Magma dynamics using FD-PDE:
a new, PETSc-based, finite-difference staggered-grid framework for solving partial differential equations

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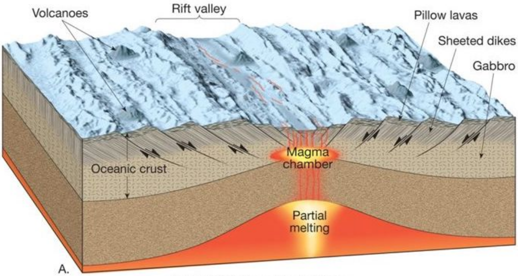
Introduction

RIFT-O-MAT (Magma-Assisted Tectonics) project seeks to understand how magmatism promotes and shapes rifts in continental and oceanic lithosphere by using models that build upon the two-phase flow theory of magma/rock interaction.

Goal: create analytical and numerical tools that are suitable for advecting thermo-chemically active material that feeds back on the two-phase flow. Emphasis on magma generation and transport, but also deformation of host rock: **diking** and **faulting**.



FD staggered grid

Why finite difference (FD) discretization on staggered grids?

- mimetic scheme (i.e., discrete differential operators mimic the properties of the continuous differential operators),
- thus conservative by construction,
- inf-sup stable, low-order stencil (fast and cheap to solve, important when you have large variations of coefficients such as viscosity),
- but more difficult to deal with boundary conditions (BCs).

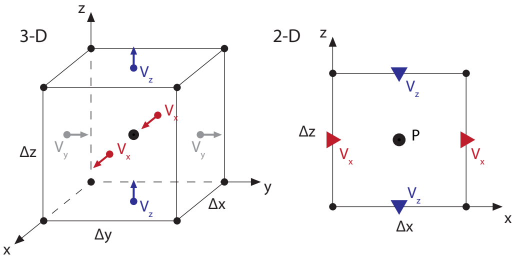


Figure: Staggered grid representation

FD staggered grid

Why develop a new code/framework?

- Separate the USER input from the discretization of partial differential equations (PDEs).
- Development should be extensible, with easy additions later on.
- Implement robust framework for testing.
- Allow for customized applications.
- The above points are common for finite element codes, BUT not so much for FD.

► **We present a new framework for FD staggered grids for solving PDEs that allows testable and extensible code for single-/two-phase flow magma dynamics.** ► **FD-PDE**

PETSc/DMStag

We build the FD-PDE framework using:

PETSc [Balay et al., 2019] - provides the building blocks (data structures and routines) for the implementation of large-scale parallel codes.
DMStag - a DM object in PETSc, which allows easy access to the staggered grid layout.
DM object - contains information on grid (topology), parallelism, coordinates, data.

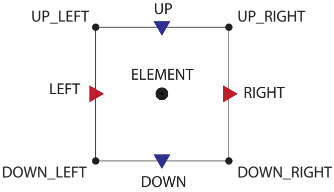


Figure: DMStag stencil

Example DMStag - a staggered grid DM object in PETSc

2-D Continuity equation: $\nabla \cdot \mathbf{v} = 0$

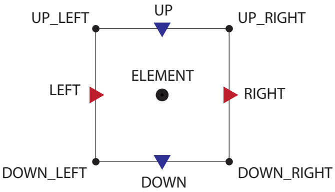
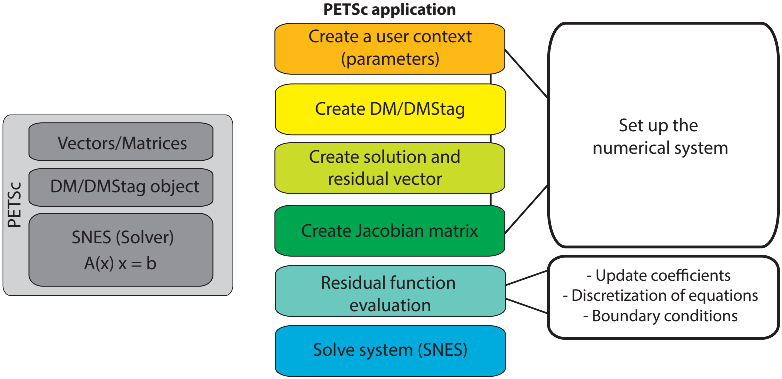


Figure: DMStag stencil

FD discretization:

