

An exactly mass conserving and pointwise divergence free velocity method: application to compositional buoyancy driven flow problems in geodynamics

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Abstract

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Key Points:

- Pointwise divergence free velocity fields are necessary for accurate advection of tracers in incompressible velocity fields.
- PDE-constrained l_2 projection exactly conserves mass of tracer data.
- High order time integration methods are unnecessary for low order spatial geodynamics numerical models.

Abstract

Tracer methods are widespread in computational geodynamics for modeling the advection of chemical data. However, they present certain numerical challenges, especially when used over long periods of simulation time. We address two of these in this work: the necessity for mass conservation of chemical composition fields and the need for the velocity field to be pointwise divergence free to avoid gaps in tracer coverage. We do this by implementing the hybrid discontinuous Galerkin (HDG) finite element method combined with a mass-conserving constrained projection of the tracer data. To demonstrate the efficacy of this system we compare it to other common finite element formulations of the Stokes system and projections of the chemical composition.

We provide a reference of the numerical properties and error convergence rates which should be observed by using these various discretization schemes. This serves as a tool for verification of existing or new implementations. We summarize these data in a reproduction of a published Rayleigh–Taylor instability benchmark, demonstrating the importance of careful choices of appropriate and compatible discretization methods for all aspects of geodynamics simulations.

Keywords: Finite element analysis, tracer methods, mantle convection, buoyancy driven convection

1 Introduction

Melting at mid-oceanic ridges causes differentiation of the Earth’s mantle with the formation of a distinct basaltic crust on top of a depleted peridotite layer. The recycling of this oceanic crust in subduction zones, where additional differentiation may occur, causes the continuous formation of chemical heterogeneity in the Earth’s mantle which adds to compositional heterogeneity that may have been formed during Earth’s formation and magma ocean solidification (e.g., Labrosse et al., 2007).

Mantle convection models that incorporate these differentiation processes can predict how any formed heterogeneity is mixed back in or retained in the mantle (Kellogg, 1992; Tackley, 2015; van Keken et al., 2002, 2014) and help decipher the processes that lead to the long term chemical evolution of the Earth as seen in geochemistry (Christensen & Hofmann, 1994; R. E. Jones et al., 2019; Samuel & Farnetani, 2003; Tucker et al., 2020; Xie & Tackley, 2004), the formation of the structure of the Earth’s mantle as imaged by seismological methods (Ballmer et al., 2016; Bull et al., 2009; Haugland et al., 2018; T. D. Jones et al., 2020), and the Earth’s thermal state and evolution (Nakagawa & Tackley, 2005; Li & McNamara, 2018; Zhong, 2006).

Implementing the chemical buoyancy term into the Stokes equations that follow from the conservation of momentum tends to be more challenging than that of thermal buoyancy because chemical diffusion is sufficiently small compared to thermal diffusion that it can be ignored. In geodynamical applications several distinct methods have been traditionally used to represent the chemical buoyancy. These include i) marker chain methods to delineate the boundary between two volumes of distinct chemical composition (Christensen & Yuen, 1984; Lin & van Keken, 2006; Schmeling, 1987); ii) tracer methods where individual tracers carry a relative proportion of the chemical buoyancy (Brandenburg et al., 2008; Christensen & Hofmann, 1994; Gerya & Yuen, 2003; O’Neill et al., 2006; Tackley & King, 2003); and iii) representing the chemical density as a composition field and solving the advection-diffusion equation with low chemical diffusivity (e.g., Hansen & Yuen, 2000; Kellogg & King, 1993), which in the presence of thermal buoyancy leads to double-diffusive convection (Turner, 1974). A comprehensive, if now slightly dated, comparison of these three methods is provided in van Keken et al. (1997).

Further complications occur if the compositionally distinct materials have different rheological behavior. In this case the continuity in stress across the interface causes a discontinuity in strainrate which is not a trivial problem to solve. See Suckale et al. (2010) for an elegant solution using a combination of ghost fluids and the level-set method.

In the past decade or so there has been significant progress improving methods for the accurate solution of thermochemical convection which are based on, among others, application of discontinuous Galerkin (DG) finite element methods (He et al., 2017), further use of level set methods (Hillebrand et al., 2014; Samuel & Evonuk, 2010), and adaptive remeshing (Davies et al., 2007; Leng & Zhong, 2011). Modeling of thermochemical convection has also become more readily available to a larger group of researchers through community codes such as ASPECT (Gassmüller et al., 2018) and the reliability of new methods has been demonstrated by careful benchmarking and error testing (e.g., Thielmann et al., 2014; Vynnytska et al., 2013).

In this paper we will focus on tracer methods. Their popularity arises primarily from their robustness when advecting sharp jumps in material properties in the absence of diffusion. In contrast, field-based methods under these circumstances are prone to instability arising as numerical oscillations or suffer from significant over-diffusion. The tracer methods are also more practical than the marker chain method for tracing chemical buoyancy over long time scales as typical mantle mixing leads to exponential growth of length of the marker chain (van Keken et al., 1997). Additionally the implementation of tracer methods is straightforward in both 2D and 3D. Each position and chemical datum pair in a population of tracers is simply advected through a velocity field using discrete time integration.

Tracer methods are not without their issues however. Pointwise chemical data associated with the tracers must be transferred, or projected, onto a mesh-based composition field before they can be used to set material properties such as buoyancy or viscosity. Various methods have been proposed for this projection, many of which depend on treating the tracers as delta-function sources within the domain. In the Dirac delta source, or ‘Stokeslet’ method (e.g., Christensen & Hofmann, 1994), direct integration of these delta functions with an associated mass per particle is used to derive the buoyancy source on the right-hand side of the Stokes system. The so-called tracer ratio and absolute methods (Tackley & King, 2003) use integrals of the delta functions to count the number of particles of a particular type per cell. Weighting these counts by either a volume fraction per particle for the absolute method or by the total number of particles per cell for the ratio method results in a mesh-based composition field.

The properties of the projected composition field vary widely depending on the algorithm. Ideally the field should be conserved both globally across the domain and locally within each cell of the mesh. Additionally the error in the field representation should converge at an optimal rate as the number of cells in the mesh increases, provided some minimum number of particles per cell is maintained. The absolute and Dirac delta methods achieve global but not local conservation. The tracer ratio method is neither locally nor globally conservative (Trim et al., 2020) but it does have the advantage that the composition field remains bounded between set limits (Tackley & King, 2003). In general however the integration of Dirac delta functions does not satisfy the smoothness, or regularity, requirements for finite elements. This causes algorithms that depend on it to typically experience reduced error convergence rates even when using nonconforming methods (e.g., Scott, 1973; Houston & Wihler, 2012). When the composition field is used to drive the flow, for example through the buoyancy or viscosity terms, this may in turn lead to suboptimal convergence of the velocity solution.

During advection tracers may drift apart (e.g., Wang et al., 2015; Trim et al., 2020), leaving gaps in coverage that may cause projection algorithms to break down when cells lack particles. This often requires the introduction (and removal) of tracers (e.g., Moresi et al., 2003), adding to the complexity of the algorithm. In incompressible flows however the

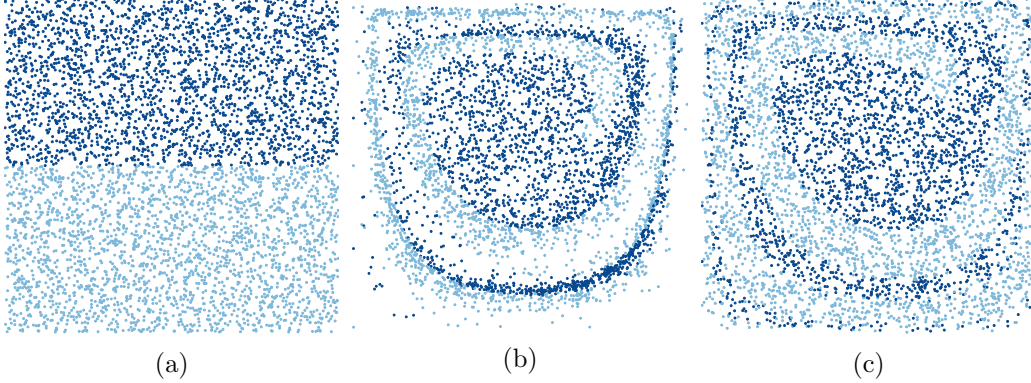


Figure 1: Example of tracers advected using a fourth order Runge–Kutta method in a forced cavity model. The geometry is a unit square and flow is forced by uniform horizontal velocity along the top boundary with free-slip boundaries elsewhere. (a) Initial configuration of the tracers. (b) Tracer distribution after 20 overturn times using a traditional Taylor–Hood finite element method. (c) as (b) but now with the new hybrid discontinuous Galerkin finite element method that guarantees the velocity field representation is pointwise divergence free.

root cause of this problem is that the discrete velocity solution is generally only divergence free in some discrete sense and not at every point in the domain. Thus over long simulations two particles may diverge even if they are initially in close proximity to each other.

Various velocity field reconstruction techniques have been proposed that maintain uniform particle distributions in the incompressible limit (Jenny et al., 2001; Wang et al., 2015; McDermott & Pope, 2008). Importantly, Maljaars et al. (2018) demonstrated that particle drift is mitigated when the incompressibility constraint is accurately satisfied. This is demonstrated in Figure 1 where initially evenly distributed particles (Figure 1a) develop significant gaps as the driven lid cavity simulation progresses when the Stokes equations are discretized using the commonly used Taylor–Hood (TH) finite element pair (Figure 1b). The use of a new hybrid discontinuous Galerkin (HDG) discretization that we will discuss further below guarantees that the incompressibility constraint is satisfied at every point in the domain. This maintains a consistent, even distribution of particles throughout the domain without the formation of gaps like those that occur with the TH discretization (Figure 1c).

The simple comparison in Figure 1 shows that, while stand-alone tracer advection algorithms are straightforward to implement, coupling them to a velocity solution may lead to significant artifacts. Here we demonstrate a holistic approach to chemical advection by tracers in geodynamic models using finite elements on 2D triangular meshes. This approach is straightforward to extend to 3D tetrahedral meshes. Our new approach requires us to reconsider the discretization of the entire system of equations. In the remainder of this paper we will demonstrate each stage individually: the advection of the tracers; the projection of their data to a chemical composition field in a conservative manner; and the appropriate spatial approximation of the velocity field such that it inherently satisfies the incompressibility constraint of the Stokes system of equations, overcoming spurious particle drift.

Advection of the composition field using tracers requires the solution of an ordinary differential equation (ODE) for each tracer in the domain. These ODEs may be discretized and numerically integrated using any appropriate method. In this work we will use (but are not limited to) flexible arbitrary order Runge–Kutta (RK) methods. We provide a brief overview of these methods in section 3.

Before solving the Stokes system we must project the tracer data to a mesh-based composition field. In section 4 we focus on the least squares projection, which preserves optimal error convergence during mesh refinement (Maljaars et al., 2018; Thielmann et al., 2014). However, it does not satisfy mass conservation so we exploit the partial differential equation (PDE) constrained least squares projection (Maljaars et al., 2019, 2020), which allows us to enforce both global and local conservation properties on the composition field (section 4.2). We provide a brief summary of tracer projection methods in Table 1.

A key benefit of this tracer projection approach is its treatment of tracer data as a point-wise approximation of a continuous field. Contrary to the ‘Stokeslet’ method composed of Dirac delta sources, this approach allows us to both add and remove tracers mid-simulation without breaking local or global mass conservation when performing the PDE constrained projection. This is not demonstrated here as the carefully selected velocity discretization, resulting lack of particle drift and near uniform mesh resolution mean that all simulations are robust without the addition or removal of particles.

Numerous methods exist for the discretization of the Stokes system but we focus in this work on the finite element (FE) method due to its ability to manage complex geometries, viscosity models, and tools for error analysis (Brenner & Scott, 2010). We summarize some of the more frequently used FE methods used in geodynamics in Table 2 but focus here on methods that produce *pointwise divergence free* velocity fields. For tracer advection in incompressible flows this has the essential property of preventing tracer ‘drift’ as demonstrated in Figure 1c. Several methods exist with this property (e.g., Cockburn et al., 2007; Evans & Hughes, 2013; Guzmán & Neilan, 2014). In this work we exploit the new HDG method (Cockburn et al., 2010; Labeur & Wells, 2012; Rhebergen & Wells, 2018a) and compare its properties to the commonly used TH scheme.

After introducing the methods we test them in section 7 using a series of computational geophysics benchmarks from the literature. We examine the impact of each specific discretization method on the accuracy of the results with the goal of demonstrating how a holistic approach is necessary to maintain accuracy and consistency in a fully coupled tracer-based model.

2 Problem definition and geometry

Let Ω be the computational domain of spatial dimension $d=2$ which accurately represents the problem geometry, for example a mantle convection cell. Furthermore let $\partial\Omega$ be the boundary of this domain with outward pointing unit normal vector $\mathbf{n}$. A depiction of this discretization is shown in Figure 2. Given an initial time $t=0$ and final time t_F , we define the time interval $t \in \mathcal{I}_t := (0, t_F]$. Subject to appropriate boundary and initial conditions we seek the velocity, pressure, and chemical compositions fields, u, p and ϕ , of the coupled problem in $\Omega \times \mathcal{I}_t$

$$-\nabla \cdot (2\eta \dot{\underline{\underline{\epsilon}}}(\mathbf{u})) + \nabla p = \mathbf{f}, \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0, \quad (2)$$

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{u}\phi) = 0. \quad (3)$$

Here η is the viscosity, $\dot{\underline{\underline{\epsilon}}}(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^\top)$ is the rate of strain tensor and $\mathbf{f}$ is the momentum source.

To discretize the domain, we subdivide Ω into non-overlapping triangles which tessellate the geometry generating a conforming mesh. We write κ to denote a triangle in the mesh $\mathcal{T}$ such that $\mathcal{T} := \{\kappa\}$. We refer to each $\kappa \in \mathcal{T}$ as an element or cell in the mesh which has measured diameter h_κ , the maximum distance between two points in the cell. We also employ the notation h to indicate that a quantity has been discretized conforming to the

Table 1: Summary of tracer data projection methods. See also sections 1 and 4.

This work		
l_2 projection		Minimizes square distance between tracer data $(X(t), \Phi(t))$ and the composition field $\phi_h(\mathbf{x}, t)$. Does not guarantee conservation. For smooth functions error converges at the optimal rate $\mathcal{O}(h^{k+1})$. When projecting into a DG FE space requires only local solves on each element.
PDE-constrained l_2 projection		l_2 projection augmented by the PDE constraint of the advection equation. HDG discretization of the variational problem <i>exactly</i> conserves the composition function. Requires a global solve over the domain.
Not implemented here		
Dirac ‘Stokeslet’ source	delta	Direct application of point source data to the right hand side of the Stokes system. Does not satisfy regularity requirements of the FE scheme. Will reduce convergence rate of the error of the velocity FE approximation to $\mathcal{O}(h)$ (Scott, 1973; Houston & Wihler, 2012). Does not provide a field representation $\phi_h(\mathbf{x}, t)$ required by the viscosity model.
Dirac delta projection		L_2 projection of tracer data to an FE space. Same issue applies in the projection of Dirac delta functions to a composition field whose FE approximation error measured in the L_2 norm will be suboptimal at a rate $\mathcal{O}(h)$. Requires a global solve over the domain if projecting into a continuous FE space.

underlying mesh. Furthermore, each cell κ has a boundary $\partial\kappa$ with corresponding outward pointing unit normal vector $\mathbf{n}_\kappa$ (see Figure 2(b)).

3 Discretization of a field by tracer data

Consider the advection equation stated in equation (3). Instead of a field, $\phi(\mathbf{x}, t)$, we use a tracer method to make discrete pointwise approximations. In this setting, we generate N_p tracers in the domain Ω such that each tracer has position $\mathbf{x}_p(t) \in \Omega$, $p = 1, \dots, N_p$. We may therefore define the set of tracer positions X inside the domain

$$X(t) := \{\mathbf{x}_p(t)\}_{p=1}^{N_p}. \quad (4)$$

Each tracer may carry arbitrary numerical data. For example, we assign the p th tracer’s datum regarding the composition field value $\phi_p(t)$, $p = 1, \dots, N_p$. So we now define the composition data associated with the tracers

$$\Phi(t) := \{\phi_p(t)\}_{p=1}^{N_p}. \quad (5)$$

An example of the discretization of the field $\phi(\mathbf{x}, t)$ by the point coordinates $X(t)$ and the interpolated data $\Phi(t) = \{\phi_p(t) = \phi(\mathbf{x}_p(t), t)\}_{p=1}^{N_p}$ is shown in Figure 3.

It is important to note that in our field discretization implementation the tracer data have no associated physical mass or volume. It is the composition field itself that carries these physical data. Therefore by this method we may add or remove tracers as necessary with no concern for breaking mass or volume conservation. However, conservation of the field itself requires consideration which we address later in section 4.

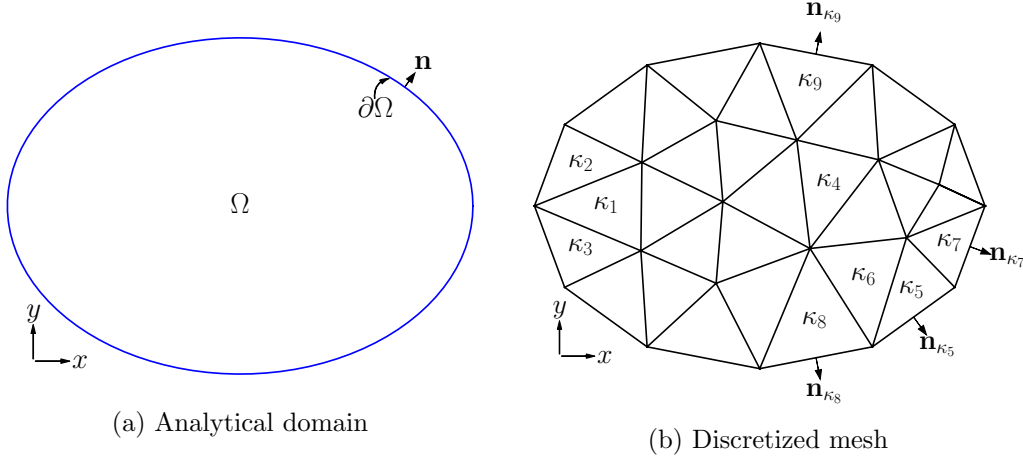


Figure 2: (a): An abstract domain Ω with boundary $\partial\Omega$ and outward pointing unit normal vector $\mathbf{n}$. (b): The discretization of Ω into a mesh comprised of tessellating triangles $\mathcal{T} = \{\kappa\}$. The first 10 triangles are labeled.

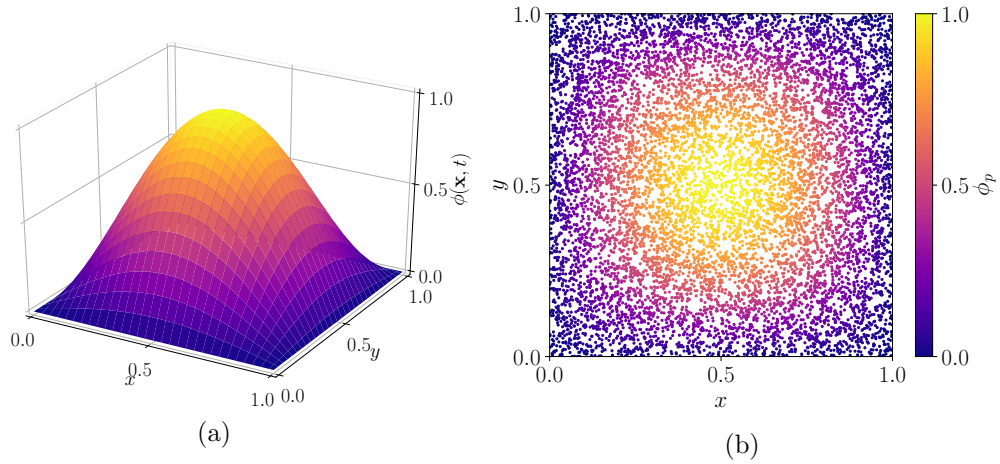


Figure 3: Pointwise discretization of a composition field by tracer data. (a): Example analytical composition field $\phi(\mathbf{x}, t)$. (b): Discretization of $\phi(\mathbf{x}, t)$ by interpolation to tracer data $\Phi(t) = \{\phi(\mathbf{x}_p, t)\}_{p=1}^{N_p}$ at positions $X(t)$.

Table 2: Summary of FE discretization schemes of the Stokes system used in this work. See also section 5 and supplementary section S3. We refer to Boffi et al. (2013) and the references cited therein for more information on FE pairs.

Demonstrated in main text	
TH	Velocity and pressure FE approximations converge at the optimal rates $\mathcal{O}(h^{p+1})$ and $\mathcal{O}(h^p)$ as measured in the L_2 norm. Globally satisfies the integral divergence free constraint $\int_{\Omega} \nabla \cdot \mathbf{u}_h \, d\mathbf{x} = 0$, however $\mathbf{u}_h$ is <i>not</i> pointwise divergence free.
HDG	Scheme coupling FE functions defined on both the cells and the facets. Velocity and pressure L_2 error converges at optimal rates. Yields a pointwise divergence free velocity approximation $\nabla \cdot \mathbf{u}(\mathbf{x}) = 0 \, \forall \mathbf{x} \in \Omega$. Can be formulated such that local components of the problem are eliminated before a global solve by static condensation.
Demonstrated in supplemental material	
DG	Nonconforming FE scheme permitting discontinuities in the solution. Velocity and pressure L_2 error converges at optimal rates. Enforces the divergence free constraint such that $\int_{\Omega} \nabla \cdot \mathbf{u}_h \, d\mathbf{x} = 0$ and $\int_{\kappa} \nabla \cdot \mathbf{u}_h \, d\mathbf{x} = 0, \kappa \in \mathcal{T}$. The resulting discontinuous velocity field $\mathbf{u}_h$ is incompatible with the PDE-constrained l_2 projection method. The degree of freedom count is typically much larger than conforming methods.
MINI	Velocity FE space enriched by the cubic vector bubble element. Allows equal order approximation of velocity and pressure ($p \geq 1$). Enforces the divergence free constraint in the global sense $\int_{\Omega} \nabla \cdot \mathbf{u}_h \, d\mathbf{x} = 0$.
P2BDG1	In some settings it is beneficial to have a discontinuous pressure approximation. This stable element pair combines the enriched velocity FE space of degree $p \geq 2$ of the MINI element with the $p-1$ degree FE DG space for the pressure. This element pair satisfies the divergence free constraint only in the global sense $\int_{\Omega} \nabla \cdot \mathbf{u}_h \, d\mathbf{x} = 0$.
P2DG0	Also permits a discontinuous pressure approximation by combining the standard $p \geq 2$ vector FE space for the velocity and $p-2$ DG FE space for the pressure. Although this yields a decrease in the number of degrees of freedom, the convergence rate of the velocity solution as measured in the L_2 norm is suboptimal $\mathcal{O}(h^p)$.

