IMPLEMENTATION OF A VOLUME-OF-FLUID METHOD IN A FINITE ELEMENT CODE WITH APPLICATIONS TO THERMOCHEMICAL CONVECTION IN A DENSITY STRATIFIED FLUID IN THE EARTH’S MANTLE

JONATHAN M. ROBEY

Department of Mathematics, U. C. Davis, Davis, CA 95616, USA

ELBRIDGE GERRY PUCKETT

Department of Mathematics, U. C. Davis, Davis, CA 95616, USA

ABSTRACT. We describe the implementation of a second-order accurate volume-of-fluid interface tracking algorithm in the open source finite element code ASPECT, which is designed to model convection in the Earth’s mantle. This involves the solution of the incompressible Stokes equations coupled to an advection diffusion equation for the temperature, a Boussinesq approximation that governs the dependence of the density on the temperature, and an advection equation for a marker indicating the two initial density states. The volume-of-fluid method is fully parallelized and is integrated with the adaptive mesh refinement algorithm in ASPECT. We present the results of several standard interface tracking benchmarks in order to demonstrate the accuracy of the method as well as the results of several benchmarks commonly used in the computational mantle convection community. Finally, we present the results of computations with and without adaptive mesh refinement of a model problem involving thermochemical convection in a computationally stratified fluid designed to provide insight into how thermal plumes, that eventually reach the Earth’s surface as ocean island basalts, originate at structures on the core-mantle boundary known as Large Low Shear wave Velocity Provinces.

Keywords: Volume-of-Fluid Method; Adaptive Mesh Refinement; Rayleigh-Bénard problem; Thermochemical Convection; Rayleigh Taylor Instability; Compositionally Stratified Fluid; Large Low Shear wave Velocity Provinces

1. INTRODUCTION

Over more than the past four decades there have been many numerical methods developed to study convection and other processes in the Earth’s mantle. In particular, there have been
a sequence of codes developed over this period of time that are now freely available to any individual who wishes to study mantle dynamics. They include HC [25, 26, 64], ConMan [36], CitCom S [43, 68, 76], Citcom CU [46, 75] and ASPECT [28, 38]. These codes, as well as others, can be downloaded from the Computational Infrastructure for Geodynamics (CIG) at U.C. Davis.  

There are a large number of problems associated with the Earth’s mantle that contain one or more interfaces in some form or another. Although there have been some very specialized computational models of interfaces in the mantle, for example, the dynamics of bubbles and plumes [40, 41, 42], it is only recently that researchers have begun to implement interface tracking algorithms in codes designed to model convection and other processes in the entirety of the Earth’s mantle; e.g., [59]. However, to our knowledge, the Volume-of-Fluid (VOF) method has not yet been implemented in a code designed to model convection in the Earth’s mantle or, more generally, used by researchers to model geodynamic flows.

In this article we describe the implementation of a second-order accurate VOF interface tracking algorithm in the open source finite element code ASPECT. ASPECT is a parallel, extendible finite element code designed to model thermal convection and other processes in the Earth’s mantle in two and three dimensions. It is built on the deal.II Finite Element Library [2, 6], which includes adaptive mesh refinement (AMR) [10] and has been shown to scale to thousands of processors [22]. ASPECT has been extended to model other processes that occur in the mantle, such as modeling grain size evolution in the mantle [17], melt generation and migration [18], as well as other problems. There is currently a very active community of researchers extending ASPECT to new problem areas and improving existing algorithms. Our VOF algorithm is fully parallelized and is designed to work efficiently with ASPECT’s AMR algorithm.

Recent studies utilizing seismic imaging have revealed large regions with anomalous seismic properties in the lower mantle. In particular, there are two dome-like regions beneath Africa and the Pacific Ocean with low shear-wave velocities that extend some 1000 km above the core-mantle boundary and have horizontal dimensions of several thousand kilometers [16, 21]. Most interpretations propose that the heterogeneities are compositional in nature, differing from the surrounding mantle, an interpretation that would be consistent with chemical geodynamic models. Based on geological and geochemical studies it has been argued that LLSVPs have persisted for billions of years [9]. In this article we compute solutions to a model problem designed to understand the dynamics of plumes that form on the LLSVPs, entrains some of the material in the LLSVP that differs from the surrounding mantle, and brings it to the Earth’s surface. The model problem consists of two horizontal layers, equal in height, in a rectangle, with a density difference of $\Delta \rho = \rho - \rho_0 \geq 0$, where $\rho_0$ is the density of the upper layer. The initial condition for the temperature is a perturbation from the well-known static temperature field, connecting the temperature boundary conditions $T_0$ at the top of the rectangle and $T_1$ at the bottom of the rectangle [72]. We study a range of density differences $\Delta \rho$ that we characterize by the non-dimensional buoyancy number $B$, which is the ratio of $\Delta \rho$ to $\rho_0 \alpha \Delta T$, where $\Delta T = T_1 - T_0$, and $\alpha$ is the volumetric coefficient of thermal expansion. The temperature perturbation initially drives the convection and, depending on the value of $B$, determines the dynamics and structure of the resulting flow field.

---

1The CIG is an NSF funded, community driven organization that advances Earth science by developing and disseminating software for geophysics and related fields.
In Section 2 we begin by describing the equations that govern thermochemical convection in the mantle and the modification to these equations that we use to model density stratification in such flows. Then, in Section 3 we describe the numerical methodology, including the underlying Finite Element Method (FEM) and the coupling of our VOF method to this FEM. In Section 4 we begin by presenting two standard interface tracking benchmarks in order to demonstrate the accuracy of the VOF method. We then present the results of two benchmarks commonly used by researchers in the computational mantle convection community. At the end of this section we present computational results of a model problem first proposed in [58], which is designed to provide insight into how thermal plumes, that are thought to eventually reach the Earth’s surface as ocean island basalts, originate at structures on the core-mantle boundary known as Large Low Shear wave Velocity Provinces (LLSVPs). We briefly discuss these latter computational results in Section 5 and, in Section 6, we present our conclusions.

### Table 1. A list of symbols used in this paper.

| Symbol | Quantity               | Unit      | Symbol | Quantity               | Unit      |
|--------|------------------------|-----------|--------|------------------------|-----------|
| \( u \) | Velocity               | \( m/s \) | \( \rho \) | Density               | \( kg \cdot m^{-3} \) |
| \( p \) | Dynamic pressure       | Pa        | \( \Delta \rho \) | Density difference    | \( kg \cdot m^{-3} \) |
| \( T_0 \) | Temperature at the top | K         | \( D \) | Compositional diffusivity | \( m^2/s \) |
| \( T_l \) | Temperature at the bottom | K       | \( \alpha \) | Thermal expansion coefficient | \( 1/K \) |
| \( T \) | Temperature            | K         | \( d \) | Vertical height of fluid layer | \( m \) |
| \( \Delta T \) | Temperature difference | K        | \( Pr \) | Prandtl number       | \( \frac{\mu}{\rho \kappa} \) |
| \( C \) | Composition            | -         | \( Le \) | Lewis number         | \( \frac{\mu}{\rho \kappa d} \) |
| \( \mu \) | Viscosity              | Pa \cdot s | \( Ra \) | Rayleigh number      | \( \frac{\rho \kappa}{\rho_0 \kappa d} \) |
| \( \kappa \) | Thermal diffusivity    | \( m^2/s \) | \( B \) | Buoyancy ratio       | \( \frac{\Delta T}{\rho \kappa d} \) |
| \( \rho_0 \) | Reference density      | \( kg \cdot m^{-3} \) |     |                        |           |

2. Thermochemical Convection with Density Stratification

In this section we present in detail the equations associated with the model problem, which we briefly described above.

### 2.1. The Dimensional Form of the Equations.

In order to study the efficacy of our implementation of a VOF algorithm in ASPECT to model processes that occur in the Earth’s mantle, we compute a problem that emphasizes the effect of a compositional density difference on thermal convection. We consider a two-dimensional flow in a horizontal fluid layer with a thickness or height \( d \). Our problem domain \( \Omega \) has width \( 3d \) and height \( d \). At a given reference temperature \( T_0 \) the region \( d/2 < y \leq d \) has a compositional density of \( \rho_0 \) and the region \( 0 \leq y < d/2 \) has a compositional density of \( \rho_0 + \Delta \rho \) where \( \Delta \rho \ll \rho_0 \).

We also introduce a composition variable \( C(x, y, t) \) defined by

\[
C = \frac{\rho - \rho_0}{\Delta \rho}.
\]
The composition $C$ is the concentration of the dense fluid as a function of space and time. The initial condition for $C$ is

$$C(x, y, t = 0) = \begin{cases} 1 & \text{for } 0 \leq y \leq d/2, \\ 0 & \text{for } d/2 < y \leq d. \end{cases}$$

(2)

The upper boundary, at $y = d$, has temperature $T_0$ and the lower boundary at $y = 0$ has temperature $T_1$. The fluid is assumed to have a constant viscosity $\mu$ which is large. The Prandtl number is assumed to be very large,

$$Pr = \frac{\mu}{\rho_0 \kappa} \gg 1,$$

(3)

where $\kappa$ is the thermal diffusivity so that inertial effects can be neglected. The fluids in the high density and low density layers are immiscible; i.e., they cannot mix by diffusion. Similarly the Lewis number is also assumed to be large,

$$Le = \frac{\kappa}{D} \gg 1 , \cdot 2.1$$

(4)

where $D$ is the diffusion coefficient for the compositional variable $C$. Thus, the discontinuous boundary between the high density and low density fluids is preserved indefinitely.

The problem we have posed requires the solution of the standard equations for thermal convection with the addition of an equation for the compositional field $C$ that tracks the density difference. The governing equations are described in detail in [61, 72].

We make the assumption that the Boussinesq approximation

$$\rho(x, y, t) = \rho_0 (1 - \alpha(T - T_0)) + \Delta \rho C.$$

(5)

holds; namely, that density differences associated with convection $\rho_0 \alpha(T_1 - T_0)$ and $\Delta \rho$ are small compared with the reference density $\rho_0$.

Conservation of mass requires

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

(6)

where $x$ and $y$ denote the horizontal and vertical spacial coordinates, oriented as shown in Figure 1, and $u$ and $v$ denote the horizontal and vertical velocity components, respectively. We use the Stokes equations

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

$$0 = -\frac{\partial P}{\partial y} + \mu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) + \rho_0 \alpha(T - T_0) g - \Delta \rho C g,$$

(7)

(8)

where $\alpha$ is the coefficient of thermal expansion, $g$ is the gravitational acceleration in the negative (downward) $y$ direction as shown in Figure 1, and $P = p + \rho_0 g y$

where $p$ is the dynamic pressure and $\rho_0 g y$ is the isostatic pressure. Conservation of energy requires

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \kappa \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right).$$

(9)
With no diffusion, i.e., $D = 0$, the composition variable $C$ satisfies the advection equation

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = 0. \quad (10)$$

### 2.2. The Nondimensional Form of the Equations.

We introduce the non-dimensional variables

$$x' = \frac{x}{d}, \quad y' = \frac{y}{d}, \quad t' = \frac{\kappa}{d^2} t, \quad t'' = \frac{\kappa}{d^2} t,$$

$$u' = \frac{d}{\kappa} u, \quad v' = \frac{d}{\kappa} v, \quad \rho' = \frac{\rho}{\rho_0},$$

$$T' = \frac{T - T_0}{T_1 - T_0}, \quad P' = \frac{d^2 P}{\mu \kappa}, \quad (11)$$

and the two nondimensional parameters, the Rayleigh number $Ra$ and the buoyancy ratio $B$

$$Ra = \frac{\rho_0 g \alpha (T_1 - T_0) d^3}{\mu \kappa}, \quad (12)$$

$$B = \frac{\Delta \rho}{\rho_0 \alpha (T_1 - T_0)}, \quad (13)$$

Substitution of equations (11)–(13) into equations (6)–(10) gives

$$\frac{\partial u'}{\partial x'} + \frac{\partial v'}{\partial y'} = 0, \quad (14)$$

$$0 = -\frac{\partial P'}{\partial x'} + \frac{\partial^2 u'}{\partial x'^2} + \frac{\partial^2 u'}{\partial y'^2}, \quad (15)$$

$$0 = -\frac{\partial P'}{\partial y'} + \frac{\partial^2 v'}{\partial x'^2} + \frac{\partial^2 v'}{\partial y'^2} + Ra T' - Ra B C, \quad (16)$$

$$\frac{\partial T'}{\partial t''} + u' \frac{\partial T'}{\partial x'} + v' \frac{\partial T'}{\partial y'} = \frac{\partial^2 T'}{\partial x'^2} + \frac{\partial^2 T'}{\partial y'^2}, \quad (17)$$

$$\frac{\partial C}{\partial t''} + u' \frac{\partial C}{\partial x'} + v' \frac{\partial C}{\partial y'} = 0. \quad (18)$$

This is the superposition of a Rayleigh-Taylor problem and a Rayleigh-Bénard problem [12, 72]. In the isothermal limit, $T_0 = T_1$, it is the classic Rayleigh-Taylor problem. If $C$ is positive, a light fluid is above the heavy fluid and in a downward gravity field the fluid layer is stable. If $\Delta \rho$ is negative, a heavy fluid lies over a light fluid and the layer is unstable. Flows will transfer the heavy fluid to the lower half and the light fluid to the upper half and the density layer will overturn. If $\Delta \rho = 0$ and hence, $B = 0$, this is the classic Rayleigh-Bénard problem for thermal convection. The governing parameter is the Rayleigh number $Ra$. If $0 < Ra < Ra_c$, the critical Rayleigh number, no flow will occur. If $Ra_c < Ra < Ra_t$ steady cellular flow will occur. If $Ra > Ra_t$ the flow becomes unsteady and thermal turbulence develops.

