The Development of a Volume-of-Fluid Interface Tracking Method for Modeling Problems in Mantle Convection

Jonathan Robey[1]

September 12, 2016

[1]Funded in part by a GAANN Fellowship

Motivation

- Mantle convection is a major area of interest in geodynamics
- Need to be able to track fluid volume/material accurately for long time without numerical smearing
  - Subduction
  - Large low-shear-velocity provinces (LLSVPs)
- Interface tracking method satisfies these requirements, and allow sub-grid resolution
- We select the Volume-of-Fluid (VoF) method

VoF Method Overview

- VoF method is a standard interface tracking method
- Interface is tracked implicitly by using volume fractions for reconstruction
- Volume fraction is a single scalar indicating the portion of the cell which is of the designated fluid
- Method is inherently conservative
- Does not require special cases for fragmenting volumes

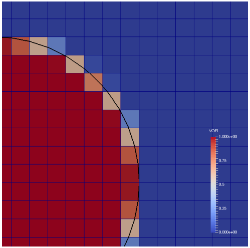


Figure: Example of VoF reconstruction of a circle

VoF Method Outline

- Initialize volume fractions
  - Start with given volume fractions or
  - Initialize volume fractions from given interface
- Begin Loop
  - Reconstruct Interface based on current volume fractions
  - Update volume fractions using an advection method based on the interface reconstruction

ELVIRA Interface Reconstruction

- Reconstructed interfaces are of the form $\vec{n} \cdot \vec{x} = d$
- Candidate normal vectors are based on slope approximations using sums of volume fractions over rows and columns
- Column sum candidates:
$$\vec{n} \in \begin{cases} (L - C, 1) \\ (C - R, 1) \\ (L - R, 2) \end{cases}$$
- Given $\vec{n}$, the intercept location d is uniquely determined by volume fraction in current cell
- Candidate error determined by ℓ_2 norm of difference from state volume fractions

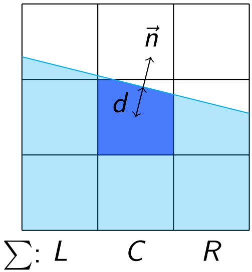


Figure: Sketch of local reconstruction region

Reconstruction Example

- Application to a circular interface with $h = \frac{r}{8}$
- Colormap indicates volume fraction
- Black contour is the reconstructed interface
- Despite discontinuous interface, visually appears continuous

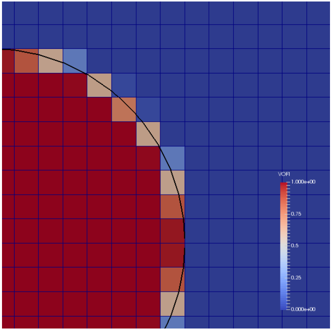


Figure: Example of reconstruction of circular interface

VoF Interface Advection

- Ω_i is cell with boundary $\partial\Omega_i$, $\vec{u}$ is velocity field, t^n is time at timestep
- f is indicator function with discretization $f^n_{h(i)} \approx \int\limits_{\Omega_i} f(\vec{x}, t^n) d\vec{x}$
- Integral form of Advection equation in conservation form discretized per cell over one timestep is

$$f^{n+1}_{h(i)} = f^n_{h(i)} + \int\limits_{t^n}^{t^{n+1}} \int\limits_{\Omega_i} f \nabla \cdot \vec{u} d\vec{x} dt - \int\limits_{t^n}^{t^{n+1}} \int\limits_{\partial\Omega_i} f \vec{u} \cdot \vec{n} d\vec{x} dt$$

- Have $\nabla \cdot \vec{u}$ and $\vec{u} \cdot \vec{n}$ to $O(h^2)$
- Incompressible Stokes Equations imply $\nabla \cdot \vec{u} = 0$; this term is retained due to the form of the advection algorithm
- Calculation for 3rd term (Flux term) of RHS on next slide