3.1 Time integration

The total derivatives of the tracer data subject to the advection equation read

$$\frac{d\phi_p}{dt} = 0, \quad (6)$$

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}(\mathbf{x}_p, t), \quad p = 1, \dots, N_p. \quad (7)$$

Clearly, once the initial composition data $\Phi(t=0)$ have been prescribed, equation (6) demands their values never change for $t > 0$. However, the approximation of the evolution of the tracers' positions should be computed from equation (7) by numerically integrating the N_p independent ODEs. See Figure 4 for a depiction of numerical advection of a tracer through a velocity field.

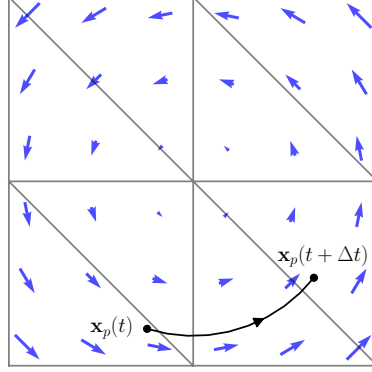


Figure 4: Example tracer advection through a velocity field. The blue arrows show a velocity field $\mathbf{u}_h(\mathbf{x})$ defined on an FE mesh. A tracer with position datum $\mathbf{x}_p(t)$ is advected to its new position at time step $\mathbf{x}_p(t + \Delta t)$.

The time derivative equation (7) must be integrated in order to compute the evolution of the tracer distribution. Precise time integration of the tracers is important to ensure a good approximation of the evolution of the composition field. In this work we will consider our implementation of the RK time integration method. We write $\text{RK}\ell$, with $\ell \in \mathbb{N}$ indicating the order of the method we use. For detailed analysis of RK methods we refer to Butcher (1987).

Given an initial time $t=0$ and final time t_F , we discretize the simulation time interval $\mathcal{I}_t$ into the points

$$\mathcal{I}_{\Delta t} = \{t_{n+1} : t_{n+1} = \min(t_n + \Delta t_n, t_F)\}. \quad (8)$$

The way in which Δt_n is chosen is a key factor in stability and accuracy of the RK method. Here we make our choice based on a form of the Courant–Friedrichs–Lewy (CFL) criterion

$$\Delta t_n = C_{\text{CFL}} \frac{h_{\min}}{\max_{\mathbf{x} \in \Omega} \mathbf{u}_h(\mathbf{x}, t_n)}, \quad (9)$$

where C_{CFL} is the constant CFL parameter and $h_{\min}$ is the smallest diameter measure of the mesh's cells. We refer to LeVeque (2007) for a comprehensive analysis of time integration methods.

3.2 Runge–Kutta method summary

The general form of the $\text{RK}\ell$ method is as follows: Find $\mathbf{x}_{p,n+1}$, $p = 1, \dots, N_p$ such that

$$\mathbf{x}_{p,n+1} = \mathbf{x}_{p,n} + \Delta t_n \sum_{i=1}^{\ell} b_i \mathbf{k}_{p,i} \quad (10)$$

where $\ell \geq 1$ and

$$\mathbf{k}_{p,i} = \mathbf{u}(\mathbf{x}_{p,n} + \Delta t_n \sum_{j=1}^{\ell} a_{ij} \mathbf{k}_{p,j}, t_n + \Delta t_n c_i). \quad (11)$$

The quantities a_{ij} , b_i and c_i are drawn from the so-called Butcher tableau (Butcher, 1987)

$$\begin{array}{c|ccc} c_1 & a_{11} & & \\ \vdots & \vdots & \ddots & \\ c_\ell & a_{\ell 1} & \cdots & a_{\ell \ell} \\ \hline & b_1 & \cdots & b_\ell \end{array} \quad (12)$$

Note that the $RK\ell$ method requires $\ell - 1$ computations of the Stokes FE solution. This expense should be considered when choosing the appropriate numerical method for the task at hand. The $RK\ell$ methods implemented for this work are shown in Table 3.

Table 3: The $RK\ell$ methods used in this work.

Method	Butcher tableau	Iteration
RK1	$\begin{array}{c c} 0 & 0 \\ \hline & 1 \end{array}$	$\mathbf{k}_{p,1} = \mathbf{u}(\mathbf{x}_{p,n}, t_n)$ $\mathbf{x}_{p,n+1} = \mathbf{x}_{p,n} + \Delta t_n \mathbf{k}_{p,1}$
RK2	$\begin{array}{c cc} 0 & 0 & \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$	$\mathbf{k}_{p,1} = \mathbf{u}(\mathbf{x}_{p,n}, t_n)$ $\mathbf{k}_{p,2} = \mathbf{u}(\mathbf{x}_{p,n} + \Delta t_n \mathbf{k}_{p,1}, t_n + \Delta t_n)$ $\mathbf{x}_{p,n+1} = \mathbf{x}_{p,n} + \frac{\Delta t_n}{2} (\mathbf{k}_{p,1} + \mathbf{k}_{p,2})$
RK3	$\begin{array}{c ccc} 0 & 0 & & \\ \frac{1}{2} & \frac{1}{2} & 0 & \\ \frac{3}{4} & 0 & \frac{3}{4} & 0 \\ \hline & \frac{2}{9} & \frac{1}{3} & \frac{4}{9} \end{array}$	$\mathbf{k}_{p,1} = \mathbf{u}(\mathbf{x}_{p,n}, t_n)$ $\mathbf{k}_{p,2} = \mathbf{u}(\mathbf{x}_{p,n} + \frac{1}{2}\Delta t_n \mathbf{k}_{p,1}, t_n + \frac{1}{2}\Delta t_n)$ $\mathbf{k}_{p,3} = \mathbf{u}(\mathbf{x}_{p,n} + \frac{3}{4}\Delta t_n \mathbf{k}_{p,2}, t_n + \frac{3}{4}\Delta t_n)$ $\mathbf{x}_{p,n+1} = \mathbf{x}_{p,n} + \Delta t_n \left(\frac{2}{9}\mathbf{k}_{p,1} + \frac{1}{3}\mathbf{k}_{p,2} + \frac{4}{9}\mathbf{k}_{p,3} \right)$
RK4	$\begin{array}{c cccc} 0 & 0 & & & \\ \frac{1}{2} & \frac{1}{2} & 0 & & \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & \\ 1 & 0 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array}$	$\mathbf{k}_{p,1} = \mathbf{u}(\mathbf{x}_{p,n}, t_n)$ $\mathbf{k}_{p,2} = \mathbf{u}(\mathbf{x}_{p,n} + \frac{1}{2}\Delta t_n \mathbf{k}_{p,1}, t_n + \frac{1}{2}\Delta t_n)$ $\mathbf{k}_{p,3} = \mathbf{u}(\mathbf{x}_{p,n} + \frac{1}{2}\Delta t_n \mathbf{k}_{p,2}, t_n + \frac{1}{2}\Delta t_n)$ $\mathbf{k}_{p,4} = \mathbf{u}(\mathbf{x}_{p,n} + \Delta t_n \mathbf{k}_{p,3}, t_n + \Delta t_n)$ $\mathbf{x}_{p,n+1} = \mathbf{x}_{p,n} + \Delta t_n \left(\frac{1}{6} (\mathbf{k}_{p,1} + \mathbf{k}_{p,4}) + \frac{1}{3} (\mathbf{k}_{p,2} + \mathbf{k}_{p,3}) \right)$

4 Projection of tracer data to a field

Let $\phi_h(\mathbf{x}, t)$ be the approximation of the true composition field $\phi(\mathbf{x}, t)$. With the tracer positions $X(t)$ and composition data $\Phi(t)$, we must define methods by which these data may be represented by $\phi_h(\mathbf{x}, t)$. We propose two methods here: the straightforward least squares (l_2) projection and the PDE-constrained l_2 projection. We summarize properties of these and other commonly used methods in Table 1.

4.1 Least squares projection

First we choose a finite dimensional space of functions $W^{h,k}$ which is composed of piecewise polynomials of degree k into which the tracer data will be projected. We will specify choices for this space after we have constructed the least squares projection operation. This l_2 projection minimizes the difference between the tracer data and its field projection in a least-squares sense. Given tracer positions $X(t)$ and composition data $\Phi(t)$, the l_2 projection operator corresponds to the following minimization problem: find $\phi_h(\mathbf{x}, t) \in W^{h,k}$ which satisfies

$$\min_{\phi_h \in W^{h,k}} \mathcal{J}(\phi_h) := \sum_p^{N_p} \frac{1}{2} (\phi_h(\mathbf{x}_p(t), t) - \phi_p(t))^2. \quad (13)$$

This corresponds to solving the following linear system: find $\phi_h(\mathbf{x}, t) \in W^{h,k}$ such that

$$\sum_{p=1}^{N_p} (\phi_h(\mathbf{x}_p(t), t) - \phi_p(t)) w_h(\mathbf{x}_p(t)) = 0 \quad (14)$$

216 for all $w_h \in W^{h,k}$.

We choose $W^{h,k}$ to be the nonconforming FE space of discontinuous piecewise polynomials, that is the standard DG FE space. We therefore write $W_{\text{DG}}^{h,k}$ to emphasize the space's characteristic and define it as follows

$$W_{\text{DG}}^{h,k} := \{v : v \text{ is square integrable in } \Omega \text{ and is composed of piecewise polynomials of degree } k \geq 0 \text{ defined on each } \kappa \in \mathcal{T}\}. \quad (15)$$

This choice offers a number of benefits. We may better approximate the discontinuity between composition phases compared with standard continuous spaces. Furthermore the linear system (14) may be written as a summation of local (i.e. cellwise) equations, that can be solved independently for each cell $\kappa \in \mathcal{T}$, i.e.: find $\phi_h(\mathbf{x}, t) \in W_{\text{DG}}^{h,k}$ such that

$$\sum_{\kappa \in \mathcal{T}} \sum_{p_\kappa=1}^{N_{p_\kappa}} (\phi_h(\mathbf{x}_{p_\kappa}(t), t) - \phi_{p_\kappa}(t)) w_h(\mathbf{x}_{p_\kappa}(t)) = 0 \quad (16)$$

217 for all $w_h \in W_{\text{DG}}^{h,k}$. Here N_{p_κ} is the number of tracers inside cell κ and $p_\kappa = 1, \dots, N_{p_\kappa}$ are
 218 the indices of the tracers which reside in the cell κ exclusively. This local solution method
 219 is typically more computationally efficient than solving the global system that would be
 220 generated by a standard continuous FE space.

221 In some geodynamical models we must constrain the composition function to reside
 222 within bounded limits. For example, $\phi_{\min} \leq \phi_h(\mathbf{x}, t) \leq \phi_{\max} \quad \forall \mathbf{x} \in \Omega$ where $\phi_{\min}$ and $\phi_{\max}$
 223 are minimum and maximum values permitted for ϕ_h , respectively. This is pertinent in the
 224 case $k \geq 1$ considering numerical oscillations will yield overshoots and undershoots in the
 225 projected composition field. See Goldfarb and Idnani (1983) for a background on quadratic
 226 programming for such problems. In our implementation we make use of `QuadProg++` to
 227 perform the box-constrained numerical optimization (Gaspero, 2020).

228 The l_2 projection scheme is not conservative. Hence, the composition field will incur a
 229 mass conservation error over time. To solve this issue we next exploit a PDE constrained l_2
 230 projection, recently introduced in Maljaars et al. (2019).

231 4.2 PDE-constrained projection

Consider again the minimization problem equation (13). We augment this problem with the constraint of the advection equation (3), so that the full problem reads: find $\phi_h(\mathbf{x}, t) \in W_{\text{DG}}^{h,k}$ which satisfies

$$\min_{\phi_h \in W_{\text{DG}}^{h,k}} \mathcal{J}(\phi_h) := \sum_p \frac{1}{2} (\phi_h(\mathbf{x}_p(t), t) - \phi_p(t))^2 \quad (17a)$$

$$\begin{aligned} \text{subject to: } & \frac{\partial \phi_h}{\partial t} + \nabla \cdot (\mathbf{u}_h \phi_h) = 0 & \text{in } \Omega, \\ & \phi_h = \phi_{\text{in}} & \text{on } \partial\Omega_{\text{in}}, \end{aligned} \quad (17b)$$

232 where $\partial\Omega_{\text{in}} = \{\mathbf{x} \in \partial\Omega : \mathbf{u}_h(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) < 0\}$ is the region of the exterior boundary where the
 233 velocity field flows into the domain Ω and ϕ_{in} is the prescribed incoming composition data
 234 on the inflow boundary. We also write $\partial\Omega_{\text{out}} = \partial\Omega \setminus \partial\Omega_{\text{in}}$ which is the outflow portion of
 235 the exterior boundary.

The implication is that the minimization problem now carries information regarding conservation of $\phi_h(\mathbf{x}, t)$ as the simulation evolves. In fact it can be shown that the HDG FE discretization of the system equation (17) *exactly conserves* ϕ_h globally and locally (to machine precision). We exploit this exact mass conservation property in this work and refer to Maljaars et al. (2019) for the details of this analysis.

For now, we will state the FE problem which solves the system equation (17). To formulate the HDG problem we require three FE spaces $W_{\text{DG}}^{h,k}$, T^h and $\bar{W}_{\text{DG}}^{h,k}$. Here $W_{\text{DG}}^{h,k}$ is the standard DG space of degree k , T^h is also a standard DG space of degree 0 (i.e. piecewise constants per cell¹) and $\bar{W}_{\text{DG}}^{h,k}$ is composed of piecewise polynomials of degree k defined on the facets of the mesh and discontinuous between facets. By multiplying equation (17b) with a Lagrange multiplier $\lambda_h \in T^h$ and applying integration by parts, which introduces an unknown flux $\bar{\phi}_h \in \bar{W}_{\text{DG}}^{h,k}$ on interior facets, the optimization problem amounts to finding the stationary points of the Lagrangian functional:

$$\begin{aligned} \mathcal{L}(\phi_h, \bar{\phi}_h, \lambda_h) = & \sum_p^{N_p} \frac{1}{2} (\phi_h(\mathbf{x}_p(t), t) - \phi_p(t))^2 \\ & + \int_{\Omega} \frac{\partial \phi_h}{\partial t} \lambda_h \, d\mathbf{x} - \sum_{\kappa \in \mathcal{T}} \int_{\kappa} \mathbf{u}_h \phi_h \cdot \nabla \lambda_h \, d\mathbf{x} \\ & + \sum_{\kappa \in \mathcal{T}} \int_{\partial\kappa \setminus \partial\Omega} \mathbf{u}_h \cdot \mathbf{n}_{\kappa} \bar{\phi}_h \lambda_h \, ds + \int_{\partial\Omega_{\text{out}}} \mathbf{u}_h \cdot \mathbf{n} \phi_h \lambda_h \, ds + \int_{\partial\Omega_{\text{in}}} \mathbf{u}_h \cdot \mathbf{n} \phi_{\text{in}} \lambda_h \, ds \\ & + \sum_{\kappa \in \mathcal{T}} \int_{\partial\kappa} \frac{1}{2} \beta (\bar{\phi}_h - \phi_h)^2 \, ds + \sum_{\kappa \in \mathcal{T}} \int_{\kappa} \frac{1}{2} \zeta (\nabla \phi_h)^2 \, d\mathbf{x}. \end{aligned} \quad (18)$$

Let us take a moment to examine the lines in equation (18). The first should be familiar from equation (17) arising from our desire to minimize the squared distance between the tracer values and the field approximation. The second and third lines are the HDG discretization of the weak formulation of the advection equation, i.e. the constraint PDE in equation (17). The first term in the final line arises from the HDG discretization where $\beta > 0$ is a parameter which prevents the problem from becoming singular when $\mathbf{u}_h \cdot \mathbf{n}_{\kappa} = 0$ by penalizing jumps between the field approximation defined on the cells ϕ_h and the facets $\bar{\phi}_h$. In all computations in this work we choose $\beta = 10^{-6}$. The final term introduces a gradient penalty parameter $\zeta \geq 0$. For $\zeta > 0$, this term penalizes the overshoot and undershoot oscillations which occur when approximating a discontinuous function of degree $p \geq 1$ where a discontinuity is not aligned with the mesh.

The FE approximation $(\phi_h, \bar{\phi}_h, \lambda_h) \in W_{\text{DG}}^{h,k} \times \bar{W}_{\text{DG}}^{h,k} \times T^h$ at the stationary points of equation (18) is computed by taking the Fréchet derivative and solving the resulting linear

¹ This choice is made as no discernible advantage is observed when employing higher order spaces (Maljaars et al., 2019).

system (Maljaars et al., 2019), that is, find $(\phi_h, \bar{\phi}_h, \lambda_h) \in W_{\text{DG}}^{h,k} \times \bar{W}_{\text{DG}}^{h,k} \times T^h$ such that

$$\begin{aligned} & \sum_{p=1}^{N_p} (\phi_h(\mathbf{x}_p(t), t) - \phi_p(t)) \delta\phi_h(\mathbf{x}_p(t)) - \sum_{\kappa \in \mathcal{T}} \int_{\partial\kappa} \beta (\bar{\phi}_h - \phi_h) \delta\phi_h \, \text{ds} \\ & + \int_{\Omega} \frac{\partial \delta\phi_h}{\partial t} \lambda_h \, \text{d}\mathbf{x} - \sum_{\kappa \in \mathcal{T}} \int_{\kappa} \mathbf{u}_h \cdot \nabla \lambda_h \delta\phi_h \, \text{d}\mathbf{x} + \int_{\partial\Omega_{\text{out}}} \mathbf{u}_h \cdot \mathbf{n} \lambda_h \delta\phi_h \, \text{ds} \\ & + \sum_{\kappa \in \mathcal{T}} \int_{\kappa} \zeta \nabla \phi_h \cdot \nabla \delta\phi_h \, \text{d}\mathbf{x} = 0, \end{aligned} \quad (19)$$

$$\begin{aligned} & \int_{\Omega} \frac{\partial \phi_h}{\partial t} \delta\lambda_h \, \text{d}\mathbf{x} - \sum_{\kappa \in \mathcal{T}} \int_{\kappa} \mathbf{u}_h \phi_h \cdot \nabla \delta\lambda_h \, \text{d}\mathbf{x} \\ & + \sum_{\kappa \in \mathcal{T}} \int_{\partial\kappa \setminus \partial\Omega} \mathbf{u}_h \cdot \mathbf{n}_{\kappa} \bar{\phi}_h \delta\lambda_h \, \text{ds} + \int_{\partial\Omega_{\text{out}}} \mathbf{u}_h \cdot \mathbf{n} \phi_h \delta\lambda_h \, \text{ds} + \int_{\partial\Omega_{\text{in}}} \mathbf{u}_h \cdot \mathbf{n} \phi_{\text{in}} \delta\lambda_h \, \text{ds} = 0, \end{aligned} \quad (20)$$

$$\sum_{\kappa \in \mathcal{T}} \int_{\partial\kappa \setminus \partial\Omega} \mathbf{u}_h \cdot \mathbf{n}_{\kappa} \lambda_h \delta\bar{\phi}_h \, \text{ds} + \sum_{\kappa \in \mathcal{T}} \int_{\partial\kappa} \beta (\bar{\phi}_h - \phi_h) \delta\bar{\phi}_h \, \text{ds} = 0, \quad (21)$$

for all $(\delta\phi_h, \delta\bar{\phi}_h, \delta\lambda_h) \in W_{\text{DG}}^{h,k} \times \bar{W}_{\text{DG}}^{h,k} \times T^h$. For numerical analysis details we refer to Maljaars et al. (2019), and for implementation and practical demonstration we refer to Maljaars et al. (in press). Although the algebra deriving this system appears daunting, the Unified Form Language (UFL) component of the FEniCS project facilitates automatic symbolic differentiation of forms like equation (18) (Alnæs et al., 2014). Furthermore we exploit the concept of static condensation by locally eliminating the unknowns ϕ_h and λ_h in favor of $\bar{\phi}_h$ on each element during matrix assembly. Therefore we only need solve for $\bar{\phi}_h$ in a global sense, thereby vastly reducing size of the underlying linear system.

A key result of this formulation is that we achieve local and global conservation of ϕ_h (Maljaars et al., 2019). Consider the component of the Fréchet derivative in all directions $\delta\lambda_h$ equation (20). To show global conservation we assign $\delta\lambda_h = 1$ to yield

$$\int_{\Omega} \frac{\partial \phi_h}{\partial t} \, \text{d}\mathbf{x} + \sum_{\kappa \in \mathcal{T}} \int_{\partial\kappa \setminus \partial\Omega} \mathbf{u}_h \cdot \mathbf{n}_{\kappa} \bar{\phi}_h \, \text{ds} + \int_{\partial\Omega_{\text{out}}} \mathbf{u}_h \cdot \mathbf{n} \phi_h \, \text{ds} + \int_{\partial\Omega_{\text{in}}} \mathbf{u}_h \cdot \mathbf{n} \phi_{\text{in}} \, \text{ds} = 0. \quad (22)$$

Since $\bar{\phi}$ is single valued across a facet, the flux at interior facets vanishes if $\mathbf{u}_h$ has continuous normal components across the facets, thus leaving us with the global conservation statement

$$\int_{\Omega} \frac{\partial \phi_h}{\partial t} \, \text{d}\mathbf{x} = - \int_{\partial\Omega_{\text{out}}} \mathbf{u}_h \cdot \mathbf{n} \phi_h \, \text{ds} - \int_{\partial\Omega_{\text{in}}} \mathbf{u}_h \cdot \mathbf{n} \phi_{\text{in}} \, \text{ds}. \quad (23)$$

This equation shows that the net change in ϕ over the domain Ω equals the total ingoing flux over the exterior boundary of the domain, thereby proving global mass conservation. Note that using nonconforming finite element methods such as standard DG FE to compute $\mathbf{u}_h$ will not inherently provide a $\mathbf{u}_h$ field with the necessary continuity requirements to obtain conservation of ϕ_h .

