Part II. Efficient and Accurate Numerical Schemes for Phase-Field Models for Two-Phase Incompressible Flows

Jie Shen

Purdue University

IMS, National University of Singapore, May 10, 2018
Outline

- Phase-field models for two-phase incompressible flows
- Extension to complex fluids
- Decoupled, energy stable numerical algorithms
- Numerical simulations
- Concluding remarks
The diffuse interface (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 \( \eta \):

Rayleigh '1892, Van der Waals '1893; Blinowski '75, Gurtin et al. '96, Jacqmin '96, Anderson & McFadden '97, Lowengrub & Truskinovsky '98, Boyer '01, Liu & S. '03, Yue, Feng, Liu & S. '04, ...
Let $F(\phi) = \frac{1}{4\eta^2}(\phi^2 - 1)^2$. Consider the mixing free energy:

$$E_{\text{mix}}(\phi) = \lambda \int_{\Omega} \left( \frac{1}{2} |\nabla \phi|^2 + F(\phi) \right) dx.$$ 

- In the 1-D case, the minimizer is: $\phi_0(x) = \tanh \frac{x}{\sqrt{2\eta}}$;

- $\lambda$ is related to the surface tension density $\sigma$: $\sigma = \frac{2\sqrt{2}\lambda}{3\eta}$. 

\[ \text{Graph: } \phi(x) = \tanh(\frac{x}{0.05}) \]
The Cahn-Hilliard phase-field equation is:

\[ \phi_t + (u \cdot \nabla) \phi = \nabla \cdot \left( \gamma \nabla \frac{\delta E_{\text{mix}}}{\delta \phi} \right) = \nabla \cdot \left( \gamma \nabla (\Delta \phi - F'(\phi)) \right). \]

- The interface will not be smeared over time.
- With the boundary conditions:

\[ \frac{\partial \phi}{\partial n} \bigg|_{\partial \Omega} = \frac{\partial (\Delta \phi - F'(\phi))}{\partial n} \bigg|_{\partial \Omega} = 0, \]

the phase-field equation leads to the desired property:

\[ \frac{d}{dt} \int_{\Omega} \phi dx = 0. \]
Phase-field model of a two-phase incompressible flow: Case of matched density

- Cahn-Hilliard phase-field equation:
  \[
  \phi_t + (u \cdot \nabla)\phi = \nabla \cdot (\gamma \nabla w),
  \]
  \[
  w = \frac{\delta E_{\text{mix}}}{\delta \phi} = -\Delta \phi + F'(\phi),
  \]
  where \( F(\phi) = \frac{1}{\eta^2} (1 - \phi^2)^2 \).

- Momentum equation:
  \[
  \rho_0 (u_t + (u \cdot \nabla)u) = \nabla \cdot (\mu (\nabla u + \nabla^t u) - pI) + f,
  \]
  where \( f \) is the capillary force which can be determined from the least action principle
  \[
  f = w \nabla \phi.
  \]

- Incompressibility:
  \[
  \nabla \cdot u = 0 \text{ (which is equivalent to } \rho_t + \nabla \cdot (u \rho) = 0).\]
Energy dissipation law

The above model is derived from an energetic variational formalism, and verifies the following energy dissipation law:

\[
\frac{d}{dt} \int_{\Omega} \left\{ \frac{\rho_0}{2} |u|^2 + \frac{\lambda}{2} |\nabla \phi|^2 + \lambda F(\phi) \right\} = -\int_{\Omega} \left\{ \mu |\nabla u|^2 + \gamma |\nabla \frac{\delta E_{\text{mix}}}{\delta \phi}|^2 \right\}.
\]

- It allows us to establish some rigorous mathematical theory about the coupled nonlinear system;
- It also enables us to design energy stable schemes, i.e., the numerical solution of which satisfies a discrete energy law.
How to deal with different density?

- If the density difference is small, one can use a Boussinesq approximation where the density difference is modeled by a gravity force.
- In the diffuse-interface model for two phase flows with different density, the incompressibility

\[ \nabla \cdot u = 0 \]

and the mass conservation

\[ \rho_t + \nabla \cdot (u \rho) = 0 \]

are no longer equivalent.