Flux Calculation

- Conservation form: $f_i^{n+1} = f_i^n + S_i + \sum_e F_e$
  where $F_e = f_e\left(\overline{\vec{u}\cdot\vec{n}}\right)$ is flux through edges where e indexes edges, S_i is the source term (divergence), and f_e is the volume fraction on the face $(\partial\Omega_i)_e \mathrm{x} [t^n, t^{n+1}]$
- Require method to obtain f_e
- Calculation of f_e done using donor region defined by method of characteristics
  - Approximation to velocity on cell face $\overline{\vec{u}\cdot\vec{n}}$ used to obtain region to be fluxed
  - Fluid volume on that region then calculated geometrically, used in calculation for flux through cell face
  - Currently we use a dimensionally split advection algorithm

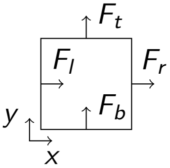


Figure: Flux sketch

VoF Interface Advection Sketch

- If dimensionally unsplit, Advection scheme will have non-zero area external to upwind cell (red)
- If dimensionally split, cannot use divergence free property of Stokes Equations, requires handling divergence term (use f_i^{n+1} as volume fraction)

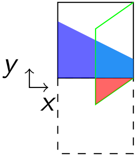


Figure: Sketch of volumes relevant to flux across right edge of cell

- Blue: Current Interface for Fluid 1
- Green: Donor Region by method of characteristics
- Cyan: Volume of Fluid 1 local to cell being advected
- Red: Volume external to cell that must be considered for the unsplit algorithm

Validation Testing

- Wish to confirm that method is implemented correctly
- Using a given velocity field, it is possible to have a known solution for all time
- Can then compute error and thus convergence rate
- Need procedure for calculating error based on true ϕ_t and calculated ϕ_c interfaces
- We approximate $E = \int\limits_{\Omega} |H(\phi_t) - H(\phi_c)| d\vec{x}$
- Test done using final implementation in ASPECT

Linear Interface Advection

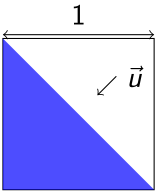


Figure: Linear interface translation problem

h	Error
0.625	$1.32630 \cdot 10^{-16}$
0.03125	$2.74613 \cdot 10^{-16}$
0.01563	$4.69034 \cdot 10^{-16}$
$7.81250 \cdot 10^{-3}$	$1.19552 \cdot 10^{-15}$
$3.90625 \cdot 10^{-3}$	$2.01992 \cdot 10^{-15}$

Table: Translation of a linear interface in a velocity field not aligned to the mesh

- Expect the error to be exact to ϵ_{mach} since the interface reconstruction algorithm, ELVIRA, reconstructs linear interfaces exactly

Circular Interface Rotation

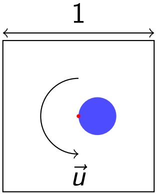


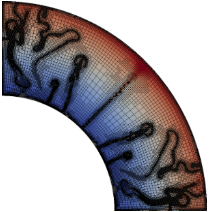
Figure: Circular interface rotation problem, the red dot is the center of rotation

h	Error	Rate
0.625	$8.08431 \cdot 10^{-3}$	
0.03125	$2.33441 \cdot 10^{-3}$	1.79
0.01563	$5.23932 \cdot 10^{-4}$	2.16
$7.81250 \cdot 10^{-3}$	$1.40612 \cdot 10^{-4}$	1.90
$3.90625 \cdot 10^{-3}$	$3.50275 \cdot 10^{-5}$	2.01

Table: Rotation of a circular interface offset from the center of rotation

- Cells are of size $h = 2^{-k}$

Implemented in Aspect



- Aspect is: An extensible code written in C++ to support research in simulating convection in the Earth's mantle
- ASPECT implements Adaptive Mesh Refinement (AMR) and Parallel capabilities to permit computation on large domains associated with mantle convection
- Pull Request pending

The Falling Block Benchmark

- Standard test problem in the geodynamics literature (Gerya and Yuen 2003)
- Composition (density) driven flow
- Rectangular region of heavy fluid (red) with viscosity $\eta = \gamma \eta_0$ sinks
- Density ratio is $\frac{\Delta\rho}{\rho_0} = \frac{100}{3200}$