If $Ra > Ra_c$ and $B$ is small, the boundary between the density differences will not block the flow driven by thermal convection. Kinematic mixing will occur and the composition will homogenize so that the density is constant. Whole layer convection will occur. If $B$ is large, the density difference boundary will block the flow driven by thermal convection. The compositional boundary will be displaced vertically but will remain intact. Layered convection will occur with the compositional boundary, the boundary between the convecting layers. In
this work the Rayleigh number $Ra$ defined in equation (12) is based on the domain thickness $d$ and this is the case for which we will show numerical computations.

3. The Numerical Methodology

In the following discussion of the numerical methodology, we will only consider the dimensionless equations (14)-(18) and drop the primes associated with the dimensionless variables. The vector form of the dimensionless equations on the 2D rectangular domain $\Omega = [0, 3] \times [0, 1]$ shown in Figure 1 are given by

\[ -\nabla^2 u + \nabla P = (-Ra \, T + Ra \, B \, C) \, g, \]
\[ \nabla \cdot u = 0, \]  
\[ \frac{\partial T}{\partial t} + u \cdot \nabla T = \nabla^2 T, \]  
\[ \frac{\partial C}{\partial t} + u \cdot \nabla C = 0, \]

where $u = (u, v)$ is the velocity and $g = (0, -1)$ is the unit vector pointing downward.

Note that the composition equation (22) is equivalent to

\[ \frac{D C}{D t} = \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = 0, \]

where

\[ \frac{D}{D t} \equiv \frac{\partial}{\partial t} + u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} \]

is the material derivative. Equation (23) implies that the composition $C$ is constant on particle paths in the flow [14]. Furthermore, since by (14) the velocity $u$ is divergence free, the composition equation (22) can be written in conservation form

\[ \frac{\partial C}{\partial t} + \nabla \cdot (u \, C) = 0, \]

\[ T' = 0 \]

\[ 0.5 \quad \partial_x T' = 0 \]

\[ \Omega \]

\[ \partial_x T' = 0 \]

\[ \uparrow \]

\[ y' \]

\[ 0 \]

\[ 0.5 \]

\[ x' \rightarrow \]
implying that the composition $C$ is a conserved quantity - it is neither created nor destroyed as it is advected in the flow field.

We assume no-flow and free-slip velocity boundary conditions on all boundaries,

$$u \cdot n = 0 \quad \text{(no-flow)},$$
$$\frac{\partial u}{\partial \tau} = 0 \quad \text{(free slip)},$$

where $n$ and $\tau$ are the unit normal and tangential vectors to the boundary respectively.

We impose Dirichlet boundary conditions for the temperature on the top and bottom of the computational domain and Neumann boundary conditions (no heat flux) on the sides of the computational domain,

$$T(x, 0, t) = 1,$$
$$T(x, 1, t) = 0,$$
$$\partial_x T(0, y, t) = 0,$$
$$\partial_x T(0, y, t) = 0.$$

The geometry of the computational domain together with the boundary conditions on the temperature are shown in Figure 1.

3.1. Decoupling of the Nonlinear System. The incompressible Stokes equations can be considered as a constraint on the temperature and composition at any given time leading to a highly nonlinear system of equations. To solve this nonlinear system, we apply the Implicit Pressure Explicit Saturation (IMPES) approach, originally developed for computing solutions of equations for modeling problems in porous media flow [34, 63], to decouple the incompressible Stokes equations (14)–(16) from the temperature and compositional equations (17)–(18). This leads to three discrete systems of linear equations, the Stokes equations, the temperature equation, and the composition equation, thereby allowing each equation to be solved easily and efficiently.

3.2. Discretization of the Stokes Equations. Let $t^k$ denote the discretized time at the $k$th time step with a time step size of $\Delta t^k = t^k - t^{k-1}$, $k = 0, 1, \ldots$ Given the temperature $T^k$ and composition $C^k$ at time $t = t^k$, we first solve for our approximation to the Stokes equations (14)–(16) to obtain the velocity $u^k = (u^k, v^k)$ and pressure $P^k$

$$-\nabla^2 u^k + \nabla P^k = (-Ra \ T^k + Ra \ B \ C^k) \ g,$$
$$\nabla \cdot u^k = 0.$$

For the incompressible Stokes equations (32)–(33), we use the standard mixed FEM method with a Taylor-Hood element [20] for the spatial approximation. We refer the interested reader to [38] for a more detailed discussion of the spatial discretization and the choice of Stokes preconditioners and solvers.

3.3. Discretization of the Temperature Equation. In all of the computations presented here we use the algorithm currently implemented in ASPECT [4] to approximate the spatial and temporal terms in the temperature equation (21). This algorithm includes an entropy
viscosity stabilization technique described in [24, 38]. If we introduce the inner product of two scalar functions \( u \) and \( v \) on \( \Omega \)

\[
(u, v)_\Omega = \int_{\Omega} u \, v \, dx \, dy
\]

and \( \Gamma_D = \{ y = 0 \} \). By multiplying the test function \( \psi(x, y) \) and taking the integration, the weak form of this spatial discretization is

\[
\left( \frac{\partial T}{\partial t} , \psi \right)_\Omega + (u \cdot \nabla T , \psi)_\Omega = - (\nabla T , \nabla \psi)_\Omega - (\nu_h(T) \nabla T , \nabla \psi)_\Omega + \left( \frac{\partial T}{\partial n} , \psi \right)_{\Gamma_D} \tag{35}
\]

where \( \nu_h(T) \) is the entropy viscosity function as defined in [38], except here we do not use a second-order extrapolation to treat the advection term \( (u \cdot \nabla T, \psi) \) and the entropy viscosity term \( (\nu_h(T) \nabla T, \nabla \psi)_\Omega \) explicitly. We use the fully implicit adaptive Backward Differentiation Formula of order 2 (BDF2) [74, 38] to discretize the temperature equation in time. Thus, the full discretization of the temperature equation is

\[
\left( \frac{1}{\Delta t^{k+1}} \left( \frac{2\Delta t^{k+1} + \Delta t^k}{\Delta t^{k+1} + \Delta t^k} T^{k+1} - \frac{\Delta t^{k+1} + \Delta t^k}{\Delta t^k} T^k + \frac{(\Delta t^{k+1})^2}{\Delta t^k(\Delta t^{k+1} + \Delta t^k)} T^{k-1} \right) , \psi \right)_\Omega \\
= - (u^k \cdot \nabla T^{k+1}, \psi)_\Omega - (\nabla T^{k+1}, \nabla \psi)_\Omega - (\nu_h^k(T) \nabla T^{k+1}, \nabla \psi)_\Omega + \left( \frac{\partial T^{k+1}}{\partial n} , \psi \right)_{\Gamma_D} . \tag{36}
\]

The entropy-viscosity function \( \nu^k_h(T) \) is a non-negative constant within each cell that only adds artificial diffusion in cells for which the local Péclet number \( Pe = Ra \cdot Pr \) is large and the solution is not smooth.

### 3.4. Discretization of the Composition Equation

In this article we use the Volume-of-Fluid (VOF) interface tracking algorithm described in Section 3.5 below to discretize the composition equation (22). Prior to our implementation of the VOF method in ASPECT the only algorithms one could use to model the solution of (22) were based on a spatial discretization of the weak form of the composition equation.

\[
\left( \frac{\partial C}{\partial t} , \psi \right)_\Omega + (u \cdot \nabla C , \psi)_\Omega = 0. \tag{37}
\]

The first advection algorithm that was implemented in ASPECT is based on the same spatial discretization as in equation (35). However, the entropy-viscosity stabilization term on the right-hand side in

\[
\left( \frac{\partial C}{\partial t} , \psi \right)_\Omega + (u \cdot \nabla C , \psi)_\Omega = - (\nu_h(C) \nabla C, \nabla \psi)_\Omega \tag{38}
\]

is computed separately for the composition field; i.e., it does not have the same value in each cell as does the entropy viscosity function \( \nu_h(T) \) for the temperature field. The adaptive BDF2 algorithm is also used for the time discretization of the composition equation, leading to the following FEM Entropy Viscosity (FEM-EV) discretization of equation (22),

\[
\frac{1}{\Delta t^{k+1}} \left( \frac{2\Delta t^{k+1} + \Delta t^k}{\Delta t^{k+1} + \Delta t^k} C^{k+1} - \frac{\Delta t^{k+1} + \Delta t^k}{\Delta t^k} C^k + \frac{(\Delta t^{k+1})^2}{\Delta t^k(\Delta t^{k+1} + \Delta t^k)} C^{k-1} , \psi \right)_\Omega \\
= - (u^k \cdot \nabla C^{k+1}, \psi)_\Omega - (\nu^k_h(C) \nabla C^{k+1}, \nabla \psi)_\Omega . \tag{39}
\]

In equation (39) the entropy viscosity function \( \nu^k_h(C) \) has the same purpose as \( \nu^k_h(T) \).
The other algorithm for modeling solutions of (22) that is implemented in ASPECT is a Discontinuous Galerkin method with a Bound Preserving limiter. See [27] for a description of this algorithm in ASPECT and a comparison with the advection method with entropy viscosity described above. Also see [58] for a comparison of these two methods with the VOF method described here and a particle method for modeling the solution of the composition equation (22).

3.5. The Volume-of-Fluid Interface Tracking Algorithm. The Volume-of-Fluid (VOF) method is an interface tracking method in which, at each time step, the interface between the two compositions, one \((C = 1)\) with density \(\rho = \rho_0 + \Delta \rho\) and the other \((C = 0)\) with density \(\rho = \rho_0\), is explicitly reconstructed in every cell that contains a portion of the interface. Given this explicit (approximate) location of the interface at the current time step one then uses this information to advance the interface in time. In this sense the VOF method approximates the compositional interface on a subgrid scale. In addition, in an incompressible flow both the VOF interface reconstruction algorithm and the VOF advection algorithm presented here conserve the volume of each of the two compositions throughout the course of the computation.

3.5.1. Background. There are a wide variety of possible VOF interface reconstruction and advection algorithms; e.g., see [51] and the references there. The VOF method was first developed at the U.S. National Labs in the 1970s [48] and have continued to be used and developed by researchers at the National Labs [33, 47, 70, 69] as well as around the world. The advantage that VOF methods have over other interface tracking algorithms is that they are designed to naturally satisfy a conservation law; namely, equation (40) below. Thus, materials that should be conserved as they move with the flow are conserved, without the need to resort to additional numerical algorithms such as the redistancing step in a Level Set method [62]. VOF methods can and have been used effectively to model a wide variety of moving interface problems, including interfaces in compressible flow with shock waves [31], interfaces with shock waves in materials in the limit of no strength effects [44, 45], jetting in meteorite impacts [57], nonconservative interface motion such as photolithography [29, 30], the transition from deflagration to detonation [50] and more than two materials; i.e., more than one interface in a cell [1, 32].

3.5.2. Description. In this article we use a two-dimensional VOF algorithm to discretize the conservation equation

\[ \frac{\partial f}{\partial t} + \nabla \cdot F(f) = 0, \]  

where \(u = (u, v)\) is the velocity field, \(f\) is the volume fraction of one of the compositional fields, say \(C = 1\), the field with density \(\rho_0 + \Delta \rho\), which we will refer to as ‘Composition 1’ or \(C_1\) for short,\(^2\) and

\[ F(f) = (F(f), G(f)) = (u f, v f) \]  

is the volume fraction flux associated with \(C_1\). In our VOF implementation in ASPECT we use the ‘Efficient Least Squares VOF Interface Reconstruction Algorithm’ (ELVIRA), which is described in detail in [51] and is based on the ideas in [49] and [52]. The ELVIRA interface reconstruction algorithm reconstructs lines on a uniform grid with square cells exactly. We

\(^2\)Throughout this section and beyond we will use the terms “volume” and “volume fraction” of \(C_1\), etc., although it is to be understood that in two dimensions the quantity in question is an area.
will explain this in more detail in Section 3.5.3 and give an example in Section 4.1.2 below. Since the ELVIRA algorithm reconstructs lines in square cells exactly it is natural to assume that the algorithm is second-order accurate on a uniform grid with identical square cells. This turns out to be true [53, 54, 55]. We use a second-order accurate operator splitting advection method [51, 58, 65] to update the values of the volume fractions in time.