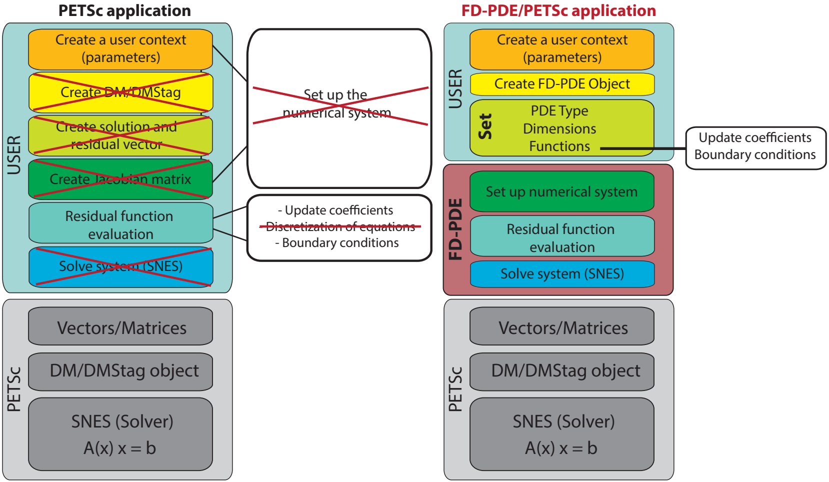
$$\frac{\partial V_x}{\partial x} + \frac{\partial V_z}{\partial z} = \frac{V_x^{\text{RIGHT}} - V_x^{\text{LEFT}}}{\Delta x} + \frac{V_z^{\text{UP}} - V_z^{\text{DOWN}}}{\Delta z} = 0$$

Solving PDEs with PETSc: typical components of a PETSc application



- many of the steps above should be skipped by the USER, while maintaining flexibility in scientific applications

Solving PDEs with PETSc and FD-PDE:



▶ the USER only needs to specify the model: PDE type, coefficients, BCs, parameters.

FD-PDE: Functionality

We have implemented the following FD-PDE Types:

1. **Stokes** (single-phase flow)
2. **StokesDarcy2Field** (two-phase flow)
3. **AdvDiff** (advection-diffusion-reaction)
4. **Composite** (coupled system)
5. **Coupled** (may couple the above FD-PDEs in various ways)

FD-PDE Example: Stokes

Conservation of mass and momentum for single-phase flow is given by Stokes equations:

$$-\nabla P + \nabla \cdot \eta \left(\nabla \mathbf{v} + \nabla \mathbf{v}^T \right) + \rho \mathbf{g} = 0 \quad (1)$$

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

Unknowns $P, \mathbf{v} = [v_x, v_z]$

- the above equations can be written in a more general way as...

FD-PDE Example: Stokes

Conservation of mass and momentum for single-phase flow is given by Stokes equations:

$$-\nabla P + \nabla \cdot A\left(\nabla \mathbf{v} + \nabla \mathbf{v}^T\right) - B = 0 \quad (1)$$

$$\nabla \cdot \mathbf{v} - C = 0 \quad (2)$$

Unknowns $P, \mathbf{v} = [v_x, v_z]$
Coefficients

$$A = \eta(\eta_0, \dot{\varepsilon}, T, P, ...)$$
$$B = -\rho \mathbf{g}$$
$$C = 0 \text{ (incompressible)}$$

Coefficients+BCs are problem dependent!

- **Separate unknowns (P,v) from coefficients (A,B,C). User has to define only the coefficients A,B,C and BCs.**

FD-PDE Example: Stokes

Discretization of Stokes equations:

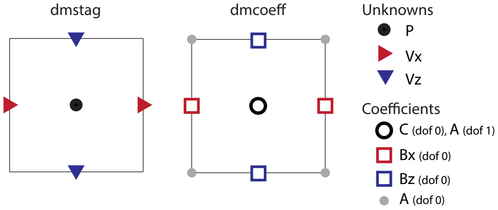


Figure: DMStag stencils for Stokes FD-PDE object.