To show local conservation we assign $\delta\lambda_h = 1$ on κ and $\delta\lambda_h = 0$ on $\Omega \setminus \kappa$

$$\int_{\kappa} \frac{\partial \phi_h}{\partial t} \, \text{d}\mathbf{x} + \int_{\partial\kappa \setminus \partial\Omega} \mathbf{u}_h \cdot \mathbf{n}_{\kappa} \bar{\phi}_h \, \text{ds} + \int_{\partial\kappa \cap \partial\Omega_{\text{out}}} \mathbf{u}_h \cdot \mathbf{n} \phi_h \, \text{ds} + \int_{\partial\kappa \cap \partial\Omega_{\text{in}}} \mathbf{u}_h \cdot \mathbf{n} \phi_{\text{in}} \, \text{ds} = 0. \quad (24)$$

The change in the composition field ϕ_h in a cell κ is determined by the incoming and outgoing fluxes over the cell boundary $\partial\kappa$, thus demonstrating local conservation in terms of the numerical flux $\mathbf{u}_h \cdot \mathbf{n} \bar{\phi}_h$.

4.3 A θ -scheme (which may be independent of θ)

Consider the semi-discrete formulation of the PDE-constrained l_2 -projection equations (19) to (21). We discretize the time derivative using a θ scheme such that

$$\phi_h^{m+\theta} = \theta \phi_h^{m+1} + (1 - \theta) \phi_h^m \quad (25)$$

where $0 \leq \theta \leq 1$ such that the time derivative is approximated by

$$\frac{\partial \phi_h}{\partial t} \approx \frac{\phi_h^{m+1} - \phi_h^m}{\Delta t_m} \quad (26)$$

Furthermore we note that

$$\frac{\partial \delta \phi_h}{\partial t} \approx \frac{\delta \phi_h^{m+1} - \delta \phi_h^m}{\Delta t_m} = \frac{\delta \phi_h^{m+1}}{\Delta t_m}, \quad (27)$$

$$\delta \phi_h^{m+\theta} = \theta \delta \phi_h^{m+1} + (1 - \theta) \delta \phi_h^m = \theta \delta \phi_h^{m+1}, \quad (28)$$

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since the Fréchet derivative of the known quantity $\delta \phi_h^m$ has no variation.

The discrete system may therefore be written

$$\begin{aligned} & \sum_{p=1}^{N_p} \left(\phi_h^{m+1}(\mathbf{x}_p^{m+1}) - \phi_p \right) \delta \phi_h^{m+1}(\mathbf{x}_p^{m+1}) - \sum_{\kappa \in \mathcal{T}} \int_{\partial \kappa} \beta \left(\bar{\phi}_h^{m+1} - \phi_h^{m+1} \right) \delta \phi_h^{m+1} \, ds \\ & + \int_{\Omega} \frac{\delta \phi_h^{m+1}}{\Delta t_m} \lambda_h \, d\mathbf{x} - \theta \sum_{\kappa \in \mathcal{T}} \int_{\kappa} \mathbf{u}_h^{m+1} \cdot \nabla \lambda_h \delta \phi_h^{m+1} \, d\mathbf{x} + \theta \int_{\partial \Omega_{\text{out}}} \mathbf{u}_h^{m+1} \cdot \mathbf{n} \lambda_h \delta \phi_h^{m+1} \, ds \\ & + \sum_{\kappa \in \mathcal{T}} \int_{\kappa} \zeta \nabla \phi_h^{m+1} \cdot \nabla \delta \phi_h^{m+1} \, d\mathbf{x} = 0, \end{aligned} \quad (29)$$

$$\begin{aligned} & \int_{\Omega} \frac{\phi_h^{m+1} - \phi_h^m}{\Delta t_m} \delta \lambda_h \, d\mathbf{x} - \sum_{\kappa \in \mathcal{T}} \int_{\kappa} (\mathbf{u}_h \phi_h)^{m+\theta} \cdot \nabla \delta \lambda_h \, d\mathbf{x} \\ & + \sum_{\kappa \in \mathcal{T}} \int_{\partial \kappa \setminus \partial \Omega} \mathbf{u}_h^{m+1} \cdot \mathbf{n}_{\kappa} \bar{\phi}_h^{m+1} \delta \lambda_h \, ds + \int_{\partial \Omega_{\text{out}}} (\mathbf{u}_h \phi_h)^{m+\theta} \cdot \mathbf{n} \delta \lambda_h \, ds \\ & + \int_{\partial \Omega_{\text{in}}} (\mathbf{u}_h \phi_h)^{m+\theta} \cdot \mathbf{n} \delta \lambda_h \, ds = 0, \end{aligned} \quad (30)$$

$$\sum_{\kappa \in \mathcal{T}} \int_{\partial \kappa \setminus \partial \Omega_{\text{in}}} \mathbf{u}_h^{m+1} \cdot \mathbf{n}_{\kappa} \lambda_h \delta \bar{\phi}_h^{m+1} \, ds + \sum_{\kappa \in \mathcal{T}} \int_{\partial \kappa} \beta \left(\bar{\phi}_h^{m+1} - \phi_h^{m+1} \right) \delta \bar{\phi}_h^{m+1} \, ds = 0. \quad (31)$$

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Recall that we have made the choice that T^h is composed of piecewise constant values on the facets of the mesh. Therefore all terms including $\nabla \lambda_h$ and $\nabla \delta \lambda_h$ vanish. Furthermore, if $\mathbf{u}_h \cdot \mathbf{n} = 0$ on $\partial \Omega$ (as is common in geodynamical simulations), this leaves us with a formulation independent of θ .

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4.4 Number of tracers per cell

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We must carefully consider the number of tracers per cell required to obtain an accurate reconstruction of $\phi_h(\mathbf{x}, t)$ from the particle data. The minimum data per cell to construct $\phi_h(\mathbf{x}, t)$ is one tracer per FE degree of freedom defined on the element. This is clear when examining equation (16) since the linear system will be underdetermined should $N_{p_{\kappa}}$ be smaller than the local dimension of the approximating function space on κ , $\dim W_{\text{DG}}^{h,k}(\kappa)$. In essence we have the requirement that

$$N_{p_{\kappa}} \geq \dim W_{\text{DG}}^{h,k}(\kappa), \quad \kappa \in \mathcal{T}. \quad (32)$$

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Although this provides a minimum bound, in practice the authors find that $N_{p_{\kappa}} \geq 15(k+1)$ is robust over long simulation times.

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5 Finite elements for the Stokes system

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In the previous sections we established the methods by which the composition field will be approximated by tracer data. Specifically in section 3 we established time integration

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methods for tracer positions and in section 4 how we project the tracer data onto the composition field $\phi_h(\mathbf{x}, t)$. In this section we show how the velocity approximation will be computed in the ODE equation (7) by means of solving a Stokes system.

We discretize the momentum and continuity equations (1) and (2) with the FE method, seeking approximations of the velocity and pressure, $\mathbf{u}_h$ and p_h in the domain Ω , respectively. This is subject to the boundary conditions $\mathbf{u}_h = \mathbf{u}_D$ on $\partial\Omega_D$ and $(2\eta\dot{\underline{\underline{\epsilon}}}(\mathbf{u}) - p\underline{\underline{I}}) \cdot \mathbf{n} = \mathbf{g}_N$ on $\partial\Omega_N$ where $\underline{\underline{I}}$ is the identity tensor. Here, $\partial\Omega_D$ and $\partial\Omega_N$, are the subdivision of $\partial\Omega$ into non-overlapping Dirichlet and Neumann components, respectively, where $\partial\Omega_D$ is not empty ($\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$, $\partial\Omega_D \cap \partial\Omega_N = \emptyset$ and $\partial\Omega_D \neq \emptyset$).

There are numerous FE methods for approximating equations (1) and (2). We will present the TH and HDG methods. A small subset of other popular methods are discussed in supplementary section S3. Furthermore for each method we summarize and state salient properties in Table 2. For extended detail see the cited monographs and references therein.

5.1 Taylor–Hood

The TH method (Taylor & Hood, 1973) is a commonly used FE method for discretizing the incompressible Stokes system. In this setting we seek the velocity approximation $\mathbf{u}_h$ in the vector space $V^{h,p}$ which comprises functions of dimension d composed of piecewise polynomials of degree $p \geq 2$ defined on each element $\kappa \in \mathcal{T}$ and continuous in Ω . This is the ‘typical’ conforming and continuous FE vector space of functions. We further define $V_{BC}^{h,p} := \{\mathbf{v} \in V^{h,p} : \mathbf{v}|_{\partial\Omega_D} = \mathbf{u}_D\}$ and $V_{BC_0}^{h,p} := \{\mathbf{v} \in V^{h,p} : \mathbf{v}|_{\partial\Omega_D} = 0\}$ which are the continuous FE function spaces satisfying arbitrary Dirichlet boundary data $\mathbf{u}_D$ and homogenized boundary data, respectively. We also seek the pressure approximation p_h in the analogous scalar space of order $p - 1$, $Q^{h,p-1}$. The TH FE problem reads: find $(\mathbf{u}_h, p_h) \in V^{h,p} \times Q^{h,p-1}$ such that

$$\int_{\Omega} 2\eta\dot{\underline{\underline{\epsilon}}}(\mathbf{u}_h) : \dot{\underline{\underline{\epsilon}}}(\mathbf{v}_h) \, d\mathbf{x} - \int_{\Omega} p_h \nabla \cdot \mathbf{v}_h \, d\mathbf{x} = \int_{\Omega} \mathbf{f} \cdot \mathbf{v}_h \, d\mathbf{x} - \int_{\partial\Omega_N} \mathbf{g}_N \cdot \mathbf{v}_h \, d\mathbf{s} \quad (33)$$

$$- \int_{\Omega} q_h \nabla \cdot \mathbf{u}_h \, d\mathbf{x} = 0 \quad (34)$$

for all test functions $(\mathbf{v}_h, q_h) \in V_{BC_0}^{h,p} \times Q^{h,p-1}$.

5.2 Hybrid discontinuous Galerkin

Introduced in Labeur and Wells (2007); Cockburn and Gopalakrishnan (2009) and developed further in Cockburn et al. (2011); Cockburn and Sayas (2014); Nguyen et al. (2010), HDG methods have recently gained popularity (Labeur & Wells, 2012; Rhebergen & Wells, 2018a; Maljaars et al., 2018, 2019; Cockburn et al., 2010; Rhebergen & Wells, 2020). One of the most attractive characteristics of the HDG method for the Stokes system is that it lends itself to a *pointwise* divergence free velocity field approximation. By this we mean that

$$\nabla \cdot \mathbf{u}_h(\mathbf{x}, t) = 0 \quad \forall \mathbf{x} \in \Omega. \quad (35)$$

This is particularly important when using tracer methods in geodynamics where advection is dependent on pointwise evaluation of an incompressible velocity field.

The term ‘hybrid’ is used to imply that the HDG method is composed of FE functions drawn from FE spaces defined on the mesh cells and the mesh facets. We refer to Rhebergen and Wells (2020) for specific choices of these spaces, their analysis and properties. In this work we use the embedded discontinuous Galerkin (EDG) HDG formulation drawing on the advantage of a pressure-robust², $H(\text{div})$ -conforming³ and pointwise divergence free approx-

² The velocity error estimates do not depend on the pressure error (Rhebergen & Wells, 2020).

³ The divergence of the velocity is piecewise continuous (square integrable).

imation with reduced degree of freedom count in the velocity component of the global linear system compared to other HDG methods (see Rhebergen & Wells, 2020).

The velocity and pressure approximations are comprised of two components:

1. $\mathbf{u}_h$ and p_h are drawn from the vector FE space $V_{\text{DG}}^{h,\mathbf{p}}$ and scalar FE space $Q_{\text{DG}}^{h,\mathbf{p}-1}$, respectively, which are continuous on each element $\kappa \in \mathcal{T}$ and discontinuous in Ω , i.e. the standard DG spaces of degree $\mathbf{p}$ and $\mathbf{p}-1$, respectively.
2. $\bar{\mathbf{u}}_h$ and $\bar{p}_h$ are drawn from $\bar{V}^{h,\mathbf{p}}$ and $\bar{Q}_{\text{DG}}^{h,\mathbf{p}}$, respectively. Here $\bar{V}^{h,\mathbf{p}}$ is the vector space of piecewise polynomials of degree $\mathbf{p}$ defined on the facets of the mesh and *continuous* between facets, and $\bar{Q}_{\text{DG}}^{h,\mathbf{p}}$ is the scalar space composed of piecewise polynomials of degree $\mathbf{p}$ defined on the facets of the mesh and *discontinuous* between facets.

To enforce Dirichlet boundary conditions we modify the vector space defined on the facets such that it satisfies the boundary data $\bar{\mathbf{u}}_h|_{\partial\Omega_D} = \mathbf{u}_D$, i.e., $\bar{V}_{\text{BC}}^{h,\mathbf{p}} := \{\bar{\mathbf{v}} \in \bar{V}^{h,\mathbf{p}} : \bar{\mathbf{v}}|_{\partial\Omega_D} = \mathbf{u}_D\}$. Furthermore we define $\bar{V}_{\text{BC}_0}^{h,\mathbf{p}} := \{\bar{\mathbf{v}} \in \bar{V}^{h,\mathbf{p}} : \bar{\mathbf{v}}|_{\partial\Omega_D} = 0\}$.

The HDG FE formulation is as follows: find $(\mathbf{u}_h, \bar{\mathbf{u}}_h, p_h, \bar{p}_h) \in V_{\text{DG}}^{h,\mathbf{p}} \times \bar{V}_{\text{BC}}^{h,\mathbf{p}} \times Q_{\text{DG}}^{h,\mathbf{p}-1} \times \bar{Q}_{\text{DG}}^{h,\mathbf{p}}$ such that

$$-\sum_{\kappa \in \mathcal{T}} \int_{\kappa} \underline{\underline{\sigma}} : \nabla \mathbf{v}_h \, d\mathbf{x} + \sum_{\kappa \in \mathcal{T}} \int_{\partial\kappa} \hat{\underline{\underline{\sigma}}} \mathbf{n}_{\kappa} \cdot \mathbf{v}_h \, d\mathbf{s} + \sum_{\kappa \in \mathcal{T}} \int_{\partial\kappa} 2\eta (\bar{\mathbf{u}}_h - \mathbf{u}_h) \cdot \hat{\underline{\underline{\sigma}}}(\mathbf{v}_h) \mathbf{n}_{\kappa} \, d\mathbf{s} = \int_{\Omega} \mathbf{f} \cdot \mathbf{v}_h \, d\mathbf{x}, \quad (36)$$

$$\sum_{\kappa \in \mathcal{T}} \int_{\partial\kappa} \hat{\underline{\underline{\sigma}}} \mathbf{n}_{\kappa} \cdot \bar{\mathbf{v}}_h \, d\mathbf{s} = \int_{\partial\Omega_N} \mathbf{g}_N \cdot \bar{\mathbf{v}}_h \, d\mathbf{s}, \quad (37)$$

$$\sum_{\kappa \in \mathcal{T}} \int_{\kappa} \mathbf{u}_h \cdot \nabla q_h \, d\mathbf{x} - \sum_{\kappa \in \mathcal{T}} \int_{\partial\kappa} \mathbf{u}_h \cdot \mathbf{n}_{\kappa} q_h \, d\mathbf{s} = 0, \quad (38)$$

$$\sum_{\kappa \in \mathcal{T}} \int_{\partial\kappa} \mathbf{u}_h \cdot \mathbf{n}_{\kappa} \bar{q}_h \, d\mathbf{s} - \int_{\partial\Omega} \bar{\mathbf{u}}_h \cdot \mathbf{n} \bar{q}_h \, d\mathbf{s} = 0, \quad (39)$$

for all $(\mathbf{v}_h, \bar{\mathbf{v}}_h, q_h, \bar{q}_h) \in V_{\text{DG}}^{h,\mathbf{p}} \times \bar{V}_{\text{BC}_0}^{h,\mathbf{p}} \times Q_{\text{DG}}^{h,\mathbf{p}-1} \times \bar{Q}_{\text{DG}}^{h,\mathbf{p}}$. Here

$$\underline{\underline{\sigma}} = -2\eta \hat{\underline{\underline{\sigma}}}(\mathbf{u}_h) + p_h \underline{\underline{I}}, \quad (40)$$

$$\hat{\underline{\underline{\sigma}}} = -2\eta \hat{\underline{\underline{\sigma}}}(\mathbf{u}_h) + \bar{p}_h \underline{\underline{I}} - \frac{\alpha}{h_{\kappa}} 2\eta (\bar{\mathbf{u}}_h - \mathbf{u}_h) \otimes \mathbf{n}_{\kappa}, \quad (41)$$

are the stress tensor and stress tensor numerical flux, respectively, where h_{κ} is the measure of the cell diameter and α is a penalty parameter similar to those found in interior penalty methods (e.g. Lew et al., 2004) chosen in this work to be $\alpha=6\mathbf{p}^2$.

At first glance, the four equations appear to demand a large increase in computational expense when compared with the TH method. However the local components, $\mathbf{u}_h$ and p_h of equations (36) and (38), may be eliminated in favor of the global components $\bar{\mathbf{u}}_h$ and $\bar{p}_h$ by the process of static condensation. Regarding preconditioning of this global system we refer to Rhebergen and Wells (2018b).

5.3 Pointwise divergence free fields

In this section we define a measure of the error in the incompressibility of our discretized velocity field $\mathbf{u}_h$. Moreover we will briefly show why the HDG formulation yields a pointwise divergence free velocity approximation unlike the TH scheme.

We define the following error norm

$$\|\mathbf{u}_h\|_{\text{div}} := \|\nabla \cdot \mathbf{u}_h\|_{L_2(\Omega)} = \left(\int_{\Omega} (\nabla \cdot \mathbf{u}_h)^2 \, d\mathbf{x} \right)^{\frac{1}{2}} \quad (42)$$

which measures the square distance of the divergence of $\mathbf{u}_h$ from the desired divergence free value.

By the TH formulation equation (34) we have that $\int_{\Omega} q_h \nabla \cdot \mathbf{u}_h \, d\mathbf{x} = 0$ for all $q_h \in Q^{h,p-1}$. In order to fulfill $\|\mathbf{u}_h\|_{\text{div}} = 0$ we need to choose $q_h = \nabla \cdot \mathbf{u}_h$. However this choice does not satisfy the regularity constraint $q_h \in Q^{h,p-1}$ given that $\nabla \cdot \mathbf{u}_h \in Q_{\text{DG}}^{h,p-1}$. In essence q_h and $\nabla \cdot \mathbf{u}_h$ are continuous and discontinuous across the elements $\kappa \in \mathcal{T}$, respectively, so that condition equation (42) cannot be satisfied.

Now consider the HDG formulation of the continuity equation equation (38). Integrating by parts we have $\sum_{\kappa \in \mathcal{T}} \int_{\kappa} q_h \nabla \cdot \mathbf{u}_h \, d\mathbf{x} = 0$ for all $q_h \in Q_{\text{DG}}^{h,p-1}$. In this setting it is valid to make the choice $q_h = \nabla \cdot \mathbf{u}_h$ and the measure $\|\mathbf{u}_h\|_{\text{div}} = 0$ is satisfied. One may further use this argument to show that $\bar{\mathbf{u}}_h$ is also pointwise divergence free (see Rhebergen & Wells, 2018a).

6 Implementation and data availability

The code developed to run all the numerical experiments in this work is available in the public repository Sime (2020). The dependencies of the code are briefly discussed in this section. For portable deployment in a Docker container we refer to Hale et al. (2017) and Hale (2020).

The core finite element computations are performed using the components of the FEniCS project (Alnæs et al., 2015). The Lagrangian–Eulerian on Particles (LEoPart) library (Maljaars et al., in press) is used in conjunction with FEniCS for managing tracer data, Runge-Kutta numerical integration, l_2 projection, PDE-constrained l_2 projection, and static condensation HDG system assembly. We further exploit the techniques described in Houston and Sime (2018) for the automatic generation of DG and HDG formulations. The PETSc (Balay et al., 2019b, 2019a) library is used for its data structures for sparse numerical linear algebra in addition to the multifrontal parallel solver MUMPS (Amestoy et al., 2000) for the direct factorization of matrices.

7 Numerical experiments

We have now established the fundamentals to be used in our tracer advection numerical experiments. We will examine our implementation of each aspect of the discretization of the incompressible Stokes system Equations (1) to (3).

As a preliminary step we verify our FE implementation of the Stokes system and advection of tracers by the $\text{RK}\ell$ method. In supplementary section S4.1 we choose velocity and pressure solutions of the Stokes system *a priori* such that we may compute the error of their respective FE approximations. On a hierarchy of successively finer grids we observe this error to converge at optimal rates as predicted by FE analysis, verifying our implementation. In a similar fashion in supplementary section S4.2 we verify our implementation of tracer advection by the $\text{RK}\ell$ method.

With this foundation the projection of tracer data to a field by the l_2 and the PDE-constrained l_2 projection is verified in section 7.1. Incorporation of these projection schemes into a coupled system where a solution is known *a priori* is examined in section 7.2. With all of these methods verified, we proceed to solve the Rayleigh–Taylor problem benchmark showcased in van Keken et al. (1997) in section 7.3. We provide more extensive experimental results in the supplementary material in section S4.4, particularly applied to other frequently used FE schemes for the Stokes system as summarized in table 2.

Throughout this section we write ‘bounded/penalized’ projection to mean that we employ box-constrained optimization and the penalized gradient ($\zeta > 0$) methods in the case of

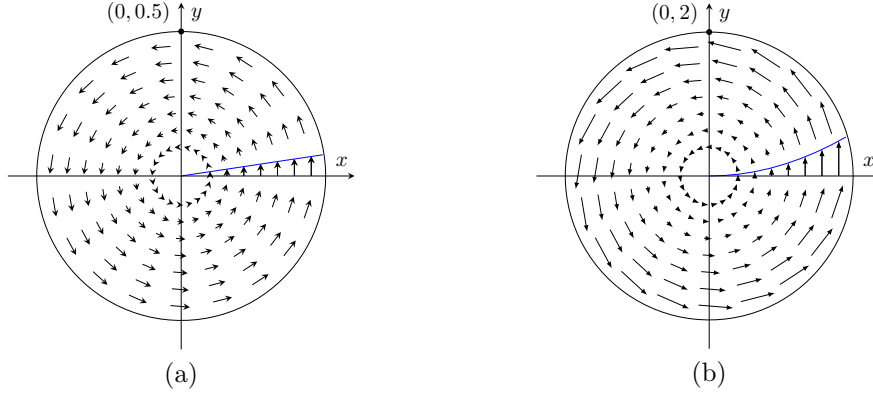


Figure 5: The domain Ω and manufactured velocity $\mathbf{u}(\mathbf{x}, t=0)$ used in (a) equation (43) and section 7.1 and (b) equation (47) and section 7.2. The blue line emphasizes linear and quadratic growth in flow speed with radius.