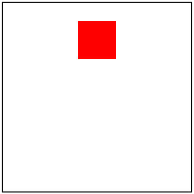
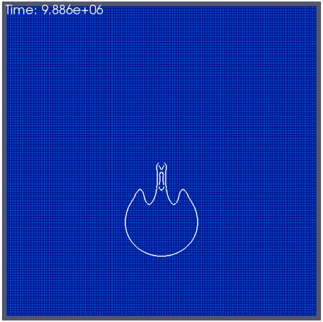
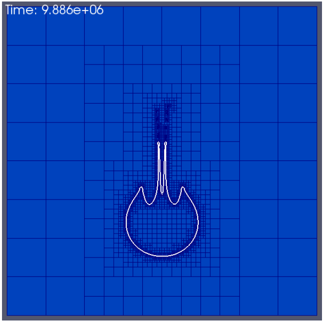


Figure: Initial Conditions; red is the heavy fluid

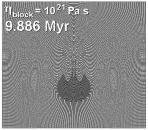
Falling Block $\eta = \eta_0$



(a) Uniform 128x128 mesh ($128^2 = 16384$ cells)



(b) AMR with maximum resolution of 512x512 (Final cell count 5,647)

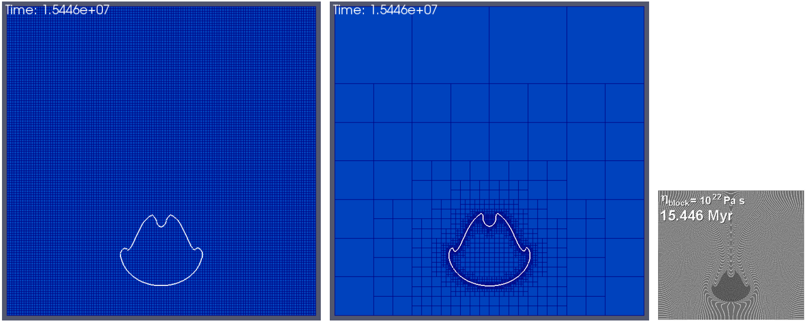


(c) (51x51 mesh, 22,500 particles (8.6p/c)) by Gerya and Yuen (2003)

AMR approximately 13 times faster than uniform mesh of equal maximum resolution

Figure: Comparison of results for the falling block problem with a constant viscosity η_0 for a uniform mesh (left), with Adaptive Mesh Refinement (AMR) (center) and the original benchmark result (right); showing the mesh and the reconstructed interface (white contour) for the new results

Falling Block $\eta = 10\eta_0$



(a) Uniform 128x128 mesh ($128^2 = 16384$ cells)

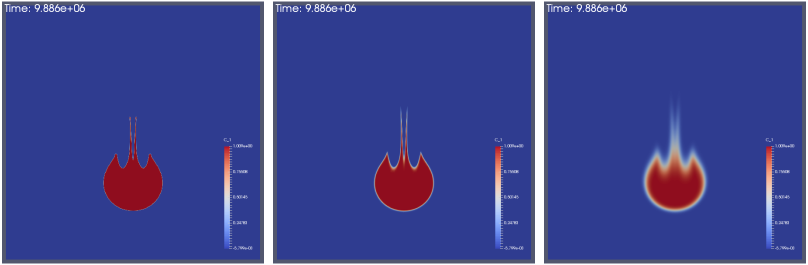
(b) AMR with maximum resolution of 512x512 (Final cell count 3,583)

(c) (51x51 mesh, 22,500 particles(8.6p/c)) by Gerya and Yuen (2003)

AMR approximately 21 times faster than uniform mesh of equal maximum resolution

Figure: Comparison of results for the falling block problem with varying viscosity for a uniform mesh (left), with Adaptive Mesh Refinement (AMR) (center) and original benchmark result (right); showing the mesh and the reconstructed interface (white contour) for the new results

