Scientific Computation of Two–Phase Ferrofluid Flows

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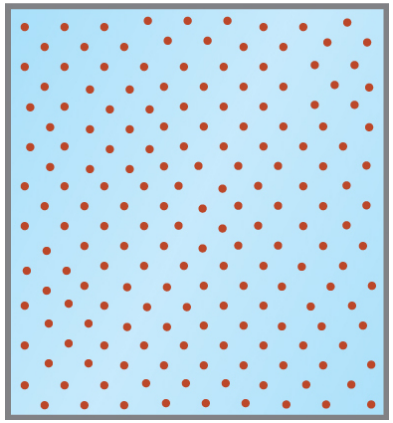
What is a Ferrofluid?

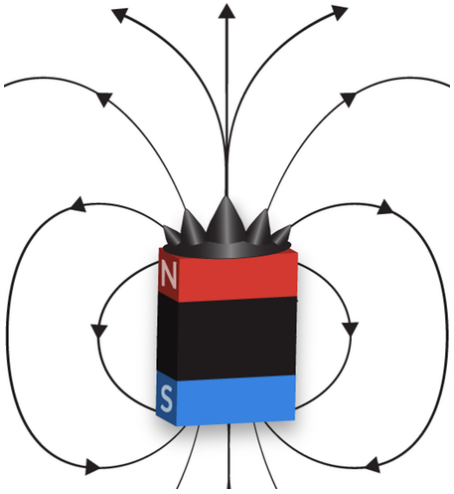
Awesome video of ferrofluids.

What is a Ferrofluid? (Backup)

A ferrofluid is a colloid of nanoscale ferromagnetic particles suspended in a carrier fluid such as oil, water, or an organic solvent.

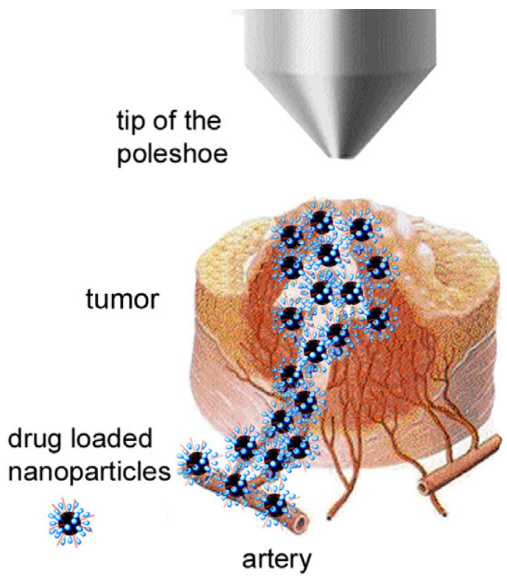


Ferrofluids become magnetized when under the effect of a magnetic field.



Applications

- Initially created to pump rocket fuel once a spacecraft entered a weightless environment.
- Commercial applications:
  - Vibration damping
  - Sensors
  - Acoustics
- Recent research areas:
  - Magnetic drug targeting
  - Adaptive deformable mirrors



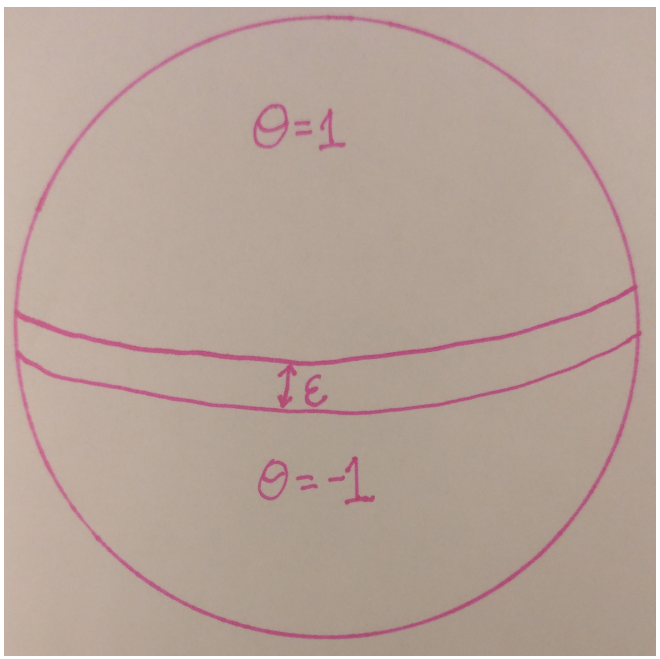
PDE Model for Two–Phase Ferrofluid Flow

- Dr. Nochetto and collaborators developed a model for two–phase ferrofluid flows and devised an energy stable numerical scheme [3].
- The model was not derived, but instead was assembled.
- Important results from [3]:
  - Proved an energy law for the PDE model.
  - Proved the numerical scheme was energy stable and the existence of a local solution.
  - For an even simpler model, they proved stability, convergence, and the existence of solutions.

