A Phase Field Approach to Modeling and Simulating Multi-Phase Flows

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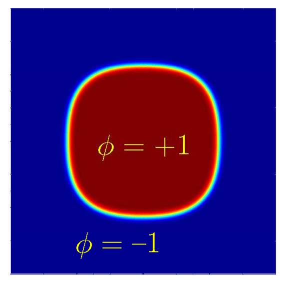
Cahn-Hilliard Mixing Energy

$$\mathcal{E}_{CH}[\phi] = \int_\Omega W(\phi, \nabla\phi)\,\mathrm{d}\mathbf{x} = \int_\Omega \gamma \left\{ \underbrace{\frac{1}{2}|\nabla\phi|^2}_{\text{"phillic"}} + \underbrace{\frac{1}{4\epsilon^2}(\phi^2-1)^2}_{\text{"phobic"}} \right\} \mathrm{d}\mathbf{x}$$

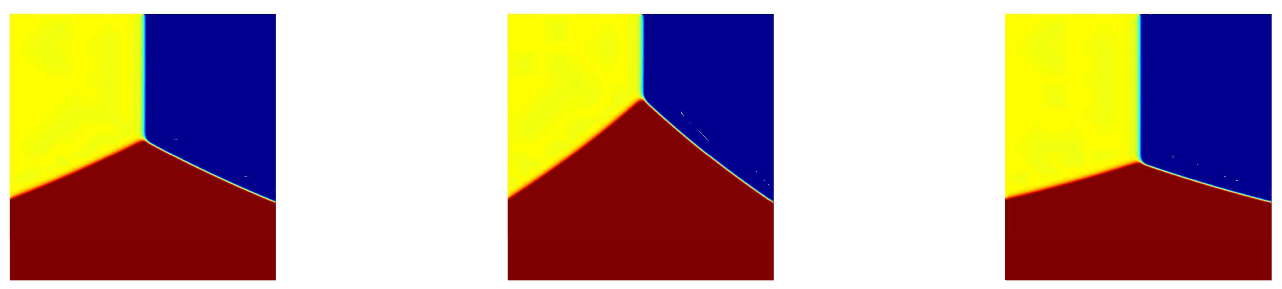


Allen-Cahn dynamics $\quad < \frac{\partial}{\partial t}\phi, \eta >_{L^2} = < \frac{\delta}{\delta\phi}\mathcal{E}_{CH}, \eta >_{L^2}$

Cahn-Hilliard dynamics $\quad < \frac{\partial}{\partial t}\phi, \eta >_{L^2} = < \frac{\delta}{\delta\phi}\mathcal{E}_{CH}, \eta >_{H^{-1}}$

Multi-Phase Modeling

We can generalize the above binary-phase to multi-phase modeling. The figures below show a simple case where we have three different phases. We prescribe different surface tensions on the interfaces so that angles of different degrees are formed at equilibrium (force balance).



Adding Fluid Dynamics

Stress due to the multi-phase structure in the fluid = Conservative force + Dissipative force

Conservative force

We define the action functional in Lagrangian coordinate ($\mathbf{X}$)

$$\mathcal{A}[\mathbf{x}] = \int_0^T \int_{\Omega_0} \left\{ \frac{1}{2}|\partial_t \mathbf{x}|^2 - \lambda \widetilde{W}(\phi, \nabla\phi) \right\} \det \frac{\partial \mathbf{x}}{\partial \mathbf{X}}\,\mathrm{d}\mathbf{X}\,\mathrm{d}t\,.$$

then apply

Principle of Least Action: $\quad \min_{\mathbf{x}} \mathcal{A}[\mathbf{x}]$

This is a variational problem with respect to the domain. We assume the corresponding Euler-Lagrange equation gives the conservative part in the momentum equation.