Component dofs are not colocated! Velocity, eta, rhs have different grid locations. But can write coefficients as:

$$A = [\text{eta\_c, eta\_n}]$$

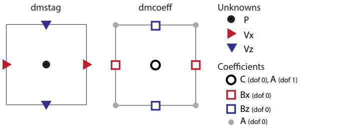
$$B = [\text{fux, fuz}]$$

$$C = \text{fp}$$

FD-PDE: other Types and Stencils

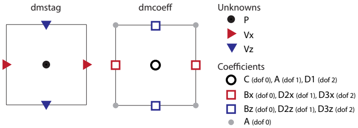
- **Stokes**

$$
\begin{aligned}
-\nabla P + \nabla \cdot A\left(\nabla \mathbf{v} + \nabla \mathbf{v}^T\right) - B &= 0 \\
\nabla \cdot \mathbf{v} - C &= 0
\end{aligned}
$$



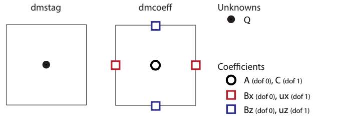
- **StokesDarcy2Field**

$$
\begin{aligned}
-\nabla P + \nabla \cdot \left(A\left(\nabla \mathbf{v} + \nabla \mathbf{v}^T\right)\right) + \nabla\left(D_1 \nabla \cdot \mathbf{v}\right) - B &= 0 \\
\nabla \cdot \mathbf{v} + \nabla \cdot \left(D_2 \nabla P + D_3\right) - C &= 0
\end{aligned}
$$



- **AdvDiff**

$$
A\left(\frac{\partial Q}{\partial t} + \nabla \cdot (\mathbf{u} Q)\right) - \nabla \cdot (B \nabla Q) + C = 0
$$



FD-PDE: Benchmarking

We verified our FD-PDE framework using:

1. **Analytical solutions**
2. **Community benchmarks**
3. **The Method of Manufactured Solutions (MMS)**

FD-PDE Benchmarking: (1) Analytical solutions

FD-PDE Stokes (single-phase flow):

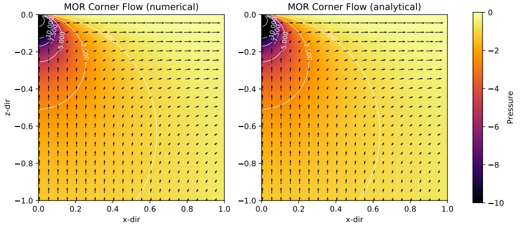


Figure: Corner flow solutions at mid-ocean ridge [Spiegelman and McKenzie, 1987].

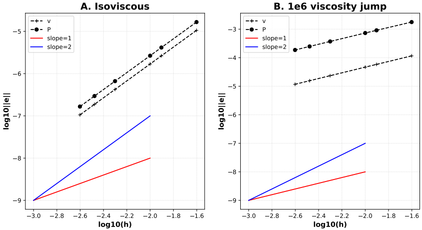
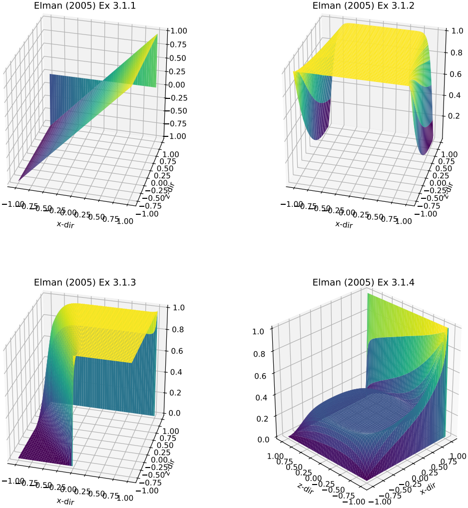


Figure: Discretization errors for the SolCx test, an analytical solution with sharp viscosity contrasts (i.e., Duretz et al. [2011]).

FD-PDE Benchmarking: (1) Analytical solutions

FD-PDE AdvDiff:

Figure: Advection-diffusion solutions from Elman et al. [2005].



FD-PDE Benchmarking: (2) Community benchmarks

Mantle convection [Blankenbach et al., 1989]

1. Non-dimensional system of equations:

$$-\nabla P + \nabla \cdot \eta \left(\nabla \mathbf{v} + \nabla \mathbf{v}^T \right) = -RaT\mathbf{k} \quad (3)$$