For simplicity of exposition we will assume the finite element grid consists entirely of square cells $\Omega_e$, of side $h$, indexed by the variable $e$, and aligned parallel to the $x$ and $y$ axes. The discretization of equation (40) proceeds as follows. Let $\Omega_e$ denote an arbitrary finite element cell in our domain $\Omega$ and let $f^k_e$ denote the discretized volume fraction in $\Omega_e$ at time $t^k$. The variable $f^k_e$ is a scalar that satisfies $0 \leq f^k_e \leq 1$ such that

$$f^k_e \approx \frac{1}{h^2} \int_{\Omega_e} f(x, y, t^k) \, dx \, dy. \quad (42)$$

Thus, the discretized volume, $V^k_e$, of $C_1$ in $\Omega_e$ at time $t^k$ is

$$V^k_e = \int_{\Omega_e} f^k_e \, dx \, dy = h^2 f^k_e. \quad (43)$$

Note that for an incompressible velocity field $\mathbf{u} = (u, v)$ we have $\nabla \cdot \mathbf{u} = 0$ and hence, the volume of ‘parcels’ or regions of $C_1$ are constant as they evolve in time.

From a mathematical point of view the variable $f(x, y)$ is the characteristic function associated with $C_1$. In other words,

$$f(x, y) = \begin{cases} f(x, y) = 1 & \text{if } (x, y) \text{ is occupied by Composition 1,} \\ f(x, y) = 0 & \text{if } (x, y) \text{ is not occupied by Composition 1.} \end{cases} \quad (44)$$

This implies $1 - f(x, y)$ is the characteristic function associated with $C_2$, the composition with density $\rho = \rho_0$. In this article we restrict ourselves to modeling the interface between two compositions. However, there is currently a great deal of research into modeling three or more interfaces in one cell with a VOF method; e.g., see [35].

In its simplest form our implementation of the VOF algorithm in ASPECT proceeds as follows.

Given the values $f^k_e$ at time $t^k$ and the velocity field at time $t^k$ we do the following to obtain the volume fractions $f^{k+1}_e$ at time $t^{k+1}$.

1. **THE INTERFACE RECONSTRUCTION STEP:** Given a cell $\Omega_e$ that contains a portion of the interface, so $0 < f^k_e < 1$ where $f^k_e$ is the volume fraction in $\Omega_e$ at time $t^k$, use the volume fractions $f^k_{e'}$ in the $3 \times 3$ block of cells $\Omega_{e'}$ centered on the cell $\Omega_e$ to reconstruct the interface in $\Omega_e$. The reconstructed interface will be a piecewise linear approximation to the true interface as shown in Figure 2 that preserves the given volume $h^2 f^k_e$ of $C_1$ in $\Omega_e$. We give a brief description of how we determine the linear approximation $\tilde{g}_e(x) = m_e x + b_e$, to the true interface in cells $\Omega_e$ for which $0 < f^k_e < 1$ in Section 3.5.3 below.
(2) COMPUTATION OF THE FLUXES: In the computations presented in this article we use a second-order accurate operator split algorithm, often referred to as Strang Splitting [65], in order to advance the interface in time. However, as mentioned above, for clarity and simplicity of exposition we will only describe a first-order accurate operator split VOF advection algorithm here. See [51] for the details of a second-order accurate operator split VOF advection algorithm.

For convenience and clarity of exposition, for the remainder of this section we will use the index notation \((i, j)\), as shown in Figures 2–4. Thus, we have nine cells with centers \((x_i', y_j')\) for \(i' = i - 1, i, i + 1\) and \(j' = j - 1, j, j + 1\) with edges indexed as shown in the figure. In the ELVIRA interface reconstruction algorithm we use the information in the 3\(\times\)3 block of cells \(\Omega_{i'j'}\) immediately adjacent to the cell \(\Omega_{ij}\) in which we wish to reconstruct the interface. Given the reconstructed interface \(\tilde{g}_e = \tilde{g}_{ij}(x)\) in

\[
\Omega_e \equiv \Omega_{ij} = [x_{i-1/2}, x_{i+1/2}] \times [y_{j-1/2}, y_{j+1/2}]
\]  

(45)

as shown in Figure 3 and the velocity \(u^k_{i±1/2,j}\) normal to the right and left edges of \(\Omega_{ij}\) at time \(t^k\), we wish to determine the volumes \(V^k_{i±1/2,j}\) of \(C_1\) that cross the right and left edges of \(\Omega_e\) in the time interval \([t^k, t^{k+1}]\). These volumes are determined

![Figure 2](image-url)

Figure 2. In our implementation of the VOF interface reconstruction algorithm the true interface, which in this example is \(g(x) = \tanh(x)\), is approximated as a line segment \(\tilde{g}_e(x) = mx + b\) in each cell \(\Omega_e\) that has a volume fraction \(f_e\) with \(0 < f_e < 1\). The approximate interface in \(\Omega_e\) is depicted as the solid red line segment in the center cell \(\Omega_e\). In this example, as with all VOF methods, the volume \(h^2 f_e^{\text{true}}\) beneath the true interface in \(\Omega_e\) is exactly equal to the volume \(h^2 f_e\) beneath the approximate interface \(\tilde{g}\) in \(\Omega_e\); i.e., \(f_e^{\text{true}} = f_e\). Note that, for convenience, we have used the notation \((x_i, y_j)\) to denote the center of the cell \(\Omega_e\), \([x_{i-1/2}, x_{i+1/2}] \times [y_{j-1/2}, y_{j+1/2}]\) to denote the cell \(\Omega_e\), etc.
Figure 3. The volume $V_{k+1/2,j}^k$ of $C_1$ in the quadrilateral outlined in green on three sides and by a portion of the solid red line on top is the flux of of $C_1$ that will cross the right-hand edge of $\Omega_e$ during the time step from time $t^k$ to $t^{k+1}$. Here $\Delta t^k = t^{k+1} - t^k$ and we have dropped the superscript $k$ from $u_{i+1/2,j}^k$ and $\Delta t^k$ for clarity. The solid red line in $\Omega_e$ is the reconstructed interface that approximates the true interface $g(x) = \tanh(x)$ in $\Omega_e$ as shown in Figure 2.

geometrically. A diagram for how to determine the volume $V_{i+1/2,j}^k$ of $C_1$ that crosses the right-hand edge of $\Omega_{ij}$ in the time interval $[t^k, t^{k+1}]$, given the assumption that $u_{i+1/2,j}^k > 0$, is outlined in green on three sides and by a portion of the solid red line on top in Figure 3.

(3) THE CONSERVATIVE UPDATE: Given the volumes $V_{i+1/2,j}^k$ of $C_1$ that cross the left and right-hand edges of $\Omega_{ij}$ in the time interval $[t^k, t^{k+1}]$ we use the following equation to determine an intermediate volume $\hat{V}_{ij}^k$ in $\Omega_{ij}$ for the first part of the two part operator split algorithm:

$$\hat{V}_{ij}^k = V_{ij}^k + V_{i-1/2,j}^k - V_{i+1/2,j}^k,$$  \hspace{1cm} (46)

where $V_{ij}^k = h^2 f_{ij}^k$ and $\hat{V}_{ij}^k$ denotes the ‘intermediate’ volume in $\Omega_{ij}$ after the first part of the operator split advection step from time $t^k$ to time $t^{k+1}$.

Given the nine intermediate volume fractions $\hat{f}_{ij}^k \equiv \hat{V}_{ij}^k / h^2$ in $\Omega_{ij}$ and the $3 \times 3$ block of cells $\Omega_{i'j'}$ surrounding $\Omega_{ij}$, together with all of the intermediate volume fractions in the $3 \times 3$ block of cells surrounding each of the cells $\Omega_{i'j'}$, reconstruct an intermediate interface $\hat{g}_{ij'}(x)$ in each cell $\Omega_{i'j'}$ and use it to geometrically determine the volumes $\hat{V}_{ij,\pm1/2}^k$ of $C_1$ that cross the top and bottom edges of $\Omega_{ij}$ in the time interval $[t^k, t^{k+1}]$ in the same manner as illustrated in Figure 3, but this time in the
The volume of \( V_{ij}^{k+1} \) in \( \Omega_{ij} \) at the new time \( t^{k+1} \) is thus,

\[
V_{ij}^{k+1} = \hat{V}_{ij}^k + \hat{V}_{i,j-1/2}^k - \hat{V}_{i,j+1/2}^k
\]  

(47)

The new volume fraction in \( \Omega_{ij} \) is now

\[
f_{ij}^{k+1} = \frac{V_{ij}^{k+1}}{h^2}
\]  

(48)

There are also unsplit VOF advection algorithms; e.g., see [51, 56].

3.5.3. The ELVIRA Interface Reconstruction Algorithm. Here we briefly describe the ELVIRA interface reconstruction algorithm [51] we used in this article. In this example we present the simplest possible case; namely, when the true interface is a line that passes through the center cell of the 3 × 3 block \( B_{ij} \) of cells \( \Omega_{i'j'} \) centered on the cell \( \Omega_{ij} \) as shown in Figure 4. The following description is intended to be easy to understand. However, the reader should be aware that there are many VOF interface reconstruction algorithms in both two [69] and three dimensions [70] and on every conceivable grid; e.g., [37], as well as numerous hybrid VOF/
Level Set algorithms [67]. See [71] and the references therein for a more complete overview
VOF methods.

In the ELVIRA algorithm the approximate interface will be a *piecewise linear* approximation
\( \tilde{g}_{ij}(x) = m_{ij} x + b_{ij} \) to the true interface in \( \Omega_{ij} \) as depicted in Figure 2. Furthermore *the approximate interface is subject to the constraint that* the volume fraction in the center cell
due to the true interface \( g(x) \) and the approximate interface \( \tilde{g}_{ij} \) are equal; i.e., \( f_{ij}^\text{true} = f_{ij} \).

Consider the example shown in Figure 4. In this example the true interface is a line
\( l(x) = mx + b \). Assume we are given the exact volume fractions \( f_{ij}' \) associated with the line \( l(x) \),
which is the true interface, in each cell \( \Omega_{i'j'} \) of the \( 3 \times 3 \) block. Then in this example the first
two column sums
\[
S_{i-1} \equiv \sum_{j'=j-1}^{j+1} f_{i-1,j'} \quad \text{and} \quad S_i \equiv \sum_{j'=j-1}^{j+1} f_{i,j'}
\]
are *exact* in the sense that
\[
S_i = \frac{1}{h^2} \int_{x_{i-1/2}}^{x_{i+1/2}} (l(x) - y_{j-3/2}) \, dx
\]
and similarly for \( S_{i-1} \), but *not* for \( S_{i+1} \). Thus, using (50) we find the difference in the column
sums \( S_i \) and \( S_{i-1} \) is
\[
h^2 (S_i - S_{i-1}) = \int_{x_{i-1/2}}^{x_{i+1/2}} (mx - b) - y_{j-3/2} \, dx - \int_{x_{i-3/2}}^{x_{i-1/2}} (mx - b) - y_{j-3/2} \, dx
\]
\[
= \left[ \int_{x_{i-1/2}}^{x_{i+1/2}} mx \, dx - \int_{x_{i-3/2}}^{x_{i-1/2}} mx \, dx \right]
\]
\[
= \frac{m}{2} \left[ \left( x_{i+1/2} \right)^2 - \left( x_{i-3/2} \right)^2 \right] - \frac{m}{2} \left[ \left( x_{i+1/2} \right)^2 - \left( x_{i-1/2} \right)^2 \right]
\]
\[
= \frac{m}{2} h \left( x_{i+1/2} - x_{i-3/2} \right)
\]
\[
= m h^2.
\]
Thus,
\[
m = S_i - S_{i-1}
\]
and we have recovered the *exact* slope \( m \) of the true interface \( l(x) \) in the center cell simply by
differencing the correct pair of column sums of volume fractions. A little thought will show
that the constraint
\[
f_{ij} = f_{ij}^\text{true}
\]
determines \( b \) uniquely, thus determining the linear approximation
\[
g_{ij}(x) = mx + b
\]
which is exactly equal to the true interface \( l(x) \). In actual fact one needs to know whether the
region containing the composition \( C_1 \) is above, below, or to the left or right of \( C_2 \). However,
there are a variety of algorithms for doing this; e.g., see [13] or [51]. This always works on a uniform grid of square cells, each of side $h$.