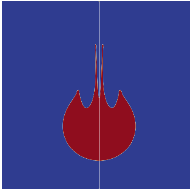
Comparison of Methods for the Falling Block



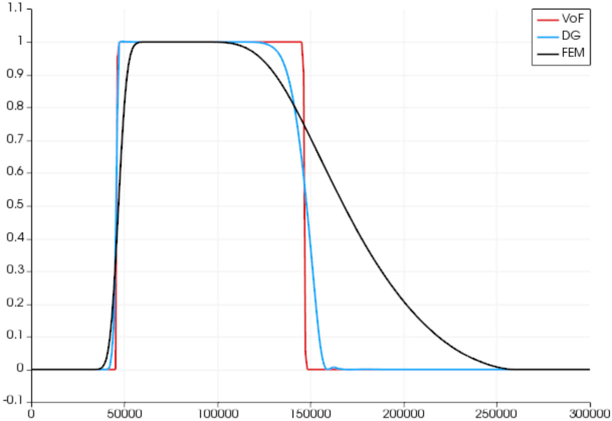
(a) VoF (b) DG (c) FEM

Figure: Comparison between VoF (left), Bounded Discontinuous Galerkin, He, Puckett, and Billen 2016 (middle), and FEM Advection method in ASPECT (right)

Comparison of Composition Profile on Center Line

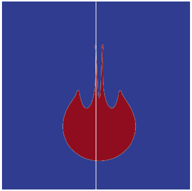


(a) Sample location

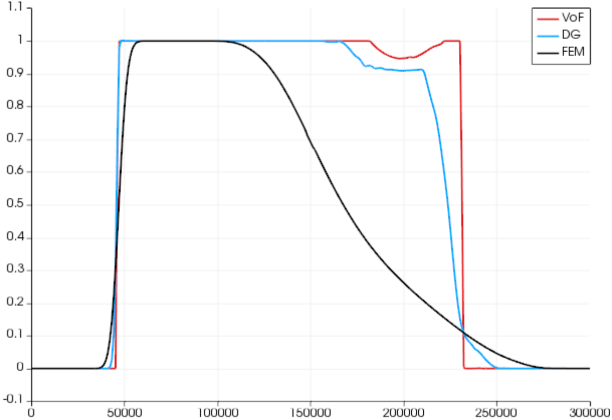


(b) Vertical profile of composition along center line ($x = 2.5 \cdot 10^5$)

Comparison of Composition Profile on Left Tail

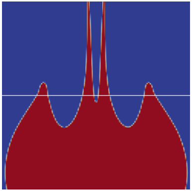


(a) Sample location

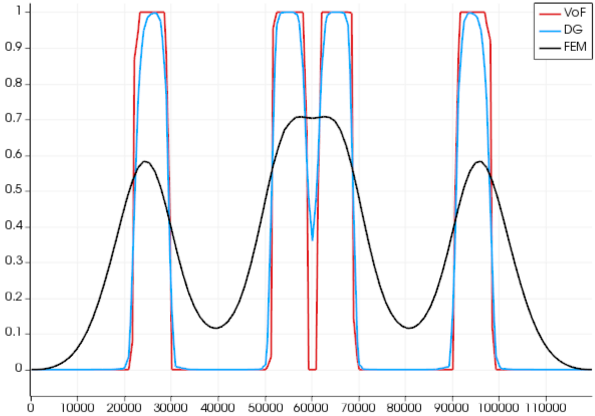


(b) Vertical profile of composition along left tail ($x = 2.45 \cdot 10^5$)