$$\nabla \cdot \mathbf{v} = 0 \quad (4)$$

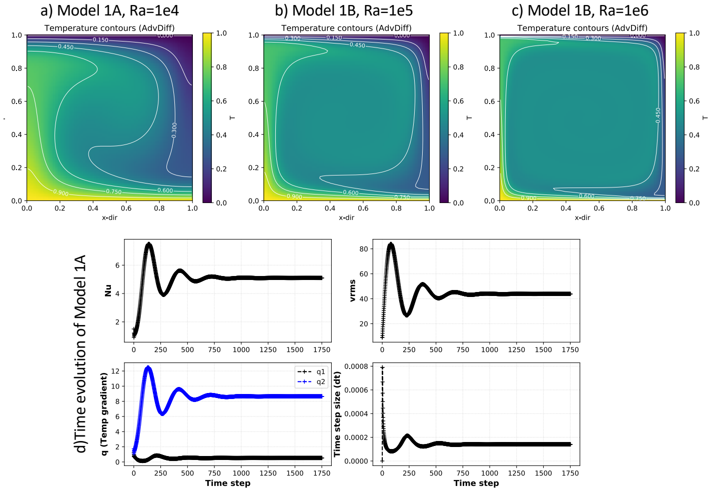
$$\frac{\partial T}{\partial t} + \nabla \cdot \mathbf{v}T - \nabla^2 T = 0 \quad (5)$$

where P-pressure, $\mathbf{v}$-velocity, T-temperature, and $Ra = \frac{\rho_0 \alpha \Delta T g h^3}{\eta_0 \kappa}$ is the Rayleigh number.

2. FD-PDE Equations: coupled Stokes+AdvDiff

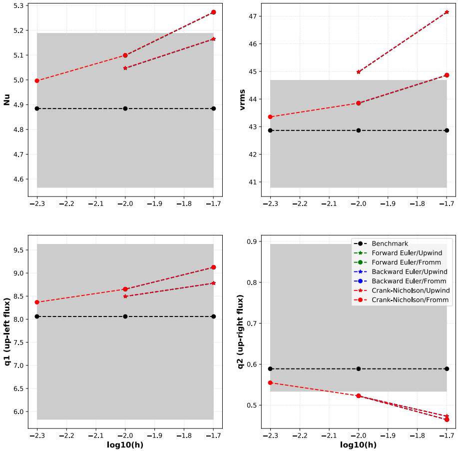
Mantle convection [Blankenbach et al., 1989]

3. Results:

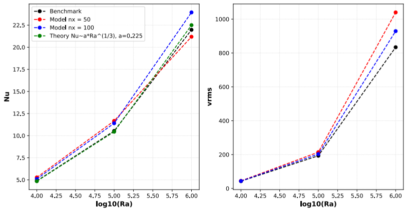


Mantle convection [Blankenbach et al., 1989]
3. Results:

a) Diagnostics Model 1A with resolution



b) Scaling Nu vs Ra



FD-PDE Benchmarking: (3) MMS

The Method of Manufactured Solutions (MMS) provides a general procedure for verifying the implementation and the quality expected by a particular numerical method [Roache, 2002].

Example 1: FD-PDE AdvDiff using MMS

$$A\left(\frac{\partial Q}{\partial t} + \nabla \cdot (\mathbf{u}Q)\right) - \nabla \cdot (B \nabla Q) + C = 0 \tag{6}$$

where Q - unknown and A, B, C, $\mathbf{u}$ (velocity) are coefficients.

Tests performed:

1. Steady-state diffusion
2. Steady-state advection-diffusion
3. Time-dependent diffusion
4. Time-dependent advection

FD-PDE Benchmarking: (3) MMS

Example 1: FD-PDE AdvDiff using MMS

MMS functions for tests 1-2:

$$
\begin{aligned}
Q_{\mathrm{MMS}} &= \cos(2\pi x)\sin(2\pi z)\\
A_{\mathrm{MMS}} &= 1.5 + \sin(2\pi x)\cos(2\pi z)\\
B_{\mathrm{MMS}} &= 1.0 + x^2 + z^2\\
C_{\mathrm{MMS}} &= -f_{\mathrm{MMS}}\\
ux_{\mathrm{MMS}} &= 1.0 + x\\
uz_{\mathrm{MMS}} &= x^2\sin(2\pi z)
\end{aligned}
$$

MMS functions for tests 3-4:

$$
\begin{aligned}
Q_{\mathrm{MMS}} &= t^3(x^2 + z^2)\\
A_{\mathrm{MMS}} &= 1.0 + \sin(2.0\pi x)\cos(2.0\pi z)\\
B_{\mathrm{MMS}} &= 0.0\\
C_{\mathrm{MMS}} &= -f_{\mathrm{MMS}}\\
ux_{\mathrm{MMS}} &= 1.0 + x\\
uz_{\mathrm{MMS}} &= x^2\sin(2\pi z)
\end{aligned}
$$

The rhs (f_{MMS}) and BCs (both Dirichlet and Neumann) are evaluated using packages for symbolic computation such as **SymPy**.

