Tutorial: Efficient and accurate numerical schemes for the phase-field model of multiphase complex fluids

Jie Shen

Department of Mathematics
Purdue University

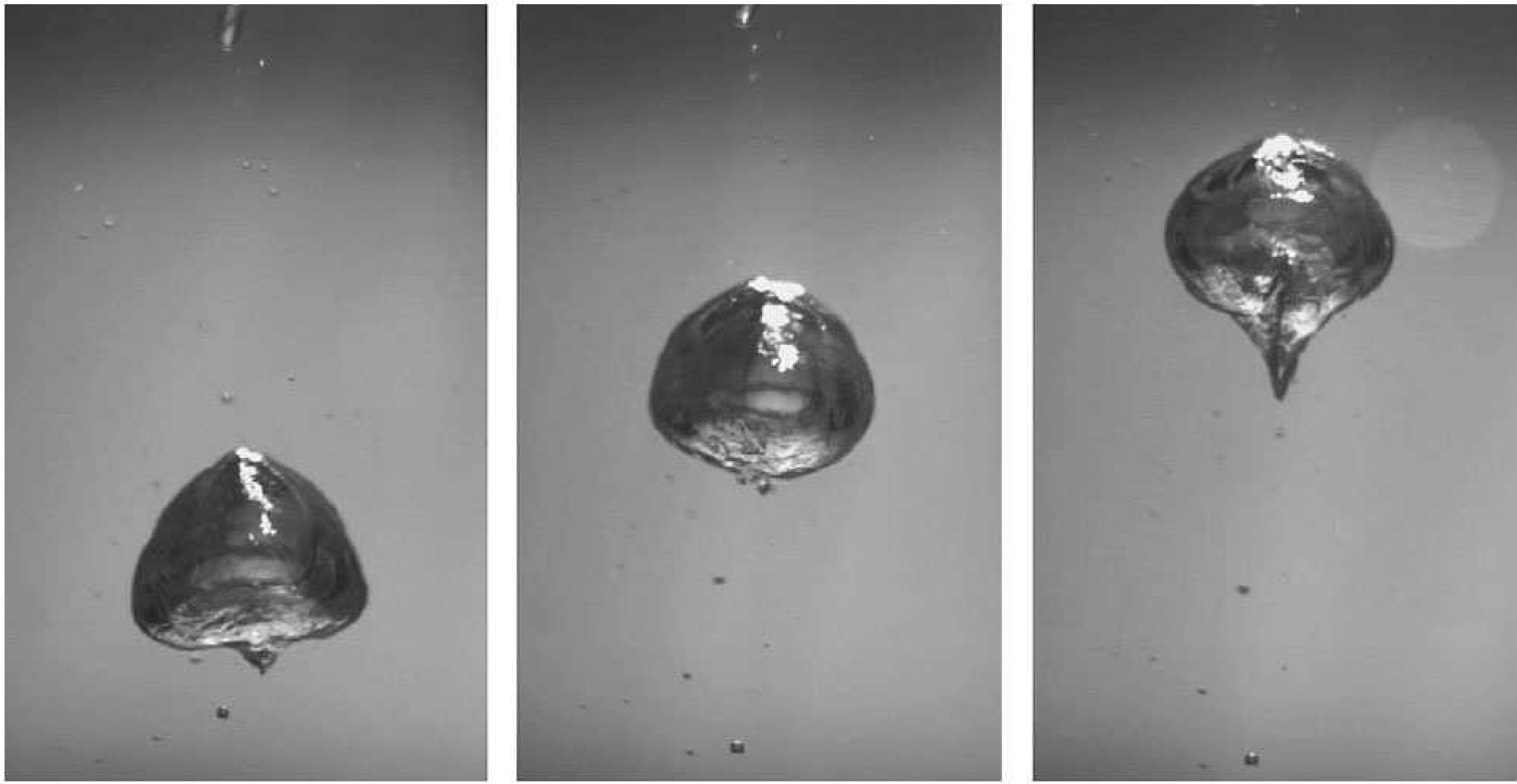
IMS, Singapore July 29-30, 2009

Outline

- Part-I: Introduction to phase field model
- Part-II: Splitting methods for incompressible flows
- Part-III: Fast spectral methods foe elliptic equations
- Part-IV: Numerical schemes for phase field model