374 l_2 and PDE-constrained l_2 projection, respectively. See section 4.2 for details. Additionally
375 for each experiment we select $C_{\text{CFL}}=1$.

376 7.1 Tracer advection and projection to a field

377 With the Stokes system FE scheme and tracer advection verified (see supplementary
378 sections S4.1 and S4.2), we examine the projection of tracer data $X(t)$ and $\Phi(t)$ to a compo-
379 sition field representation. The manufactured examples in this section are inspired by those
380 shown in Maljaars et al. (2019). Here, two different sources of error are to be considered:

- 381 1. The temporal approximation of the tracers' positions.
- 382 2. The spatial approximation of the composition field representation.

Let Ω be the unit disc of radius $r=0.5$ centered at $r_0=(0,0)$. We define the rotational and time varying velocity field

$$\mathbf{u} = \begin{pmatrix} -y \\ x \end{pmatrix} \left(\cos^2 t + \frac{1}{2} \right). \quad (43)$$

This velocity field is shown in Figure 5 at $t=0$. It can be shown that the period of one rotation of any tracer in this velocity field occurs at $t=2\pi$. We examine two cases of a smooth and non-smooth composition field

$$\text{Smooth:} \quad \phi(\mathbf{x}, t) = \sin(2\pi x_\theta) \sin(2\pi y_\theta), \quad (44)$$

$$\text{Non-smooth:} \quad \phi(\mathbf{x}, t) = \begin{cases} 1 & \text{if } \theta_{\text{rot}} > 0, \\ 0 & \text{if } \theta_{\text{rot}} \leq 0, \end{cases} \quad (45)$$

where

$$\begin{aligned} \theta(\mathbf{x}, t) &= - \left(t + \frac{1}{4} \sin(2t) \right), \\ \begin{pmatrix} x_\theta \\ y_\theta \end{pmatrix} &= \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}, \\ \theta_{\text{rot}} &= \arctan2(y_\theta, x_\theta), \end{aligned} \quad (46)$$

383 and $\arctan2(\cdot, \cdot)$ is the standard two argument arctangent function (defined in supplemen-
384 tary section S1). The initial conditions $\phi(\mathbf{x}, t=0)$ in both cases are shown in Figure 6.

The smooth case is designed to test the error convergence rate of the projected tracer data through time. The non-smooth case gives an indication of the performance of the projection methods when modeling chemical phase interfaces by a discontinuity in the composition function. For example those which may require bounded/penalized projection to yield physically relevant composition field approximations to mitigate the impact of overshoots and undershoots (see sections 4.1 and 4.2).

We measure two components of the error in this experiment:

1. $\|\phi - \phi_h\|_{L_2(\Omega)}$: The spatial error of the composition field approximation,
2. $\epsilon_{\Delta\phi} = \int_{\Omega} (\phi_h(\mathbf{x}, t) - \phi_h(\mathbf{x}, 0)) \, d\mathbf{x}$: The mass conservation error.

We compute the projected composition over a period of one rotation for the smooth, non-smooth, and non-smooth and bounded/penalized functions (see Figure 6 for examples using the PDE-constrained projection). In the bounded/penalized case we use box-constrained optimization in the l_2 projection and we select $\zeta=25$ in our PDE-constrained l_2 projection operator. Per mesh cell we generate 25 tracers by drawing their initial positions from a random uniform distribution defined in the cell's geometry.

The error through time for each of the smooth and non-smooth cases is shown in Figure 7. Here we see in the smooth case that a comparison between the error using the l_2 and PDE-constrained l_2 projection methods is indistinguishable at this scale. In the case of l_2 projection method $\epsilon_{\Delta\phi}$ is converging. However, the difference in the mass conservation properties between the two methods is obvious as the PDE-constrained l_2 method conserves ϕ_h to machine precision.

In the non-smooth case the composition field approximation error from the l_2 and PDE-constrained l_2 projection methods is very similar. However, the $k=1$ and $k=2$ high order approximations show no great benefit over the low order $k=0$ approximation. This is expected as the interface discontinuity is not aligned with the mesh, yielding suboptimal convergence rates. See for example the four ‘dips’ in error corresponding to the interface discontinuity approximately lining up with the mesh constructed in our experiment. Despite this suboptimal convergence ϕ_h is conserved in the case of PDE-constrained l_2 projection by measurement of $\epsilon_{\Delta\phi}$. The l_2 projection shows no evidence of $\epsilon_{\Delta\phi}$ converging with increased approximation order.

In the non-smooth and bounded/penalized case we see similar results to the non-smooth and unbounded/unpenalized case. However, we have that the errors in the approximation of the composition field are slightly larger when using both projection methods.

The convergence properties in the smooth initial condition case after one rotation at time $t=2\pi$ are shown in supplementary Figure S5. Evidently we recover optimal rates and recover exact mass conservation $\epsilon_{\Delta\phi}$ when using the PDE-constrained projection. Not shown are the convergence properties of the non-smooth cases since the exact field is recovered at $t=2\pi$ in even the lowest order FE approximation.

7.2 Coupled manufactured solution

We have demonstrated and verified: the spatial approximation of the Stokes subsystem FE solution in supplementary section S4.1, the temporal approximation of the advected tracers’ positions in supplementary section S4.2 and the spatiotemporal approximation of the projection of the tracer values to a FE function representation in section 7.1.

Now we examine the fully coupled case where the tracers representing the composition data are advected based on the FE approximation of the Stokes subsystem, which in turn also depends on the projection of the tracer data onto an FE function space. Analytical

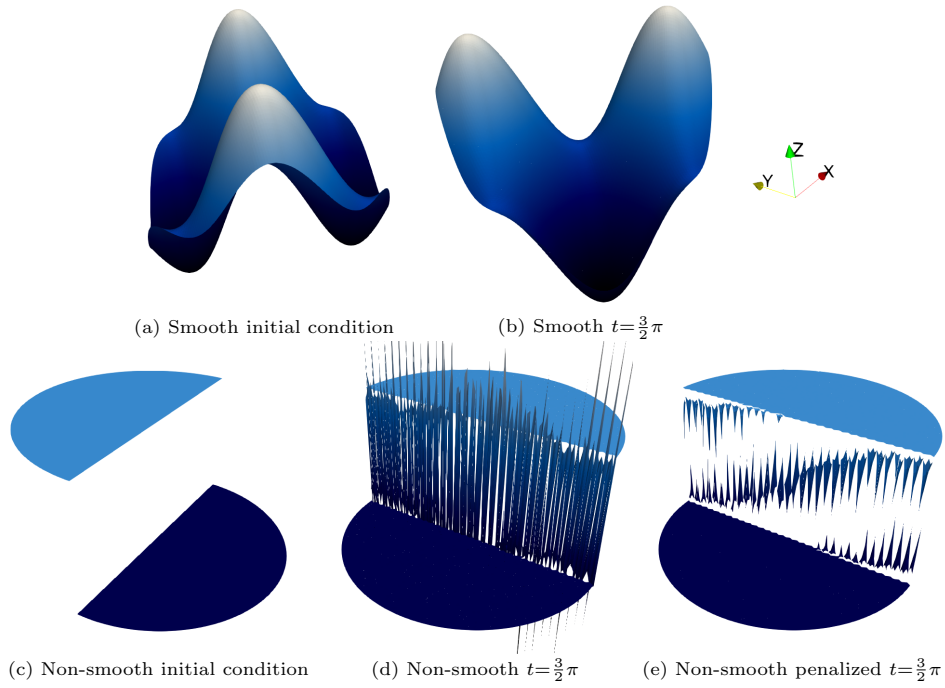


Figure 6: The smooth and non-smooth functions used in the manufactured field advection example in section 7.1. Shown are the initial $\phi_h(\mathbf{x}, t=0)$ and evolved $\phi_h(\mathbf{x}, t=\frac{3}{2}\pi)$ fields as computed by the PDE-constrained projection method where $k=2$. Note in (d) the non-smooth case projection yields large overshoots and undershoots. (e) Using a penalized gradient method ($\zeta=25$) reduces the severity of these overshoots and undershoots. The convergence of the error of these functions is quantified in Figure 7.

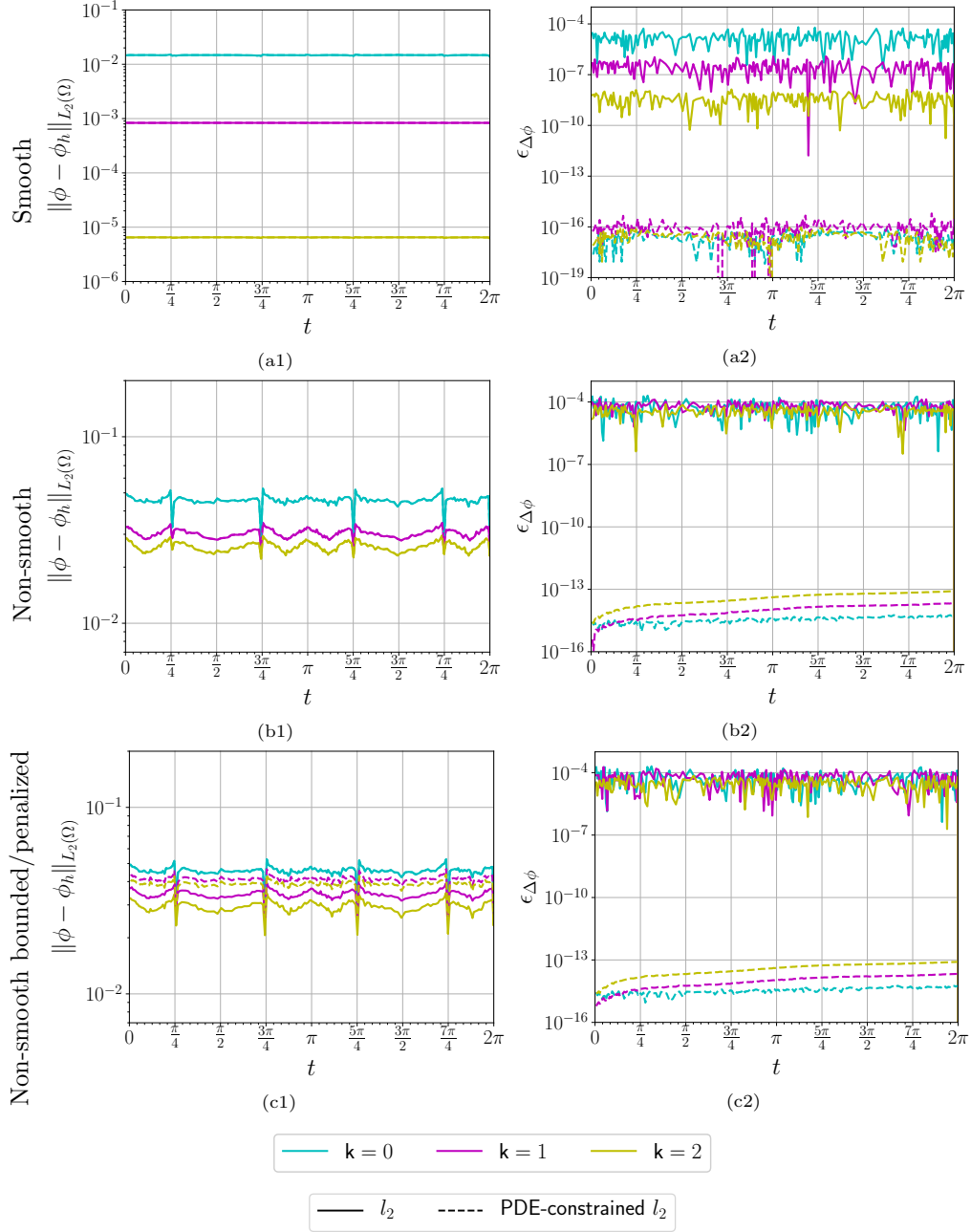


Figure 7: Computed error from the field advection manufactured solution experiment described in section 7.1. The left column shows composition field approximation error measured in the L_2 norm with time. The right column shows and mass conservation error with time. The disc geometry is discretized with a mesh such that $\max_{\kappa \in \mathcal{T}} h_\kappa \approx \frac{1.42}{32}$ and $\min_{\kappa \in \mathcal{T}} h_\kappa = \frac{1}{32}$. In (a1) and (b1) the L_2 error difference between l_2 and PDE-constrained l_2 projection is indistinguishable at this scale. This is also true in (c1) for the $k=0$ case. We show evidence for optimal convergence of the smooth function approximation in supplementary Figure S5. Projection of the non-smooth composition function is achieved with suboptimal convergence rates, to be expected from the inability to resolve the intraelement discontinuity. In (a2), (b2) and (c2) we achieve exact mass conservation by PDE-constrained projection (to machine precision), even when error convergence of the non-smooth composition field is suboptimal.

solutions for such problems are extremely difficult to derive in the context of geodynamics simulations. Therefore we manufacture the following problem.

Let $\Omega := \{(x, y) : \sqrt{x^2 + y^2} < 2\}$ be the disc of radius 2. We compute the FE approximation of the Stokes system (equations (1) and (2)) in Ω where we prescribe the velocity and pressure fields

$$\begin{aligned}\mathbf{u}(\mathbf{x}, t) &= \sqrt{x^2 + y^2} \begin{pmatrix} -y \\ x \end{pmatrix} \left(\cos^2 t + \frac{1}{2} \right), \\ p(\mathbf{x}, t) &= 0.\end{aligned}\tag{47}$$

Furthermore two composition functions are defined to be advected through the velocity field:

$$\text{Smooth:} \quad \phi(\mathbf{x}, t) = \exp \left(-\frac{(x_\theta - x_0)^2 + (y_\theta - y_0)^2}{2\xi} \right), \tag{48}$$

$$\text{Non-smooth:} \quad \phi(\mathbf{x}, t) = \begin{cases} 1 & \theta_{\text{rot}} > 0, \\ 0 & \theta_{\text{rot}} \leq 0. \end{cases} \tag{49}$$

Here, $\xi=0.1$, $(x_0, y_0)=(0.25, 0)$ is the initial center point of the Gaussian function and

$$\begin{aligned}\theta(\mathbf{x}, t) &= -\sqrt{x^2 + y^2} \left(t + \frac{1}{4} \sin(2t) \right), \\ \begin{pmatrix} x_\theta \\ y_\theta \end{pmatrix} &= \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}, \\ \theta_{\text{rot}} &= \arctan 2(y_\theta, x_\theta).\end{aligned}\tag{50}$$

The velocity field is shown in Figure 5(b) and the smooth and non-smooth composition functions are shown in Figure 8.

In the Stokes system we set the viscosity and momentum source to

$$\eta = 1, \quad \mathbf{f} = \mathbf{r} + \phi \hat{\mathbf{g}}, \tag{51}$$

where $\hat{\mathbf{g}}=(0, -1)^\top$ is the unit vector acting in the direction of gravity and

$$\mathbf{r} = \frac{3}{\sqrt{x^2 + y^2}} \begin{pmatrix} y \\ -x \end{pmatrix} \left(\cos^2 t + \frac{1}{2} \right) - \phi \hat{\mathbf{g}} \tag{52}$$

is the conservation of momentum equation residual of the true solution⁴.

We measure the following errors:

1. $\|\mathbf{u}(\mathbf{x}, t) - \mathbf{u}_h(\mathbf{x}, t)\|_{L_2(\Omega)}$: velocity field approximation error,
2. $\|\mathbf{u}_h(\mathbf{x}, t)\|_{\text{div}}$: divergence free constraint error,
3. $\|\phi(\mathbf{x}, t) - \phi_h(\mathbf{x}, t)\|_{L_2(\Omega)}$: composition field approximation error,
4. $\epsilon_{\Delta\phi} = \int_{\Omega} (\phi_h(\mathbf{x}, t) - \phi_h(\mathbf{x}, 0)) \, d\mathbf{x}$: mass conservation error.

Example solutions using the PDE-constrained projection at $t=\frac{\pi}{2}$, the error functionals computed in the simulation time domain $t \in \mathcal{I}_t = (0, \frac{\pi}{2}]$ and their convergence rates at final time $t=\frac{\pi}{2}$ are shown in Figures 8 to 10, respectively. Here we demonstrate the second order HDG ($p=1$, $k=1$, $\ell=2$) and third order HDG and TH ($p=2$, $k=2$, $\ell=3$) methods. In each case the initial tracer configuration is generated with 25 tracers per mesh cell where $X(t=0)$ is drawn from a random distribution defined on the cells' geometries.

In the case of the smooth composition field we observe optimal convergence rates of the numerical methods. However, in the non-smooth case the inability to represent the intraelement discontinuity in the composition function yields suboptimal convergence rates. These suboptimal results are expected and follow from our findings in section 7.1 and Figure 7.

⁴ We use the true value of ϕ in the construction of the residual, $\mathbf{r}$, prescribed by equations (48) and (49).

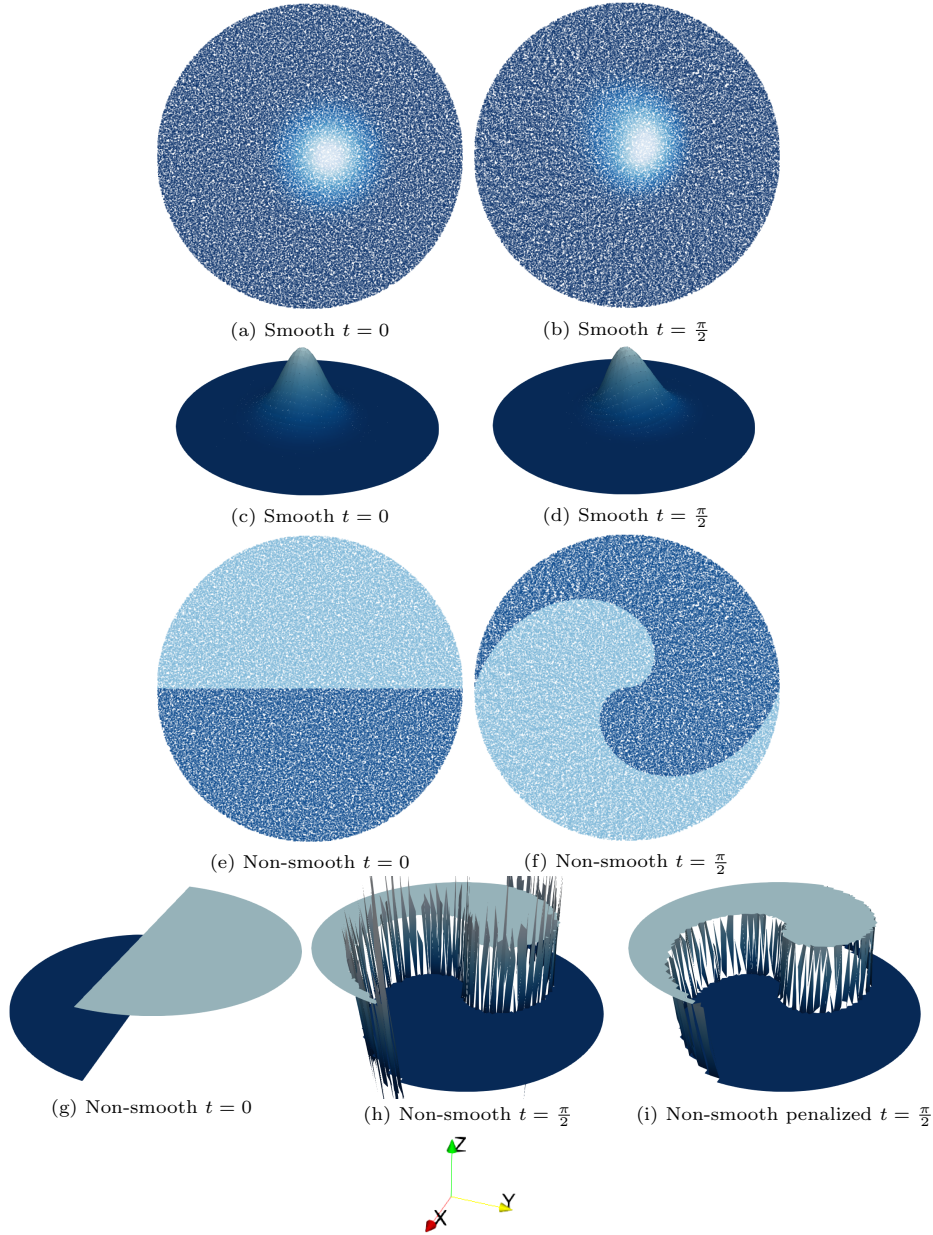


Figure 8: The smooth and non-smooth functions used in the manufactured solution example equations (48) and (49) described in section 7.2. Shown are the initial $t=0$ and evolved $t=\frac{\pi}{2}$ particle distributions $X(t)$, $\Phi(t)$, and fields $\phi_h(\mathbf{x}, t)$ computed by PDE-constrained projection. Note in (h) the non-smooth case with no penalization of the gradient in the projection ($\zeta=0$) yields large undershoots and overshoots. The convergence of the error of these functions is quantified in Figure 9.