However, there are a few caveats: There are three ways to difference the column sums,

$$
m_{x,l} = (S_i - S_{i-1})$$
$$m_{x,c} = \frac{(S_{i+1} - S_{i-1})}{2}$$
$$m_{x,r} = (S_{i+1} - S_i)$$

and three ways to difference the row sums

$$m_{y,l} = (R_j - R_{j-1})$$
$$m_{y,c} = \frac{(R_{j+1} - R_{j-1})}{2}$$
$$m_{y,r} = (R_{j+1} - R_j)$$

where the row sums are defined by

$$R_{j-1} \equiv \sum_{i' = i-1}^{i+1} f_{i',j-1}, \quad R_j \equiv \sum_{i' = i-1}^{i+1} f_{i',j} \quad \text{and} \quad R_{j+1} \equiv \sum_{i' = i-1}^{i+1} f_{i',j+1}$$

In order to determine the best linear approximation to the true interface we compare the the volume fractions $f_{x,l}^{i',j'}$, $f_{x,c}^{i',j'}$, $f_{x,r}^{i',j'}$, ..., $f_{y,r}^{i',j'}$ due to each of the six lines

$$g_{x}^{l} = m_{x}^{l} x + b_{x}^{l} \quad \quad g_{y}^{l} = m_{y}^{l} x + b_{y}^{l}$$
$$g_{x}^{c} = m_{x}^{c} x + b_{x}^{c} \quad \quad g_{y}^{c} = m_{y}^{c} x + b_{y}^{c}$$
$$g_{x}^{r} = m_{x}^{r} x + b_{x}^{r} \quad \quad g_{y}^{r} = m_{y}^{r} x + b_{y}^{r}$$

we obtain from each of the six slopes in (55) and (56) in the $3 \times 3$ block $B_{ij}$ centered on the cell of interest $\Omega_{ij}$ and use the line that minimizes the difference between the given volume fractions and the volume fractions due to the lines in (58). We now explain this procedure in a bit more detail.

3.5.4. Approximating an Unknown Interface. Suppose $g(x)$ is an unknown interface that passes through the center cell $\Omega_{ij}$ of a $3 \times 3$ block of cells $B_{ij}$ containing nine square cells $\Omega_{i',j'}$, each of side $h$, centered on $\Omega_{ij}$. Furthermore, assume the only information we have are the nine exact volume fractions $f_{i',j'}$ in the cells $\Omega_{i',j'}$ due to $g(x)$. For example, in Figure 2 the ‘unknown’ interface is $g(x) = \tanh(x)$, which is the blue curve, and the volume fractions are nonzero only in cells that either contain the curve or are below it. We want to find a line segment $\tilde{g}_{ij}(x) = m_{ij} x + b_{ij}$ that is a second-order accurate approximation to $g(x)$, in the following sense,

$$\max |g(x) - \tilde{g}_{ij}(x)| \leq \tilde{C} h^2 \quad \text{for all } x \in [x_{i-1/2}, x_{i+1/2}],$$

where $\tilde{C}$ is a constant that is independent of $h$.

First we define a way to measure the error $E(\tilde{m})$ between the volume fractions $f_{i',j'}$, we are given that are due to the unknown interface and the approximate volume fractions $\tilde{f}_{i',j'}$ due
to a line segment \( \tilde{g}(x) = \tilde{m}x + \tilde{b} \) that passes through the center cell \( \Omega_{ij} \) and the \( 3 \times 3 \) block \( B_{ij} \) centered on \( \Omega_{ij} \),

\[
E(\tilde{m}) = \sum_{i'=i-1}^{i+1} \sum_{j'=j-1}^{j+1} (f_{i'j'} - \tilde{f}_{i'j'})^2 .
\] (60)

Note that this is the square of the two norm on vector spaces \( \mathbb{R}^n \) from linear algebra, where in our case \( n = 9 \), [66].

Now take the volume fractions we are given, namely \( f_{i'j'} \), and form all six of the slopes in (55) and (56) and the six candidate lines in (58) from these slopes. Remember that the ’y intercept’ \( b \) for each of the lines in (58) is determined by the constraint \( f_{ij}^{\text{true}} = f_{ij} \). Each of the six line produces nine volume fractions in the \( 3 \times 3 \) block \( B_{ij} \). For example, given the slope \( m^{x,c} \) defined in (55) we obtain the line \( g^c = m^c x + b^c \) defined in (58), which in turn gives us nine volume fractions \( f^x_{i'j'} \) for \( i' = i - 1, i, i + 1 \) and \( j' = j - 1, j, j + 1 \). Now compute \( E(\tilde{m}^c) \) and repeat this procedure for each of the other lines in (58) with slopes computed as in (55) and (56). Finally, take the line from (58) that minimizes the error defined in (60); i.e., pick the slope from (55) and (56), call it \( \tilde{m} \), that satisfies

\[
E(\tilde{m}) = \min \{ E(m^c), E(m^r), \ldots, E(m^y) \} .
\] (61)

The line

\[
\tilde{g} = \tilde{m} x + \tilde{b}
\] (62)

is the linear approximation to the true interface \( g(x) \) in \( \Omega_{ij} \) that we use in the VOF algorithm in this article. In [53] and [55] it is proven that this algorithm produces a second-order accurate approximation in the sense of (59) to the interface provided that

\[
h \leq \frac{2}{33 \sigma_{\text{max}}}
\] (63)

where \( \sigma_{\text{max}} \) denotes the maximum curvature of the interface, \( h \) is the grid size, and the volume fractions due to the true interface are exact.

3.5.5. Implementation of the VOF method in ASPECT. In the work described in this article we implemented the VOF algorithm described above in ASPECT. We will now describe our implementation for square, two dimensional, cells \( \Omega_e \) in physical space (often referred to as the ‘real’ cell in ASPECT) and show computational results for such cells. First note that the VOF method is essentially a specialized version of a Finite Volume Method, which is equivalent to a Discontinuous Galerkin (DG) method with values \( f_e \) that are constant on each cell \( \Omega_e \). Approaching the VOF algorithm from this point of view, we note that both methods require the computation of the flux of the volume of \( C_1 \), or, equivalently, the volume fraction of \( C_1 \), across each of the edges of \( \Omega_e \).

In a VOF method it is natural to use the method of characteristics to calculate the flux of \( C_1 \) through each of the cell edges. This is done by tracing backward in time along a linear approximation to each characteristic in order to identify the total volume that will cross a given edge and then computing that portion of the volume associated with the fluid that is being tracked as shown in Figure 3: i.e., by computing the volume fraction of \( C_1 \) in the total volume that will cross that edge. See [15] and [39] for examples of computing a second-order accurate flux in this manner in a finite volume discretization of (40), rather than a VOF discretization of (40), as well as higher resolution versions of these algorithms. In our
computation of the volume fraction flux we make use of several algorithms that we developed for the interface reconstruction step. We will describe these algorithms in more detail below.

There are a number of approaches one can consider for obtaining the velocities on the $k$th edge from the approximate FEM solution of the incompressible Stokes equations. Two approaches are (1) a point sample of the normal velocity on the $k$th edge and (2) the velocity integrated

$$\int_{\partial \Omega_{e,k}} u \cdot n_k \, ds$$

along the $k$th edge of $\Omega_e$, where $n_k$ denotes the unit normal to the $k$th edge of $\Omega_e$. For a finite volume method, (1) and (2) are both reasonable approximations to the edge velocities. However, the latter method (64) is a closer analogue to the type of procedure one would choose for a finite element method.

We now describe our implementation of the computation of the volume flux of $C_1$, on a square cell $\Omega_e$ of side $h$. (When we employ AMR, $h$ denotes the length of each side of the most finely resolved cells in the FEM grid.) All of the information that we use to describe the interface in a real cell $\Omega_e$; namely, its distance $d_e$ to the center of the cell and the unit normal $n_e$ to the interface, is stored with respect to the interface’s location relative to the center of the unit cell $\hat{\Omega}_e$ associated with $\Omega_e$ when $\Omega_e$ is mapped to $\hat{\Omega}_e$ as depicted in Figure 5. In particular,
the interface in the unit cell $\Omega_e$ is given by

$$
\mathbf{n}_e \cdot (\mathbf{x} - \mathbf{x}_e) = d_e
$$

(65)

where $\mathbf{x}_e$ is the center of $\Omega_e$, $d_e$ is the distance of the interface from the center $\mathbf{x}_e$ of $\Omega_e$, and $\mathbf{n}_e$ is a unit vector that is perpendicular to the approximate (linear) interface in $\Omega_e$, with the convention that $\mathbf{n}_e$ always points away from the region containing Composition 1. The location of the interface is stored by recording $\mathbf{n}_e$ and $d_e$ for each cell $\Omega$ that contains a portion of the interface. For the case when the velocity field is perpendicular to a cell edge, say $\partial \Omega_{e,k}$, for some $k = 1, 2, 3, 4$, let $\mathbf{n}_k$ be the unit normal vector to the $k$th edge $\partial \Omega_{e,k}$ of the unit cell $\Omega_e$, and let $V_F$ denote the total volume flux (i.e., the volume of $C_1$ and $C_2$) that will flux / advect across $\partial \Omega_{e,k}$.

As shown in Figure 5, with only a few computationally inexpensive transformations we can use the same algorithm we used to compute the volume fraction on a cell $\Omega_e$ in the reconstruction step to compute the volume flux of $C_1$ across each of the edges of $\Omega_e$. If we map $V_F$ from $\hat{\Omega}_e$ to another unit cell $\hat{\Omega}_I$ and assuming the velocity is perpendicular to the $k$th cell edge $\partial \hat{\Omega}_{e,k}$ of $\hat{\Omega}_e$, we find that the interface within the unit cell $\hat{\Omega}_I$ is given by

$$
\mathbf{n}_I \cdot (\mathbf{x} - \mathbf{x}_I) = d_I
$$

where $\mathbf{x}_I$ is the center of $\hat{\Omega}_I$ as shown in Figure 5. The values of $\mathbf{n}_I$ and $d_I$ in terms of $\mathbf{n}_e$, $\mathbf{n}_k$, and $d_e$ are given by

$$
\mathbf{n}_I = \mathbf{n}_e + \left( \frac{V_F}{V_e} - \mathbf{n}_e \cdot \mathbf{n}_k \right) \mathbf{n}_k,
$$

(66)

$$
d_I = d_e - \left( \frac{1}{2} + \frac{V_F}{2V_e} \right) (\mathbf{n}_e \cdot \mathbf{n}_k).
$$

(67)

where $V_e$ is the volume of $\Omega_e$ (the upwind cell for this edge), and $\mathbf{n}_k$ is the outward pointing normal of the cell edge $\partial \Omega_{e,k}$.

Given the assumptions we have made regarding a uniform square grid, we have a constant Jacobian, so the volumes on the unit cell and the volume in physical space are related by a constant multiple. For a given interface, there is a simple formula to calculate the volume of $C_1$ on the side opposite the unit normal $\mathbf{n}$; e.g., see [60]. In our notation this formula is

$$
f(\mathbf{n},d) = \begin{cases}
1 & \frac{1}{2} \leq \bar{d} \\
1 - \frac{(\bar{d} - \frac{1}{2})^2}{2m(1-m)} & \frac{1}{2} - m \leq \bar{d} \leq \frac{1}{2} \\
\frac{1}{2} + \frac{d}{(1-m)} & m - \frac{1}{2} \leq \bar{d} \leq \frac{1}{2} - m \\
\frac{(d+\frac{1}{2})^2}{2m(1-m)} & \frac{1}{2} - m < \bar{d} < \frac{1}{2} \\
0 & \bar{d} \leq -\frac{1}{2}
\end{cases}
$$

(68)

Where $m = 1 - \frac{\|\mathbf{n}\|_\infty}{\|\mathbf{n}\|_1}$ and the components of $\mathbf{n}$ are parallel to sides of the unit cell $\hat{\Omega}_e$, and $\bar{d} = \frac{d}{\|\mathbf{n}\|_1}$. We use (68) to compute the flux of $C_1$ across the RH edge, which is $f(\mathbf{n}_I, d_I) V_F$. In general we use an analogous procedure to compute the (volume) flux of $C_1$ across the other edges of $\Omega_e$. 
3.5.6. Volume Correction. In our current implementation of the VOF advection algorithm we use a dimensionally split algorithm as described in Section 3.5.2 above. Consequently, we cannot assume that the velocity at the intermediate step is divergence free due to the decoupling of the cell edges from one spatial dimension to the other. This decoupling removes the guarantee that the volume fractions retain the bound $0 \leq f \leq 1$, since there is no guarantee that the velocity is divergence free during the intermediate step. Since the reconstruction algorithm requires $0 \leq f \leq 1$, it is therefore necessary to modify the advection algorithm.