- quasi-incompressible models (with mass averaged velocity) which enforce the mass conservation: Lowengrub & Truskinovsky '98; S., Wang & Yang '12; Guo, Lin & Lowengrub '14.
- Incompressible models (with volume averaged velocity): Boyer '01; S. & Yang '11; Abel et al. '12; Liu, S. & Yang '14.
An incompressible model (Abel, Garcke & Grün ’12)

- Cahn-Hilliard phase-field equation:
  \[ \phi_t + (u \cdot \nabla)\phi = \nabla \cdot (\gamma \nabla \frac{\delta E_{mix}}{\delta \phi}). \]

- Momentum equation:
  \[ \rho(u_t + u \cdot \nabla u) + J \cdot \nabla u = \nabla \cdot (\mu(\nabla u + \nabla^T u) - pI) + \frac{\delta E_{mix}}{\delta \phi} \nabla \phi, \]
  where \( J \) is the relative mass flux such that \( \rho_t + \nabla \cdot (\rho u + J) = 0 \), and is assumed, by Fick’s law, to take the form
  \[ J = -\frac{\rho_1 - \rho_2}{2} \gamma \nabla \frac{\delta E_{mix}}{\delta \phi}. \]

- Incompressibility: \( \nabla \cdot u = 0 \) (\( u \) is volume-averaged velocity).
- It also satisfies the energy law:
  \[ \frac{d}{dt} \int_{\Omega} \left\{ \frac{\rho}{2} |u|^2 + \frac{\lambda}{2} |\nabla \phi|^2 + \lambda F(\phi) \right\} = - \int_{\Omega} \left\{ \mu |\nabla u|^2 + \gamma |\nabla \frac{\delta E_{mix}}{\delta \phi}|^2 \right\}. \]
Let $\phi = 1$ representing the liquid crystal drop (represented by director $d$) and $\phi = -1$ representing the Newtonian fluid. Mixing energy density:
\[
 f_{\text{mix}}(\phi, \nabla \phi) = \frac{\lambda}{2} |\nabla \phi|^2 + \frac{\lambda}{4\eta^2}(\phi^2 - 1)^2,
\]
(penalized Oseen-Frank) Bulk elastic energy density for isotropic liquid crystals:
\[
 f_{\text{bulk}} = K \left[ \frac{1}{2} \nabla d : (\nabla d)^T + \frac{(|d|^2 - 1)^2}{4\delta^2} \right],
\]
Planar anchoring energy density:
\[
 f_{\text{anch}} = \frac{A}{2} (d \cdot \nabla \phi)^2,
\]
Total energy:
\[
 E(\phi, d, \nabla \phi, \nabla d) = \int_{\Omega} f_{\text{mix}} + \left( \frac{1 + \phi}{2} \right)^2 f_{\text{bulk}} + f_{\text{anch}}
\]
Since the density difference is small, a Boussinesq approximation can be used.

\[
\begin{align*}
\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi &= \nabla \cdot (M_1 \nabla \frac{\delta E}{\delta \phi}) \quad \text{(Cahn-Hilliard),} \\
\frac{\partial d}{\partial t} + \mathbf{v} \cdot \nabla d &= -M_2 \frac{\delta E}{\delta d}, \\
\nabla \cdot \mathbf{v} &= 0, \\
\rho_0 \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) &= -\nabla p + \nabla \cdot \left[ \mu (\nabla \mathbf{v} + \nabla \mathbf{v}^T) + \tau^e \right] + g(\rho),
\end{align*}
\]

where $M_1$ is the inter-facial mobility and $M_2$ determines the relaxation time of $d$, and
\[
\frac{\delta E}{\delta \phi} = \lambda \left[ -\nabla^2 \phi + \frac{\phi(\phi^2 - 1)}{\eta^2} \right] + \frac{1}{2} f_{bulk} - A \nabla \cdot [(d \cdot \nabla \phi) d],
\]

\[
\frac{\delta E}{\delta d} = -K \left[ -\nabla \cdot \left( \frac{1 + \phi}{2} \nabla d \right) + \frac{1 + \phi}{2} \frac{(d^2 - 1) d}{\delta^2} \right] - A(d \cdot \nabla \phi) \nabla \phi.
\]

\[
\tau^e = -\lambda (\nabla \phi \otimes \nabla \phi) - K \left( \frac{1 + \phi}{2} \right)^2 (\nabla d) \cdot (\nabla d)^T - A(d \cdot \nabla \phi) d \otimes \nabla \phi.
\]

