A Volume-of-Fluid Interface Tracking Method for Modelling the Advection of Compositional Fields with Sharp Boundaries in the Mantle Convection Code ASPECT

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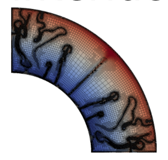
Section 1: Overview of Volume of Fluid Algorithm

- Methodology designed to conservatively advect the interface between two (immiscible) materials while maintaining a sharp interface



- Implemented as an extension to ASPECT [2], a parallel extensible code written in C++ to support research in modeling convection in the Earth's mantle.

Incompressible Stokes Equations:

$$\eta\nabla^2\vec{u} = \nabla P + \rho\vec{g}$$

$$\nabla\cdot\vec{u} = 0$$

Temperature Advection-Diffusion Equation:

$$\frac{\partial T}{\partial t} + \vec{u}\cdot\nabla T = \frac{k}{\rho c}\nabla^2 T$$

With Boussinesq Approximation:

$$\rho = \rho_0(1-\alpha(T-T_0))$$

- Implementation is second-order accurate, which is its design rate

- Method consists of two steps: Reconstruction and Advection

Reconstruction

- For accuracy, performance, and ease of implementation, we implemented the ELVIRA interface reconstruction algorithm [3]

- ELVIRA has been proven to be second-order accurate [4,5]; it is designed to reproduce linear interfaces exactly

- Since ELVIRA was designed to reproduce linear interfaces exactly, one validation problem was to advect a linear interface with constant velocity to machine precision

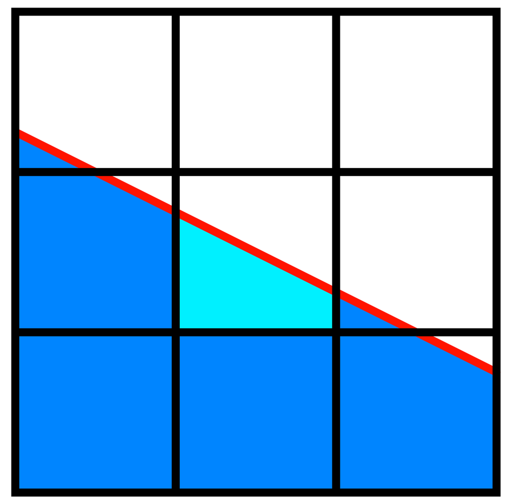


Figure 1.1a: Example 3x3 reconstruction Cyan volume matches data exactly Deviation of blue volume from the given data is minimized Red line in center cell is reconstructed interface

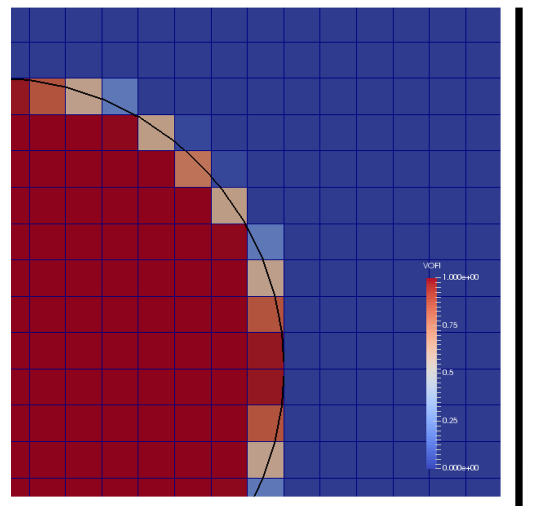


Figure 1.1b: Example of reconstruction of a circular interface with cells of side length one eighth of the circle's radius

Advection

- We use the reconstructed interface to calculate the fluxes for the advection step using the method of characteristics

- Formulated as a variation on Discontinuous Galerkin for implementation with the ASPECT FEM library

- Use of conservative advection update results in an inherently conservative method