Modeling a Two–Phase Fluid

- In order to track both fluids, a diffuse interface is used.
- The phase variable θ is introduced, which takes values in $[-1, 1]$.
- The evolution of θ is given by a modified Cahn–Hilliard equation:

$$\begin{cases} \theta_t + \operatorname{div}(\mathbf{u}\theta) + \gamma\Delta\psi = 0 & \text{in } \Omega \\ \psi - \epsilon\Delta\theta + \frac{1}{\epsilon}f(\theta) = 0 & \text{in } \Omega \\ \partial_\eta\theta = \partial_\eta\psi = 0 & \text{on } \Gamma, \end{cases}$$



where

- $0 < \epsilon << 1$ is related to the interface thickness,
- $\gamma > 0$ is the constant mobility,
- ψ is the chemical potential,
- $f(\theta)$ is the truncated double well potential.

Modeling of the Magnetic Field

- Instead of using the magnetostatics equations, a simplified approach was used.
- Define the magnetic field by

$$\mathbf{h} := \mathbf{h}_a + \mathbf{h}_d,$$

where

  - $\mathbf{h}_a$ – smooth harmonic (curl–free and div–free) applied magnetizing field,
  - $\mathbf{h}_d$ – demagnetizing field.

- Then the magnetic field is induced via the scalar potential φ by

$$\mathbf{h} = \nabla\varphi,$$

along with,

$$-\Delta\varphi = \operatorname{div}(\mathbf{m} - \mathbf{h}_a) \quad \text{in } \Omega, \qquad \partial_\eta\varphi = (\mathbf{h}_a - \mathbf{m}) \cdot \eta \quad \text{on } \Gamma.$$

Modeling of Ferrohydrodynamics

- A simplified version of Shliomis model is used, which couples an advection–reaction equation for the magnetization $\mathbf{m}$:

$$\mathbf{m}_t + (\mathbf{u} \cdot \nabla)\mathbf{m} = -\frac{1}{\mathscr{T}}(\mathbf{m} - \varkappa_\theta \mathbf{h}),$$

with the Navier–Stokes equations of incompressible fluids for the velocity–pressure pair $(\mathbf{u}, p)$:

$$\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u} - \mathrm{div}(\nu_\theta \mathbf{T}(\mathbf{u})) + \nabla p = \mu_0 (\mathbf{m} \cdot \nabla)\mathbf{h} + \frac{\lambda}{\epsilon}\theta \nabla \psi,$$

$$\mathrm{div}\mathbf{u} = 0,$$

where

  - $\mathscr{T}$ is the relaxation time of the ferrofluid,
  - $\varkappa_\theta$ is the magnetic susceptibility of the phase variable,
  - ν_θ is the viscosity of the phase variable,
  - μ_0 is the constitutive parameter related to the Kelvin force,
  - $\frac{\lambda}{\epsilon}\theta \nabla \psi$ is the capillary force.

- This is supplemented with a no–slip condition on the boundary:

$$\mathbf{u} = 0 \quad \text{on } \Gamma.$$

- The model reads: Consider a bounded convex polygon/polyhedron domain $\Omega \subset \mathbb{R}^d$ ($d = 2$ or 3) with boundary Γ. The evolution of the system is given by the following set of equations in strong form in Ω

$$\theta_t + \operatorname{div}(\mathbf{u}\theta) + \gamma\Delta\psi = 0, \tag{1a}$$

$$\psi - \epsilon\Delta\theta + \frac{1}{\epsilon}f(\theta) = 0, \tag{1b}$$

$$\mathbf{m}_t + (\mathbf{u}\cdot\nabla)\mathbf{m} = -\frac{1}{\mathscr{T}}(\mathbf{m} - \varkappa_\theta \mathbf{h}), \tag{1c}$$