Part-I: Phase field model for two-phase incompressible flows

Air bubbles rising in a polymetric flow



Typical “sharp-interface” formulation for two-phase flows

• Use a marker function $\phi(x,t)$ to identify the two fluids — ϕ is advected by the fluid velocity:

$$\frac{\partial \phi}{\partial t} + (u \cdot \nabla)\phi = 0.$$

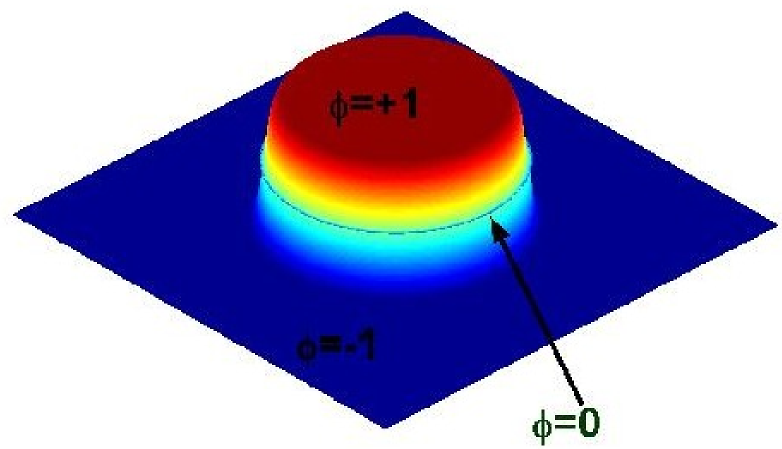
• Use a singular delta function “$\sigma H \delta(\mathbf{n})\mathbf{n}$” (H: mean curvature of the interface) to represent the surface tension:

$$\rho(u_t + (u \cdot \nabla)u) + \nabla p = \nabla \cdot \mu(\nabla u + \nabla^t u) + \sigma H \delta(\mathbf{n})\mathbf{n}.$$

Levelset method (ϕ: distance function), volume-of-fluid method (ϕ: discontinuous Heaviside function) ...

The diffusive phase-field approach

Use a phase function $\phi(x,t) = \pm 1$ to label the two fluids (e.g., $\phi = 1$ in one fluid and $\phi = -1$ in the other) with a transitional layer of thickness η:



Rayleigh '1892, Van der Waals '1893; Blinowski '75, Gurtin et al. '96, Jacqmin '96, Anderson & McFadden '97, Lowengrub & Truskinovsky '98, Liu & S. '03, ...

Governing equations for the fluids

The momentum equation:

$$\rho(u_t + (u \cdot \nabla)u) = \nabla \cdot \tau,$$

with $\tau = -pI + \mu(\nabla u + \nabla^t u) + \tau^e$; where τ^e is the extra elastic stress induced by the capillary force near the interface;

Incompressibility:

$$\nabla \cdot u = 0;$$

(The mass conservation $\rho_t + (u \cdot \nabla)\rho = 0$ will be replaced by an equation for the phase-field ϕ.)

Elastic stress

Elastic mixing energy:

$$W(\phi) = \lambda \int_{\Omega} \{\frac{1}{2}|\nabla\phi|^2 + \frac{1}{4\eta^2}(\phi^2 - 1)^2\}\, dx.$$

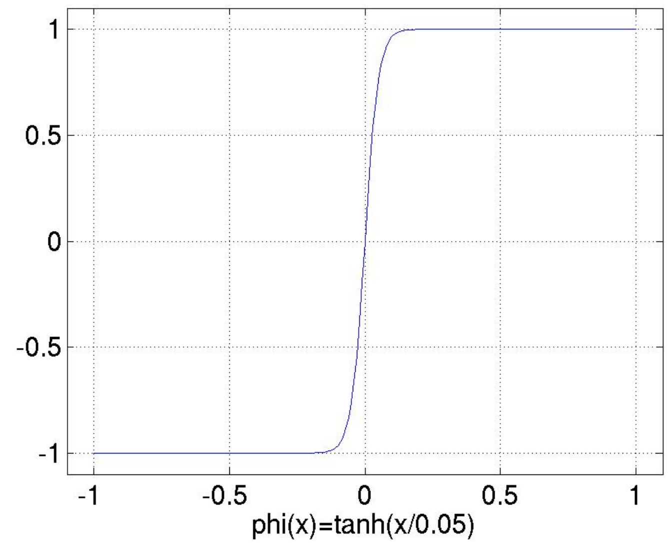
• The two parts represent, respectively, the “hydrophilic” and “hydrophobic” tendency of the two fluids;

• λ: mixing energy density which can be related to the traditional surface energy density σ;

• From the least action principle, one can derive

$$\tau^e = -\lambda(\nabla\phi \otimes \nabla\phi).$$

η: capillary width of the transition layer. In the 1-D case, it can be shown that the minimizer is: $\phi_0(x) = \tanh \frac{x}{\sqrt{2}\eta}$;



- In the 1-D case, setting the surface tension energy $\sigma = W(\phi_0)$, we find: $\sigma = \frac{2\sqrt{2}\lambda}{3\eta}$.