First, note that the equation that governs the advection of the characteristic function $f$ is

$$\frac{\partial}{\partial t} f + \mathbf{u} \cdot \nabla f = 0.$$  \hspace{1cm} (69)

Using (20) we obtain a modified form of (69),

$$\overbrace{\frac{\partial}{\partial t} f + \nabla \cdot (\mathbf{u} f)}^{\text{Advection}} - \overbrace{\bar{f} (\nabla \cdot \mathbf{u})}^{\text{Correction}} = 0$$  \hspace{1cm} (70)

Note that in (70) the first term is a conservation law for $f$. If (20) is satisfied exactly then the correction term in (70) will be zero. However, in the case of a dimensionally split algorithm the assumption that the velocity $\mathbf{u}$ is divergence free, even to $O(h^q)$ for some integer $q \geq 2$, breaks down. One expects this to add a small error to the computation. However, since the VOF interface reconstruction algorithm requires $f$ to satisfy $0 \leq f \leq 1$ it is necessary to retain this correction term.

We approximate (70) by

$$f_{e}^{n+1} V_{e} = f_{e}^{n} V_{e} + \sum_{k} f_{k} U_{k} - \bar{f}_{e} \sum_{k} U_{k},$$  \hspace{1cm} (71)

where $e$ is an index that ranges over all cells $\Omega_{e}$, $V_{e}$ is the volume of $\Omega_{e}$, $k$ is an index that ranges over the cell edges of $\Omega_{e}$, $f_{k}$ is the volume fraction of $C_{1}$ that will be fluxed across the $k$th edge as described in the caption to Figure 5, and

$$U_{k} = \Delta t \int_{\partial \Omega_{e,k}} \tilde{u}_{k} \cdot \mathbf{n}_{k} \, ds.$$  \hspace{1cm} (72)

where $\tilde{u}_{k}$ is a time centered approximation to the velocity $\mathbf{u}$ on the $k$th edge,

$$\tilde{u}_{k} = \frac{\mathbf{u}^{n+1} + \mathbf{u}^{n}}{2}.$$  

The term $\bar{f}_{e}$ in (71) can be one of several approximations to the volume fraction $f_{e}$ in $\Omega_{e}$. The two simplest cases are (1) $\bar{f}_{e} = f_{e}^{old}$, i.e., an explicit correction term, and (2) $\bar{f}_{e} = f_{e}^{new}$, i.e., an implicit correction term. In the results shown here we use the explicit term $\bar{f}_{e} = f_{e}^{old}$.

Since we are using Strang splitting, (71) is evaluated once for each spatial dimension in the problem at each time step, alternating the order of the dimensions in the subsequent time step.
3.5.7. Model Coupling Procedure. Having now described our implementation the VOF method in ASPECT, it is necessary to establish how the computed \( C \) field may be used by the other portions of the model in cases where the tracked fluid is not a passive tracer.

There is a significant reduction in the complexity of the implementation and duplication of work if the \( C \) field can be discretized in the same manner as what are known as “compositional fields” in ASPECT [5]. Furthermore, in order to avoid interfering with the values on neighboring cells, we prefer to use a discontinuous element. For a number of reasons, often relating to the physical interpretation of the quantity \( C \), it is also desirable to ensure that it will always be bounded; e.g., \( 0 \leq C \leq 1 \).

A basic implementation can be done by directly discretizing the volume fraction data on a discontinuous \( P_0 \) element, which is equivalent to a least squares approximation to the composition field implied by the reconstructed interface. Attempting to obtain an ideal approximation using a higher order element such as DG \( Q_1 \) or DG \( P_1 \) is more difficult, especially if the bounds on the composition \( C \) are respected, since the result of an unconstrained least squares approximation for such an element is almost certain to violate these bounds. Furthermore, the unconstrained least squares computation can be expected to be both more complex and more expensive. Thus, any approximation using a non-constant DG element will require a heuristic approach.

In our implementation, in order to generate a DG \( Q_1 \) element approximation to the \( C \) field that is implied by the reconstructed interface, we apply the following constraints.

1. The gradient of the element is in the same direction as the normal of the interface.
2. The gradient is as large as possible while maintaining \( 0 \leq C \leq 1 \) everywhere.
3. In order to maintain conservation of mass the volume fraction implied by the DG \( Q_1 \) element approximation to the \( C \) field must match the volume fraction \( f_e \) in the VOF approximation to the \( C \) field; i.e.,

\[
\int_{\Omega_e} C(x) \, dx = f_e V_e
\]

where \( V_e \) is the volume of \( \Omega_e \).

On a square mesh, for a cell with the reconstructed interface

\[
\mathbf{n}_e \cdot (\mathbf{x} - \mathbf{x}_e^\varepsilon) = d_e \tag{73}
\]

the above constraints result in the approximation on the unit cell being

\[
C(x) = f_e - 1 - 2 f_e - 0.5 \frac{\mathbf{n}_e \cdot (\mathbf{x} - \mathbf{x}_e^\varepsilon)}{||\mathbf{n}_e||_1} \tag{74}
\]

If we use a DG \( Q_1 \) element, the use of the above equation produces a bilinear approximation to the VOF method’s reconstructed \( C \) field, with little additional computational cost over the \( P_0 \) approximation.
3.5.8. Coupling with the AMR Algorithm. The dealii library [3] upon which ASPECT is built manages the AMR algorithm through the p4est library [11]. Dealii, and hence, ASPECT provides a mechanism for setting the refinement criteria; both when to refine a cell and when to coarsen a cell. Since reconstructing and advecting the interface across different levels of refinement both increases algorithm complexity and decreases the accuracy with which the interface is resolved, in this work we ensure that the interface is always on the finest level of refinement. This approach requires that the cells that contain the interface, including the case where the interface is on a cell boundary, and any cell that shares a vertex with any of those cells must also be at the finest level of refinement.

The criteria for refining a cell that we have adopted is a two step algorithm that requires one pass over the entire mesh and one pass over a subset of the entire mesh. In the first step we check every cell in the entire mesh making a list of all cells that contain a part of the interface. More specifically, we regard all cells $\Omega_e$ that satisfy $\epsilon_{vof} < f_e < 1 - \epsilon_{vof}$, where $\epsilon_{vof}$ is a small parameter, to contain a portion of the interface. In addition, all cells $\Omega_e$ that have a neighboring cell $\Omega'_e$ that shares a face with $\Omega_e$ and differ in volume fraction sufficiently (e.g., $|f_e - f'_e| > \epsilon_{vof}$) are also added to this list. In the computational results shown in Section 4 we use the value $\epsilon_{vof} = 10^{-6}$. In the second pass over a subset of the entire grid we make a list of all cells that share a vertex with any cell already in the list of cells that contain a portion of the interface and also flag each of these cells for refinement. These flags are then passed to dealii, and thus on to p4est, which handles the details of the refinement of these cells and the coarsening of those cells that no longer need to be at the finest level of refinement.

Given that the time step $\Delta t$ is constrained by a CFL condition, the interface can move at most $\sigma$ cell widths where $\sigma \leq 1$ is the CFL number. This permits the reduction of the frequency with which we conduct the remeshing procedure to $N$ time steps where $N < \frac{W-2}{2\sigma}$ and $W$ is the minimum width of the maximally refined band of cells. (See, for example, any of the AMR computations in the second (b) and fourth (d) frames in Figures 12–23 for explicit examples of $W$.) For the refinement strategy described above, the safest assumption is that $W = 4$. This takes into consideration the case where the interface is at the cell boundary. A band of larger width $W > 4$ would both require a more complex algorithm to find the necessary cells to flag and would increase the number of refined cells. Thus, there is a balance between cost associated with the frequency of running the algorithm to flag cells for refinement and cost of having a larger value of $W$. This balance is problem dependent.

4. Numerical Results

In this section we present our numerical results. First, in Section 4.1 we compute two test problems with prescribed velocity fields to verify the accuracy of our implementation of the VOF algorithm [51]. Then, in Section 4.2, we compute some mantle convection benchmarks to verify the accuracy of the coupling to the mantle convection code. Finally, in Section 4.3, we apply the algorithm to a problem of interest in the field of geodynamics.

4.1. Interface Tracking Benchmark Problems. In this section, we compute two test problems with known exact solutions to ensure that our the implementation of the VOF algorithm converges at its design rate. In particular, in Subsection 4.1.2 we compute one of
4.1.1. Definition of the Error Measurement. Since each volume fraction \( f_e \) is constant on its grid cell \( \Omega_e \), we use \( P_0 \) elements to store the value of the volume fraction \( f_e \) on each \( \Omega_e \). Given a fixed grid with cells \( \Omega_e \) indexed by \( e \) we define the error between the exact \( f_e^{\text{exact}} \) and computed \( f_e^{\text{comp}} \) volume fractions by

\[
\text{Error} (f_e^{\text{exact}} - f_e^{\text{comp}}) = \sum_e |f_e^{\text{exact}} - f_e^{\text{comp}}| V(\Omega_e)
\]

(75)

where \( V(\Omega_e) \) denotes the volume of \( \Omega_e \). Note that this is the \( L^1 \) norm of the difference between \( f_e^{\text{exact}} \) and \( f_e^{\text{comp}} \) with weight \( V(\Omega_e) \).

4.1.2. Advection of a Linear Interface in a Constant Velocity Field. Our first VOF benchmark problem is the advection of a linear interface in a constant velocity field as shown in Figures 6 and 7. The computational domain is \([0, 1] \times [0, 1]\) and the initial interface given by \( y = 1 - x \).

At each time step \( t^k \to t^{k+1} \) the interface is advanced the velocity field \( \mathbf{u} = (-\frac{25}{100}, -\frac{24}{100}) \), and then compared with the exact solution, for which the interface is given by \( y = \frac{51}{100} - x \). In this computation we used a CFL number of \( \sigma = \frac{1}{2} \), which resulted in, for example, of a total of 23 time steps on the least refined grid of \( h = 2^{-16} \).

Since the ELVIRA interface reconstruction method reproduces lines exactly, we expect the error in the computations to be exact to machine precision \( \epsilon_{\text{mach}} \approx 10^{-16} \). The results of computations for \( h = ... \) are given in Table 2. We note that in all cases the error is \( O (\epsilon_{\text{mach}}) \).

4.1.3. Rotation of a Circular Interface. The second benchmark problem is the advection of a circle containing composition 1 in a rotating velocity field as shown in figure 8. In this problem
Figure 7. On the left is the initial condition as reconstructed by our VOF method. On the right is a comparison between the exact and computed interface at \( t = 1 \), with the exact interface in blue and the computed interface in black. It is apparent that the two interfaces are visually indistinguishable.

Figure 8. Circular interface rotation benchmark problem, the red dot is the center of rotation

Table 3. Rotation of a circular interface offset from the center of rotation

| \( h \) | Error   | Rate   |
|--------|---------|--------|
| \( 2^{-4} \) | \( 6.03897 \cdot 10^{-3} \) |        |
| \( 2^{-5} \) | \( 1.74516 \cdot 10^{-3} \) | 1.79   |
| \( 2^{-6} \) | \( 3.92745 \cdot 10^{-4} \) | 2.15   |
| \( 2^{-7} \) | \( 1.05605 \cdot 10^{-4} \) | 1.89   |
| \( 2^{-8} \) | \( 2.63464 \cdot 10^{-5} \) | 2.00   |
| \( 2^{-9} \) | \( 6.48952 \cdot 10^{-6} \) | 2.02   |

the angular velocity is \( \pi \) radians per unit time with an end time of \( t = 2.0 \). Note that the center of rotation is not at the center of the circle, but rather it lies on the boundary of the circle. Since our reconstruction and advection algorithms, are designed to be second-order accurate, we expect the approximate interface to be a second-order accurate approximation to the true circle. The \( L^1 \) error in the volume fractions \( f_c \) for this benchmark for six computations
with increasing grid resolution \( h = 2^{-4}, 2^{-5}, \ldots, 2^{-9} \) is shown in Table 3. In each of these computations we used a CFL number of \( \sigma = \frac{1}{2} \).

**4.2. Mantle Convection Benchmark Problems.** In this section we compute two ‘benchmark’ problems that are well-known and frequently used in the computational mantle convection community to demonstrate that our VOF interface tracking algorithm can reproduce previously published computational results of the same problem. In our view the first problem, commonly known as the “van Keken problem” or the “van Keken isoviscous Rayleigh-Taylor problem” is not a reasonable ‘benchmark’, since the problem is mathematically ill-posed. In other words, it is unstable [12] and perturbations due to different numerical methods can yield vastly differing results. In fact, in [58] we demonstrated that it suffices to change only the algorithm with which the composition variable \( C \) is advected in order to obtain clearly different results at the same output time. For example, see Figure 11 of [58] or compare Figures 5(c)–(d) of [59] to our results here or in [58] or to the results in [73].

**4.2.1. The van Keken Isoviscous Rayleigh-Taylor Problem.** In this section, we present our computation of the van Keken isoviscous Rayleigh-Taylor problem [73]. In spite of the fact that the problem is unstable and hence ill-posed, it has become a standard ‘benchmark’ in the computational geodynamics community. In this problem a less dense (buoyant) fluid lies beneath a denser fluid, with a perturbed interface between the two layers. The problem is computed in a \([D, 1]\) computational domain where \( D = 0.9142 \) is the width of the domain. The initial discontinuity between the two compositional/density layers is given by

\[
C(x, y, t = 0) = \begin{cases} 
0, & \text{if } 0 \leq y < 0.2 + 0.02 \cos \left( \pi \frac{x}{D} \right), \\
1, & \text{otherwise}.
\end{cases}
\]
Figure 10. Computed solution of the van Keken isoviscous Rayleigh-Taylor problem at time $t = 2000$ on a uniform grid of $128 \times 128$ cells. Compare with the computational results in [38], [59], and [73].