Comparison of Composition Profile above Main Body

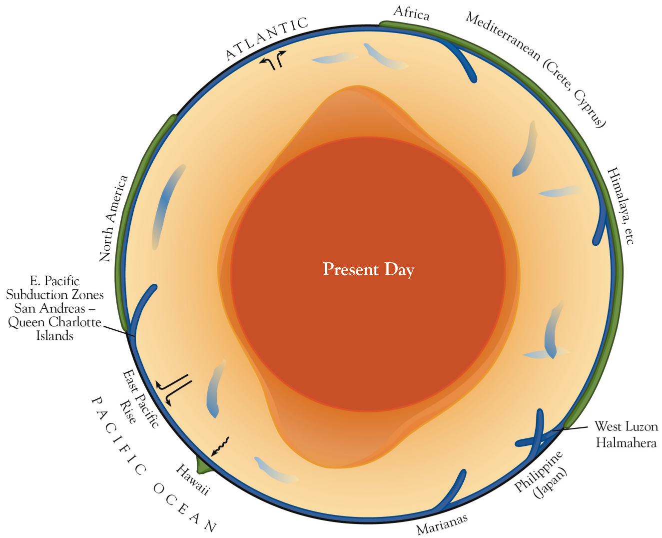


(a) Sample location



(b) Horizontal profile of composition just above main body ($y = 2 \cdot 10^5$)

Mantle Cartoon



Mantle Convection Equations

$$-\frac{\partial P}{\partial x} + \mu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) = 0 \tag{1a}$$

$$-\frac{\partial P}{\partial y} + \mu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) = -g\rho \tag{1b}$$

$$\nabla \cdot \vec{u} = 0 \tag{1c}$$

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

$$\frac{\partial C}{\partial t} + \nabla \cdot (C\vec{u}) = 0 \tag{3}$$

$$\rho = \rho_0(1 - \alpha_v(T - T_0)) \tag{4}$$

Density Stratified Convection

- Related to active research project with Professors Puckett, Billen, Turcotte, Kellogg and Dr He
- Three nondimensional parameters:
  - $B = \frac{\Delta\rho}{\rho_0 \alpha_v \Delta T}$ Chemical buoyancy
  - $Ra = \frac{g \rho_0^2 \alpha_v \Delta T b^3 c_p}{\mu k} \approx 10^5$
  - $a = \frac{d_1}{d_2} = 1$
- Due to experience with test runs, two initial perturbations used
  - Sinusoidal temperature perturbation, amplitude $0.05\Delta T$
  - Sinusoidal interface perturbation of amplitude $0.01b = 0.01(d_1 + d_2)$

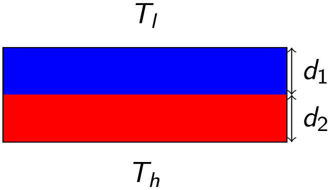
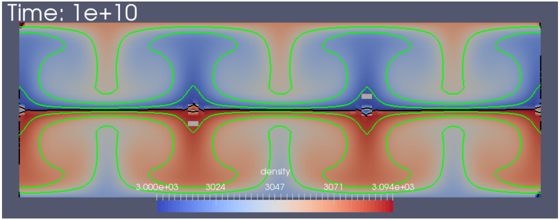
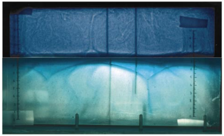


Figure: Initial Conditions: density of red fluid is $\rho_0 + \Delta\rho$ and density of blue fluid is ρ_0 with $\Delta T = T_h - T_l$

Stratified convection for DSF problem



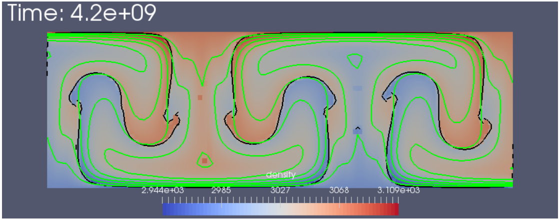
(a) Density colormap with temperature contours (green) and reconstructed interface (black) superimposed for computation with $B = 0.7$



(b) Stratified convection from experiment ($B = 2.4$, $Ra_l = 2.2 \cdot 10^5$, $Ra_h = 8 \cdot 10^6$) by Davaille (1999, Fig. 1f) Note: $d_1 \neq d_2$ in this experiment