Governing equation for the phase function

Pure transport equation: $\phi_t + (u \cdot \nabla)\phi = 0$ —- No mecanism to keep the interface profile.

It is therefore natural to "relax" it:

$$\phi_t + (u \cdot \nabla)\phi = \gamma \Delta \frac{\delta W}{\delta \phi}, \quad (\text{or } -\gamma \frac{\delta W}{\delta \phi}),$$

where the free energy W is once again:

$$W(\phi) = \int_\Omega \{\frac{1}{2}|\nabla \phi|^2 + \frac{1}{4\eta^2}(\phi^2 - 1)^2\} \, dx.$$

- γ is a relaxation parameter related to the relaxation time scale of the system;
- The thickness of the interface will remain to be of order η;
- Topological changes are handled seamlessly;
- In many situations, it can be shown that when $\lambda \sim$ surface tension $\cdot$ capillary width, the phase equation will approach, as $\gamma, \eta \to 0$, to the transport equation:

$$\phi_t + u \cdot \nabla\phi = 0.$$

Cahn-Hilliard dynamics

The Cahn-Hilliard phase equation:

$$\phi_t + (u \cdot \nabla)\phi = \gamma \Delta(-\Delta \phi + f(\phi))$$

with $f(\phi) = \frac{1}{\eta^2}(\phi^2 - 1)\phi$ and the boundary condition:

$$\frac{\partial \phi}{\partial n}|_{\partial\Omega} = 0; \qquad \frac{\partial(\Delta\phi - f(\phi))}{\partial n}|_{\partial\Omega} = 0.$$

We observe that

$$\frac{d}{dt}\int_\Omega \phi dx = 0,$$

but fourth-order spatial derivatives are involved.

Allen-Cahn dynamics

The Allen-Cahn phase equation:

$$\phi_t + (u \cdot \nabla)\phi = -\gamma(-\Delta\phi + f(\phi))$$

with the boundary condition:

$$\frac{\partial \phi}{\partial n}|_{\partial\Omega} = 0.$$

In this case,

$$\frac{d}{dt}\int_\Omega \phi dx = -\int_\Omega f(\phi) dx \neq 0.$$

Remedy: adding a Lagrange multiplier $\xi(t)$:

$$\phi_t + (u \cdot \nabla)\phi = \gamma(\Delta\phi - f(\phi) + \xi(t)),$$

$$\frac{d}{dt}\int_\Omega \phi dx = 0.$$

The complete set of governing equations

Find $u,\ p,\ (\phi, \xi)$ such that

$$\rho(u_t + (u\cdot\nabla)u) + \nabla p = \nabla\cdot\mu(\nabla u + \nabla^t u) - \lambda\nabla\cdot(\nabla\phi\otimes\nabla\phi);$$

$$\nabla\cdot u = 0;$$

$$\phi_t + (u\cdot\nabla)\phi = \gamma(\Delta\phi - f(\phi) + \xi(t)),$$

$$\frac{d}{dt}\int_\Omega \phi dx = 0;$$

$$(\rho,\mu) = \frac{1+\phi}{2}(\rho_1,\mu_1) + \frac{1-\phi}{2}(\rho_2,\mu_2);$$

μ: viscosity, λ: surface tension coefficient, γ: elastic relaxation coefficient, η: interfacial width.

Energy laws

Unfortunately, the above system does not admit an energy law. However, energy law can be derived in several “approximate” situations.

- Using a Boussinesq approximation in the momentum eqn:

$$\rho_0(u_t + (u\cdot\nabla)u) + \nabla p = \nabla\cdot\mu(\nabla u + \nabla^t u) - \lambda\nabla\cdot(\nabla\phi\otimes\nabla\phi) + g(\rho)$$

Multiplying the momentum eqn by u and the phase eqn by $\lambda(\frac{\delta W}{\delta\phi} - \xi(t)) = \lambda(-\Delta\phi + f(\phi) + \xi(t))$, using the identity:

$$(\nabla\cdot(\nabla\phi\otimes\nabla\phi), u) = (\Delta\phi\nabla\phi + \frac{1}{2}\nabla|\nabla\phi|^2, u) = ((u\cdot\nabla\phi), \Delta\phi - f(\phi)),$$

one obtains

$$\frac{d}{dt}\int_\Omega\{\frac{\rho}{2}|u|^2 + \frac{\gamma\lambda}{2}|\nabla\phi|^2 + \lambda F(\phi)\} = -\int_\Omega\{\mu|\nabla u|^2 + \gamma\lambda|\Delta\phi - f(\phi) - \xi(t)|^2\}$$

which ensures the wellposedness of the system, and makes it possible to prove the numerical stability.

