CHiMaD Phase Field Workshop V Draft Benchmark Problems

July 13, 2017

1 Stokes incompressible flow in 2D

Flow of a liquid can be incorporated into phase field models, so we present this benchmark problem for incompressible fluid flow through a channel (the flow of many liquids can be modeled as incompressible). The flow of a fluid can generally be modeled via the Navier-Stokes equations. When length scales are small, fluid velocities are low, and/or viscosity is large, such that the Reynolds number $Re << 1$, inertial forces are small compared with viscous forces, resulting in a simplification of Navier-Stokes flow to Stokes flow.

In this problem, two variables are used: the fluid velocity, $\mathbf{u}$, which is a vector field, and the fluid pressure, p, which is a scalar field. The Stokes momentum equation is given as

$$\mu\nabla^2\mathbf{u} + \nabla p - \rho\mathbf{g} = 0, \tag{1}$$

where ρ is the density, assumed constant in this problem, μ is the dynamic viscosity, and $\mathbf{g}$ is the acceleration due to gravity. To fully describe fluid flow, the momentum balance equation (Eq. 1) is supplemented with the continuity equation for mass flow,

$$\frac{d\rho}{dt} + \nabla\cdot(\rho\mathbf{u}) = 0; \tag{2}$$

this simplifies to

$$\nabla\cdot\mathbf{u} = 0 \tag{3}$$

for incompressible flow. Use $\rho = 100$, $\mu = 1$, and $\mathbf{g} = (0, -0.001)$.

In this problem, we consider flow in a 2D channel (a) without and (b) with an obstruction. The computational domain for case (b) is shown in Fig. 1. The domain and boundary conditions, etc., for case (a) are the same as that in case (b), but without the obstruction.

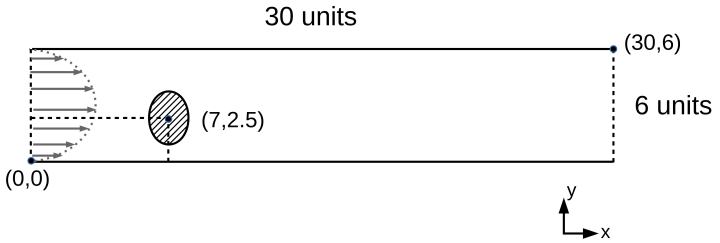


Figure 1: Schematic illustration of the 2D computational domain and inlet boundary condition (indicated by arrows) for the Stokes flow benchmark problem with an obstruction (case (b)).

All solid surfaces, including the boundary for the obstruction, have no-slip boundary conditions, that is, $u_x = u_y = 0$. The inlet velocity, on the left boundary, follows a parabolic profile described by

$$\mathbf{u}(0, y) = -0.001(y - 3)^2 + 0.009. \tag{4}$$

The outlet velocity (on the right boundary) is left to the solver to determine, as is the pressure over the entire domain. However, we specify that the pressure at point (30, 6) is zero. Finally, the obstruction is described by an ellipse centered at (7, 2.5). The semi-major axis (in the y-direction) is $a = 1.5$, and the semi-minor axis (in the x-direction) is $b = 1$.

For both case (a) and case (b), find the steady-state pressure and velocity distributions given these boundary conditions. Plot the pressure and all three vector components of the velocity over the lines $y = 5$ and $x = 7$. Perform a mesh convergence study to illustrate the effect of mesh size on the solution.

2 Coupled electrostatics and Cahn-Hilliard dynamics

Diffusion of a charged species is often modeled with the phase field approach, such as for batteries, electrodeposition, and electromigration. This benchmark problem incorporates the first benchmark problem for spinodal decomposition [1] and extends it to incorporate coupling with electrostatics.

In this problem, two variables are used: c, the concentration field of our charged species, and Φ, the electric potential field. The free energy of the system is given as

$$F = \int_V \left[\frac{\kappa}{2} |\nabla c|^2 + f_{chem}(c) + f_{elec}(c, \Phi) \right] \, dV, \tag{5}$$

where κ is the gradient energy coefficient, f_{chem} is the chemical free energy, and f_{elec} is the electrostatic coupling energy. Here, f_{chem} is a symmetric double-well function with minima between $0 < c < 1$,

$$f_{chem} = \rho (c - c^\alpha)^2 (c^\beta - c)^2, \tag{6}$$

where ρ controls the height of the double-well and c^α and c^β are the compositions at which the energy is minimum. In addition, the electrostatic coupling energy is given as

$$f_{elec} = \frac{k \, c \, \Phi}{2}, \tag{7}$$

where k is a constant.