Figure: Preliminary qualitative comparison of stratified convection computation to experiment by Davaille (1999) Note: we have not yet attempted to explicitly duplicate Daville's experimental parameters

Full depth convection for DSF problem

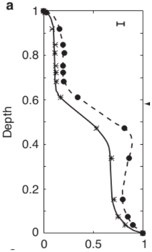


(a) Density colormap with temperature contours (green) and reconstructed interface (black) superimposed for computation with $B = 0.4$

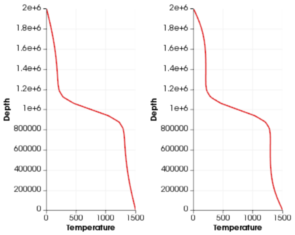
(b) Full depth convection from experiment ($B = 0.2$, $Ra_l = 9 \cdot 10^4$, $Ra_h = 9 \cdot 10^6$) by Davaille (1999, Fig. 1b) Note: $d_1 \neq d_2$ in this experiment

Figure: Preliminary comparison of full depth convection computation to experiment by Davaille (1999) Note: we have not yet attempted to explicitly duplicate Davaille's experimental parameters

Comparison of temperature vs depth for the stratified convection case



(a) Stratified convection from experiment ($B = 2.4$) by Davaille (1999, Fig 1a)



(b) Stratified convection from VoF model ($B = 0.7$)

Figure: Comparsion of upwelling temperature-depth plots to experimental temperature-depth plots from Davaille (1999). Note: These are preliminary results and no attempt has been made to match the experimental values of the Rayleigh number Ra, bouyancy parameter B, viscosity ratio γ, and depth ratio $a = \frac{d_1}{d_2}$.

Conclusion

- The VoF method has been successfully implemented, in Aspect for 2D rectangular meshes including AMR and parallel

Future Work

- Implementation of a 3D interface reconstruction, and use of the 3D formulas for volume frction and interface location in Scardovelli and Zaleski (2000), which would allow the examination of the behavior of 3D systems.
- Improve volume fraction calculation to permit use of non-parallelogram meshes.
- Examination of other interface reconstruction approaches, such as the moment of fluid algorithm that allows the tracking of multiple materials.
- Examination of alternate advection algorithms; i.e. for flux fraction calculation to the donor region approach commonly used. This is likely to require significant additional information.

End

Thank You!

Interface Tracking Method List

- Lagrangian (particles, auxiliary Lagrangian mesh)
  - Many hard/unsolved difficulties
  - Fragmentation complex
- Indicator field
  - Trivial approach
  - Highly subject to numerical distortion
- Level Set
  - Maintains sharp interface
  - Requires solution of Hamilton Jacobi Equation
  - Best current approach requires modern methods for shock wave problems (cutting edge in FEM)
  - Time stepping requires frequent expensive reinitialization in practice, even with state of art method
- Volume-of-Fluid
  - Maintains sharp interface
  - Local data dependence
  - Inherently conservative (based on Cons. of Fluid Equation)

Particle vs VoF

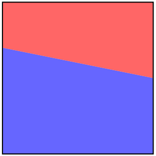


Figure: VoF

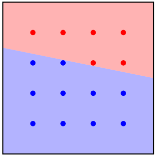


Figure: Particles

Reconstruction Methods

- SLIC (1st order)
  - One or two interfaces both parallel to same cell edge
  - Heuristic based
- LVIRA (2nd order)
  - Find interface of form $\vec{n} \cdot \vec{x} = d$
  - Select based on least volume error of extension to surrounding cells
  - d selected to preserve volume fraction
- ELVIRA (2nd order)
  - Same criteria as LVIRA, but selecting from specified list of candidates for $\vec{n}$
- Other
  - MoF: Track and use additional moment data for reconstruction
  - CLSVoF: Track and use a level set for reconstruction, reinitialize level set based on VoF data

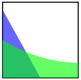
Multi-material (> 2) VoF

- Known extension of current approach
- Active area of interest in National Labs
- Current methodology reliant on MoF reconstruction
- Implementation much more complex than 2 fluid