Dissipative force

We consider the dissipation relation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}^{\text{total}}[\mathbf{u}, p, \phi] = -\Delta[\mathbf{u}, p, \phi]$$

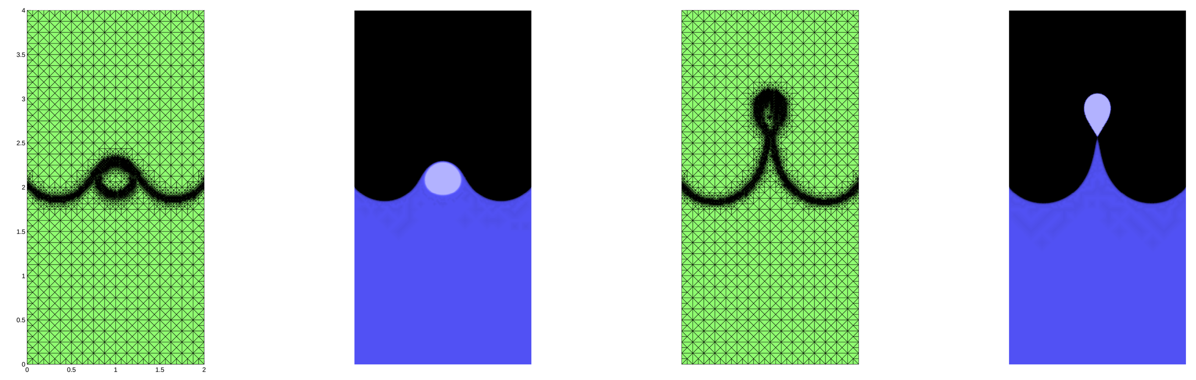
where $\mathcal{E}^{\text{total}}$ is the total energy of the system (with the primitive variables: velocity $\mathbf{u}$, pressure p and phase field function ϕ). Δ is the functional of dissipation.
Then we apply

Principle of Minimum Dissipation: $\quad \min_{\mathbf{u},p,\phi} \Delta$

This is a variational problem with respect to the functions. We assume the corresponding Euler-Lagrangian equation gives the dissipative part int the momentum equation.

A Multi-Phase Fluid Simulation

Rising fluid bubble:



Numerical Ingredients:

- Adaptive Mesh Refinement (AMR).
- Pressure Schur Complement (PSC) method for fluid equations.
- Krylov subspace type solver with Algebraic Multigrid (AMG) preconditioner.

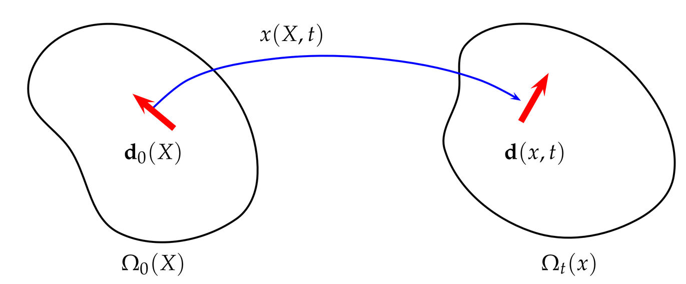
Solid immersed in a fluid

The classical result of **Jeffery's orbit** states that an ellipsoid particle immersed in a shear flow will experience a time-periodic tumbling motion. The method was based on explicit construction from ellipsoidal harmonics.

Alternatively, we consider the following equation which describes the transport dynamics

$$\partial_t \mathbf{d} + \mathbf{u}\cdot\nabla\mathbf{d} - \mathbf{\Omega}\mathbf{d} - (2\alpha - 1)\mathbf{A}\mathbf{d} = 0. \qquad (1)$$

where $\mathbf{d}$ is a vector field describing the orientation of particles immersed in the fluid. $\mathbf{A} = \frac{\nabla\mathbf{u}+(\nabla\mathbf{u})^T}{2}$ and $\mathbf{\Omega} = \frac{\nabla\mathbf{u}-(\nabla\mathbf{u})^T}{2}$ characterize the stretching and rotating effect. The parameter $2\alpha - 1 = \frac{r^2-1}{r^2+1}$ with r being the aspect ratio of the ellipsoids take shape effect into account.