This initial condition has a (discontinuous) interface along the curve

$$y = 0.2 + 0.02 \cos \left( \frac{\pi x}{D} \right).$$  

(77)
4.2.2. The Gerya-Yuen Sinking Box Benchmark. Following the original authors, we pose the Gerya-Yuen 'sinking box' problem \cite{23} in dimensional form. The problem is defined on a 500 km \times 500 km two-dimensional Cartesian computational domain. A small horizontally centered 100 km \times 100 km square is placed with its top edge 50 km below the top of the domain so that the initial location and dimension of the box is defined by the composition field \( C(x,t) \) as follows:

\[
C(x,0) = \begin{cases} 
1, & \text{if } (x,y) \in [200 \text{ km}, 300 \text{ km}] \times [350 \text{ km}, 450 \text{ km}], \\
0, & \text{otherwise}.
\end{cases}
\]  

(78)

The block’s density is \( \rho_1 = 3300 \text{ kg/m}^3 \), while the background density is \( \rho_1 = 3300 \text{ kg/m}^3 \). We approximate the solution of the incompressible Stokes equations (i.e., equations (6)–(8) without the term \( \rho_0 \alpha (T - T_0)g \) in equation (8)) with these initial conditions and holding the following parameters fixed:

\[
\begin{align*}
g &= (0, 9.8) \text{ m/s}^2, & \text{acceleration due to gravity} \\
L &= 500 \text{ km} & \text{domain height and width} \\
\mu &= 10^{21} \text{ Pa} \cdot \text{s} & \text{viscosity} \\
\rho_0 &= 3200 \text{ kg/m}^3, & \text{background density} \\
\rho_1 &= 3300 \text{ kg/m}^3, & \text{small box density}
\end{align*}
\]  

(79)

4.3. Computations of Thermochemical Convection in a Density Stratified Fluid. We now present the results of our computations of the model problem for thermochemical convection with density stratification, the equations for which were presented in Section 2. In these computations the Rayleigh number is fixed at \( Ra = 10^5 \) and we vary only the buoyancy ratio as follows: \( B = 0.0, 0.1, 0.2, \ldots, 1.0 \) and \( B = 2.0 \). The domain for all of the
computational results shown below is a two-dimensional rectangular region that we denote by
\( \Omega = [0, 3] \times [0, 1] \) as shown in Figure 1.

The initial conditions for the temperature \( T \) are,
\[
T(x, 0) = \begin{cases} 
(1 - 5y) + A \sin(10 \pi y) \left( 1 - \cos(\frac{5}{3} k \pi x) \right) & \text{if } 0 \leq y \leq \frac{1}{10}, \\
(5 - 5y) + A \sin(10 \pi y) \left( 1 - \cos(\frac{5}{3} k \pi x + \pi) \right) & \text{if } \frac{9}{10} \leq y \leq 1, \\
0.5 & \text{otherwise,}
\end{cases}
\]
where the period of the perturbation \( k = 1.5 \) and the amplitude of the perturbation \( A = 0.05 \). Note that \( A = 0.05 \) ensures that \( 0 \leq T(x,y;0) \leq 1 \) throughout the entire computational domain. The initial conditions for the composition are,
\[
C(x, y; t = 0) = \begin{cases} 
1 & \text{if } 0 \leq y < \frac{1}{2}, \\
0 & \text{if } \frac{1}{2} \leq y \leq 1
\end{cases}
\]
and the boundary conditions for the velocity and temperature are as specified in (26)–(31).

All of the results shown below were computed twice: once on a fixed, uniform grid with
192 \times 64 square cells each with side \( h = 64^{-1} \) and then on the same underlying grid but with
the addition of two levels of an adaptively refined mesh, on and in, a neighborhood of the
interface. Each level of refinement increases the grid resolution by a factor of two; i.e., \( h \to h^2 \)
with two levels of refinement.

5. DISCUSSION

In Section 4.1 we demonstrated that our implementation of the VOF method in ASPECT
is second-order accurate on smooth flows in the norm defined in (75). In Section 4.2 we
demonstrated that the method correctly reproduces two benchmarks from the computational mantle
convection literature. We now present a detailed discussion of the results of our
computations of thermochemical convection in density stratified flow shown in Section 4.3.
This model problem is designed to study the basic physics underlying the formation of thermal plumes that form at LLSVPs, entrain some of the material in the LLSVP, and bring it to the
Earth’s surface. It is also a two dimensional analog of the experimental results of Davaille [19] and Le Bars and Davaille [7, 8].

5.1. Computations of Thermochemical Convection in a Density Stratified Fluid.
Examining the results in Section 4.3 of our computations of thermochemical convection in a
density stratified fluid for values of the nondimensional buoyancy parameter \( B = 0.0, 0.1, 0.2, \ldots, 1.0 \)
and \( B = 2.0 \) at Rayleigh number \( Ra = 10^5 \), we note a fundamental change in the dynamics
and structure of the flow field as \( B \) increases from \( B = 0.0 \) to \( B = 2.0 \). First, considering only
the extreme values \( B = 0.0 \) and \( B = 2.0 \), we observe the following difference in the qualitative behavior of the interface. For \( B = 0.0 \) (Figure 12), which is the classic Rayleigh-Bénard problem in which there is no difference in the densities of the two fluids (i.e., \( \Delta \rho = 0 \)), the height of the convection cells is equal to the height of the domain \( \Omega \) and we observe the steady cellular convection structure with three \( 1 \times 1 \) counter rotating cells as predicted by the analysis in Section 6.21 of [72]. That the flow is steady, (i.e., independent of time) in Figure 12 is apparent after comparing the temperature fields at \( t' = 1.97 \cdot 10^{-2} \) and \( t' = 2.36 \cdot 10^{-2} \).
Figure 12. Computations with $B = 0.0$ and $Ra = 10^5$ on an underlying uniform grid of $196 \times 64$ square cells at $t' = 1.97 \cdot 10^{-2}$ and $t' = 2.36 \cdot 10^{-2}$. The background color is the temperature, which varies from $T = 0.0$ (dark blue) to $T = 1.0$ (dark red).
Figure 13. Computations with $B = 0.1$ and $Ra = 10^5$ on an underlying uniform grid of $196 \times 64$ square cells at $t' = 1.97 \cdot 10^{-2}$ and $t' = 2.36 \cdot 10^{-2}$. The background color is the temperature, which varies from $T = 0.0$ (blue) to $T = 1.0$ (dark red).
(a) $B = 0.2$ at $t' = 1.97 \cdot 10^{-2}$ ON A UNIFORM GRID of $196 \times 64$ cells.

(b) $B = 0.2$ at $t' = 1.97 \cdot 10^{-2}$ with two levels of AMR.

(c) $B = 0.2$ at $t' = 2.36 \cdot 10^{-2}$ ON A UNIFORM GRID of $196 \times 64$ cells.

(d) $B = 0.2$ at $t' = 2.36 \cdot 10^{-2}$ with two levels of AMR.

Figure 14. Computations with $B = 0.2$ and $Ra = 10^5$ on an underlying uniform grid of $196 \times 64$ square cells at $t' = 1.97 \cdot 10^{-2}$ and $t' = 2.36 \cdot 10^{-2}$. The background color is the temperature, which varies from $T = 0.0$ (blue) to $T = 1.0$ (dark red).
Figure 15. Computations with $B = 0.3$ and $Ra = 10^5$ on an underlying uniform grid of $196 \times 64$ square cells at $t' = 1.97 \cdot 10^{-2}$ and $t' = 2.36 \cdot 10^{-2}$. The background color is the temperature, which varies from $T = 0.0$ (dark blue) to $T = 1.0$ (dark red).
(a) $B = 0.4$ at $t' = 1.97 \cdot 10^{-2}$ ON A UNIFORM GRID of $196 \times 64$ cells.

(b) $B = 0.4$ at $t' = 1.97 \cdot 10^{-2}$ with two levels of AMR.

(c) $B = 0.4$ at $t' = 2.36 \cdot 10^{-2}$ ON A UNIFORM GRID of $196 \times 64$ cells.

(d) $B = 0.4$ at $t' = 2.36 \cdot 10^{-2}$ with two levels of AMR.

Figure 16. Computations with $B = 0.4$ and $Ra = 10^5$ on an underlying uniform grid of $196 \times 64$ square cells at $t' = 1.97 \cdot 10^{-2}$ and $t' = 2.36 \cdot 10^{-2}$. The background color is the temperature, which varies from $T = 0.0$ (dark blue) to $T = 1.0$ (dark red).
Figure 17. Computations with $B = 0.5$ and $Ra = 10^5$ on an underlying uniform grid of $196 \times 64$ square cells at $t' = 1.97 \cdot 10^{-2}$ and $t' = 2.36 \cdot 10^{-2}$. The background color is the temperature, which varies from $T = 0.0$ (dark blue) to $T = 1.0$ (dark red).
Figure 18. Computations with $B = 0.6$ and $Ra = 10^5$ on an underlying uniform grid of $196 \times 64$ square cells at $t' = 1.97 \cdot 10^{-2}$ and $t' = 2.36 \cdot 10^{-2}$. The background color is the temperature, which varies from $T = 0.0$ (dark blue) to $T = 1.0$ (dark red).
(a) $B = 0.7$ at $t' = 1.97 \cdot 10^{-2}$ ON A UNIFORM GRID of 196 × 64 cells.

(b) $B = 0.7$ at $t' = 1.97 \cdot 10^{-2}$ with two levels of AMR

(c) $B = 0.7$ at $t' = 2.36 \cdot 10^{-2}$ ON A UNIFORM GRID of 196 × 64 cells.

(d) $B = 0.7$ at $t' = 2.36 \cdot 10^{-2}$ with two levels of AMR

Figure 19. Computations with $B = 0.7$ and Ra = $10^5$ on an underlying uniform grid of 196 × 64 square cells at $t' = 1.97 \cdot 10^{-2}$ and $t' = 2.36 \cdot 10^{-2}$. The background color is the temperature, which varies from $T = 0.0$ (dark blue) to $T = 1.0$ (dark red).
Figure 20. Computations with $B = 0.8$ and $Ra = 10^5$ on an underlying uniform grid of $196 \times 64$ square cells at $t' = 1.97 \cdot 10^{-2}$ and $t' = 2.36 \cdot 10^{-2}$. The background color is the temperature, which varies from $T = 0.0$ (dark blue) to $T = 1.0$ (dark red).
Figure 21. Computations with $B = 0.9$ and $Ra = 10^5$ on an underlying uniform grid of $196 \times 64$ square cells at $t' = 1.97 \cdot 10^{-2}$ and $t' = 2.36 \cdot 10^{-2}$. The background color is the temperature, which varies from $T = 0.0$ (dark blue) to $T = 1.0$ (dark red).
Figure 22. Computations with $B = 1.0$ and $Ra = 10^5$ on an underlying uniform grid of $196 \times 64$ square cells at $t' = 1.97 \cdot 10^{-2}$ and $t' = 2.36 \cdot 10^{-2}$. The background color is the temperature, which varies from $T = 0.0$ (dark blue) to $T = 1.0$ (dark red).
Figure 23. Computations with $B = 2.0$ and $Ra = 10^5$ on an underlying uniform grid of $196 \times 64$ square cells at $t' = 1.97 \cdot 10^{-2}$ and $t' = 2.36 \cdot 10^{-2}$. The background color is the temperature, which varies from $T = 0.0$ (dark blue) to $T = 1.0$ (dark red).
Note that for $B = 0$ each of the three $1 \times 1$ convection cells overturn at the same fixed rate. On the other hand, for $B = 2.0$ the magnitude of $\Delta \rho$ prevents the denser fluid from reaching the top of the domain and producing overturns, and hence convection cells, on the scale of the height of the domain. Rather, the structure of the flow shown in Figure 23 consists of six (roughly) square counter rotating $\frac{1}{2} \times \frac{1}{2}$ cells below $y = 0.5$ and a similar structure above $y = 0.5$. Thus, for $B = 2.0$ we observe a permanently stratified convection structure. Furthermore, from $B = 0.7$ in Figure 19 and, perhaps, from $B = 0.4$ in Figure 16 or $B = 0.5$ in Figure 17, on; i.e., as $B \rightarrow 2.0$ from below with $B > B_c$ where $0.3 < B_c \leq 0.7$, it appears that at the times shown the flow is tending continuously toward the stratified convection pattern shown in Figure 23.