The above system admits an energy law:

\[
\partial_t \left( \frac{\rho_0}{2} \int_{\Omega} \left| u \right|^2 + E \right) = - \int_{\Omega} \left( \nu \left| \nabla u \right|^2 + M_1 \left| \nabla \frac{\delta E}{\delta \phi} \right|^2 + M_2 \left| \frac{\delta E}{\delta d} \right|^2 \right) + g(\rho) u.
\]
Numerical issues and approaches

- Coupling of $p$ to $(u, \phi)$ can be handled by a projection-type method which decouples the computation of pressure from that of $(u, \phi)$.
- **Stiffness in the phase equation** — use the SAV approach to treat $f(\phi)$ explicitly while maintaining stability.
- There exist some energy law preserving schemes which are usually fully implicit, leading to nonlinear coupled systems at each time step — **decouple** the computation of $\phi$, $u$ and $p$ while preserving the energy law.
- **Interface needs to be resolved** — Use a **moving mesh** approach to redistribute more points near the interface.
\[ \frac{\partial u}{\partial t} - \nu \Delta u + u \cdot \nabla u + \nabla p = f, \quad \text{in} \quad Q = \Omega \times (0, T], \]
\[ \text{div} u = 0, \quad \text{in} \quad Q, \quad u|_{t=0} = u_0, \]

with appropriate boundary conditions:

\[ u|_{\Gamma_1} = 0, \quad \text{(no-slip)}; \]
\[ u \cdot n|_{\Gamma_2} = 0, \quad (\sigma \cdot n)|_{\Gamma_2} = 0 \quad \text{(free-slip)}; \]
\[ \sigma \cdot n|_{\Gamma_3} = g \quad \text{or} \quad (-\nu \nabla u + pl) \cdot n|_{\Gamma_3} = g \quad \text{(open boundary)}; \]

where \( \sigma = -\nu(\nabla u + \nabla u^T) + pl. \)
A generalized Stokes (or linearized Navier-Stokes) problem

\[ \frac{1}{\Delta t} u^{n+1} - \nu \Delta u^{n+1} + \nabla p^{n+1} = h^{n+1}, \]

\[ \text{div} u^{n+1} = 0, \]

needs to be solved at each time step!

- Not as easily solvable as a Poisson equation (but could be made equally efficient in many situations with a sophisticated multigrid method);
- Inf-sup condition is needed.
Decoupled approach: Splitting schemes

**Pioneer work:** The projection method, proposed by Chorin and Temam in late 60’s, decouples the computation of pressure and velocity — very efficient but the accuracy is not satisfactory.

**Notations:**
- \( \frac{Du_{n+1}}{\Delta t} = \frac{1}{\Delta t}(\beta qu_{n+1} - \sum_{j=0}^{q-1} \beta_j u_{n-j}) \): q-th order BDF approximation to \( u_t(\cdot, t_{n+1}) \).
- \( p^{*,n+1} \): (q – 1)-th order extrapolation for \( p(\cdot, t_{n+1}) \).
  - \( q = 1 \): \( Dv_{k+1} = v_{k+1} - v_k \), \( p^{*,k+1} = 0 \);
  - \( q = 2 \): \( Dv_{k+1} = \frac{3}{2} v_{k+1} - 2v_{k} + \frac{1}{2} v_{k-1} \), \( p^{*,k+1} = p_{k} \).
Pressure-correction Method

\[
\begin{aligned}
\left\{ \begin{array}{l}
\frac{1}{\Delta t} (\beta q \tilde{u}^{n+1} - \sum_{j=0}^{q-1} \beta_j u^{n-j}) - \nu \Delta \tilde{u}^{n+1} + \nabla p^{*,n+1} = h(t_{n+1}), \\
\tilde{u}^{n+1} |_{\partial \Omega} = 0,
\end{array} \right.
\end{aligned}
\]

\[
\left\{ \begin{array}{l}
\frac{\beta q (u^{n+1} - \tilde{u}^{n+1})}{\Delta t} + \nabla (p^{n+1} - p^{*,n+1}) = 0, \\
\text{div} u^{n+1} = 0, \quad u^{n+1} \cdot n |_{\partial \Omega} = 0.
\end{array} \right.
\]