Flow map

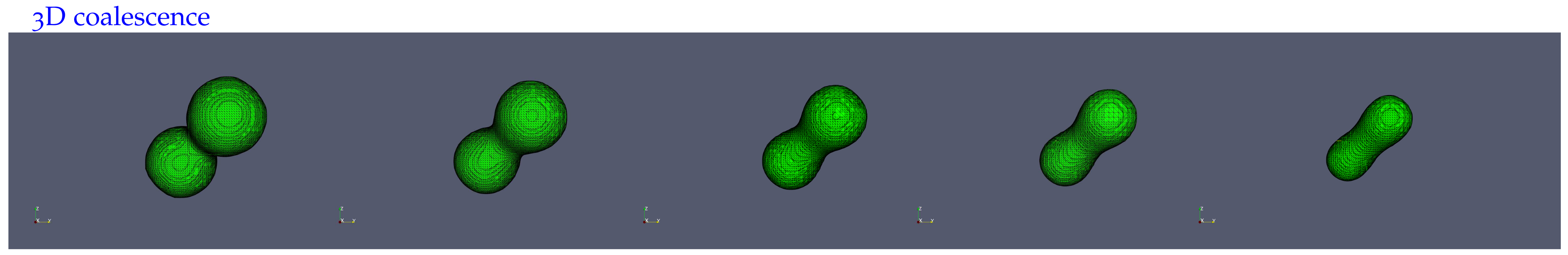
Theorem 1 *Under a shear flow $\mathbf{u} = (0, 0, \kappa y)$, there is an explicit solution of (1) as follows*

$$\begin{aligned} \mathbf{d} &= (\cos\theta, \cos\varphi\sin\theta, \sin\varphi\,\sin\theta)^T \\ \frac{\mathrm{d}}{\mathrm{d}t}\varphi &= -\kappa\frac{a^2\sin^2\varphi + b^2\cos^2\varphi}{a^2+b^2} \\ \frac{\mathrm{d}}{\mathrm{d}t}\theta &= \frac{\kappa(a^2-b^2)\sin\theta\cos\theta\sin\varphi\cos\varphi}{a^2+b^2} \end{aligned}$$

i.e. we can recover Jeffery's orbit from the dynamical equation.

However, both Jeffery's original work and the dynamical equation (1) above assume there is no slip between the solid and the surrounding fluid. However, this might not be always true, especially in multi-phase problems, e.g. the moving contact line problem. Also this apparent slip is negligible in the macroscopic scale but may play a crucial role in microfluidics. All these motivate us to study the slip effect.

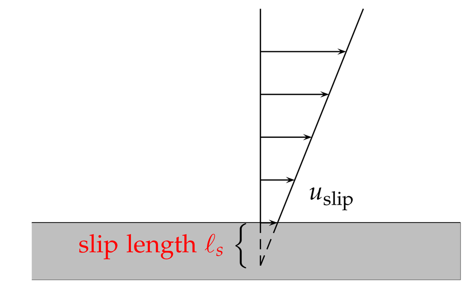
3D coalescence



Slip between fluid and solid

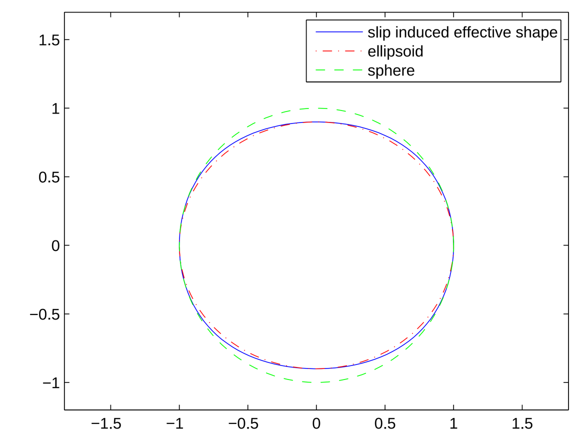
Slip from a Kinematic Perspective

We relate the slip effect to the particle shape by adopting the notion of **slip length**. There are two boundaries for a slippery solid body: the physical boundary where slip occurs and the imaginary one where the velocity is extrapolated to zero, i.e. there is no slip.