Conservative Advection:

$$\frac{\partial C}{\partial t} + \nabla\cdot(C\vec{u}) = 0$$

Conservative update calculation

$$C_i^{n+1} = C_i^n + (F_L - F_R + F_B - F_T)$$

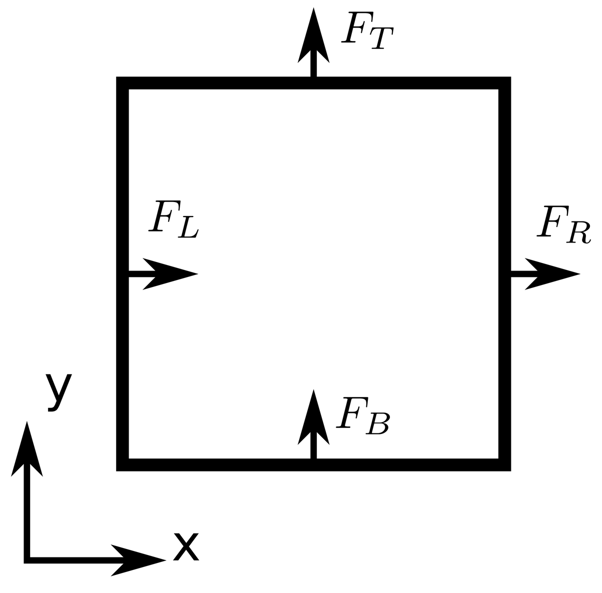


Figure 1.2: Sketch of Flux locations on example cell

Section 2: Falling Block Test Problem

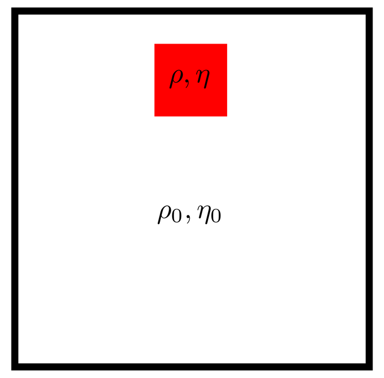


Figure 2.1: Initial Conditions

$\rho = 3.3\cdot 10^3$

$\rho_0 = 3.2\cdot 10^3$

$\eta = \eta_0 = 10^{21}$

- Benchmark from Gerya and Yuen [1]
- Incompressible Stokes equations with forcing term
- Comparison of 3 methods: Volume of Fluid (VoF), Bound Preserving Discontinuous Galerkin (BPDG), and the default ASPECT advection method with entropy viscosity to preserve bounds.
- Computations are on an AMR mesh with maximum resolution equivalent to a uniform 512x512 mesh
- Contour and line plots below show the diffusion of the interface for each method