An alternative formulation

For problems with large density ratio, we are not aware of an energy law for the phase-field model, making it difficult to design stable numerical algorithms.

Using the relation $\rho = \frac{1+\phi}{2}\rho_1 + \frac{1-\phi}{2}\rho_2$, we can eliminate ϕ, leading to the following system (see also Korteweg 1908):

$$\rho(u_t + (u \cdot \nabla)u) + \nabla p = \nabla \cdot \mu(\rho)D(u) - \lambda \nabla \cdot (\nabla \rho \otimes \nabla \rho)$$

$$\nabla \cdot u = 0;$$

$$\rho_t + (u \cdot \nabla)\rho = \gamma(\Delta \rho - F'(\rho)),$$

where $F(\rho) = \frac{1}{4\eta^2}(\rho - \rho_1)^2(\rho - \rho_2)^2$.

- The above system can be viewed as a system with ρ acting as the phase variable; still no energy law.

- Let $\sigma = \sqrt{\rho}$. Using the "original" mass conservation "$\rho_t + (u \cdot \nabla)\rho = 0$, we can show

$$\rho(u_t + (u \cdot \nabla)u) = \sigma(\sigma u)_t + (\rho u \cdot \nabla)u + \frac{1}{2}\nabla \cdot (\rho u)u.$$

- Using the above in the momentum eqn., we can establish the following energy law:

$$\frac{d}{dt}\int_\Omega \{\frac{1}{2}|\sigma u|^2 + \frac{\gamma\lambda}{2}|\nabla\rho|^2 + \lambda F(\rho)\} = -\int_\Omega \{\mu|\nabla u|^2 + \gamma\lambda|\Delta\rho - f(\phi)|^2\}$$

- A Lagrange multiplier can be added to conserve the total mass.

Main numerical difficulties and our approach

• Coupling between velocity and pressure — use a suitable projection-type scheme to decouple the pressure from the velocity

• Stiffness of the phase equation for $\eta << 1$ — stabilized semi-implicit discretization to alleviate the stiffness

• Cases with large density ratio where Boussinesq approximation is no longer valid — a suitable penalty or projection scheme involving only pressure Poisson equation (with constant coefficients).

• Fine resolution needed to resolve the interface with thickness η — a high resolution spectral discretization in space coupled with a moving mesh method.

Numerical stiffness of the phase equation

A simple semi-implicit discretization:

$$\frac{\phi^{n+1} - \phi^n}{\delta t} - \gamma \Delta \phi^{n+1} = -\frac{\gamma(|\phi^n|^2 - 1)\phi^n}{\eta^2}.$$

leads to a time step constraint $\delta t \lesssim \eta^2$.

A simple fix: Use the stabilized semi-implicit scheme:

$$\frac{\phi^{n+1} - \phi^n}{\delta t} - \gamma(\Delta - \frac{C_s}{\eta^2} I)\phi^{n+1} = -\frac{\gamma(|\phi^n|^2 - 1 + C_s)\phi^n}{\eta^2}.$$

- Numerical evidence shows that with a suitable choice of C_s (usually ~ 1), the time step can be enlarged significantly for small η.

- A second-order version can be devised easily.

An alternative approach — splitting:

$$\phi_t - \gamma(\Delta\phi - \frac{1}{\eta^2}(\phi^2 - 1)\phi) = 0, \quad t \in (t_n, t_{n+1})$$

can be approximated by solving two sub problems: the first being the linear system

$$\phi_t - \gamma\Delta\phi = 0, \quad t \in (t_n, t_{n+\frac{1}{2}})$$

and the second is an ODE

$$\phi_t + \frac{\gamma}{\eta^2}(\phi^2 - 1)\phi = 0, \quad t \in (t_{n+\frac{1}{2}}, t_{n+1})$$

which can be solved exactly.

- A second-order version can be derived using the Strang splitting;
- Easy to solve and stable for large δt;
- The two substeps do not preserve the interface profile, leading to large splitting errors;
- Can not be extended to the Cahn-Hilliard case;
- Our numerical experiments indicate that the stabilized semi-implicit scheme leads to more accurate results.