$$-\Delta\varphi = \operatorname{div}(\mathbf{m} - \mathbf{h}_a), \tag{1d}$$

$$\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u} - \operatorname{div}(\nu_\theta \mathbf{T}(\mathbf{u})) + \nabla p = \mu_0(\mathbf{m}\cdot\nabla)\mathbf{h} + \frac{\lambda}{\epsilon}\theta\nabla\psi, \tag{1e}$$

$$\operatorname{div}\mathbf{u} = 0, \tag{1f}$$

for every $t \in [0, t_F]$, where $\mathbf{T}(\mathbf{u}) = \frac{1}{2}(\nabla\mathbf{u} + \nabla\mathbf{u}^T)$ denotes the symmetric gradient and $\mathbf{h} = \nabla\varphi$. The system (1) is supplemented with the boundary conditions

$$\partial_\eta\theta = \partial_\eta\psi = 0, \quad \mathbf{u} = 0, \quad \text{and} \quad \partial_\eta\varphi = (\mathbf{h}_a - \mathbf{m})\cdot\eta \quad \text{on } \Gamma. \tag{2}$$

Define the backward difference operator $\delta f^k = f^k - f^{k-1}$.

For given smooth initial data $\{\Theta^0, \mathbf{M}^0, \mathbf{U}^0\}$ and timestep τ, compute $\{\Theta^k, \Psi^k, \mathbf{M}^k, \Phi^k, \mathbf{U}^k, P^k\} \in \mathbb{G}_h \times \mathbb{Y}_h \times \mathbb{M}_h \times \mathbb{X}_h \times \mathbb{U}_h \times \mathbb{P}_h$ for every $k \in \{1, ..., K\}$ that solves

$$\left(\frac{\delta\Theta^k}{\tau}, \Lambda\right) - (\mathbf{U}^k\Theta^{k-1}, \nabla\Lambda) - \gamma(\nabla\Psi^k, \nabla\Lambda) = 0, \tag{3a}$$

$$(\Psi^k, \Upsilon) + \epsilon(\nabla\Theta^k, \nabla\Upsilon) + \frac{1}{\epsilon}(f(\Theta^{k-1}), \Upsilon) + \frac{1}{\eta}(\delta\Theta^k, \Upsilon) = 0, \tag{3b}$$

$$\left(\frac{\delta\mathbf{M}^k}{\tau}, \mathbf{Z}\right) - \mathcal{B}_h^m(\mathbf{U}^k, \mathbf{Z}, \mathbf{M}^k) + \frac{1}{\mathscr{T}}(\mathbf{M}^k, \mathbf{Z}) = \frac{1}{\mathscr{T}}(\varkappa_\theta \mathbf{H}^k, \mathbf{Z}), \tag{3c}$$

$$(\nabla\Phi^k, \nabla X) = (\mathbf{h}_a^k - \mathbf{M}^k, \nabla X), \tag{3d}$$

$$\left(\frac{\delta\mathbf{U}^k}{\tau}, \mathbf{V}\right) + \mathcal{B}_h(\mathbf{U}^{k-1}, \mathbf{U}^k, \mathbf{V}) + (\nu_\theta \mathbf{T}(\mathbf{U}^k), \mathbf{T}(\mathbf{V})) - (P^k, \mathrm{div}\mathbf{V}) = \mu_0 \mathcal{B}_h^m(\mathbf{V}, \mathbf{H}^k, \mathbf{M}^k) + \frac{\lambda}{\epsilon}(\Theta^{k-1}\nabla\Psi^k, \mathbf{V}), \tag{3e}$$

$$(Q, \mathrm{div}\mathbf{U}^k) = 0. \tag{3f}$$

Numerical Implementation Details

Discretization of the Numerical Scheme:

- Time Discretization: Backward Euler is used.
- Space Discretization: A mix of Continuous and Discontinuous Galerkin is used, approximating the spaces with polynomials of degree 2 in each variable (i.e. $\mathcal{Q}_2$ elements).
  - Continuous: Cahn–Hilliard, Magnetic potential, and Navier Stokes equations.
  - Discontinuous: Magnetization equations.

