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

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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.
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: $\nabla \cdot \mathbf{v} = 0$

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

- Create a user context (parameters)
- Create DM/DMStag
- Create solution and residual vector
- Create Jacobian matrix
- Residual function evaluation
- Solve system (SNES)

Set up the numerical system
- Update coefficients
- Discretization of equations
- Boundary conditions

PETSc application

PETSc

Vectors/Matrices
DM/DMStag object
SNES (Solver) $A(x) \ x = b$

Many of the steps above should be skipped by the USER, while maintaining flexibility in scientific applications.
PETSc/DMStag ▶ FD-PDE Framework

Solving PDEs with PETSc and FD-PDE:

PETSc application

- Create a user context (parameters)
- Create DM/DMStag
- Create solution and residual vector
- Create Jacobian matrix
- Residual function evaluation
- Solve system (SNES)

FD-PDE/PETSc application

- Create a user context (parameters)
- Create FD-PDE Object
- Set PDE Type
  - Dimensions
  - Functions
- Set up numerical system
- Residual function evaluation
- Solve system (SNES)
- Update coefficients
- Boundary conditions

- Vectors/Matrices
- DM/DMStag object
- SNES (Solver)
  - A(x) x = b

▶ the USER only needs to specify the model: PDE type, coefficients, BCs, parameters.
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)
Conservation of mass and momentum for single-phase flow is given by Stokes equations:

\[-\nabla P + \nabla \cdot \eta \left( \nabla \mathbf{v} + \nabla \mathbf{v}^T \right) + \rho \mathbf{g} = 0\]  \hspace{1cm} (1)
\[\nabla \cdot \mathbf{v} = 0\]  \hspace{1cm} (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:

\[-\nabla P + \nabla \cdot A \left( \nabla \mathbf{v} + \nabla \mathbf{v}^T \right) - B = 0\]  
\[\nabla \cdot \mathbf{v} - C = 0\]

Unkowns \( P, \mathbf{v} = [v_x, v_z] \)

Coefficients

\[A = \eta(\eta_0, \dot{\varepsilon}, T, P, ...)]\]

\[B = -\rho g\]

\[C = 0 \text{ (incompressible)}\]

 Côefficients+BCs are problem dependent!

- Separate unknowns \((P, \mathbf{v})\) 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 collocated! Velocity, eta, rhs have different grid locations. But can write coefficients as:

\[
A = [\text{eta}_c, \text{eta}_n] \\
B = [\text{fux}, \text{fuz}] \\
C = \text{fp}
\]
**FD-PDE: other Types and Stencils**

- **Stokes**
  \[-\nabla P + \nabla \cdot A \left( \nabla v + \nabla v^T \right) - B = 0 \]
  \[\nabla \cdot v - C = 0\]

- **StokesDarcy2Field**
  \[-\nabla P + \nabla \cdot \left( A \left( \nabla v + \nabla v^T \right) \right) + \nabla \left( D_1 \nabla \cdot v \right) - B = 0 \]
  \[\nabla \cdot v + \nabla \cdot (D_2 \nabla P + D_3) - C = 0\]

- **AdvDiff**
  \[A \left( \frac{\partial Q}{\partial t} + \nabla \cdot (uQ) \right) - \nabla \cdot (B \nabla Q) + C = 0\]
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].
Mantle convection [Blankenbach et al., 1989]

1. Non-dimensional system of equations:

\[-\nabla P + \nabla \cdot \eta \left( \nabla \mathbf{v} + \nabla \mathbf{v}^T \right) = -Ra T k\]  \hspace{1cm} (3)

\[\nabla \cdot \mathbf{v} = 0\]  \hspace{1cm} (4)

\[\frac{\partial T}{\partial t} + \nabla \cdot \mathbf{v} T - \nabla^2 T = 0\]  \hspace{1cm} (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:

- a) Model 1A, \( Ra=1 \times 10^4 \)
- b) Model 1B, \( Ra=1 \times 10^5 \)
- c) Model 1B, \( Ra=1 \times 10^6 \)
- d) Time evolution of Model 1A
FD-PDE Benchmarking: (2) Community benchmarks

Mantle convection [Blankenbach et al., 1989]

3. Results:

a) Diagnostics Model 1A with resolution

b) Scaling Nu vs Ra
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

\[
A \left( \frac{\partial Q}{\partial t} + \nabla \cdot (uQ) \right) - \nabla \cdot (B \nabla Q) + C = 0
\]  

(6)

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

Tests performed:

1. Steady-state diffusion
2. Steady-state advection-diffusion
3. Time-dependent diffusion
4. Time-dependent advection
Example 1: FD-PDE AdvDiff using MMS

MMS functions for tests 1-2:

\[
\begin{align*}
Q_{\text{MMS}} &= \cos(2\pi x) \sin(2\pi z) \\
A_{\text{MMS}} &= 1.5 + \sin(2\pi x) \cos(2\pi z) \\
B_{\text{MMS}} &= 1.0 + x^2 + z^2 \\
C_{\text{MMS}} &= -f_{\text{MMS}} \\
u_{x\text{MMS}} &= 1.0 + x \\
u_{z\text{MMS}} &= x^2 \sin(2\pi z)
\end{align*}
\]