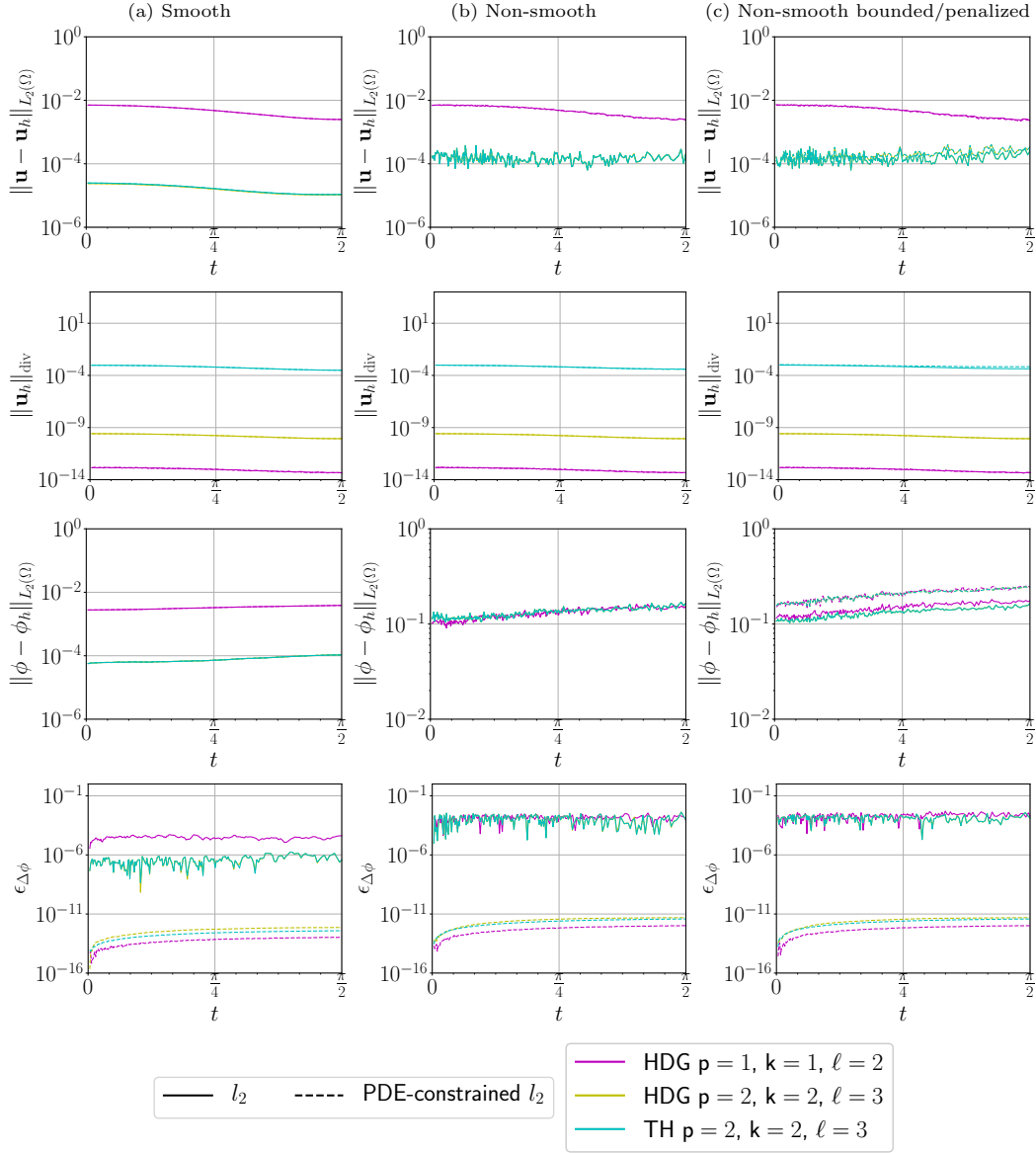


Figure 9: Coupled manufactured solution computed error. The disc geometry is discretized with a mesh such that $\max_{\kappa \in \mathcal{T}} h_{\kappa} \approx \frac{1.42}{32}$ and $\min_{\kappa \in \mathcal{T}} h_{\kappa} = \frac{1}{32}$. The velocity and composition field approximation errors using the third order HDG ($p=2$) and TH methods are indistinguishable at this scale. From the data in columns (b) and (c) we observe no benefit using higher order methods to approximate a discontinuous composition field. In all cases the PDE-constrained l_2 projection method preserves exact mass conservation and the HDG method provides pointwise divergence free velocity fields (to machine precision).

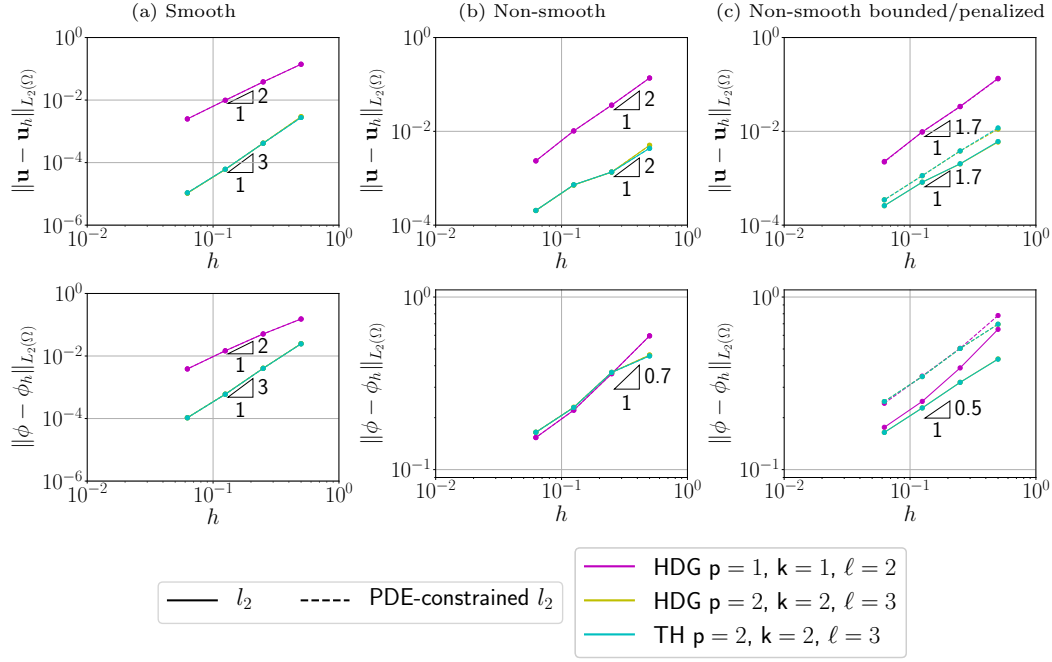


Figure 10: Coupled manufactured solution error functionals convergence rates measured at $t = \frac{\pi}{2}$. The cell measure here is selected such that $h = \min_{\kappa \in \mathcal{T}} h_{\kappa}$. The difference between the $p=2$ HDG and TH methods, in addition to the l_2 and PDE-constrained l_2 projection, are indistinguishable at this scale. (a) Optimal convergence rates are observed in the approximation of the smooth composition field. (b) Inadequate representation of intraelement discontinuities causes convergence rates to be suboptimal in the non-smooth case. (c) Use of bounded/penalized projection to alleviate impact of undershoots in the composition field projection has a small detrimental impact on convergence rates with the benefit of a more robust solver for the Stokes system.

7.3 Rayleigh–Taylor instability

In the previous section we demonstrated and validated: the exact conservation of the composition function; the pointwise divergence free velocity approximation; and the optimal convergence rates of the numerical approximation for smooth problems. We now turn to the Rayleigh–Taylor instability benchmark from van Keken et al. (1997) which is an example relevant to geodynamics simulations.

The Rayleigh–Taylor instability problem models the buoyancy driven evolution of a compositionally light material which initially resides below a compositionally denser layer. The chemical composition field is constructed such that $\phi=0$ and $\phi=1$ correspond to the immiscible light and dense materials, respectively. A key challenge lies in simulating the moving discontinuity at the interface between these immiscible materials.

In all of the numerical experiments in this section we employ bounded/penalized projection methods of the tracer data. As in the previous section, the initial tracers’ positions are drawn from a random distribution defined on the mesh cells’ geometries where we generate 25 tracers per mesh cell.

7.3.1 Problem definition

The domain Ω is the rectangle with bottom left and top right corners positioned at $(0, 0)$ and $(H=1, L=0.9142)$, respectively. The chemical composition function is constructed such that

$$\phi(\mathbf{x}, t) = \begin{cases} 0 & \forall x \in \text{light material}, \\ 1 & \forall x \in \text{dense material}. \end{cases} \quad (53)$$

The viscosity of the light and dense materials are the constant values η_{light} and η_{dense} , respectively. We construct the global viscosity function from the composition function such that

$$\eta = \eta_{\text{light}} + \phi (\eta_{\text{dense}} - \eta_{\text{light}}). \quad (54)$$

The initial state of the composition field introduces a perturbation of the system from equilibrium

$$\phi(\mathbf{x}, t = 0) = \begin{cases} 0 & y < d_b + \frac{1}{50} \cos\left(\frac{\pi x}{L}\right), \\ 1 & \text{otherwise}. \end{cases} \quad (55)$$

Here $d_b=0.2$ is the thickness of the initial compositionally light (buoyant) material layer.

The velocity boundary conditions are set as follows:

1. No flow condition $u=(0, 0)^\top$ on the top and bottom boundaries $y=0$ and $y=H$.
2. Free-slip condition $\mathbf{u} \cdot \mathbf{n}=0$ and $\left((2\eta\hat{\underline{\underline{e}}}(\mathbf{u}) - p\underline{\underline{I}}) \cdot \mathbf{n}\right) \cdot \boldsymbol{\tau}=0$ on the left ($x=0$) and right ($x=L$) boundaries, respectively, where $\boldsymbol{\tau}$ is a unit vector tangential to the boundary.

The momentum source is prescribed such that $\mathbf{f}=\phi\hat{\mathbf{g}}$, where $\hat{\mathbf{g}}=(0, -1)^\top$ is the unit vector acting in the direction of gravity.

7.3.2 Computed snapshots

The mesh of triangles is constructed from 160×160 equally spaced and bisected quadrilaterals. This mesh is then displaced to approximately align the facets with the discontinuity required by the initial condition equation (55). Each triangle is initially seeded with 25 tracers giving rise to a total of $N_p = 1\,280\,000$ tracers in the domain. The initial tracer data is assigned by pointwise interpolation of equation (55), i.e. $\Phi(t = 0) = \{\phi(\mathbf{x}_p(t = 0), t = 0)\}_{p=1}^{N_p}$.

In Figure 11 the Stokes system is discretized by the $p=1$ HDG scheme. The composition field is constructed by exploiting PDE-constrained l_2 projection of the tracer data onto the

$\mathbf{k} \in \{0, 1\}$ DG FE space. The time integration of the particle advection is computed using the RK3 method, although this order of accuracy is superfluous given the second order Stokes and composition field approximation.

In this first experiment we examine the cases where $\eta_{\text{dense}}=1$ and $\eta_{\text{light}} \in \{1, 0.1, 0.01\}$. We show the tracer distribution and projected composition field snapshots at time $t=1500$ in Figure 11 (Cf. van Keken et al., 1997).

7.3.3 The impact of a pointwise divergence free field

A key message of this work is the benefit of pointwise divergence free velocity field approximations yielded from HDG FE solutions. The initial tracer configuration which interpolates the initial condition equation (55) is shown in Figure 12. Also shown is the tracer distribution of the composition data computed from PDE-constrained l_2 projection method where the velocity field is approximated using either the TH or the HDG FE scheme at time $t \approx 634$ where $\eta_{\text{dense}} = 1$ and $\eta_{\text{light}} = 0.01$. This is the final time step after which the TH scheme fails due to the lack of sufficient tracer data in the mesh cells. This is evident from the large empty spaces in the tracer distribution using TH. We also see ‘bunching’ of the tracers close to the interface discontinuity. Compare this with the pointwise divergence free velocity approximation of the HDG FE scheme, in which the tracers remain well distributed owing to this numerical property.

7.3.4 Relative error convergence of functionals

We examine three viscosity contrast scenarios where $\eta_{\text{dense}} = 1$ and $\eta_{\text{light}} \in \{1, 0.1, 0.01\}$. Based on our findings in sections 7.1 and 7.2 we expect that sharp discontinuities in the composition field will have a negative impact on error convergence rates. The composition field appears in both the viscosity and momentum source terms in the Stokes system. Therefore we pay close attention to the difference in convergence rates in the smooth and non-smooth viscosity cases, $\eta_{\text{light}}=1$ and $\eta_{\text{light}} \in \{0.1, 0.01\}$, respectively.

The functional of interest is the root-mean-square velocity

$$u_{\text{rms}} = \sqrt{\frac{\int_{\Omega} \mathbf{u} \cdot \mathbf{u} \, d\mathbf{x}}{\int_{\Omega} d\mathbf{x}}}. \quad (56)$$

We measure u_{rms} at final time t_F where

$$t_F = \begin{cases} 100 & \eta_{\text{light}} = 1.0, \\ 50 & \eta_{\text{light}} = 0.1, \\ 10 & \eta_{\text{light}} = 0.01. \end{cases} \quad (57)$$

Using the computed numerical data we evaluate the relative error changes between mesh refinement levels where $\mathcal{T}$ is a mesh consisting of $m \in \{20^2, 40^2, 80^2, 160^2\}$ bisected quadrilaterals, evenly dividing the domain into $2m$ triangles. Inside each triangle 25 tracers per cell are generated to form the initial condition equation (55) such that there are 20 000, 80 000, 320 000 and 1 280 000 tracers in the mesh, respectively. In each case we use the PDE-constrained l_2 projection to generate the composition field representation of the tracer data. The relative error in our computation of u_{rms} is measured as follows

$$\epsilon_{\text{rel}}(u_{h,\text{rms}}) = \left| \frac{u_{h,\text{rms}} - u_{2h,\text{rms}}}{u_{h,\text{rms}}} \right|, \quad (58)$$

where $u_{h,\text{rms}}$ and $u_{2h,\text{rms}}$ correspond to fine and coarse approximations of u_{rms} on meshes with cell diameter h and $2h$, respectively, and $h = \min_{\kappa \in \mathcal{T}} h_{\kappa}$.

The computed root-mean-square velocity functional values with mesh (and implicitly time step by the CFL criterion) refinement are shown in supplementary Figure S6. The relative error is shown in Figure 13.

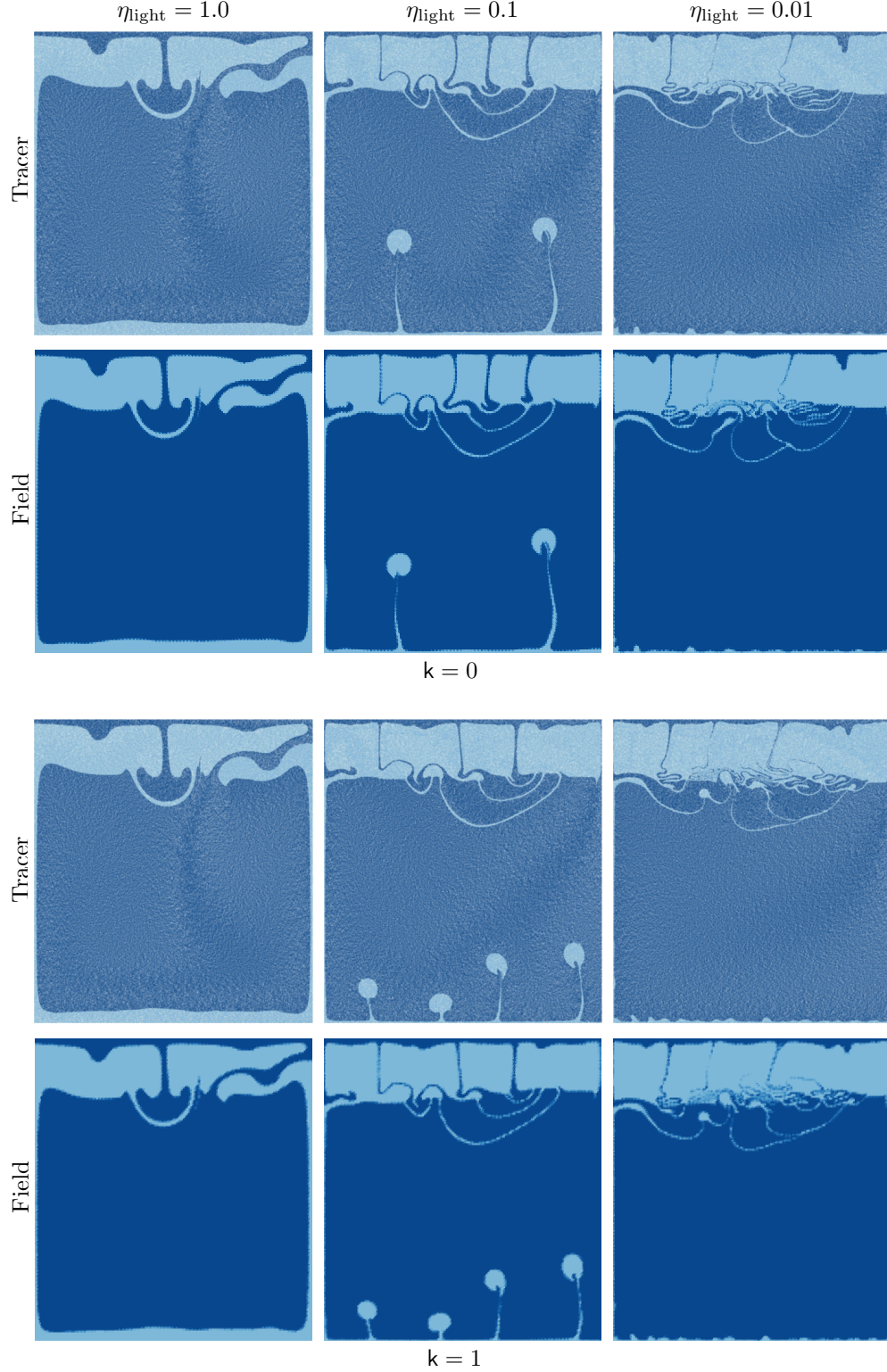


Figure 11: Snapshots of the Rayleigh–Taylor instability benchmark at $t=1500$ (Cf. van Keken et al., 1997). Shown are the tracer distributions, tracer data and their PDE-constrained l_2 projection onto the composition field space $W_{\text{DG}}^{h,k}$ of degree $k \in \{0, 1\}$. Dark and light colors correspond to dense ($\phi, \phi_p=1$) and light ($\phi, \phi_p=0$) material, respectively. In all cases the Stokes system is solved using the $p=1$ HDG scheme on a mesh of 160×160 bisected quadrilaterals with 1 280 000 tracers and $\eta_{\text{dense}}=1$. For more details see section 7.3.2.

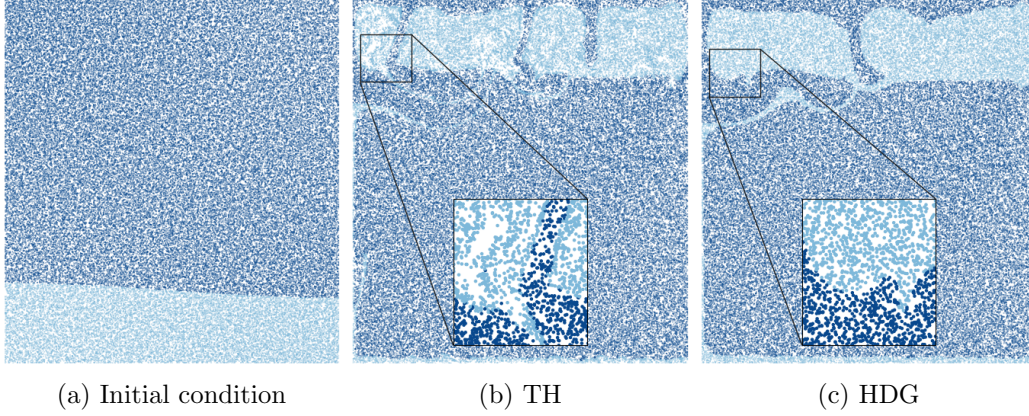


Figure 12: Tracer distribution in the Rayleigh–Taylor instability problem where $\eta_{\text{dense}}=1$ and $\eta_{\text{light}}=0.01$. Dark and light colors correspond to compositionally dense $\phi_p=1$ and light $\phi_p=0$, $p=1, \dots, N_p$, material, respectively. The mesh comprises 40×40 equally sized bisected quadrilaterals. Each triangle hosts 25 uniform randomly distributed tracers at its initial state giving rise to $N_p=80\,000$. (a) The initial condition equation (55), (b) the TH solution at time $t \approx 634$ where there are large empty spaces between tracers and ‘bunching’ close to the interface discontinuity, (c) the HDG solution at time $t \approx 634$ where the tracers have remained evenly distributed.

The convergence rates of the relative changes in error are suboptimal as expected from the inability to resolve intraelement discontinuities. The choice of $\ell \geq 2$ in the $\text{RK}\ell$ method plays only a small role in the approximation error. Although the RK4 method may appear to yield high order rates of convergence, in each case this is only featured in the $m=80$ and $m=40$ comparison. Examining the rates at $m=160$ the approximation error benefit of RK4 over its lower order counterparts is small considering its computational cost (three solutions of the Stokes equations).

Although the TH and HDG methods compare favorably at equivalent approximation order ($p=2$), one must bear in mind that over long time periods the TH results will be severely affected by the lack of a pointwise divergence free field approximation (see section 7.3.3 and Figure 12 for example). Evidently the higher order approximation of the composition field, $k=1$, offers no obvious advantage over the $k=0$ field representation. Although this is to be expected for the field representation of a discontinuity as examined in sections 7.1 and 7.2.

7.3.5 Comparison of Stokes finite element formulations

Here we provide a reference of the various FE methods for the Stokes system when used in the Rayleigh–Taylor instability benchmark. The mesh is generated as described in the previous section. With each FE discretization scheme we are interested in the error incurred by the divergence free velocity approximation $\|\mathbf{u}_h\|_{\text{div}}$ as well as the mass conservation error through time $\varepsilon_{\Delta\phi}$. We employ the RK3 method for time integration in all experiments in this section.