Fixed Point Solver:

- A Picard–like iteration is used.
- Utilizes the "lagging" of the velocity $\mathbf{U}$ to solve each subsystem.
- Iterates until a fixed point for $\mathbf{U}^k$ is reached.
- Given $\mathbf{U}^{k-1}$
  1) Compute Θ^k and Ψ^k substituting $\mathbf{U}^{k-1}$ for $\mathbf{U}^k$.
  2) Next compute $\mathbf{M}^k$ and Φ^k using (Θ^k, Ψ^k) from the previous iteration and substituting $\mathbf{U}^{k-1}$ for $\mathbf{U}^k$.
  3) Finally, compute $\mathbf{U}^k$ and P^k using $(\Theta^k, \Psi^k, \mathbf{M}^k, \Phi^k)$ from the previous two iterations.
  4) Repeat steps 1-3 using $\mathbf{U}^k$ from the previous iteration as input until $\mathbf{U}^k$ does not change between iterations.

Semester Plan

- Implement and unit test solvers for each subsystem in "isolation".
  - Cahn–Hilliard (3a)–(3b)
  - Navier–Stokes (3e)–(3f)
  - Magnetization (3c)–(3d)
- Combine the solvers using a Picard iteration to implement the full two phase ferrofluid flow.

Adaptive Mesh Refinement

For adaptive refinement, we used a method of marking cells for refinement known as Dofler marking. Our adaptive refinement procedure is:

- Compute the element indicator η_T on each element, where

$$\eta_T^2 = h_T \int_{\partial T} \left| \left[\!\left[\frac{\partial \Theta}{\partial \eta} \right]\!\right] \right|^2 dS \quad \forall T \in \mathcal{T}_h,$$

  and $[\![\cdot]\!]$ is the jump across the face.
- Order the elements from highest to lowest based on their element indicator value.
- Compute the set of elements whose error makes up 55 percent of the total error for refinement, starting with the higher valued elements.
- Compute the set of elements whose error makes up 5 percent of the total error for coarsening, starting with the lowered valued elements.
- Refine/coarsen the mesh and transfer the solution from the old mesh to the new mesh.

We enforce a limit on the number of times an element can be refined. This procedure is performed every 5 iterations and on the initial condition.

Cahn–Hilliard Matrix Structure

- Rearranging the system we have that

$$\left(\Theta^k, \Lambda\right) - \tau\gamma(\nabla\Psi^k, \nabla\Lambda) = \left(\Theta^{k-1}, \Lambda\right) + \tau(\mathbf{U}^k\Theta^{k-1}, \nabla\Lambda),$$
$$(\Psi^k, \Upsilon) + \epsilon(\nabla\Theta^k, \nabla\Upsilon) + \frac{1}{\eta}(\Theta^k, \Upsilon) = \frac{1}{\eta}(\Theta^{k-1}, \Upsilon) - \frac{1}{\epsilon}(f(\Theta^{k-1}), \Upsilon).$$

- This leads to the following block matrix form

$$\begin{pmatrix} M & -\tau\gamma K \\ \epsilon K + \frac{1}{\eta}M & M \end{pmatrix} \begin{pmatrix} \Theta^k \\ \Psi^k \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix},$$

where M and K are the usual mass and stiffness matrices and f and g are the respective right hand sides.

Reduced Phase System

- We eliminate the chemical potential by adding $\tau\gamma KM^{-1}$ the second row to the first.
- Doing so yields the following reduced phase system

$$\left(M + \tau\epsilon\gamma KM^{-1}K + \frac{\tau\gamma}{\eta}K\right)\Theta^k = f + \tau\gamma KM^{-1}g.$$

- The chemical potential is then found by solving

$$M\Psi^k = g - \left(\epsilon K + \frac{1}{\eta}M\right)\Theta^k.$$

Solving the Reduced Phase System

- In order to precondition the reduced phase system, we consider the following preconditioner

$$P = M + \tau\gamma\epsilon K \text{diag}(M)^{-1} K + \tau\frac{\gamma}{\eta} K.$$

- When solving with GMRES, we then use an incomplete LU preconditioner of the preconditioner matrix P.
- Note: We never explicitly compute the matrix $M + \tau\epsilon\gamma K M^{-1} K + \frac{\tau\gamma}{\eta} K$. When solving with GMRES, you only need the action of the matrix. This allows us to not compute the inverse of M as we can compute its action on a vector x,

$$y = M^{-1} x,$$

by solving

$$My = x$$

using CG.

- Finally, we solve for the chemical potential using CG by using the action of the inverse of M.

Cahn–Hilliard Solver Verification

We verify the solver using three unit tests.

1) A flat initial profile with no forcing and adaptive refinement.