In simulations (yet to implement) we would like to calculate the **slip-induced shape** and derive the coefficient of aspect ratio $\widetilde{r}$ in the dynamical equation (1).

Our approach is to asymptotically calculate the velocity "around" a slightly slippery sphere (the green line in the figure on right), determine the induced effective shape, and then find a corresponding slightly different nonslip ellipsoid (red line) that can produce the same (in the asymptotic sense) velocity in the vicinity. This ellipsoid will provide us with the effective aspect ratio $\widetilde{r}$.

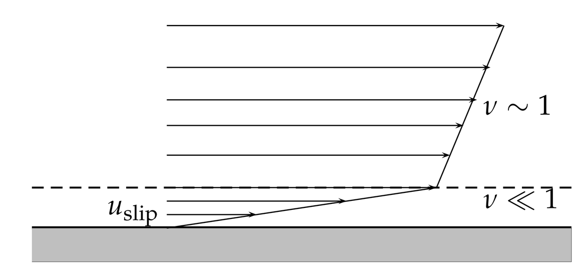


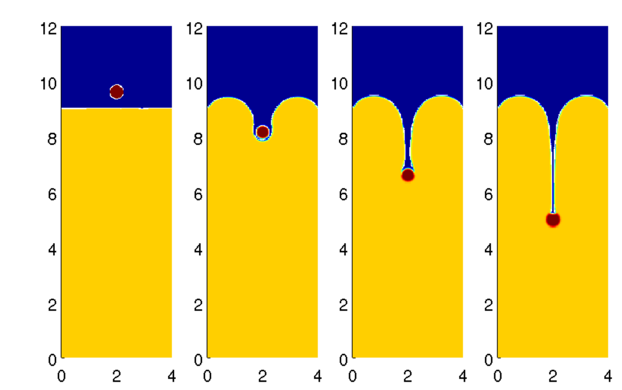
Slip from an Energetic Perspective

Slip means extra dissipation in energy.

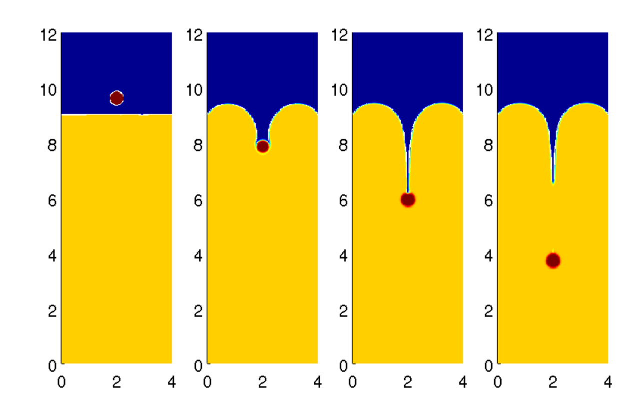
$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \frac{1}{2}\rho\,|\mathbf{u}|^2\mathrm{d}\mathbf{x} \\ &= -\int_\Omega \nu|\nabla\mathbf{u}|^2\mathrm{d}\mathbf{x} - \beta\int_{\partial\Omega} u_{\text{slip}}^2\,\mathrm{d}S \end{aligned}$$

The second boundary dissipative term can be obtained by assuming a bulk dissipation in a thin layer near the fluid-solid interface and passing the layer width to the limit of zero, as is illustrated blow.





a nonslip solid ball falling in a two-phase Stokesian flow



a slippery solid ball falling in a two-phase Stokesian flow

The implementation of this idea in the numerical simulation is relatively easy since we can have a variable viscosity that depends on the phase field function. We present the simulation result on the left, a contrast of the dynamics of a falling slippery solid sphere to that of a nonslip one, in a binary-phase Stokesian flow.

Ongoing or Future Work

1. Calibrating physical parameters.
2. Application to falling spheres in stratified fluids.
3. Application to moving contact line.
4. Parallel code for full 3D simulations.
   An example is on the left.

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