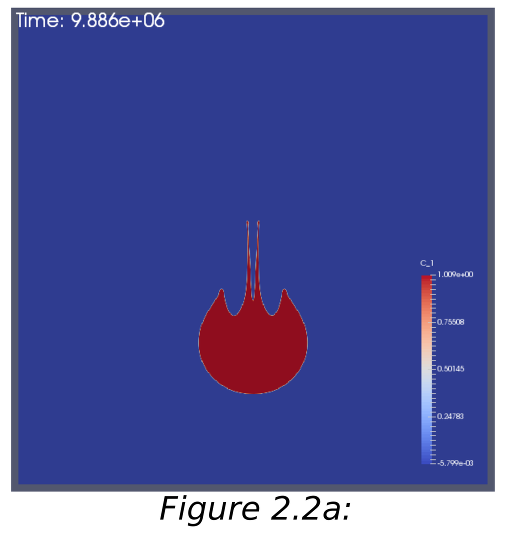


Figure 2.2a: VoF

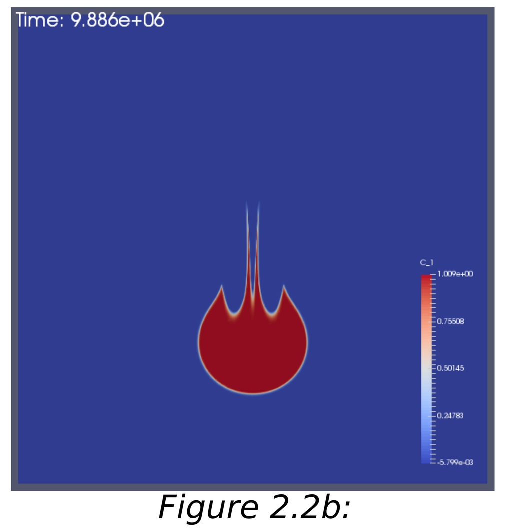


Figure 2.2b: BPDG

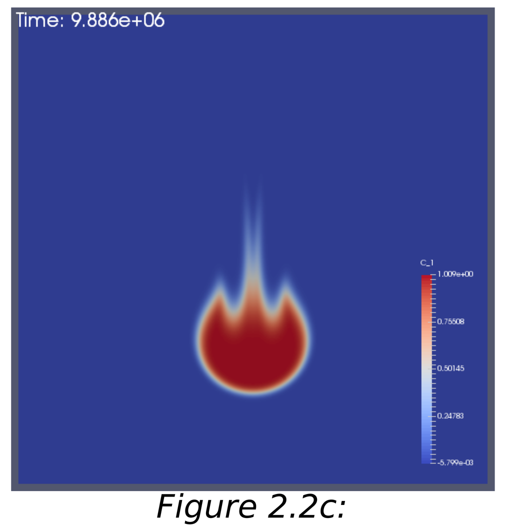


Figure 2.2c: Default ASPECT advection with entropy viscosity

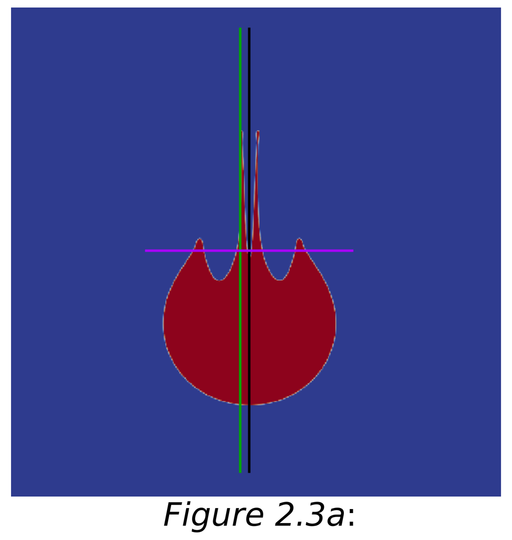


Figure 2.3a: Locations for compostion line plots on VoF colormap

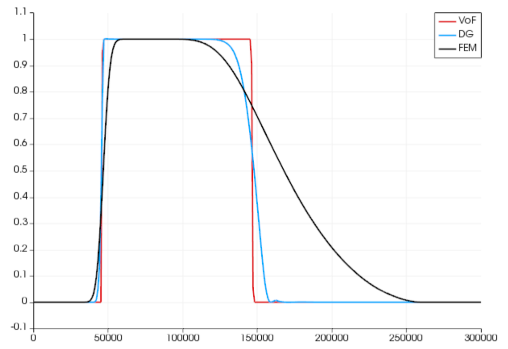


Figure 2.3b: Composition along vertical center line (black)

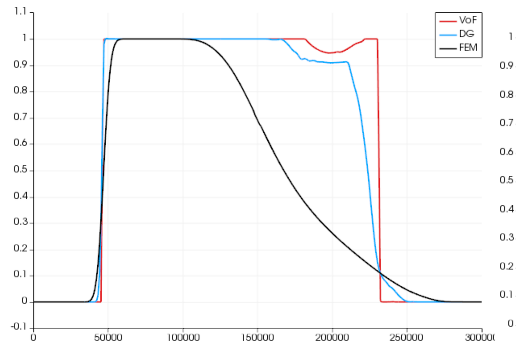


Figure 2.3c: Composition along left tail (vertical) (green)

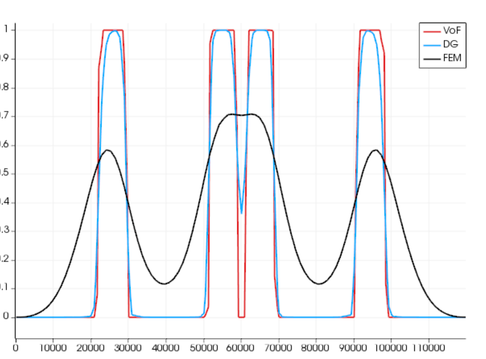


Figure 2.3d: Composition just above tail bifurcation (horizontal)