The time evolution of the system is described by the Cahn-Hilliard equation with the additional constraint that the Poisson equation must be satisfied at every point in the system at each time step (Refs. [2, 3]). To avoid a lengthy derivation, we simply present the equations below and suggest the readers study the given references. The Cahn-Hillard equation is given as

$$\frac{\partial c}{\partial t} = \nabla \cdot \left\{ M \nabla \left(2\rho (c - c^\alpha)(c^\beta - c)(c^\alpha + c^\beta - 2c) - \kappa \nabla^2 c + k \, \Phi \right) \right\}, \tag{8}$$

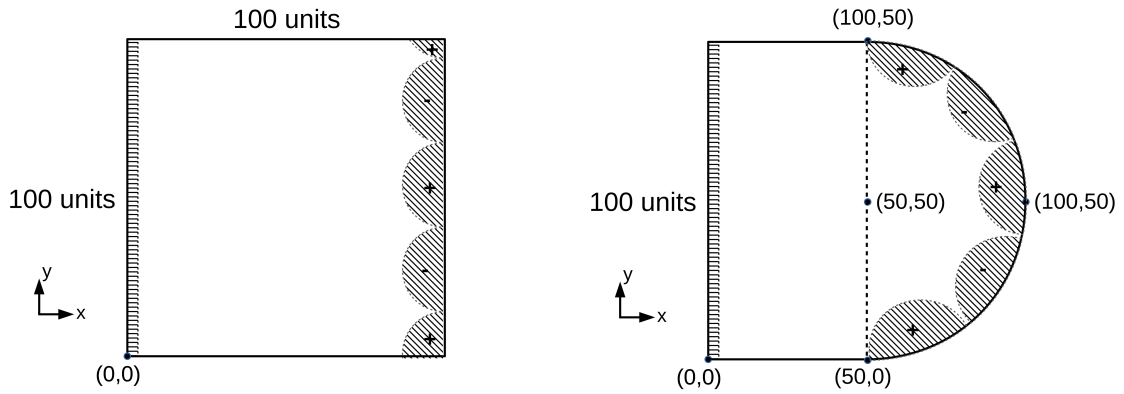
where M is the mobility. The dynamics of electric relaxation occur at a much faster time scale than the diffusion of the charged species. In this case, the Poisson equation is solved at each time step,

$$\nabla^2 \Phi = \frac{-k \, c}{\epsilon}, \tag{9}$$

where ϵ is the permittivity.

As in the spinodal benchmark problem, $c^\alpha = 0.3$, $c^\beta = 0.7$, $\kappa = 2$, $\rho = 5$, and $M = 5$. In addition, $k = 0.09$ and $\epsilon = 9$.

In this problem, the system consists of a domain which is grounded on one side and with a voltage applied on the other. Two different 2D computational domains are given, shown in Fig. 2 (the boundary conditions for Φ are schematically illustrated). The first consists of a square domain (Fig. 2a), while the second consists of a half-circle with a radius of 50 units and centered at (50, 50), which is attached to a rectangle of 50 units wide by 100 units tall (Fig. 2b). The curved boundary is the right-hand boundary, while the straight domain edges from (0, 0) to (50, 0) and (0, 100) to (50, 100) are the bottom and top boundaries, respectively.



(a) (b)

Figure 2: Schematic illustration of the 2D computational domains and boundary conditions of Φ (indicated by hatching) for the electrochemical benchmark problem.

We impose $\nabla c \cdot \hat{\mathbf{n}} = 0$ on all boundaries, where $\hat{\mathbf{n}}$ is the unit normal vector, while $\Phi = 0$ for the left boundary, $\nabla\Phi \cdot \hat{\mathbf{n}} = 0$ for the top and bottom boundaries, and the right boundary is given by

$$\Phi(x|_{boundary}, y) = \sin(y/7), \tag{10}$$

where $x|_{boundary} = 100$ for the square domain, and varies from 50 to 100 for the other domain. The initial condition for c is specified by

$$\begin{aligned} c\left(x,y\right) &= c_0 + c_1 \Big[\cos\left(0.2x\right)\cos\left(0.11y\right) + \left[\cos\left(0.13x\right)\cos\left(0.087y\right)\right]^2 \\ &\quad + \cos\left(0.025x - 0.15y\right)\cos\left(0.07x - 0.02y\right)\Big], \end{aligned} \tag{11}$$

where $c_0 = 0.5$ and $c_1 = 0.04$ (you may recognize this as the initial conditions for the spinodal decomposition benchmark problem with a slightly different parameterization).

Find the equilibrium distributions of c and Φ by evolving the system. Use synchronization times of $t = 5$, 10, 20, 50, 100, 200, 400, and 1000 to visualize the c and Φ fields during evolution and to plot horizontal line cuts through the center of the domain for c. Plot the total free energy of the system as a function of time.

References

[1] A. Jokisaari, P. Voorhees, J. E. Guyer, J. Warren, and O. Heinonen, "Benchmark problems for numerical implementations of phase field models," *Computational Materials Science*, vol. 126, pp. 139–151, 2017.

[2] J. E. Guyer, W. J. Boettinger, J. A. Warren, and G. B. McFadden, "Phase field modeling of electrochemistry. I. Equilibrium," *Physical Review E*, vol. 69, no. 2, p. 021603, 2004.

[3] J. E. Guyer, W. J. Boettinger, J. A. Warren, and G. B. McFadden, "Phase field modeling of electrochemistry. II. Kinetics," *Physical Review E*, vol. 69, no. 2, p. 021604, 2004.