The functional of interest is again the root-mean-square velocity u_{rms} computed from the Stokes FE approximation equation (56). We set $\eta_{\text{dense}}=1$ and prescribe final time t_F

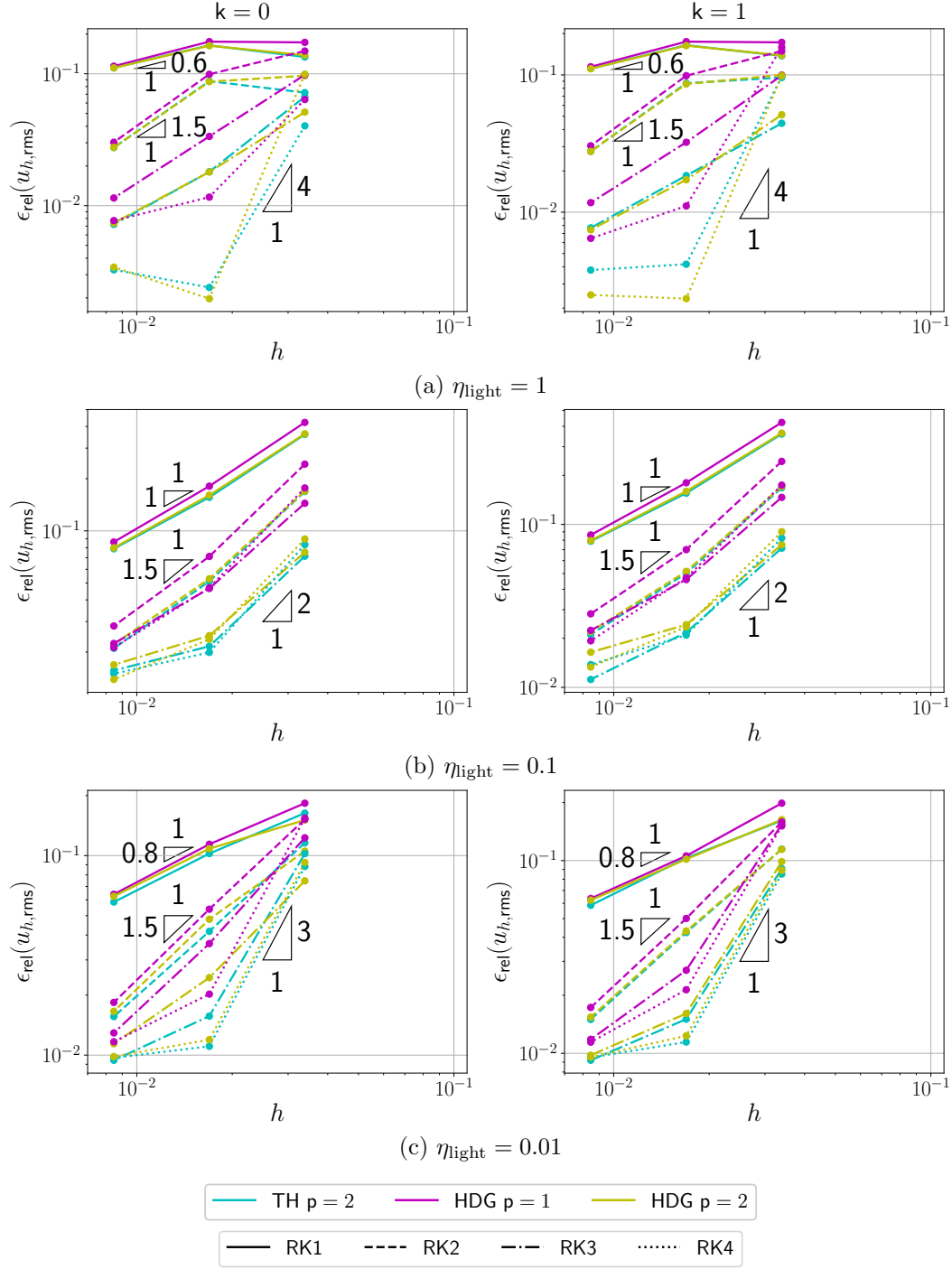


Figure 13: Measured relative error in u_{rms} computed from the Rayleigh–Taylor instability benchmark. Here we see we can best achieve approximately second order error convergence rates. The expense of higher order RK methods ($\ell \geq 3$) and composition field function spaces $k \geq 1$ is not warranted unless intraelement discontinuities may be precisely resolved. PDE-constrained l_2 projection is used to generate the composition field representation of the tracer data. The left and right columns show cases where the composition field function belongs to the $k = 0$ and $k = 1$ DG FE spaces, respectively.

and η_{light} according to

$$t_F = \begin{cases} 500 & \eta_{\text{light}} = 1, \\ 200 & \eta_{\text{light}} = 0.1, \\ 60 & \eta_{\text{light}} = 0.01. \end{cases} \quad (59)$$

These time intervals capture the period over which the bulk of the light material rises to the top of the domain showing large changes in u_{rms} . To see measured computations of u_{rms} over larger time intervals we refer to van Keken et al. (1997) and Maljaars et al. (in press).

We show results computed using $p=2$ TH and $p \in \{1, 2\}$ HDG FE schemes for the Stokes system. The cases where $k=0$ and $k=1$ are shown in Figures 14 and 15, respectively. Further results using other common FE schemes for the Stokes system (particularly those in table 2) are shown in supplementary section S4.4.

Some key observations are as follows:

1. Of the methods demonstrated, solely the HDG scheme offers pointwise divergence free velocity field approximations. One should expect that using a non-pointwise divergence free discretization would lead to failure over long time simulations as exhibited in section 7.3.3. In fact, we find that even over short time simulations the TH scheme for the Stokes system is insufficient as a robust solver for the Rayleigh–Taylor benchmark with tracers. Our implementation fails to complete the TH simulations successfully due to insufficient tracer data in mesh cells, even in the isoviscous $\eta_{\text{light}}=1$ case.
2. In the TH scheme, larger viscosity contrasts incur larger $\|\mathbf{u}\|_{\text{div}}$ error. This should be expected as rapid changes in viscosity will be difficult to resolve for a high order conforming FE method.
3. A comparison of the l_2 and PDE-constrained l_2 projection methods appear to yield only subtle differences in the evaluation of u_{rms} . However, using the non-conserving l_2 projection method breaks the physical law demanded by the conservation model.
4. Projection of the tracer data into the $k=1$ space appears to offer little to no benefit over the $k=0$ space. This is expected as discussed in section 7.1 for non-smooth composition fields.

8 Conclusion

Using the HDG Stokes and PDE-constrained l_2 tracer projection numerical scheme we have the following attractive properties:

1. Exact mass conservation of the composition field.
2. A pointwise divergence free velocity field which mitigates tracer dispersion.
3. Optimal convergence rates of the approximation error as measured in the L_2 norm provided regularity is satisfied.
4. The ability to add and remove tracers without worrying about conservation (not demonstrated here).

Acronyms

CFL	Courant–Friedrichs–Lewy
DG	discontinuous Galerkin
EDG	embedded discontinuous Galerkin
FE	finite element
HDG	hybrid discontinuous Galerkin
ODE	ordinary differential equation

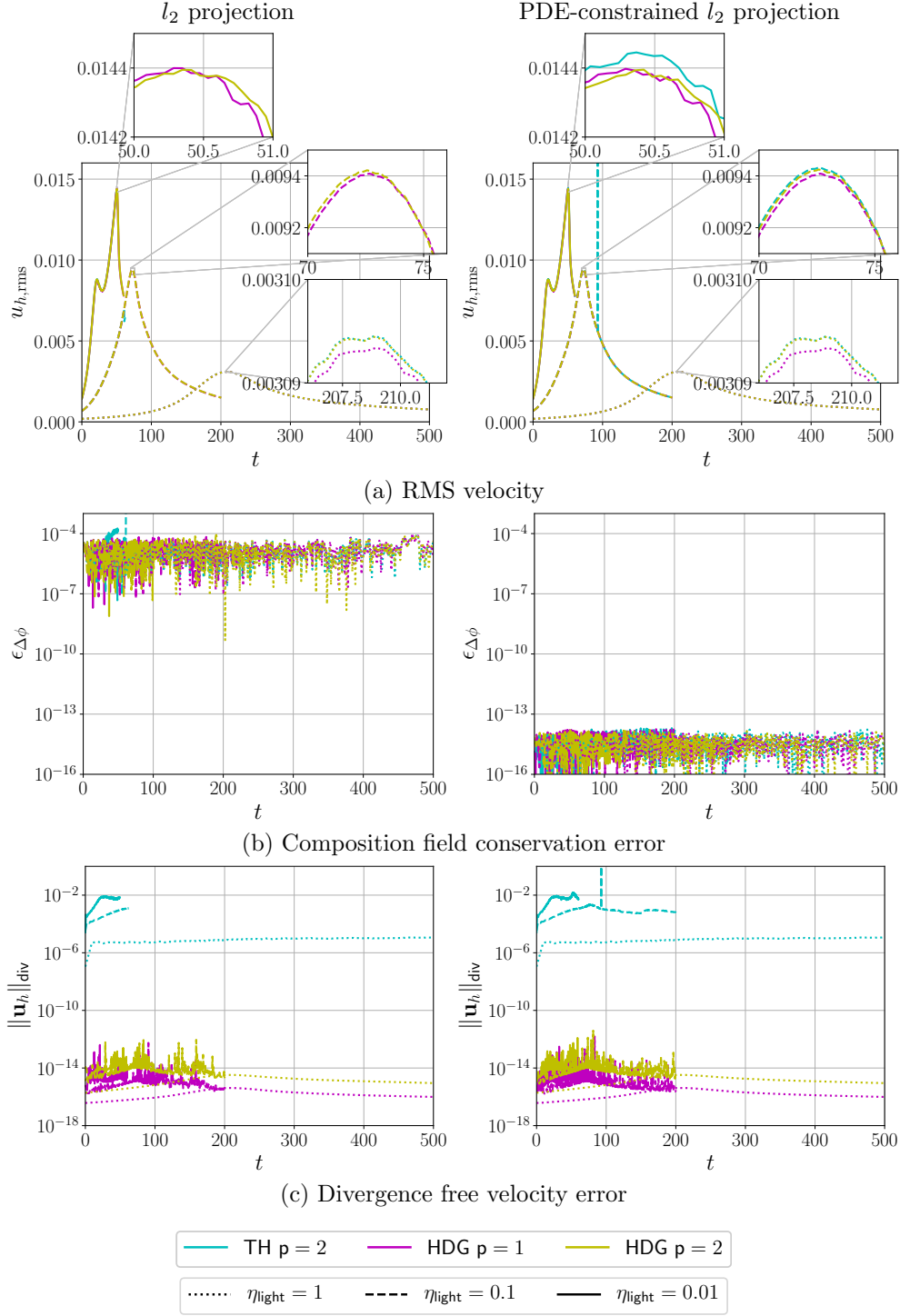


Figure 14: Rayleigh–Taylor instability benchmark data where $k=0$. Using the TH and HDG methods combined with l_2 and PDE-constrained l_2 projection we compare the evolution of: (a) the root mean square velocity, (b) the mass conservation error and (c) the error in the divergence free velocity constraint. In all cases we see that in (b) PDE-constrained projection provides exact mass conservation (to machine precision). Furthermore in (c) the HDG FE method provides pointwise divergence free velocity field approximations. The TH method does not provide a robust solution framework prematurely ending our simulations (Cf. Figure 12). See section 7.3.5 for details.

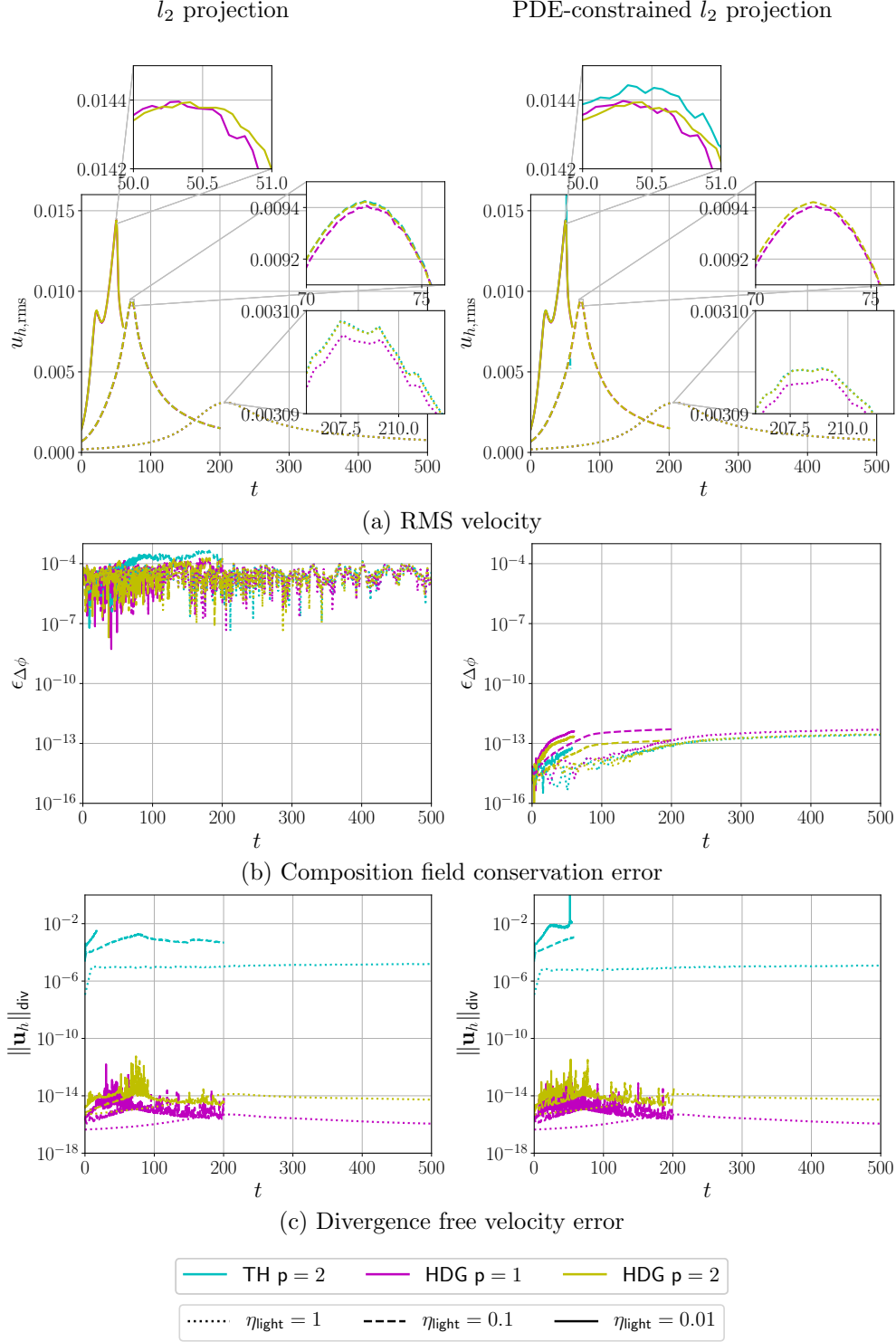


Figure 15: Rayleigh–Taylor instability benchmark data where $k = 1$. As in Figure 14 we compare the evolution of: (a) the root mean square velocity, (b) the mass conservation error and (c) the error in the divergence free velocity constraint in the TH and HDG methods. Again we see that in (b) and (c) that PDE-constrained projection provides exact mass conservation and the HDG FE method provides pointwise divergence free velocity field approximations to machine precision, respectively. See section 7.3.5 for details.

PDE partial differential equation

RK Runge–Kutta

TH Taylor–Hood

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The code developed to run all the numerical experiments in this work and a list of its dependencies is available in the public repository Sime (2020) (see section 6 for details).

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Supplementary Material

S1 Two argument tangent function

The two argument arctangent function is defined as follows

$$\arctan2(y, x) := \begin{cases} \arctan\left(\frac{y}{x}\right) & \text{if } x > 0, \\ \arctan\left(\frac{y}{x}\right) & \text{if } x < 0 \text{ and } y \geq 0, \\ \arctan\left(\frac{y}{x}\right) & \text{if } x < 0 \text{ and } y < 0, \\ \frac{\pi}{2} & \text{if } x = 0 \text{ and } y > 0, \\ -\frac{\pi}{2} & \text{if } x = 0 \text{ and } y < 0, \\ \text{undefined} & \text{if } x = 0 \text{ and } y = 0. \end{cases} \quad (\text{S1})$$

S2 Comparison of Taylor–Hood (TH) and hybrid discontinuous Galerkin (HDG) elements

A summary of the global degrees of freedom arising from the finite elements used by the TH and HDG schemes is depicted in Table S1.

S3 Other Stokes finite element schemes

In this section we provide a summary of the formulations for a small subset of other popular FE methods used to approximate the solution of the Stokes system. These formulations and corresponding finite element pairs are implemented and available in Sime (2020).

S3.1 MINI

Given two linear function spaces $\mathcal{U}$ and $\mathcal{W}$, we may define the new linear space $\mathcal{V}$ as the set of all functions which are derived from the linear sum of the two contributing spaces $\mathcal{U}$ and $\mathcal{W}$. I.e. $\mathcal{V} = \{v = u + w \text{ for all } u \in \mathcal{U} \text{ and } w \in \mathcal{W}\} = \mathcal{U} \oplus \mathcal{W}$.

The MINI element is constructed by defining $\mathcal{V}^{h,p} = V^{h,p} \oplus \mathcal{B}^{h,3}$ where $\mathcal{B}^{h,3}$ is the cubic vector bubble element. This yields the advantage of stable equal order polynomial approximation of both the (enriched) velocity and the pressure FE spaces. For example this allows us to choose $V^{h,p}$ and $Q^{h,p}$. We refer to Alnæs et al. (2015); Arnold et al. (1984) for details and implementation examples.

The FE problem reads: $(\mathbf{u}_h, p_h) \in \mathcal{V}^{h,p} \times Q^{h,p}$ such that equations (33) and (34) are satisfied for all $(\mathbf{v}_h, q_h) \in \mathcal{V}^{h,p} \times Q^{h,p}$.

S3.2 P2BDG1

In some geodynamical processes, a discontinuous or singular solution of the pressure field may be permissible. The P2BDG1 FE element comprises an enriched velocity and non conforming discontinuous pressure FE solutions. We seek $\mathbf{u}_h$ in the standard conforming vector FE space of functions enriched by cubic bubble functions, $\mathcal{V}^{h,2}$ as defined in section S3.1 where $\mathbf{p} = 2$. $Q_{\text{DG}}^{h,1}$ is the discontinuous space of scalar FE functions defined and linear in $\kappa \in \mathcal{T}$ with no requirement for continuity in Ω .

As in the previous sections, the FE problem reads: $(\mathbf{u}_h, p_h) \in \mathcal{V}^{h,2} \times Q_{\text{DG}}^{h,1}$ such that equations (33) and (34) are satisfied for all $(\mathbf{v}_h, q_h) \in \mathcal{V}^{h,2} \times Q_{\text{DG}}^{h,1}$. For details see Boffi et al. (2013).

TH	HDG	embedded discontin- uous Galerkin (EDG)-HDG	EDG
	$\bar{V}_{\text{DG}}^{h,1}$	$\bar{V}^{h,1}$	$\bar{V}^{h,1}$
			
	$\bar{Q}_{\text{DG}}^{h,1}$	$\bar{Q}_{\text{DG}}^{h,1}$	$\bar{Q}^{h,1}$
			
$V^{h,2}$	$\bar{V}_{\text{DG}}^{h,2}$	$\bar{V}^{h,2}$	$\bar{V}^{h,2}$
			
$Q^{h,1}$	$\bar{Q}_{\text{DG}}^{h,2}$	$\bar{Q}_{\text{DG}}^{h,2}$	$\bar{Q}^{h,2}$
			
$V^{h,3}$	$\bar{V}_{\text{DG}}^{h,3}$	$\bar{V}^{h,3}$	$\bar{V}^{h,3}$
			
$Q^{h,2}$	$\bar{Q}_{\text{DG}}^{h,3}$	$\bar{Q}_{\text{DG}}^{h,3}$	$\bar{Q}^{h,3}$
			

Table S1: The degrees of freedom arising in the global Stokes finite element (FE) problem on triangle elements. Here we assume the local degrees of freedom in the EDG/HDG problems have been eliminated by static condensation. Each dot corresponds to a global degree of freedom. Note that degrees of freedom defined on the triangles' facets and vertices are shared between neighboring elements and facets.

835 S3.3 Suboptimal P2DG0

836 One may formulate using a discontinuous pressure space without enriching the velocity
 837 space with bubble functions using the P2DG0 FE pair. The price paid however is suboptimal
 838 convergence of the FE approximation. The FE approximation of a standard TH element
 839 converges to the true solution at a rate of $\mathcal{O}(h^{p+1})$ when measured in the L_2 norm. In the
 840 case that we choose $Q_{\text{DG}}^{h,p-2}$ to be discontinuous and $V^{h,p}$ to be continuous with $p = 2$ we
 841 observe suboptimal convergence rates of $\mathcal{O}(h^p)$.

842 Despite these suboptimal convergence rates, the method may be attractive due to the
 843 reduced number of degrees of freedom arising in the underlying linear system, compared
 844 with the P2BDG1 method, for example. The FE problem reads: find $(\mathbf{u}_h, p_h) \in V^{h,2} \times Q_{\text{DG}}^{h,0}$
 845 such that equations (33) and (34) are satisfied for all $(\mathbf{v}_h, q_h) \in V^{h,2} \times Q_{\text{DG}}^{h,0}$. For details see
 846 Auricchio et al. (2004); Boffi et al. (2013).

847 S3.4 Discontinuous Galerkin

848 The discontinuous Galerkin (DG) method further removes the requirement that the
 849 velocity finite element space be composed of functions which are continuous in Ω . This
 850 provides some key benefits:

- 851 1. A richer space of functions in which the approximations $\mathbf{u}_h$ and p_h are sought.
- 852 2. Upwind stabilization as a component of the formulation leading to reduced suscepti-
 853 bility to numerical oscillations incurred by boundary layers.
- 854 3. Piecewise discontinuous approximation of functions.

855 However, these benefits come at a cost. The number of degrees of freedom in discontinuous
 856 Galerkin (DG) FE spaces is larger than conforming continuous FE spaces of the same
 857 polynomial order. Furthermore the variational formulation is complicated to implement since
 858 it contains interfacet flux terms. In this work we get around the implementation difficulty
 859 by using automatic generation of DG formulations using the `dolfin_dg` library (Houston &
 860 Sime, 2018).

