerical implementation of the markers-in-bulk and markers-in-chain methods outlined above, together with the simulation results of the especially designed benchmarks that demonstrate the relative successes and limitations of these methods.