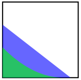
Error Approximation: L1 Interface Error

- L^1 Error is $E = \int_{\Omega} |H(\phi_t) - H(\phi_c)| d\vec{x}$
- Prohibitive in practice, use approximation by Iterated Midpoint Quadrature (Cell to 32x32 subcells) (psuedometric)
- Heaviside H is discontinuous, smooth for better behavior of quadrature
- How to smooth H:
  - Heaviside w/ Midpoint quadrature can be interpreted as difference in f based only on value at cell center
  - If ϕ is signed level set, can easily get $O(h^3)$ volume approximation on subcell using initialization procedure
  - Volume differences on subcell exact difference from linear interface approximation in the most common case(21c)

(a) Disjoint



(b) Intersect



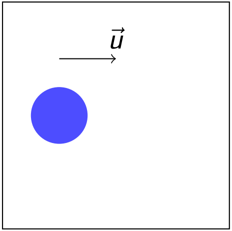
(c) Simple

Figure: Cases for Error Approximation

Error Approximation: L1 Field Error

- Want measurement of "state error" - Error in current model state
- For VoF, model state is restricted to volume fraction data
- Have procedure to generate volume fractions from known interface (initialization)
- ℓ_1 norm weighted by cell measure obvious means to compare volume fraction data, i.e. $E = \|\{f_i\} - f_I(\phi_t)\|_1$ note $\{f_i\} = f_I(\phi_c)$.
- Converges to the L^1 norm as $h \to 0$

Circular Interface Translation



(a) Circular interface translation problem

Figure: Sketches of rate of convergence tests

Circular Interface Linear Advection

k	L1 Interface Error	Rate	L1 Field Error	Rate
5	$2.52391 \cdot 10^{-3}$		$1.98931 \cdot 10^{-3}$	
6	$7.90262 \cdot 10^{-4}$	1.68	$6.46623 \cdot 10^{-4}$	1.62
7	$2.30100 \cdot 10^{-4}$	1.78	$1.83052 \cdot 10^{-4}$	1.82
8	$6.55917 \cdot 10^{-5}$	1.81	$5.45257 \cdot 10^{-5}$	1.75

Table: Mesh Aligned Translation of a Circular Interface with $\sigma = \frac{1}{2}$

Circular Interface Linear Advection

k	L1 Interface Error	Rate	L1 Field Error	Rate
5	$5.14405 \cdot 10^{-3}$		$4.73691 \cdot 10^{-3}$	
6	$1.79281 \cdot 10^{-3}$	1.52	$1.61010 \cdot 10^{-3}$	1.56
7	$4.80234 \cdot 10^{-4}$	1.90	$4.33513 \cdot 10^{-4}$	1.89
8	$1.31839 \cdot 10^{-4}$	1.86	$1.19947 \cdot 10^{-4}$	1.85

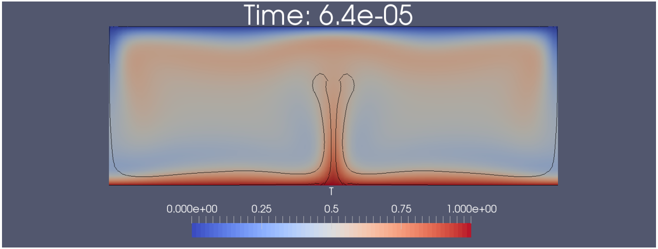
Table: Mesh Aligned Translation of a Circular Interface with $\sigma = \frac{1}{32}$