The features at either end of the interval $B = [0.0, 2.0]$ are consistent with the diagrams - obtained from experiments - on the left and right of Figure 1 in [8], although in the diagram on the right the authors have only drawn three cells above and three cells below the centerline and, in both drawings, the cells appear to be more rectangular than square in shape. We assume that these diagrams are simply rough sketches of the dynamics of what the authors of [8] refer to as “Whole Layer” (left) and “Stratified” (right) convection. Perhaps, also, these diagrams are for different values of the other two nondimensional parameters the authors varied in the work described in the sequence of papers [7, 8] and [19]; namely, the ratio $a$ of the height of the lower layer to the height of the entire domain and the ratio $\gamma$ of viscosity of the lower layer to that of the upper layer. In the work we present in Section 4.3 we did not vary these other two parameters; they were held fixed at $a = 0.5$ and $\gamma = 1.0$. In short, we conclude that our computational results correctly correspond qualitatively to what the authors of [8] observe in their experiments when the nondimensional parameters $a$ and $\gamma$ are held fixed at $a = 0.5$ and $\gamma = 1.0$. Finally, note the similarity of the two counter rotating convection cells on the right in Figures 12c–12d and 13c–13d to the structure of the flow in Figure 4(a) of [7].

It is possible to obtain additional insight into the structure and dynamics of the flow for various values of $B$ from the results shown in Figures 12–23. As $B$ increases from 0.0 to 0.1, 0.2, and 0.3 in Figures 12–15 we observe that the rate of overturn decreases, until for $B = 0.3$ the denser material has just reached the top of the domain at $t' = 2.36 \cdot 10^{-2}$ (Figures 15c and 15d), whereas for smaller values of $B$ the overturn has passed beyond the top of the domain by $t' = 2.36 \cdot 10^{-2}$. For $B = 0.4$ we can see from Figures 16c and 16d, that the fluid does not reach a full overturn by $t' = 2.36 \cdot 10^{-2}$ suggesting that there may be a transition between the qualitative dynamics of the flow at some $B_c$ in the range $0.3 \leq B \leq 0.4$. In [8] the authors find $B_c = 0.302$ when the viscosity ratio is $\gamma = 6.7$.

For $0.5 \leq B \leq 1.0$ in Figures 17–22 the general interface structures are similar, although with smaller volumes for the “pinched” regions that are produced during the transition from “Whole Layer” convection to “Stratified” flow. As shown in Figure 23, for $B = 2.0$, the stratification is sufficiently strong that the pinched structures do not form, although a standing wave does form as a slight perturbation from the initial location of the interface at $y = \frac{1}{2}$ with boundaries at $x \approx 0.5, 1.5, 2.5$.

5.1.1. A qualitative comparison to the experiments Davaille and Le Bars. In this section we briefly make some additional qualitative comparisons of our computational results to the
A qualitative comparison of the computations presented in this paper to the experimental results of Davaille [19] and Le Bars & Davaille [7, 8]. The grayscale regions correspond to boundaries of the qualitative regions shown in Figure 3 of [19] and Figure 2 of [8] for $a = 0.5$. The experimental data is from Table 3 of [19] and Table 3 of [7] with $a = 0.5$ as is the case for all of the computations in this article. The terms “Stratified”, “Dynamic Topography”, and “Whole Layer” used to describe the qualitative state of the flow are the same as those used by the authors of [7, 8] and [19].

Before doing so however, it is first necessary to make several caveats concerning this comparison. First, as we mentioned above, in the experiments the authors varied two additional nondimensional parameters; namely, (1) the ratio $a$ of the height of the lower layer to the height of the entire domain and (2) the ratio $\gamma$ of the viscosity of the fluid that initially occupies the lower layer to the viscosity that initially occupies the upper layer. In our computations, shown in Section 4.3, we kept these parameters fixed at $a = 0.5$ and $\gamma = 1.0$. Second, in the experiments the two fluids are miscible, whereas in our computations the two fluids are immiscible. In both cases there is no surface tension at the boundary between the two fluids.

The general transition between one type of structure and another (e.g., “Whole Layer” convection to “Stratified Convection”) is similar to that found in the experiments shown in [8],
although the precise location of the transition may differ. A rough comparison is show in Figure 24. The different grayscale backgrounds in Figure 24 correspond to the grayscale regions in Figure 3 of [19] and Figure 2 of [8] for $a = 0.5$. In the results presented in this paper we do not continue the computation for a sufficiently long times to confirm that in the $0.3 \leq B \leq 0.5$ regime the flow oscillates before beginning an overturn. However, the observed behavior does produce structures that match those described in [8] for the length of time for which we do have computational results. This difference may be in part due to the fact that in [8] the two fluids also vary in viscosity ratio $\gamma$, and Rayleigh number $Ra$.

5.1.2. Numerical artifacts that occur when the interface is underresolved. Since the VOF method maintains a sharp interface between the two compositional fields, it is able to capture features that are approximately on the order of the grid scale $h$. However, in cases where the structures formed by the interface become sufficiently small, for example, a thin column of fluid of width $2h$, the interface reconstruction algorithm might produce numerical artifacts that are “characteristic” of the combination of the particular reconstruction algorithm and advection algorithm one chooses to use in the VOF method. Here we briefly examine of the nature of one particular numerical artifact that appears frequently in Section 4.3.

The most common numerical artifact in the computational results shown in Section 4.3 is the tendency for the reconstructed interface to form ‘droplets’ that are diamond shaped and generally occupy a square of four cells, each edge having two square cells of side $h$. For example, droplets such as these appear in Figure 13a. In the computations shown in Section 4.3 these droplets typically resolve into a thin vertical column of fluid of approximately $2h - 4h$ in width with a length that is nearly the entire height of the computational domain. For example Figures 13a and Figure 13b, in which the more refined computation in Figure 13b appears to be sufficiently well-resolved to draw the conclusion that a thin column of fluid is forming in the locations where in Figure 13a there are only a few droplets and no real indication of what the flow “should” look like. Or the droplets may resolve into a thin finger that is shorter than the height of the computational domain such as in Figures 18c 18d, 19c and 19d.

We note that if a feature of the interface is underresolved, it can help the user determine if additional refinement is required. In some instances, perhaps after making a second, more refined computation, it will be clear that additional refinement is necessary, sometimes even more refined than the second computation was. For example see Figures 13c and 13d, neither of which appear sufficiently well resolved to accept the computation in Figure 13d as well resolved enough to determine the true nature of the flow. On the other hand, there are instances when the numerical artifact is sufficiently small so as not to affect the dynamics of the interface that are of interest and additional resolution might not be required. For example, depending on the user and the underlying scientific application, this might be the case for Figures 20c, 20d, 21c, and 21d, even though under magnification the fingers in the refined computations shown in Figures 20d and 21d do not yet appear fully resolved. In other words, depending on the application, these computations may or may not be well resolved enough

---

3It is important to recognize that this is not a failing of the VOF method in general or of the specific interface reconstruction and advection algorithms we have chosen for our work here, since whenever a computation is underresolved, all numerical methods will exhibit some sort of numerical artifact or artifacts that are “characteristic” of that particular method.
for the user to arrive at conclusions appropriate for their application concerning the flow at this point in time.

In conclusion, we emphasize that the required degree of resolution for a given computation will depend on the purpose of the computation and the user’s need for fine detail as opposed to general qualitative information concerning the flow.

6. Conclusions

We have implemented a Volume-of-Fluid (VOF) interface tracking method in the open source finite element code ASPECT, which is designed to model convection and other processes in the Earth’s mantle. Our VOF method works efficiently and effectively in ASPECT’s parallel environment and with its adaptive mesh refinement (AMR) algorithm. We show that the VOF method reproduces linear interfaces in a constant flow to machine precision and is second-order accurate when we use it to compute a standard, smooth, interface tracking benchmark problem. We also demonstrate that the method shows excellent agreement with two benchmark problems from the computational mantle convection literature. In particular, in the second of these benchmarks we use AMR to allow us to compute at a much higher effective resolution at lower computational cost than would otherwise be possible.

Finally, we use the new interface tracking methodology to study a problem involving thermochemical convection in density stratified flow. This model problem is relevant to the study of structures at the core mantle boundary known as Large Low Shear Velocity Provinces (LLSVPs). Recent studies utilizing seismic imaging have revealed large regions with anomalous seismic properties in the lower mantle. There are two dome-like regions beneath Africa and the Pacific with low shear-wave velocities that extend some 1000 km above the core-mantle boundary and have horizontal dimensions of several thousand kilometers [16, 21]. Most interpretations propose that the heterogeneities are compositional in nature, differing from the surrounding mantle, an interpretation that would be consistent with chemical geodynamic models. Based on geological and geochemical studies it has been argued that LLSVPs have persisted for billions of years [9].

The model problem is designed to study the basic physics underlying the formation of thermal plumes that bring some of this material to the Earth’s surface. In our computations of we use AMR to obtain an effective grid resolution of 768 × 256 square cells overlaying the fluid interface on an underlying grid of 192 × 64 square cells. This increase in resolution confirms that for a certain range of the nondimensional buoyancy parameter B at Rayleigh number $Ra = 10^5$ our computations of the interface have converged well enough to interpret with confidence the large scale dynamics of the two regions of differing densities.

In conclusion, the results of the work presented here demonstrate that our VOF interface tracking method should perform well on a number of problems of interest to the computational mantle convection community.
ACKNOWLEDGEMENTS

This work was supported by the National Science Foundation’s (NSF) SI2-SSE Program under Award number 1440811. The development of ASPECT was supported by the Computational Infrastructure for Geodynamics (CIG) under NSF Award numbers 0949446 and 1550901. The computations were made under the auspices of CIG on the U.C. Davis Division of Mathematical and Physical Sciences distributed computing cluster Peloton.

REFERENCES

[1] Anbarlooei, H. R., Mazaheri, K., 2011. Moment of fluid interface reconstruction method in axisymmetric coordinates. International Journal for Numerical Methods in Biomedical Engineering 27 (10), 1640–1651.
[2] Arndt, D., Bangerth, W., Davydov, D., Heister, T., Heltai, L., Kronbichler, M., Maier, M., Pelteret, J.-P., Turcksin, B., Wells, D., 2017. The deal.II library, version 8.5. Journal of Numerical Mathematics 25 (3), 137–146.
[3] Arndt, D., Bangerth, W., Davydov, D., Heister, T., Heltai, L., Kronbichler, M., Maier, M., Pelteret, J.-P., Turcksin, B., Wells, D., 2017. The deal.II library, version 8.5. Journal of Numerical Mathematics.
[4] Bangerth, W., Dannberg, J., Gassmoeller, R., Heister, T., et al., March 2017. ASPECT. URL http://www.math.clemson.edu/~heister/manual.pdf
[5] Bangerth, W., Dannberg, J., Gassmöller, R., Heister, T., et al., 2017. ASPECT: Advanced Solver for Problems in Earth’s ConvecTion, User Manual. CIG.
[6] Bangerth, W., Hartmann, R., Kanschat, G., 2007. deal.II – a general purpose object oriented finite element library. ACM Trans. Math. Softw. 33 (4), 24/1–24/27.
[7] Bars, M. L., Davaille, A., 2004. Large interface deformation in two-layer thermal convection of miscible viscous fluids. J. Fluid Mech. 499, 75110.
[8] Bars, M. L., Davaille, A., 2005. Thermochemical convection in two superimposed miscible viscous fluids. In: Gutkowski, W., Kowalewski, T. (Eds.), Mechanics of the 21st Century, Proceedings of the 21st International Congress of Theoretical and Applied Mechanics. Springer Verlag, pp. FM7–12126.
[9] Burke, K., Steinberger, B., Torsvik, T. H., Smethurst, M. A., 2008. Plume generation zones at the margins of large low shear velocity provinces on the core–mantle boundary. Earth and Planetary Science Letters 265 (1), 49–60.
[10] Burstedde, C., Wilcox, L. C., Ghattas, O., 2011. pdet: Scalable algorithms for parallel adaptive mesh refinement on forests of octrees. SIAM Journal on Scientific Computing 33 (3), 1103–1133.
[11] Burstedde, C., Wilcox, L. C., Ghattas, O., 2011. pdet: Scalable algorithms for parallel adaptive mesh refinement on forests of octrees. SIAM Journal on Scientific Computing 33 (3), 1103–1133.
[12] Chandrasekhar, S., 1961. Hydrodynamic and Hydromagnetic Stability. Dover, New York.
[13] Chorin, A. J., 1985. Curvature and solidification. J. Comput. Phys. 57, 472–490.
[14] Chorin, A. J., Marsden, J. E., 1993. A Mathematical Introduction to Fluid Mechanics, 4th Edition. No. 4 in Texts in Applied Mathematics. Springer-Verlag, New York, qA901.C53 1992.
[15] Colella, P., 1990. Multidimensional upwind methods for hyperbolic conservation laws. J. Comput. Phys. 87, 171–200.
[16] Cottaar, S., Romanowicz, B., 2012. An unusually large ULVZ at the base of the mantle near Hawaii. Earth and Planetary Science Letters 355, 213–222.