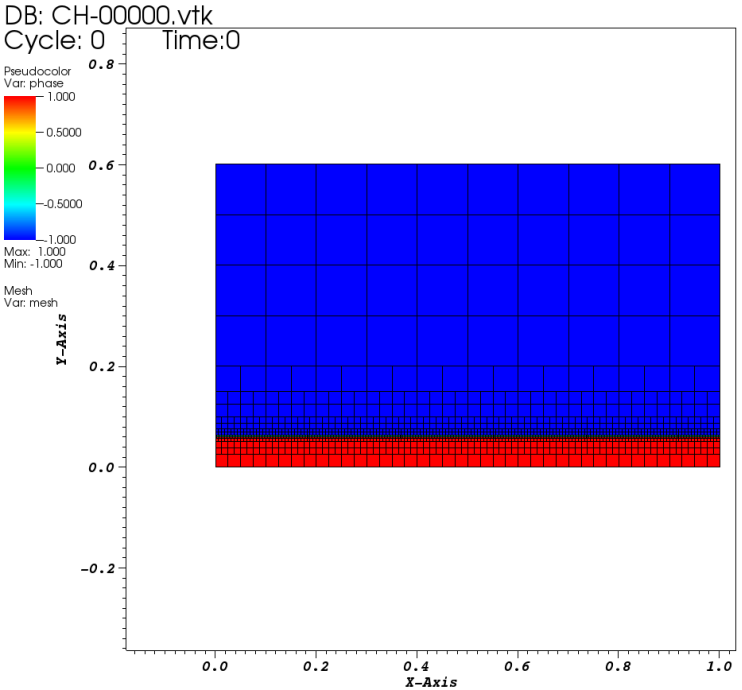
2) A circular profile with no forcing and adaptive refinement.

3) A forced solution on a series of globally refined grids. This is done to compute the convergence rate.

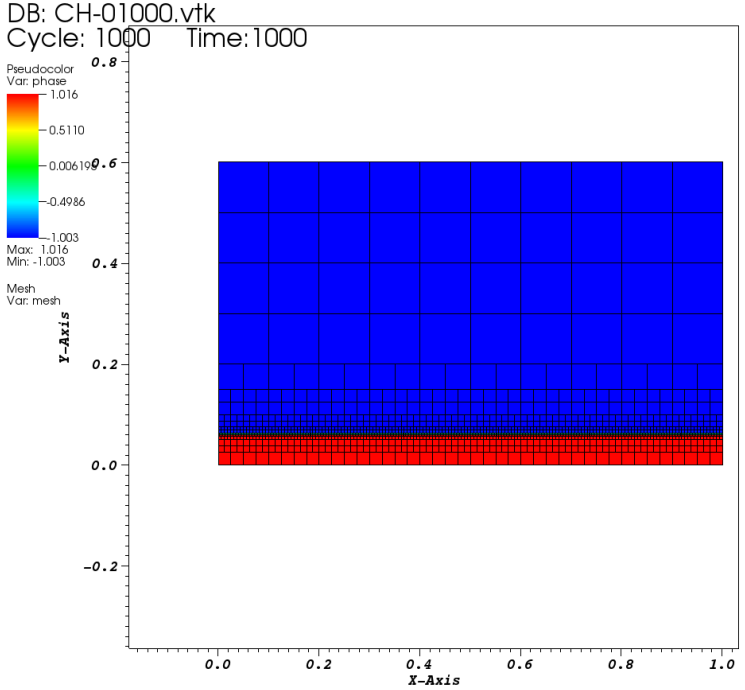
The initial condition for the flat profile was

$$f(x,y) = \begin{cases} -1 & y > .06 \\ 1 & \text{otherwise} \end{cases}.$$

The maximum level of refinement was 5 and the initial data was refined 20 times. Model parameters were chosen as $\epsilon = .001$, $\gamma = .2$, $\eta = .000001$. The error of the solution stayed approximately constant over 1000 time steps.