FD-PDE Benchmarking: (3) MMS

Example 1: FD-PDE AdvDiff using MMS

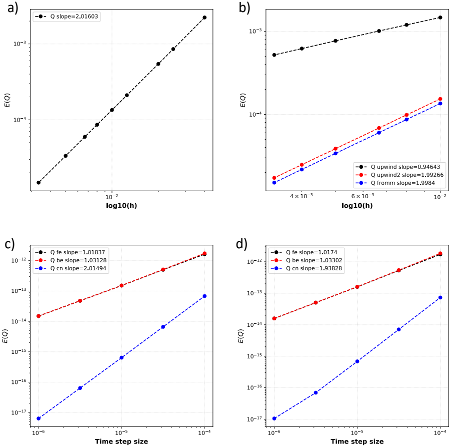


Figure: Results of the AdvDiff MMS tests: a) Steady-state diffusion, spatial errors, *h* is grid spacing. b) Steady-state advection-diffusion, spatial errors. Each color line represents a different advection scheme: upwind (FOU), upwind2 (SOU), fromm (Fromm). c) Time-dependent diffusion, temporal errors. Each color line represents a different time-stepping scheme: fe (forward Euler), be (backward Euler), cn (Crank-Nicholson). d) Time-dependent advection, temporal errors.

FD-PDE Benchmarking: (3) MMS

Example 2: StokesDarcy2Field using MMS [Rhebergen et al., 2014]

1. Non-dimensional system of equations:

$$-\nabla P + \frac{1}{2}\nabla \cdot \left(\nabla \mathbf{v}_s + \nabla \mathbf{v}_s^T\right) + \nabla\left(\alpha \nabla \cdot \mathbf{v}_s\right) + \phi \mathbf{e}_3 = \mathbf{0} \qquad (7)$$

$$\nabla \cdot \mathbf{v}_s - \nabla \cdot \left[k\left(\nabla P - \mathbf{e}_3\right)\right] = 0 \qquad (8)$$

where P-dynamic pressure, $\mathbf{v}_s$-solid velocity, ϕ-porosity, $\alpha = \frac{1}{2}\left(r_\zeta - \frac{2}{3}\right)$-compaction viscosity, $k = \frac{R^2}{\alpha+1}\left(\frac{\phi}{\phi_0}\right)^n$ is permeability, $R = \delta/H$ is a scaled compaction length (δ), and $\mathbf{e}_3$ is unit vector in direction of gravity.

Example 2: StokesDarcy2Field using MMS [Rhebergen et al., 2014]

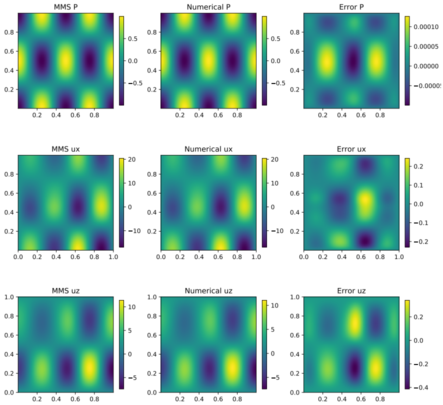
2. Pick MMS functions for $P, \mathbf{v}_s$ and coefficient k:

$$k^{MMS} = \frac{k^* - k_*}{4\tanh(5)}\left(2 + \tanh(10x-5) + \tanh(10z-5) + \frac{2(k^*-k_*) - 2\tanh(5)(k^*+k_*)}{k_* - k^*}\right),$$
$$P^{MMS} = -\cos(4\pi x)\cos(2\pi z),$$
$$v_x^{MMS} = k\frac{\partial P}{\partial x} + \sin(\pi x)\sin(2\pi z) + 2,$$
$$v_z^{MMS} = k\frac{\partial P}{\partial z} + \frac{1}{2}\cos(\pi x)\cos(2\pi z) + 2.$$

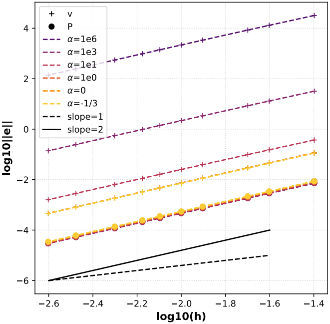
where $k_* = 0.5$ and $k^* = 1.5$.