Prior to stating the variational formulation we introduce some notation. We write $\mathcal{E}_I$
 to be the set of cell edges which reside on the interior of the mesh, i.e. $\mathcal{E}_I = \cup_{\kappa \in \mathcal{T}} \partial\kappa \setminus \partial\Omega$.
 On an interior edge, we arbitrarily label the neighboring cells κ^+ and κ^- . Given a function,
 w , which is continuous in both κ^+ and κ^- , and discontinuous on $\kappa^+ \cap \kappa^-$, we write $w^\pm$ to
 denote the evaluation of the trace of w from $\kappa^\pm$, respectively. We therefore define the jump
 and average operators

$$\llbracket \underline{\sigma} \rrbracket = \frac{1}{2} (\underline{\sigma}^+ + \underline{\sigma}^-), \quad \llbracket \mathbf{u} \rrbracket = \mathbf{u}^+ \otimes \mathbf{n}_\kappa^+ + \mathbf{u}^- \otimes \mathbf{n}_\kappa^-. \quad (\text{S2})$$

In the DG setting, $Q_{\text{DG}}^{h,p-1}$ is the scalar space of piecewise polynomials of degree $p - 1$,
 $p \geq 1$ defined on each element $\kappa \in \mathcal{T}$ with no requirement for their continuity in the global
 domain Ω . The vector space $V_{\text{DG}}^{h,p}$ is similarly defined by piecewise polynomials defined
 on $\kappa \in \mathcal{T}$ of degree p . There are many flavors of DG methods which are defined by their
 prescribed interelement flux functions. We will exploit the interior penalty Galerkin method:

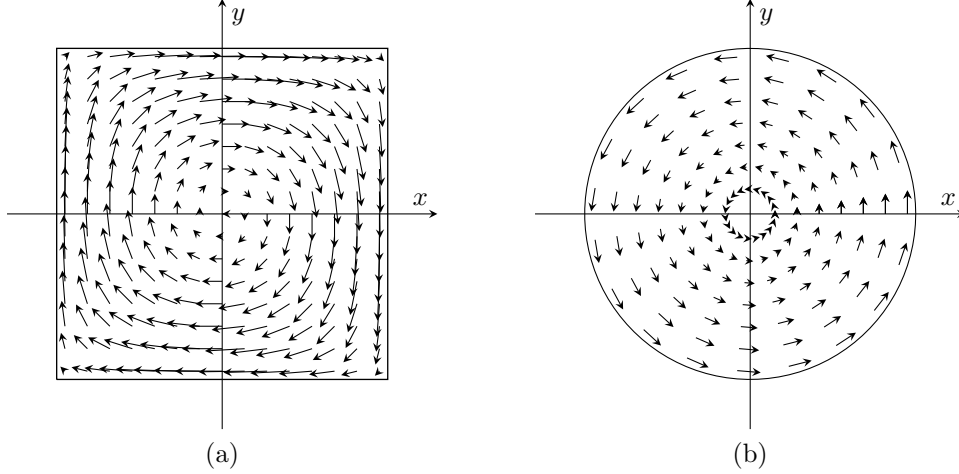


Figure S1: The domain Ω and manufactured velocity u used in (a) section S4.1 equation (S5), (b) sections S4.2 and 7.1 equation (S6) at time $t = 0$.

we seek $(\mathbf{u}_h, p_h) \in V_{\text{DG}}^{h,p} \times Q_{\text{DG}}^{h,p-1}$ such that

$$\begin{aligned} & \sum_{\kappa \in \mathcal{T}} \int_{\kappa} \underline{\underline{\sigma}}_h : \underline{\underline{\dot{\varepsilon}}}(\mathbf{v}_h) \, d\mathbf{x} - \sum_{e \in \mathcal{E}_I} \int_e \llbracket \mathbf{u}_h \rrbracket : \{2\eta \underline{\underline{\dot{\varepsilon}}}(\mathbf{v}_h)\} \, ds \\ & + \sum_{e \in \mathcal{E}_I} \int_e \{ \underline{\underline{\sigma}}_h \} : \llbracket \mathbf{v}_h \rrbracket \, ds + \sum_{e \in \mathcal{E}_I} \int_e \frac{C_{\text{IP}} p^2}{h_e} \{2\eta\} \llbracket \mathbf{u}_h \rrbracket : \llbracket \mathbf{v}_h \rrbracket \, ds \\ & + \mathcal{A}_{\partial\Omega}(\mathbf{u}_h, \mathbf{v}_h) = \int_{\Omega} \mathbf{f} \cdot \mathbf{v}_h \, d\mathbf{x}, \end{aligned} \quad (\text{S3})$$

$$\sum_{\kappa \in \mathcal{T}} \int_{\kappa} \mathbf{u}_h \cdot \nabla q_h \, d\mathbf{x} - \sum_{\kappa \in \mathcal{T}} \int_{\partial\kappa} \mathbf{u}_h \cdot \mathbf{n} q_h \, ds = 0, \quad (\text{S4})$$

for all $(\mathbf{v}_h, q_h) \in V_{\text{DG}}^{h,p} \times Q_{\text{DG}}^{h,p-1}$. Here $\underline{\underline{\sigma}}_h = 2\eta \underline{\underline{\dot{\varepsilon}}}(\mathbf{u}_h) - p_h \underline{\underline{I}}$ is the stress tensor where $\underline{\underline{I}}$ is the identity tensor, h_e is the length of the edge e , $C_{\text{IP}} > 0$ is the interior penalty parameter (chosen in this work to be $C_{\text{IP}} = 20$) and $\mathcal{A}_{\partial\Omega}(\cdot, \cdot)$ encapsulates the FE formulation associated with the weak imposition of boundary conditions on $\partial\Omega$ (see Houston and Sime (2018) for details). A summary of analysis of DG methods for elliptic FE problems is given in Arnold et al. (2001) and its application to the linear Stokes system in Cockburn et al. (2002).

Consider the partial differential equation (PDE)-constrained l_2 projection method of tracers shown in section 4.2. The lack of (normal) continuity of the DG FE function $\mathbf{u}_h$ on $\mathcal{E}_I$ is not consistent with the HDG numerical scheme for the projection. Therefore we should not expect to see optimal results in the case that $k > 0$. Indeed we observe this in our numerical experiments in section S4.4.

S4 Numerical methods verification

S4.1 Stokes system

Our first numerical experiment serves to demonstrate the spatial error convergence properties of the FE methods for the velocity approximation of the Stokes system listed in section 5. Let Ω be the square with bottom left and top right corners at positions $(-1, -1)$

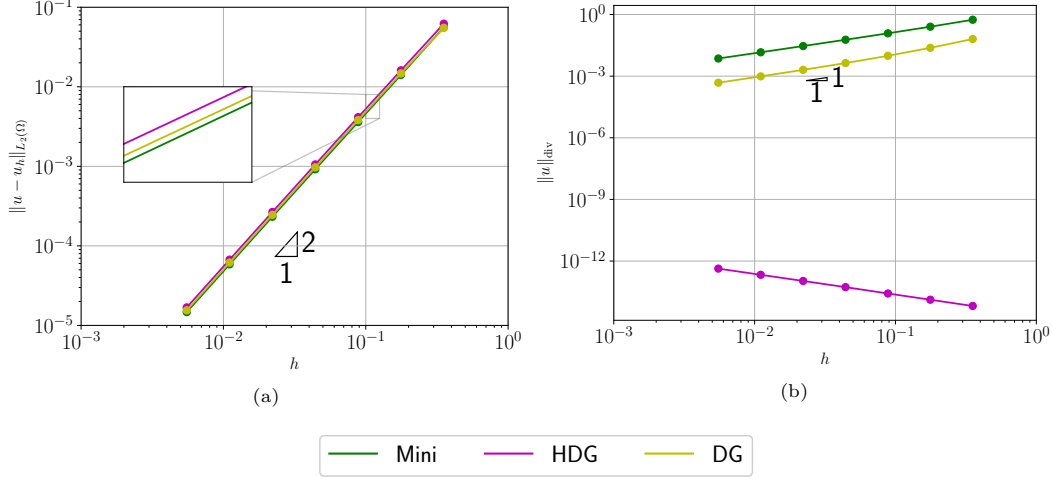


Figure S2: Convergence of the Stokes system discretized by second order FE methods ($p=1$) with h -refinement. (a) velocity FE solution error measured in L_2 norm, (b) FE velocity incompressibility error.

and $(1, 1)$, respectively. We manufacture the following solution

$$\mathbf{u} = \begin{pmatrix} 2y(1-x^2) \\ -2x(1-y^2) \end{pmatrix}, \quad p = 0, \quad (\text{S5})$$

which retains the properties $\mathbf{u} \cdot \mathbf{n} = 0$ on $\partial\Omega$ and $\nabla \cdot \mathbf{u} = 0$. Using this solution we construct the corresponding value of $\mathbf{f} = 4(y, -x)^\top$.

For each of the methods discussed in sections S3 and 5 we compute the FE approximation of the Stokes system equations (1) and (2) on a sequence of meshes of increasing resolution. We may then compare the FE approximation to the true solution to measure the error incurred by each method and its rate of convergence. These rates of convergence are then compared with theoretical results for validation.

The key functionals we measure are as follows:

1. $\|\mathbf{u} - \mathbf{u}_h\|_{L_2(\Omega)} = \sqrt{\int_{\Omega} (\mathbf{u} - \mathbf{u}_h)^2 \, \mathrm{d}\mathbf{x}}$: a measure of the distance of the FE approximation from the true solution.
2. $\|\mathbf{u}_h\|_{\text{div}} = \sqrt{\int_{\Omega} (\nabla \cdot \mathbf{u}_h)^2 \, \mathrm{d}\mathbf{x}}$: a global measure of the local deviation of the divergence free constraint of the continuity equation equation (2).

These functionals measured from the experiment data are shown for second order methods in Figure S2 and third order methods in Figure S3. Examining these results we see that each method converges at the rate expected according to theory. However we see one clear distinction from the HDG method. The measure of the HDG error $\|\mathbf{u}_h\|_{\text{div}}$ is zero within numerical tolerance of the functional's floating point evaluations.

S4.2 Tracer advection

In this numerical experiment we test the time integration of equation (7) using the $\text{RK}\ell$ method. Taking inspiration from van Keken et al. (1997) a single tracer is advected through a time varying velocity field known *a priori*. We compose a rotational velocity field which

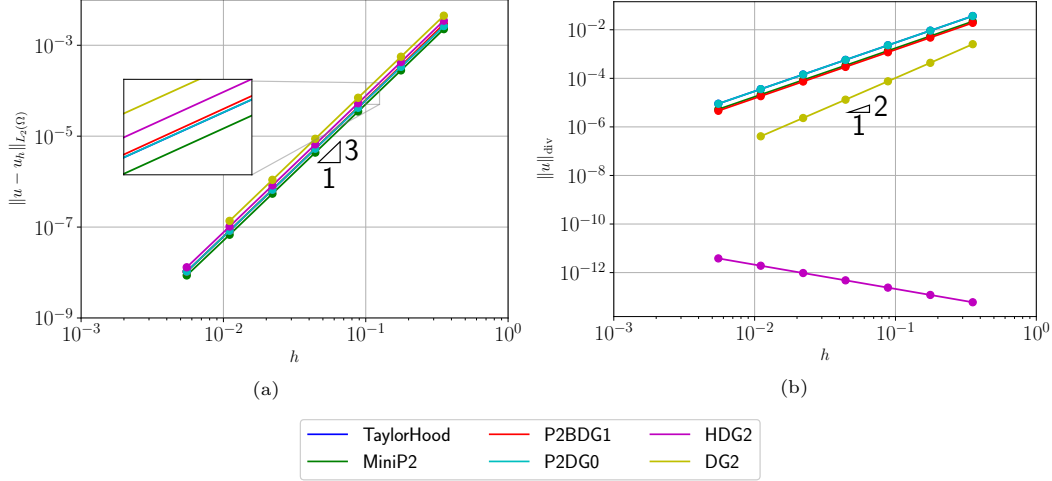


Figure S3: Convergence of the Stokes system discretized by third order FE methods ($p=2$) with h -refinement. (a) velocity FE solution error measured in L_2 norm, (b) FE velocity incompressibility error.

is exactly represented in a vector FE function space of degree $p \geq 1$. We may measure the error in the position of tracers advected in this field to ensure that the rates of convergence of the error match with the theory validating our implementation.

Let Ω be the unit disc of radius $r = 0.5$ centered at $r_0 = (0, 0)$. We define the rotational and time varying velocity field

$$\mathbf{u} = \begin{pmatrix} -y \\ x \end{pmatrix} \left(\cos^2 t + \frac{1}{2} \right). \quad (\text{S6})$$

This velocity field is shown in Figure S1 at $t=0$. It can be shown that the period of one rotation of any tracer in this velocity field occurs at $t=2\pi$.

We place a single tracer at position $\mathbf{x}_p(t=0) = (0.5, 0.0)$. We then advect this tracer through the velocity field for a period of one rotation. Its final position $\mathbf{x}_p(t=2\pi)$ is measured for comparison with the true solution using the following measure

$$\left\| \mathbf{x}_p(t=2\pi) - (0.5, 0.0)^T \right\|_2 = \sqrt{(\mathbf{x}_p(t=2\pi) - (0.5, 0.0)^T)^2}. \quad (\text{S7})$$

We expect the rate at which $\mathbf{x}_p(t=2\pi)$ converges to the true solution in the 2-norm measure to be the same as the order of the Runge–Kutta (RK) scheme we employ. We choose the time step size based on the Courant–Friedrichs–Lewy (CFL) criterion equation (9) which directly relates the time step size to the smallest measure of the mesh cells' diameters, $h_{\min}$. We can therefore present convergence rate results in terms of $h_{\min}$.

We construct a hierarchy of meshes based on refinements of an initial coarse mesh. On each of these meshes we solve the proposed experiment and choose $C_{\text{CFL}} = 1$. The results of our numerical experiment are shown in Figure S4. Indeed we find that our implementation exhibits expected error convergence rates.

S4.3 Tracer data projection

Error convergence data of the smooth composition field equation (44) approximation at simulation time $t = 2\pi$ is shown in Figure S5. See section 7.1 for details.

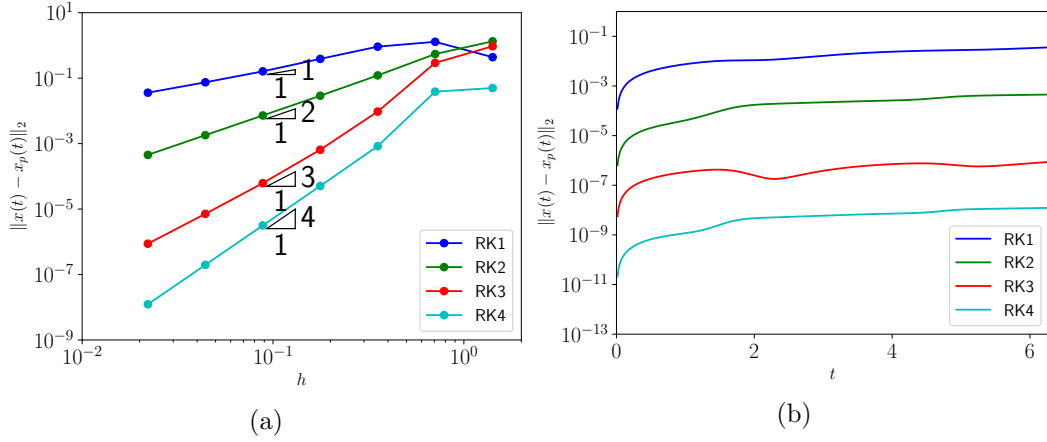


Figure S4: Convergence of the temporal integration of a tracer's path in a prescribed velocity field with h -refinement (and implicitly Δt refinement). (a) Convergence of tracer position error after one rotation measured in the 2-norm. (b) Measured 2-norm error of the tracer position through time where $h = 2.221 \times 10^{-2}$.

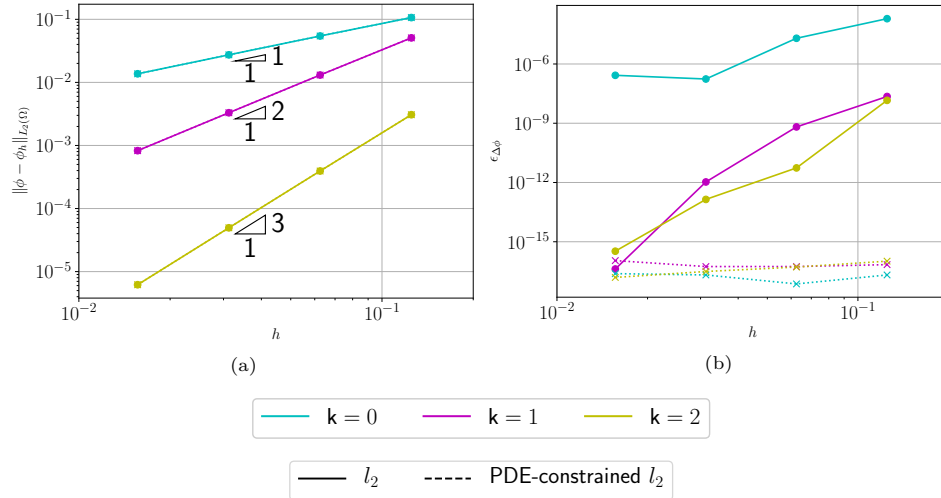


Figure S5: Error convergence data at time $t = 2\pi$ of the manufactured advection of the smooth initial data case. (a) The composition field error measured in the L_2 norm where the l_2 and PDE-constrained l_2 projection results are indistinguishable at this scale, (b) mass conservation error.

S4.4 Rayleigh–Taylor instability benchmark

Computed values of the u_{rms} functional at given times are shown in Figure S6. Additional results computed with various FE methods are provided for reference in Figures S7 to S12. These data serve as an extension of those shown in Figures 14 and 15.

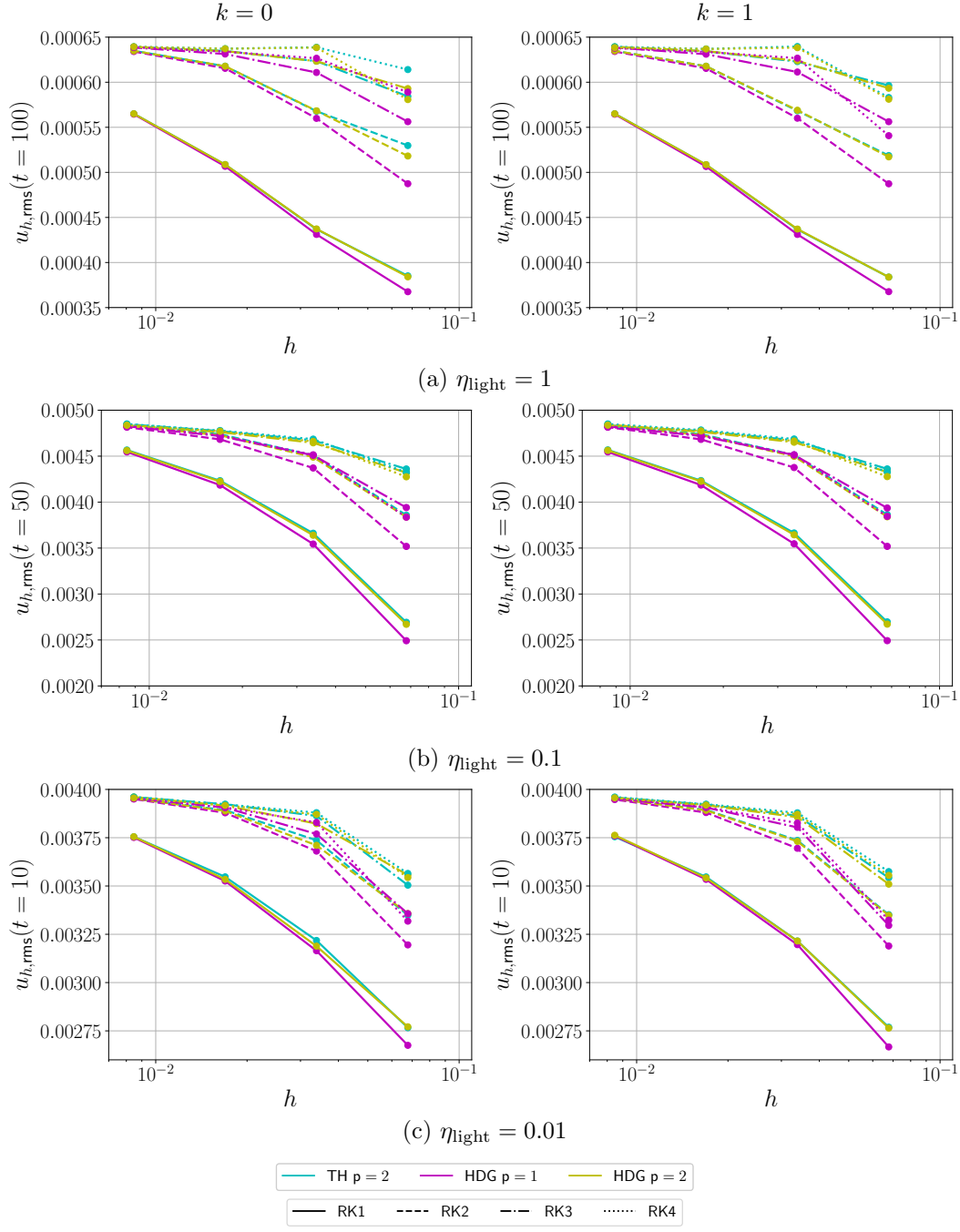


Figure S6: Measured root-mean-square velocities computed from the Rayleigh–Taylor instability benchmark. PDE-constrained l_2 projection is used to generate the composition field representation of the tracer data. The left and right columns show cases where the composition field function belongs to the $W_{DG}^{h,k=0}$ and $W_{DG}^{h,k=1}$ spaces, respectively.