Circular Interface Linear Advection

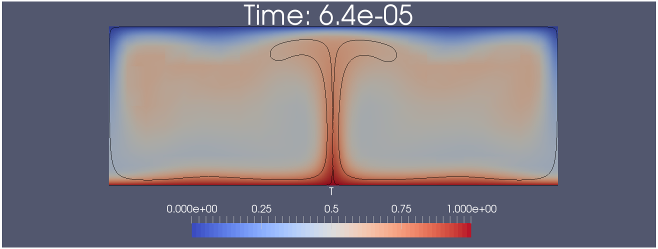
k	L1 Interface Error	Rate	L1 Field Error	Rate
5	$1.89618 \cdot 10^{-3}$		$1.26228 \cdot 10^{-3}$	
6	$3.82585 \cdot 10^{-4}$	2.31	$2.36274 \cdot 10^{-4}$	2.42
7	$9.07219 \cdot 10^{-5}$	2.08	$3.31707 \cdot 10^{-5}$	2.83
8	$2.07321 \cdot 10^{-5}$	2.13	$6.34625 \cdot 10^{-6}$	2.39

Table: Mesh Aligned Translation of a Circular Interface with $\sigma = 1$

Convection



(a) Uniform 96x32 mesh



(b) AMR mesh with maximum resolution 384x128

Contour comparison

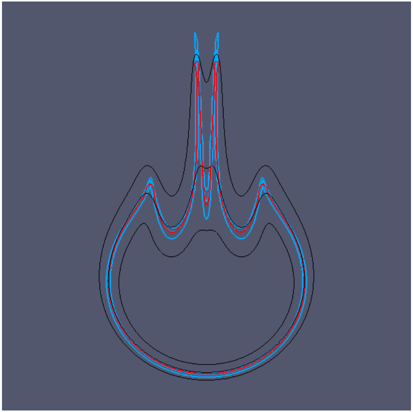
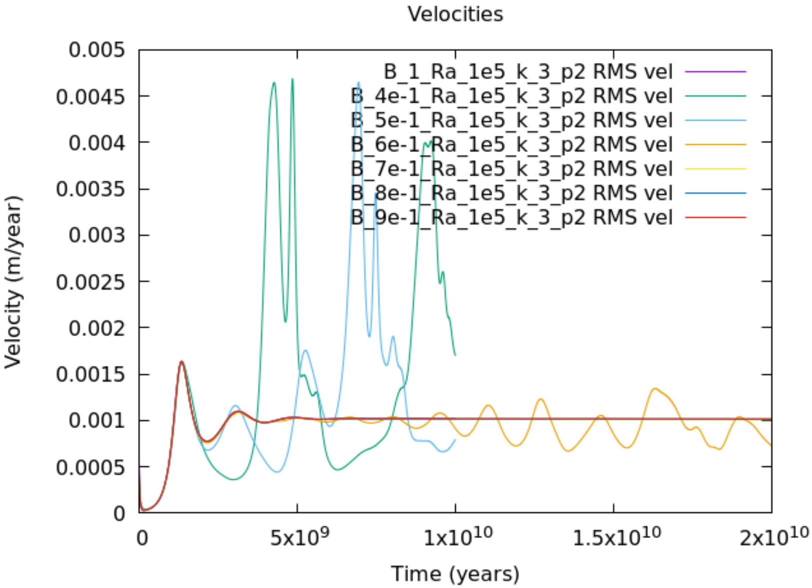


Figure: Contours for interface approximation for different methods: VoF (red), DG $\{0.1, 0.5, 0.9\}$(cyan), and FEM $\{0.1, 0.5, 0.9\}$(black)

Parameter Survey



Lit Search FEM Volume of Fluid

- Interface Advection Schemes (Triangle/Tetrahedron): Dimitrios Pavlidis et al. (2015). "Compressive advection and multi-component methods for interface-capturing". In: *International Journal for Numerical Methods in Fluids* 80.4, pp. 256–282. DOI: 10.1002/fld.4078. URL: http://dx.doi.org/10.1002/fld.4078
- Finite Element VoF method (Triangle/Tetrahedron): Zhihua Xie et al. (2016). "A balanced-force control volume finite element method for interfacial flows with surface tension using adaptive anisotropic unstructured meshes". In: *Computers & Fluids*. ISSN: 0045-7930. DOI: http://dx.doi.org/10.1016/j.compfluid.2016.08.005. URL: http://www.sciencedirect.com/science/article/pii/S0045793016302511