[17] Dannberg, J., Eilon, Z., Faul, U., Gassmiller, R., Moulid, P., Myhill, R., 2017. The importance of grain size to mantle dynamics and seismological observations. Geochemistry, Geophysics, Geosystems 18 (8), 3034–3061.

[18] Dannberg, J., Heister, T., 2016. Compressible magma/mantle dynamics: 3d, adaptive simulations in ASPECT. Geophysical Journal International 207 (3), 1343–1366.

[19] Davaille, A., 1999. Two-layer thermal convection in miscible viscous fluids. J. Fluid Mech. 379, 223–253.

[20] Donea, J., Huerta, A., 2005. Steady Transport Problems. John Wiley and Sons.

[21] French, S. W., Romanowicz, B., 2015. Broad plumes rooted at the base of the Earth’s mantle beneath major hotspots. Nature 525 (7567), 95–99.

[22] Gassmoller, R., 2016. Open source support for massively parallel, generic finite element methods. Poster presented at the 2016 NSF SI2 PI Workshop.

URL http://maxim.ucsd.edu/suave/index.html?file=si2n.cxml

[23] Gerya, T. V., Yuen, D. A., 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.

[24] Guermond, J.-L., Pasquetti, R., Popov, B., 2011. Entropy viscosity method for nonlinear conservation laws. J. Comput. Phys. 230 (11), 4248 – 4267, Special issue High Order Methods for CFD Problems.

[25] Hager, B., O’Connell, R., 1981. A simple global model of plate dynamics and mantle convection. Journal of Geophysical Research: Solid Earth 86 (B6), 4843–4867.

[26] Hager, B. H., Clayton, R. W., 1989. Constraints on the structure of mantle convection using seismic observations, flow models, and the geoid. In: Mantle Convection, Plate Tectonics and Global Dynamics. Gordon and Breach Science Publishers, pp. 657–763.

[27] He, Y., Puckett, E. G., Billen, M. I., 2017. A discontinuous Galerkin method with a bound preserving limiter for the advection of non-diffusive fields in solid Earth geodynamics. PEPI 263, 23–37.

[28] Heister, T., Dannberg, J., Gassmoller, R., Bangerth, W., 2017. High accuracy mantle convection simulation through modern numerical methods. II: Realistic models and problems. Geophysical Journal International 210 (2), 833–851.

[29] Helmsen, J. J., Colella, P., Puckett, E. G., 1997. Non-convex profile evolution in two dimensions using volume of fluids. Technical Report LBNL-40693, Lawrence Berkeley National Laboratory.

[30] Helmsen, J. J., Colella, P., Puckett, E. G., Dorr, M., January 1996. Two new methods for simulating photolithography development in three dimensions. In: Proceeedings of the 10th SPIE Optical/Laser Microlithography Conference. Vol. 2726. SPIE, San Jose, CA, pp. 253–261.

[31] Henderson, L. F., Colella, P., Puckett, E. G., March 1991. On the refraction of shock waves at a slowfast gas interface. J. Fluid Mech. 224, 1–27.

[32] Hill, R. N., Shashkov, M., 2013. The symmetric moment-of-fluid interface reconstruction algorithm. J. Comput. Phys. 249, 180 – 184.

[33] Hirt, C. W., Nichols, B. D., 1981. Volume of Fluid (VOF) method for the dynamics of free boundaries. J. Comput. Phys. 39, 201–225.

[34] Huber, R., Helmig, R., 1999. Multiphase flow in heterogeneous porous media: A classical finite element method versus an implicit pressure–explicit saturation-based mixed finite element–finite volume approach. International Journal for Numerical Methods in Fluids
29 (8), 899–920.

[35] Jemison, M., Sussman, M., Shashkov, M., 2015. Filament capturing with the multime-rial-moment-of-fluid method. J. Comput. Phys. 285, 149–172.

[36] King, S., Raefsky, A., Hager, B., 1990. ConMan: Vectorizing a finite element code for incompressible two-dimensional convection in the Earth’s mantle. Physics of the Earth and Planetary Interiors 59 (3), 195–207.

[37] Kothe, D. B., Puckett, E. G., Williams, M. W., 1999. Robust finite volume modeling of 3-d free surface flows on unstructured meshes. In: Proceedings of the 14th AIAA Computational Fluid Dynamics Conference. American Institute of Aeronautics and Astronautics, Norfolk, VA, pp. 1–6.

[38] Kronbichler, M., Heister, T., Bangerth, W., 2012. High accuracy mantle convection simulation through modern numerical methods. Geophysical Journal International 191 (1), 12–29.

[39] LeVeque, R. J., April 1996. High-resolution conservative algorithms for advection in incompressible flow. SIAM J. Numer. Anal. 33 (2), 627–665.

[40] Manga, M., 1996. Mixing of heterogeneities in the mantle: Effect of viscosity differences. Geophysical Research Letters 23 (4), 403–406.

[41] Manga, M., Stone, H., 1994. Interactions between bubbles in magmas and lavas: effects of bubble deformation. Journal of Volcanology and Geothermal Research 63 (3), 267–279.

[42] Manga, M., Stone, H. A., O’Connell, R. J., 1993. The interaction of plume heads with compositional discontinuities in the earth’s mantle. Journal of Geophysical Research: Solid Earth 98 (B11), 19979–19990.

[43] McNamara, A., Zhong, S., 2004. Thermochemical structures within a spherical mantle: Superplumes or piles?: Thermochemical structures. Journal of Geophysical Research: Solid Earth 109 (B7), n/a–n/a.

[44] Miller, G. H., Puckett, E. G., February 1994. Edge effects in molybdenum-encapsulated molten silicate shock wave targets. J. Appl. Phys. 75 (3), 1426–1434.

[45] Miller, G. H., Puckett, E. G., August 1996. A high-order Godunov method for multiple condensed phases. J. Comput. Phys. 128 (1), 134–164.

[46] Moresi, L., Gurnis, M., 1996. Constraints on the lateral strength of slabs from three-dimensional dynamic flow models. Earth and Planetary Science Letters 138 (1), 15–28.

[47] Nichols, B. D., Hirt, C. W., Hotchkiss, R. S., August 1980. SOLA-VOF: a solution algorithm for transient fluid flow with multiple free boundaries. Technical Report LA-8355, Los Alamos National Laboratory.

[48] Noh, W. F., Woodward, P. R., June 28–July 3 1976. SLIC (Simple Line Interface Calculation). In: van de Vooren, A. I., Zandbergen, P. J. (Eds.), Proceedings of the Fifth International Conference on Numerical Methods in Fluid Dynamics. Vol. 59 of Lecture Notes in Physics. Springer-Verlag, Twente University, Enschede, pp. 330–340.

[49] Pilliod, J. E., September 1992. An analysis of piecewise linear interface reconstruction algorithms for volume-of-fluid methods. MS Thesis, Graduate Group in Applied Mathematics, University of California, Davis.

[50] Pilliod, J. E., Puckett, E. G., 1998. An unsplit, second-order accurate Godunov method for tracking deflagrations and detonations. In: Houwing, A. F. P., Paull, A., Boyce, R. R., Danehy, P. M., Hannemann, H., Kurtz, J. J., McIntyre, T. J., McMahon, S. J., Mee, D. J., Sandeman, R. J., Tanno, H. (Eds.), Proceedings of the 21st International Symposium on Shock Waves. Vol. II. Panther Publishing, Fyshwick, Australia, pp. 1053–1058.

[51] Pilliod, J. E., Puckett, E. G., September 2004. Second-order accurate volume-of-fluid algorithms for tracking material interfaces. J. Comput. Phys. 199 (2), 465–502.
Puckett, E. G., 1991. A volume-of-fluid interface tracking algorithm with applications to computing shock wave refraction. In: Proceedings of the Fourth International Symposium on Computational Fluid Dynamics. pp. 933–938.

Puckett, E. G., February 2010. On the second-order accuracy of volume-of-fluid interface reconstruction algorithms: Convergence in the max norm. CAMCoS 5 (1), 99–148.

Puckett, E. G., October 2010. A volume-of-fluid interface reconstruction algorithm that is second-order accurate in the max norm. CAMCoS 5 (2), 199–220.

Puckett, E. G., January 2014. On the second-order accuracy of volume-of-fluid interface reconstruction algorithms II: An improved constraint on the cell size. CAMCoS 8 (1), 123–158.

Puckett, E. G., Almgren, A. S., Bell, J. B., Marcus, D. L., Rider, W. J., January 1997. A high-order projection method for tracking fluid interfaces in variable density incompressible flows. J. Comput. Phys. 130 (2), 269–282.

Puckett, E. G., Miller, G. H., 1996. The numerical computation of jetting impacts. In: Sturtevant, B., Shepherd, J. E., Hornung, H. (Eds.), Proceedings of the 20th International Symposium on Shock Waves. Vol. II. World Scientific, New Jersey, pp. 1467–1472.

Puckett, E. G., Turcotte, D. L., He, Y., Lokavarapu, H., Robey, J. M., Kellogg, L. H., 2017. New numerical approaches for modeling thermochemical convection in a compositionally stratified fluid. Physics of the Earth and Planetary Interiors (online November 11, 2017).

Samuel, H., Evonuk, M., 2010. Modeling advection in geophysical flows with particle level sets. Geochemistry, Geophysics, Geosystems 11 (8).

Scardovelli, R., Zaleski, S., 2000. Analytical relations connecting linear interfaces and volume fractions in rectangular grids. Journal of Computational Physics 164 (1), 228 – 237.

Schubert, G., Turcotte, D. L., Olson, P., 2001. Mantle convection in the Earth and planets. Cambridge University Press.

Sethian, J. A., June 1999. Level Set Methods and Fast Marching Methods: Evolving Interfaces in Computational Geometry, Fluid Mechanics, Computer Vision, and Materials Sciences, 2nd Edition. Vol. 3 of Cambridge Monographs on Applied and Computational Mathematics. Cambridge University Press, Cambridge, U.K. ; New York.

Sheldon, J., Cardwell Jr, W., et al., 1959. One-dimensional, incompressible, noncapillary, two-phase fluid flow in a porous medium. Petroleum Transactions, AIME 216, 290–296.

Steinberger, B., 2000. Plumes in a convecting mantle: Models and observations for individual hotspots. Journal of Geophysical Research: Solid Earth 105 (B5), 11127–11152.

Strang, W. G., 1968. On the construction and comparison of difference schemes. SIAM J. Numer. Anal. 5 (3), 506–517.

Strang, W. G., 2016. Introduction to Linear Algebra, 5th Edition. Cambridge Wellsely Press.

Sussman, M. S., Puckett, E. G., 2000. A coupled level set and volume of fluid method for computing 3D and axisymmetric incompressible two-phase flows. J. Comput. Phys. 162, 301–337.

Tan, E., Choi, E., Thoutireddy, P., Gurnis, M., Aivazis, M., 2006. Geoframework: Coupling multiple models of mantle convection within a computational framework: Geoframework-mantle convection models. Geochemistry, Geophysics, Geosystems 7 (6), n/a–n/a.
[69] Torrey, M. D., Cloutman, L. D., Mjolsness, R. C., Hirt, C. W., December 1985. NASA-VOF2D: A computer program for incompressible flows with free surfaces. Technical Report LA-10612-MS, Los Alamos National Laboratory.

[70] Torrey, M. D., Mjolsness, R. C., Stein, L. R., July 1987. NASA-VOF3D: A three-dimensional computer program for incompressible flows with free surfaces. Technical Report LA-11009-MS, Los Alamos National Laboratory.

[71] Tryggvason, G., Scardovelli, R., Zaleski, S., 2011. Direct Numerical Simulations of Gas-Liquid Multiphase Flows, 1st Edition. Cambridge Monographs on Applied & Computational Mathematics. Cambridge University Press, Cambridge.

[72] Turcotte, D. L., Schubert, G., 2014. Geodynamics, 3rd Edition. Cambridge University Press.

[73] van Keken, P. E., King, S. D., Schmeling, H., Christensen, U. R., Neumeister, D., Doin, M.-P., 1997. A comparison of methods for the modeling of thermochemical convection. Journal of Geophysical Research: Solid Earth 102 (B10), 22477–22495.

[74] Wanner, G., Hairer, E., 1991. Solving ordinary differential equations II. Vol. 14 of Springer Series in Computational Mathematics. Springer-Verlag Berlin Heidelberg.

[75] Zhong, S., 2006. Constraints on thermochemical convection of the mantle from plume heat flux, plume excess temperature, and upper mantle temperature. Journal of Geophysical Research 111 (B4).

[76] Zhong, S., Zuber, M., Moresi, L., Gurnis, M., 2000. Role of temperature-dependent viscosity and surface plates in spherical shell models of mantle convection. Journal of Geophysical Research: Solid Earth 105 (B5), 11063–11082.