Time step 0

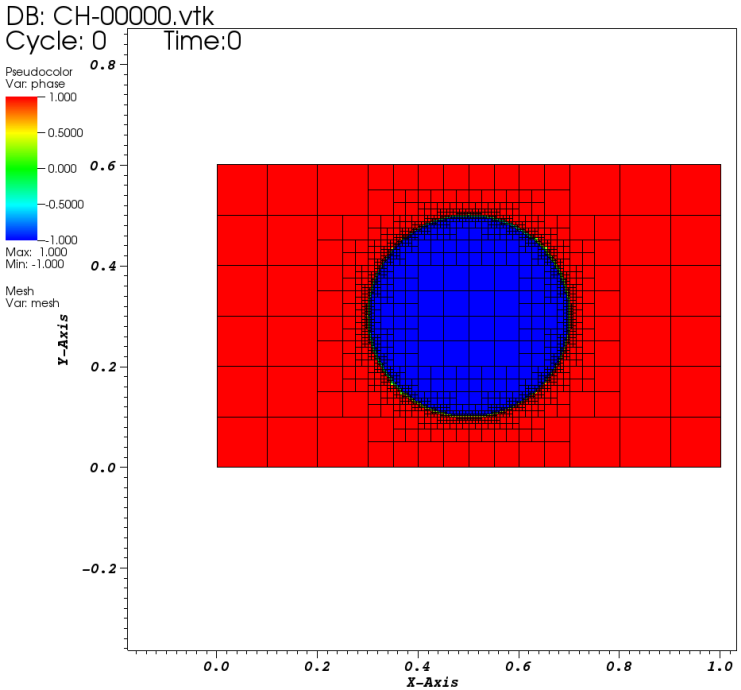


Time step 1000

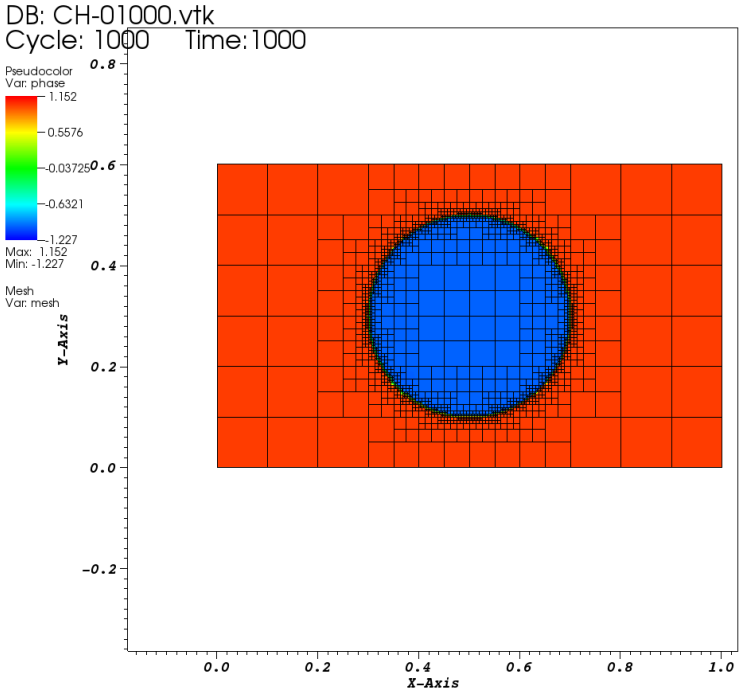
The initial condition for the circular profile was

$$f(x,y) = \begin{cases} -1 & (x,y) \in B((.5,.3),.2) \\ 1 & \text{otherwise} \end{cases}.$$

The maximum level of refinement was 5 and the initial data was refined 20 times. Model parameters were chosen as $\epsilon = .001$, $\gamma = .2$, $\eta = .000001$. The error of the solution stayed approximately constant over 1000 time steps.



Time step 0



Time step 1000

The forcing function chosen was $f(x, y) = \cos(2\pi x)cos(2\pi y)$ and $\Omega = [-1, 1]^2$. Model parameters were chosen as $\epsilon = .2$, $\gamma = .2$, $\eta = .000001$. The error was computed after 1000 iterations.

n cells		H^1-error			L^2-error		
2	16	4.264e+00	-	-	3.109e-01	-	-
3	64	8.079e-01	5.28	2.40	2.658e-02	11.70	3.55
4	256	2.038e-01	3.96	1.99	3.310e-03	8.03	3.01
5	1024	5.104e-02	3.99	2.00	4.125e-04	8.02	3.00
6	4096	1.277e-02	4.00	2.00	5.152e-05	8.01	3.00

This is the convergence rate that we expect for both the H^1 and L^2 error for Q_2 elements.