3. Calculate MMS BCs and right-hand-side for the system of equations, assuming no body forces.

Example 2: StokesDarcy2Field using MMS [Rhebergen et al., 2014]



MMS and numerical solutions



Convergence errors as a function of grid spacing h

- **Velocity errors depend on α. However, the dependency is reduced with different scaling parameters.**

FD-PDE Benchmarking: (3) MMS

Example 3: StokesDarcy2Field+AdvDiff for porosity evolution

1. Non-dimensional system of equations:

$$-\nabla P + \nabla \cdot \eta(\nabla \mathbf{v}_s + \nabla \mathbf{v}_s^T) + \nabla(\xi \nabla \cdot \mathbf{v}_s) + \phi \mathbf{e}_3 = \mathbf{0} \quad (9)$$

$$\nabla \cdot \mathbf{v}_s - \nabla \cdot \left[\left(\frac{\phi}{\phi_0} \right)^n (\nabla P - \mathbf{e}_3) \right] = 0 \quad (10)$$

$$\frac{\partial(1-\phi)}{\partial t} + \nabla \cdot (1-\phi)\mathbf{v}_s = 0 \quad (11)$$

where P-dynamic pressure, $\mathbf{v}_s$-solid velocity, ϕ-porosity, η, ζ-shear and bulk viscosity, $\xi = \zeta - \frac{2}{3}\eta$ is compaction viscosity, ϕ_0 is reference porosity, and $\mathbf{e}_3$ is unit vector in direction of gravity.

FD-PDE Benchmarking: (3) MMS

Example 3: StokesDarcy2Field+AdvDiff for porosity evolution

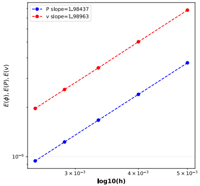
2. Pick MMS for $\phi, P, \mathbf{v}_s$ also as function of time:

$$
\begin{aligned}
Q_{\mathrm{MMS}} &= t^3(x^2 + z^2) \\
\phi_{\mathrm{MMS}} &= 1 - Q_{\mathrm{MMS}} \\
P_{\mathrm{MMS}} &= P^* \cos(m\pi x)\cos(m\pi z) \\
\Psi_{\mathrm{MMS}} &= \Psi^*[1 - \cos(m\pi x))(1 - \cos(m\pi z)] \\
\mathcal{U}_{\mathrm{MMS}} &= -\mathcal{U}^* \cos(m\pi x)\cos(m\pi z) \\
v_{x\,\mathrm{MMS}} &= \frac{\partial \Psi}{\partial z} + \frac{\partial \mathcal{U}}{\partial x} \\
v_{z\,\mathrm{MMS}} &= -\frac{\partial \Psi}{\partial x} + \frac{\partial \mathcal{U}}{\partial z}
\end{aligned}
$$

where we take $P^* = 1.0$, $\psi^* = 1.0$, $\mathcal{U}^* = 1.0$, and $m = 2$.
On the boundary of the domain, $\partial\Omega$, we impose: $\mathbf{v}_s = \mathbf{v}_{s\mathrm{MMS}}$, $P = P_{\mathrm{MMS}}$ and $\phi = \phi_{\mathrm{MMS}}$.

Example 3: StokesDarcy2Field+AdvDiff for porosity evolution

1. Spatial convergence test



2. Temporal convergence test

a) constant P, v

b) Reference MMS functions

c) time-dependent variable P,v

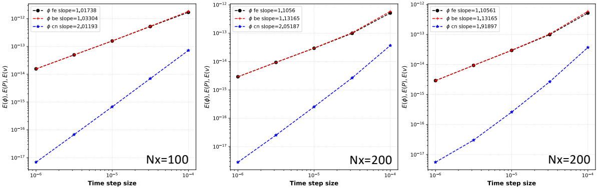


Figure: Results for the coupled Stokes-Darcy porosity evolution test. 1. Spatial discretization errors for P, $\mathbf{v}_s$. 2. Temporal discretization errors for ϕ. a) constant $P_{\text{MMS}} = 1.0$, $\mathbf{v}_{s\,\text{MMS}} = [1.0, 1.0]$, b) reference MMS functions above, c) time-dependent $P_{\text{MMS}}, \mathbf{v}_{s\,\text{MMS}}$ (provided on request). h-grid spacing, Nx-grid cells in one direction.

Summary and Future work

We built a FD-PDE framework that:

- allows for fast application development (user focuses primarily on problem specifics),
- is flexible: can build single or coupled PDEs,
- is highly testable and extensible.

Future work:

- build models with complex physics for scientific applications (i.e., two-phase flow mid-ocean ridge model with free surface, visco-elasto-plastic rheologies).

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