MMS functions for tests 3-4:

\[
\begin{align*}
Q_{\text{MMS}} &= t^3(x^2 + z^2) \\
A_{\text{MMS}} &= 1.0 + \sin(2.0\pi x) \cos(2.0\pi z) \\
B_{\text{MMS}} &= 0.0 \\
C_{\text{MMS}} &= -f_{\text{MMS}} \\
u_{x\text{MMS}} &= 1.0 + x \\
u_{z\text{MMS}} &= x^2 \sin(2\pi z)
\end{align*}
\]

The rhs \(f_{\text{MMS}}\) and BCs (both Dirichlet and Neumann) are evaluated using packages for symbolic computation such as **SymPy**.
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.
Example 2: StokesDarcy2Field using MMS [Rhebergen et al., 2014]

1. Non-dimensional system of equations:

\[-\nabla P + \frac{1}{2} \nabla \cdot (\nabla v_s + \nabla v_s^T) + \nabla (\alpha \nabla \cdot v_s) + \phi \mathbf{e}_3 = 0\] 

\[\nabla \cdot v_s = \nabla \cdot [k (\nabla P - \mathbf{e}_3)] = 0\]

where \(P\)-dynamic pressure, \(v_s\)-solid velocity, \(\phi\)-porosity,
\(\alpha = \frac{1}{2} (r_\zeta - \frac{2}{3})\)-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 (\(\delta\)), 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 $P$, $v_s$ and coefficient $k$:

$$
k_{MMS} = \frac{k^* - k_\ast}{4 \tanh(5)} \left(2 + \tanh(10x - 5) + \tanh(10z - 5) + \frac{2(k^* - k_\ast) - 2 \tanh(5)(k^* + k_\ast)}{k^* - k_\ast}\right),
$$

$$
P_{MMS} = -\cos(4\pi x) \cos(2\pi z),
$$

$$
v_{x\ MMS} = k \frac{\partial P}{\partial x} + \sin(\pi x) \sin(2\pi z) + 2,
$$

$$
v_{z\ MMS} = k \frac{\partial P}{\partial z} + \frac{1}{2} \cos(\pi x) \cos(2\pi z) + 2.
$$

where $k_\ast = 0.5$ 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 $\alpha$. However, the dependency is reduced with different scaling parameters.
Example 3: StokesDarcy2Field+AdvDiff for porosity evolution

1. Non-dimensional system of equations:

\[-\nabla P + \nabla \cdot \eta (\nabla v_s + \nabla v_s^T) + \nabla (\xi \nabla \cdot v_s) + \phi e_3 = 0\]  \hspace{1cm} (9)

\[\nabla \cdot v_s - \nabla \cdot \left[ \left( \frac{\phi}{\phi_0} \right)^n (\nabla P - e_3) \right] = 0\]  \hspace{1cm} (10)

\[\frac{\partial (1 - \phi)}{\partial t} + \nabla \cdot (1 - \phi)v_s = 0\]  \hspace{1cm} (11)

where $P$-dynamic pressure, $v_s$-solid velocity, $\phi$-porosity, $\eta$, $\zeta$-shear and bulk viscosity, $\xi = \zeta - \frac{2}{3}\eta$ is compaction viscosity, $\phi_0$ is reference porosity, and $e_3$ is unit vector in direction of gravity.
Example 3: StokesDarcy2Field+AdvDiff for porosity evolution

2. Pick MMS for $\phi, P, v_s$ also as function of time:

$$Q_{\text{MMS}} = t^3(x^2 + z^2)$$
$$\phi_{\text{MMS}} = 1 - Q_{\text{MMS}}$$
$$P_{\text{MMS}} = P^* \cos(m\pi x) \cos(m\pi z)$$
$$\psi_{\text{MMS}} = \psi^* [1 - \cos(m\pi x))(1 - \cos(m\pi z)]$$
$$\Psi_{\text{MMS}} = \Psi^* [1 - \cos(m\pi x))(1 - \cos(m\pi z)]$$
$$U_{\text{MMS}} = -U^* \cos(m\pi x) \cos(m\pi z)$$
$$v_{x\text{MMS}} = \frac{\partial \psi}{\partial z} + \frac{\partial U}{\partial x}$$
$$v_{z\text{MMS}} = - \frac{\partial \psi}{\partial x} + \frac{\partial U}{\partial z}$$

where we take $P^* = 1.0, \psi^* = 1.0, U^* = 1.0,$ and $m = 2.$

On the boundary of the domain, $\partial \Omega,$ we impose: $v_s = v_{s\text{MMS}}, P = P_{\text{MMS}}$ and $\phi = \phi_{\text{MMS}}.$
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 $P$, $v$

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