Figure 2.4a: Contour Comparsion

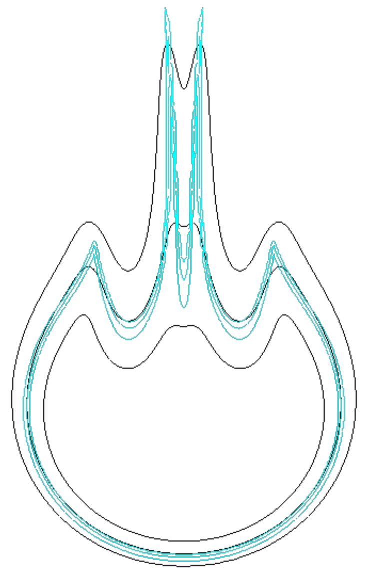
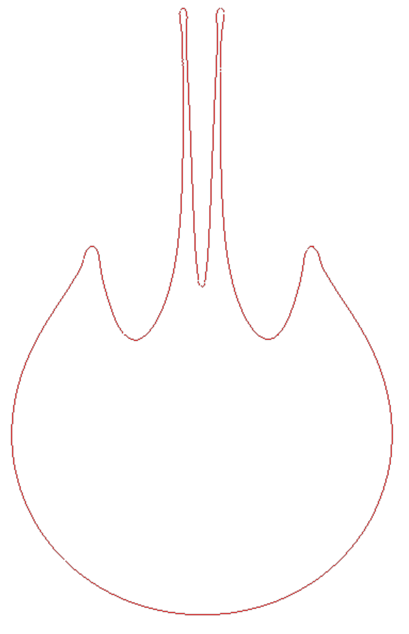


Figure 2.4b: VoF Contour isolated



Red:Reconstructed interface for VoF (subgrid resolution)

Blue: 0.1, 0.5, and 0.9 contours for BPDG

Black: 0.1, 0.5, and 0.9 contours for default ASPECT

Conclusions

- ASPECT's advection method (black) is too diffusive to effectively capture the upper interface and tail (Figures 2.3b-d)

- The most prominent discrepancy is the resolution of the tail (Figure 2.3d)

- BPDG (blue) resolves the interface reasonably well though it is spread across multiple cells (Figures 2.3b-d)

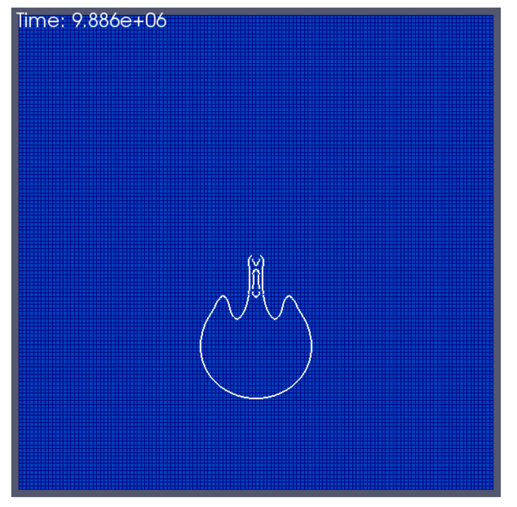
- VoF (red) tracks the interface with subgrid resolution as designed (Figures 2.3b-d)

Section 3: Performance with AMR

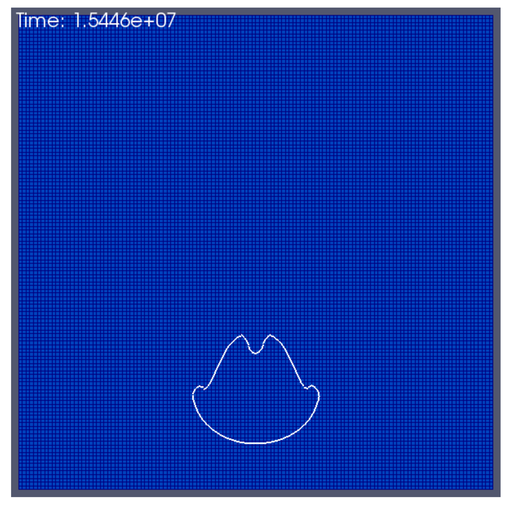
- The general structure of the falling box is over both coarse uniform and fine AMR meshes