Navier–Stokes Block Matrix Structure

The system has following block matrix form

$$\begin{pmatrix} F & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} \mathbf{U}^k \\ P^k \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix},$$

where

$$F = (\mathbf{U}^k, \mathbf{V}) + \tau \mathcal{B}_h(\mathbf{U}^{k-1}, \mathbf{U}^k, \mathbf{V}) + \tau(\nu_\theta \mathbf{T}(\mathbf{U}^k), \mathbf{T}(\mathbf{V})),$$

$$B = (Q, \mathrm{div}\mathbf{U}^k),$$

and

$$f = (\mathbf{U}^{k-1}, \mathbf{V}) + \tau \mu_0 \mathcal{B}_h^m(\mathbf{V}, \mathbf{H}^k, \mathbf{M}^k) + \tau \frac{\lambda}{\epsilon}(\Theta^{k-1} \nabla \Psi^k, \mathbf{V}).$$

We would like to use the block preconditioner

$$P = \begin{pmatrix} F & 0 \\ B & -S \end{pmatrix}$$

where S is the the Schur Complement $S = B^T F^{-1} B$. This preconditioner is desirable as it has the property that

$$P^{-1} \begin{pmatrix} F & B^T \\ B & 0 \end{pmatrix} = \begin{pmatrix} I & F^{-1} B^T \\ 0 & I \end{pmatrix}.$$

Since we don't want to compute inverse matrices, we instead consider the following approximation for P^{-1}

$$P^{-1} \approx \begin{pmatrix} \tilde{F}^{-1} & 0 \\ \tilde{S}^{-1} B \tilde{F}^{-1} & -\tilde{S}^{-1} \end{pmatrix}$$

where $\tilde{F}^{-1}$ is computed as an inverse action and $\tilde{S}^{-1}$ is the Least Squares Commutator [1] defined as

$$\tilde{S}^{-1} = (B\text{diag}(M)^{-1} B^T)^{-1} (B\text{diag}(M)^{-1} F \text{diag}(M)^{-1} B^T)(B\text{diag}(M)^{-1} B^T)^{-1},$$

and M is the mass matrix for the velocity.

The preconditioner was implemented to compute $Y = P^{-1}X$, where X, Y are block vectors. It does so in three steps.

- Compute
$$Y_0 = \tilde{F}^{-1} X_0.$$
- Then compute in a temporary vector N
$$N = X_1 - BX_0 = X_1 - B\tilde{F}^{-1} X_0.$$
- Finally compute
$$Y_1 = S^{-1}N = S^{-1}(X_1 - B\tilde{F}^{-1} X_0).$$

Using this preconditioner the system is solved using GMRES.

Navier–Stokes Solver Verification

We verify the solver using the following forced solution

$$\mathbf{u}(x, y, t) = \begin{pmatrix} t \sin(\pi x) \sin(\pi(y + .5)) \\ t \cos(\pi x) \cos(\pi(y + .5)) \end{pmatrix}, \quad p(x, y, t) = \sin(2\pi(x - y) + t),$$

on $\Omega = [0, 1]^2$. The model parameters are $\mu = 1$, $\lambda = .05$, $\epsilon = .2$. The system was solved until $t = 2$ with 1000 time steps. The system was solved on a uniformly refined grid with levels $3, 4, 5$.

n cells		L^2-error
3	64	0.642479
4	256	0.642518
5	1024	0.64252

Deliverables

- Cahn–Hilliard solver and unit tests
- Navier–Stokes solver and unit test
- Summary of the capabilities of the code will be published on the github repo
- List of software requirements
- Instructions on how to run each of the codes and how to alter initial conditions and forcing functions

Figure References

- Slide 1: https://youtu.be/wHZDgSFzQ_s?t=12
- Slide 2:
  - https://www.researchgate.net/profile/Vikram_Raghavan2/post/What_is_the_effect_of_magnetic_field_on_alignment_of_ferro_fluid_droplet/attachment/59d622166cda7b8083a1b9a2/AS%3A273810673078272%401442292959057/download/Effect+of+Magnetic+field.jpg
  - https://ksr-ugc.imgix.net/assets/003/310/641/f0ef73d1fd99f6aa5d96872168478df4_original.png?v=1424378871&w=680&fit=max&auto=format&lossless=true&s=c183d857603c12de82a71f3139283d9e
  - https://opentextbc.ca/chemistry/wp-content/uploads/sites/150/2016/05/CNX_Che_11_05_Colloid.jpg
- Slide 3: [2]
- Slide 12: [3]
- Slide 13: [3]
- Slide 18: [3]

References I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