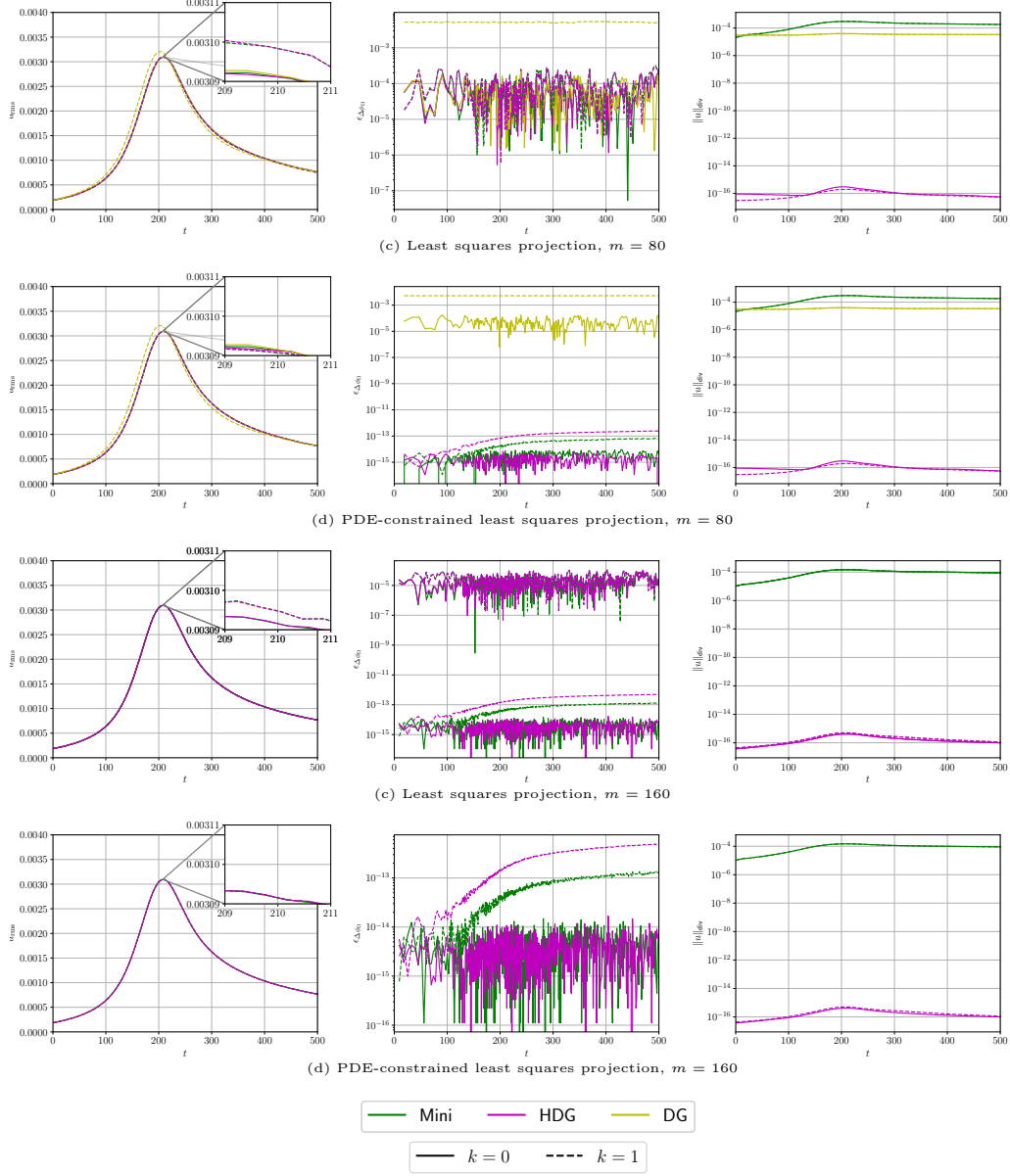


Figure S7: Example 4: $\eta_{\text{light}} = 1$, second order approximation of the Stokes system.

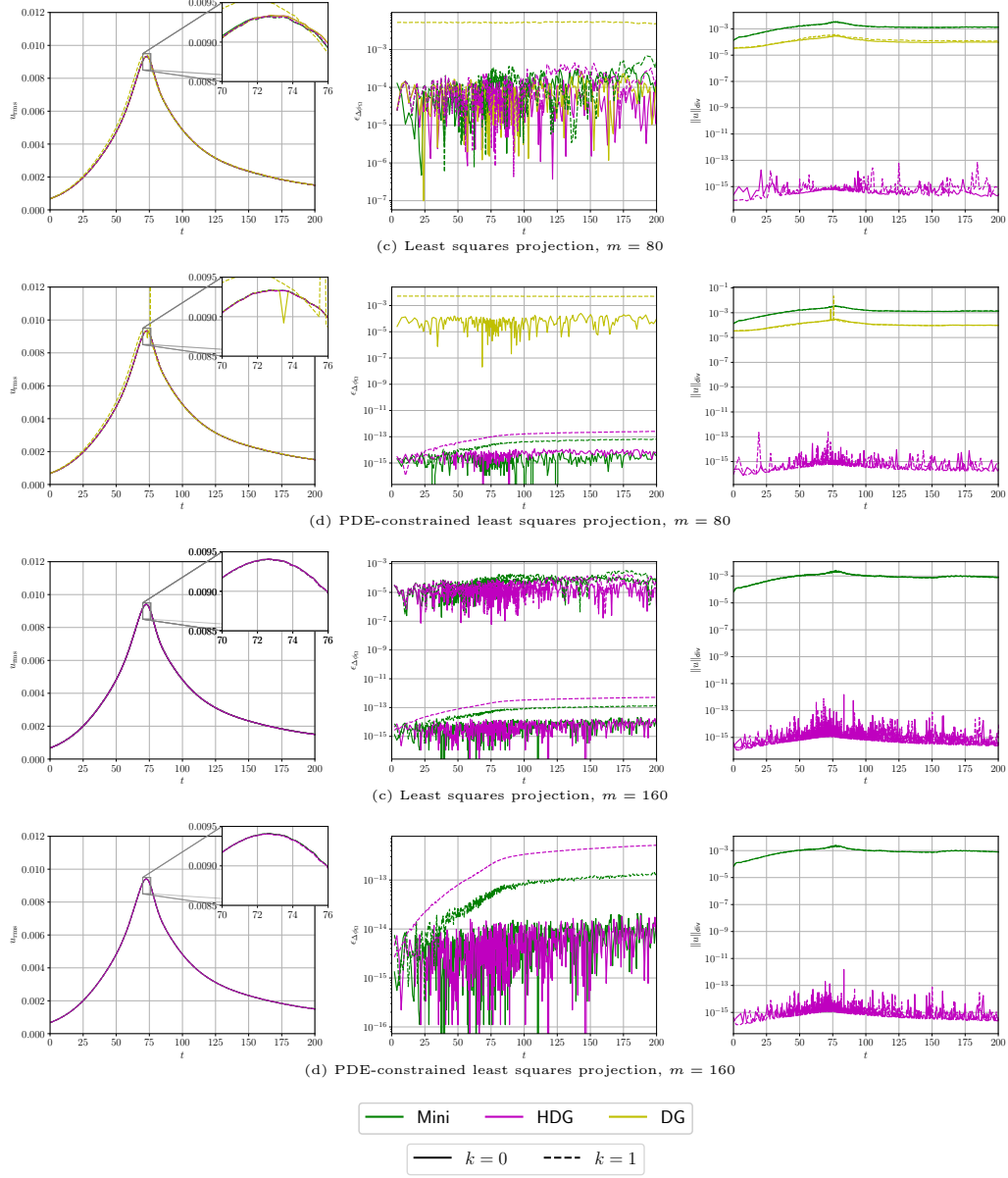


Figure S8: Example 4: $\eta_{\text{light}} = 0.1$, second order approximation of the Stokes system.

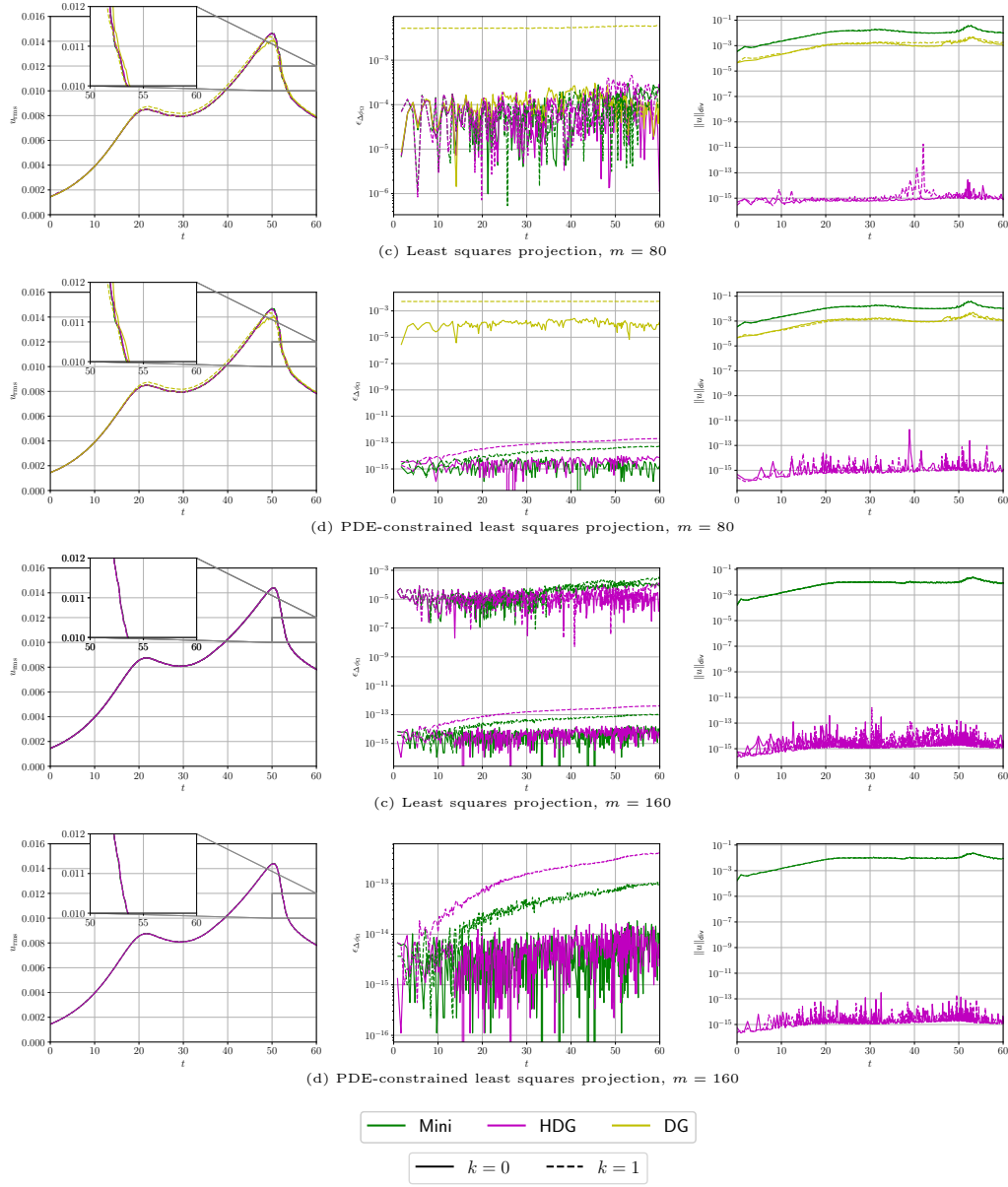


Figure S9: Example 4: $\eta_{\text{light}} = 0.01$, second order approximation of the Stokes system.

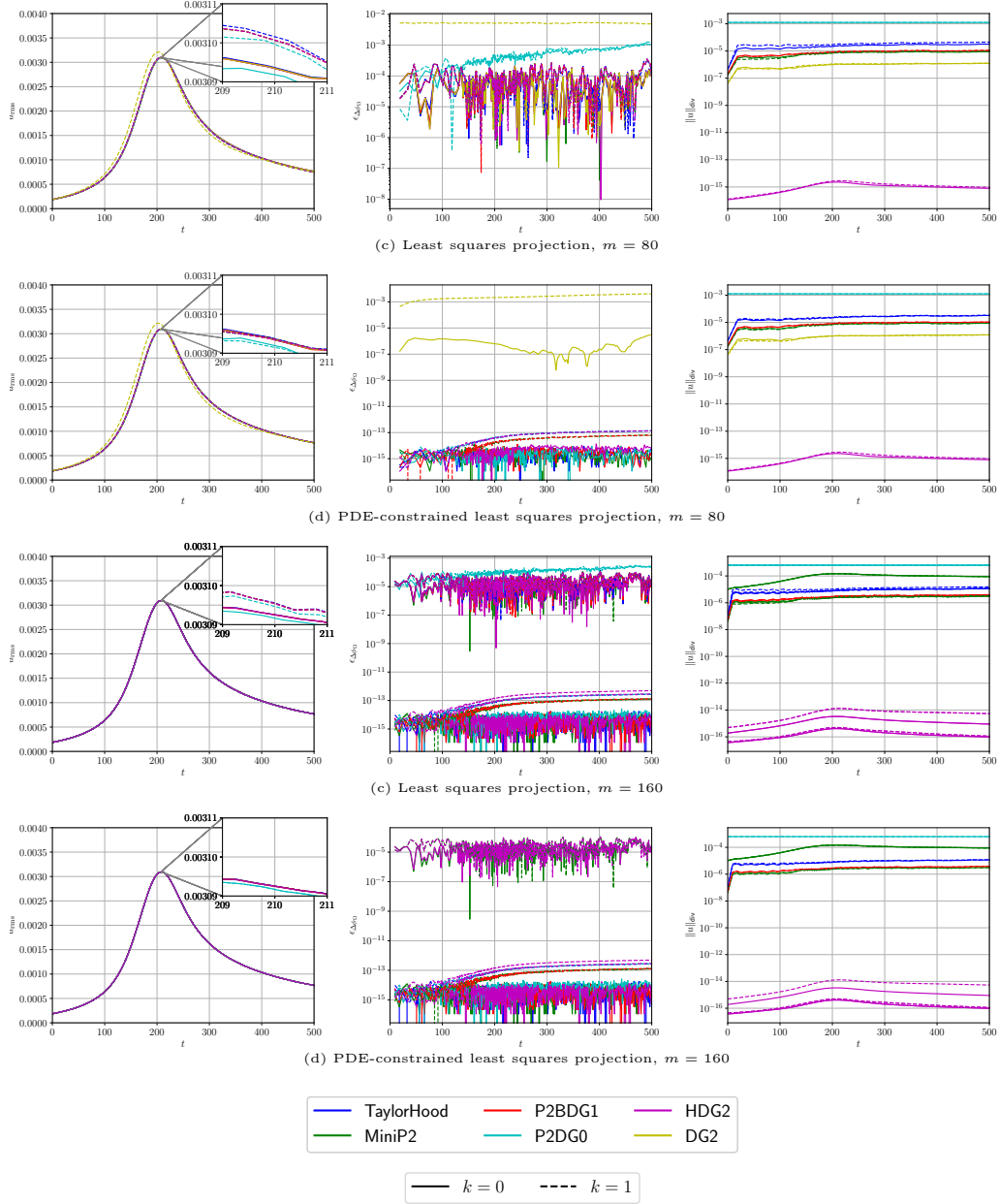


Figure S10: Example 4: $\eta_{\text{light}} = 1$, third order approximation of the Stokes system.

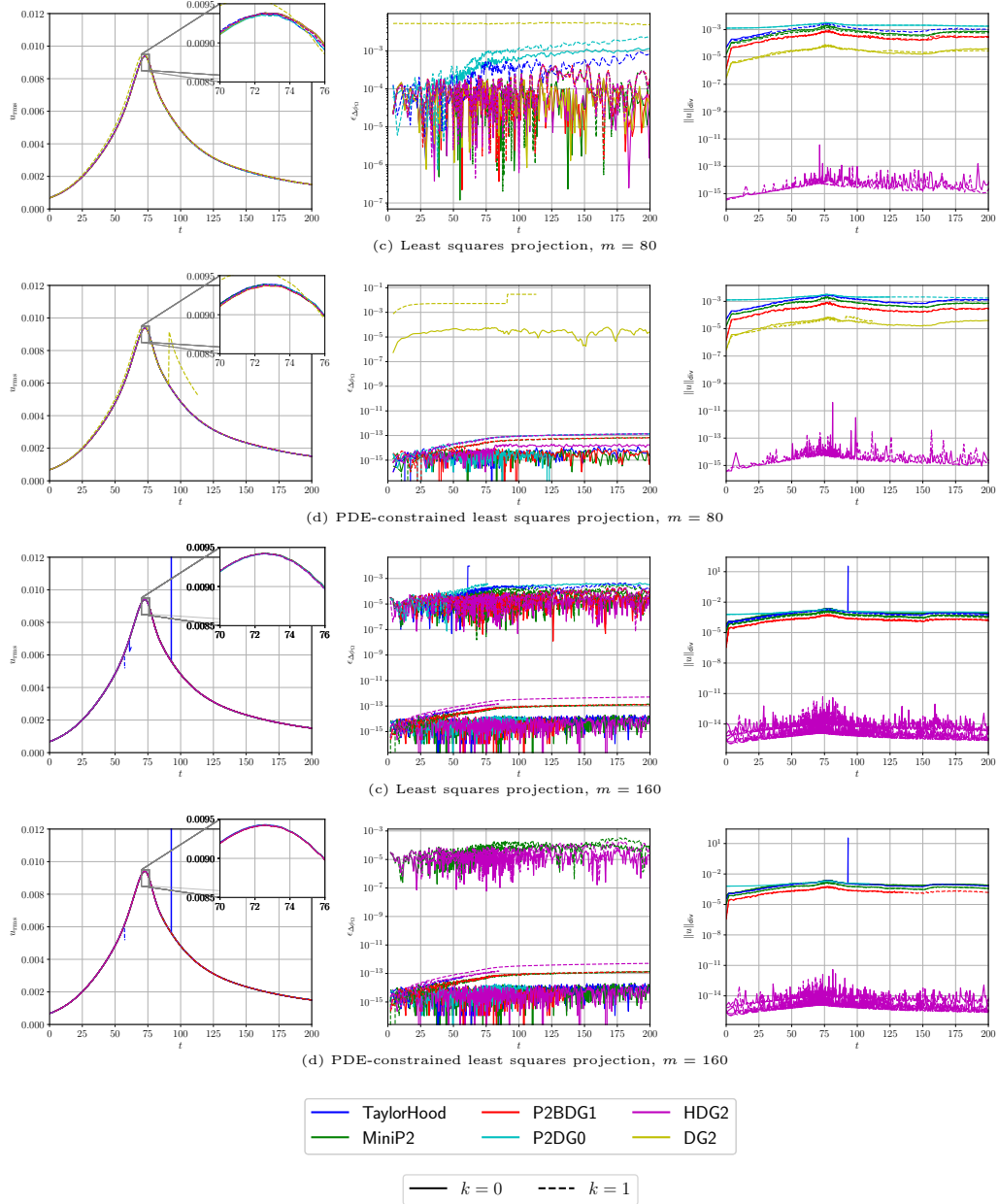


Figure S11: Example 4: $\eta_{\text{light}} = 0.1$, third order approximation of the Stokes system.

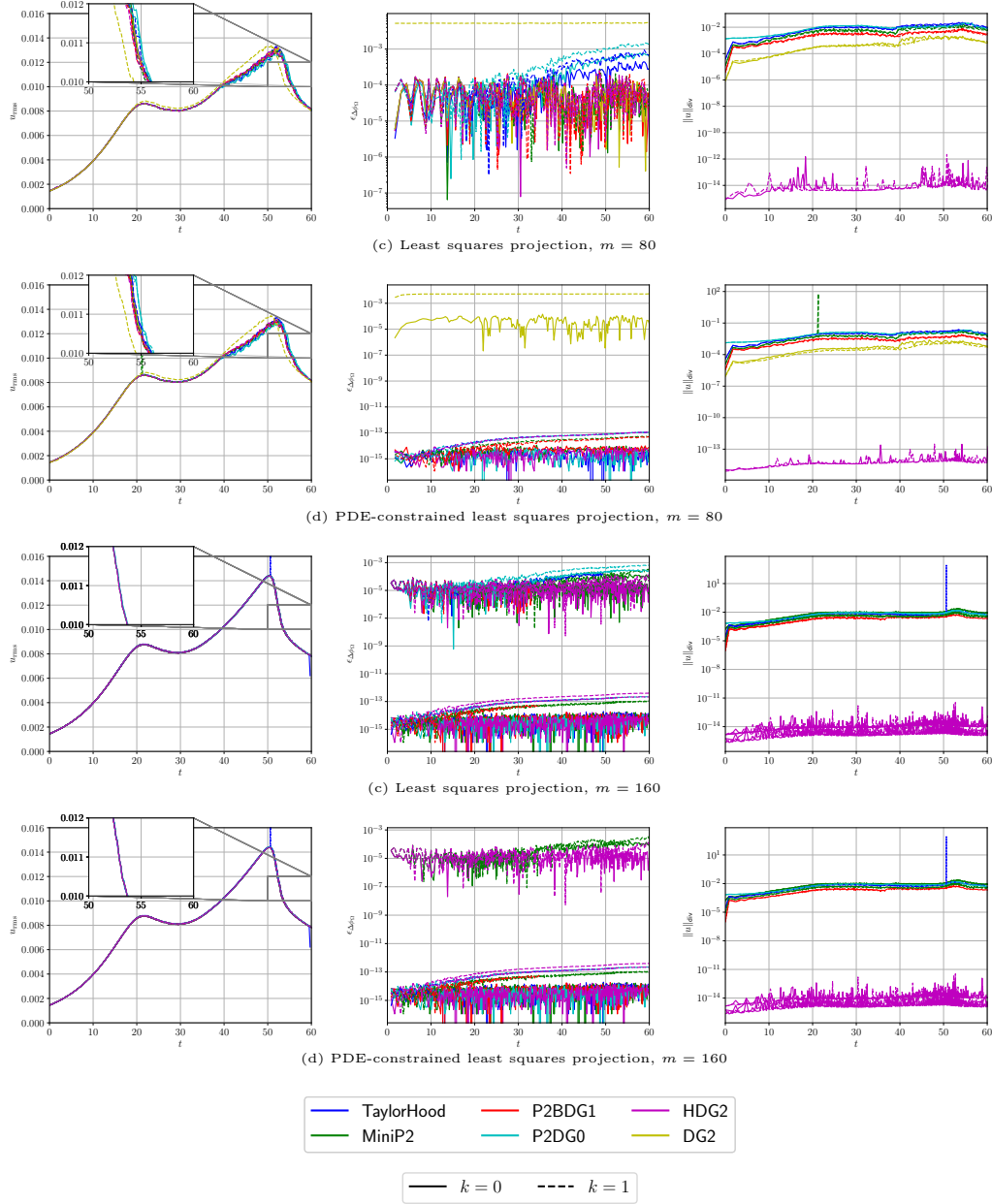


Figure S12: Example 4: $\eta_{\text{light}} = 0.01$, third order approximation of the Stokes system.