- Greater resolution resolves smaller structures

η = η₀ | η = 10η₀

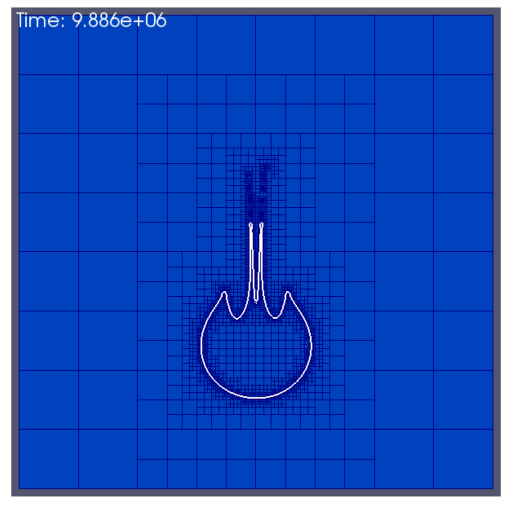


0.40 hrs (1.43e3 sec)

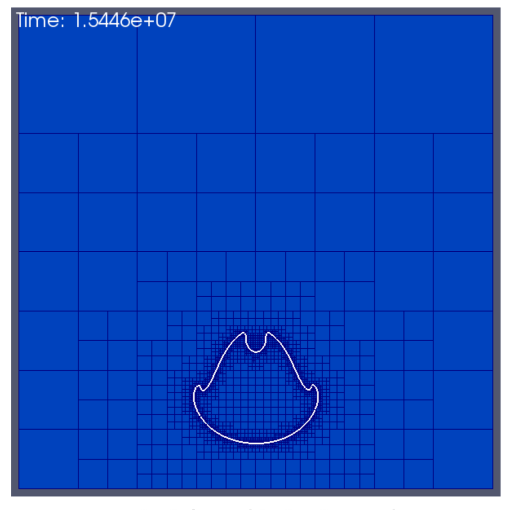


0.84 hrs (3.03e3 sec)

Uniform Refinement 128x128



1.9 hrs (7e3 sec)



2.6 hrs (9.2e3 sec)

AMR Maximum Refinement 512x512

- Refinement criterion specified by requiring that cells including and neighboring the interface must be at maximum level of refinement (a requirement which is entirely local to the neigborhood of the cell in question and therefore easily used as a refinement strategy with minimal computational cost)

- For the falling block problems, AMR reduces computation time by a factor of 12-21 as compared to the equivalent uniform mesh. (Estimated based on the CFL condition and expecting a linear increase in the computation time proportional to the number of cells)

Section 5: Conclusions and Future Work

Conclusions

- Our VoF implementation performs well on all of the test problems considered

- The VoF method eliminates the numerical diffusion associated with compositional advection methods

Future Work

- Modifications necessary to correctly handle non-Cartesian meshes and 3D.

- Dimensionally unsplit advection computation

- More than two fluids

References

[1] Gerya, T. V., and D. A. Yuen (2003), Characteristics-based marker-in-cell method with conservative finite-differences schemes for modeling geological flows with strongly variable transport properties, Physics of the Earth and Planetary Interiors, 140(4), 293–318, doi:http://dx.doi.org/10.1016/j.pepi.2003.09.006.

[2] Kronbichler, M., T. Heister, and W. Bangerth (2012), High accuracy mantle convection simulation through modern numerical methods, Geophysics Journal International, 191, 12–29.

[3] Pilliod Jr., J. E., and E. G. Puckett (2004), Second-order accurate volume-of-fluid algorithms for tracking material interfaces, Journal of Computational Physics, 199(2), 465–502, doi:http://dx.doi.org/10.1016/j.jcp.2003.12.023.

[4] Puckett, E. (2010a), A volume-of-fluid interface reconstruction algorithm that is second-order accurate in the max norm, Communications in Applied Mathematics and Computational Science, 5(2), 199–220.

Supported by the U. S. National Science Foundation under Award No. ACI - 1440811