The second step reduces to a Pressure Poisson equation — only a sequence of Poisson-type equations need to be solved at each time step.
The second step is nothing but the Helmholtz decomposition of $u^{n+1}$, i.e., $u^{n+1}$ is the orthogonal projection of $\tilde{u}^{n+1}$ onto

$$H = \{ u \in L^2(\Omega) : \nabla \cdot u = 0, \ u \cdot n|_{\partial \Omega} = 0 \}.$$

The pressure approx. satisfies an artificial Neumann B.C.

$$q = 1 : \frac{\partial p^{n+1}}{\partial n}|_{\partial \Omega} = 0; \quad q = 2 : \frac{\partial p^{n+1}}{\partial n}|_{\partial \Omega} = \frac{\partial p^0}{\partial n}|_{\partial \Omega}$$

— numerical boundary layer and a loss of accuracy.

Error estimates: (proved by many in various forms)

$$\|u^n - u(t_n)\|_0 + \Delta t(\|u^n - u(t_n)\|_1 + \|p^n - p(t_n)\|_0) \leq c\Delta t^2.$$
D. PRESSURE ERROR: TIME STEP=0.05, SCHEME 1.3-1.4.

E. PRESSURE ERROR: TIME STEP=0.025, SCHEME 1.3-1.4.

F. PRESSURE ERROR: TIME STEP=0.0125, SCHEME 1.3-1.4.

B. VELOCITY ERROR: TIME STEP=0.025, SCHEME 1.3-1.4.
Reducing the effect of the artificial Neumann pressure boundary condition

\[
\begin{align*}
\frac{1}{\Delta t} (\beta_q \tilde{u}^{n+1} - \sum_{j=0}^{q-1} \beta_j u^{n-j}) - \nu \Delta \tilde{u}^{n+1} + \nabla p^{*,n+1} &= h(t_{n+1}), \\
\tilde{u}^{n+1} |_{\partial \Omega} &= 0;
\end{align*}
\]

Eliminating \( \tilde{u}^{n+1} \) from above, one finds that the correct way to update \( p^{n+1} \) is:

\[
p^{n+1} = \phi^{n+1} + p^{*,n+1} - \nu \text{div} \tilde{u}^{n+1}.
\]
A striking fact is that \textit{a priori} the following estimate holds (even for $q = 1$):

$$\|\text{div}\tilde{u}^n\|_0 \leq c\Delta t^{3/2}, \quad q = 1, 2,$$

which leads to \textbf{Improved error estimates:}

$$\|u^n - u(t_n)\|_1 + \|p^n - p(t_n)\|_0 \leq c\Delta t^{3/2}.$$

\textbf{Figure:} Plots of the pressure errors: standard form and rotational form
Figure: Convergence rates of 2nd-order pressure-correction schemes: standard form and rotational form with spectral method
The large errors at the corners are due to the domain singularity. Consider \( \Omega = (0, 2\pi) \times (-1, 1) \) with periodic condition in \( x \).

**Figure:** Pressure error in a channel: (L) standard; (R) rotational
Let \( \bar{\phi}^{n+1} := 2\phi^n - \phi^{n-1} \), \( \bar{u}^{n+1} := 2u^n - u^{n-1} \) and \( \hat{u}^{n+1} = 2u^n - u^{n-1} \) or \( \tilde{u}^{n+1} \).

\[
\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\delta t} + \hat{u}^{n+1} \cdot \nabla \bar{\phi}^{n+1} = \gamma \Delta w^{n+1},
\]

\[
w^{n+1} = -\lambda \Delta \phi^{n+1} + \frac{\lambda r^{n+1}}{\sqrt{E_1[\bar{\phi}^{n+1}]} + \delta} F'(\bar{\phi}^{n+1}),
\]

\[
\frac{3r^{n+1} - 4r^n + r^{n-1}}{2\Delta t} = \int_{\Omega} \frac{F'(\bar{\phi}^{n+1})}{2\sqrt{E_1[\bar{\phi}^{n+1}]} + \delta} \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\Delta t} \, dx;
\]

\[
\rho_0\left\{ \frac{3\bar{u}^{n+1} - 4u^n + u^{n-1}}{2\delta t} + \bar{u}^{n+1} \cdot \nabla \bar{u}^{n+1} \right\}
\]

\[
- \nu \Delta \bar{u}^{n+1} + \nabla p^n - w^{n+1} \nabla \bar{\phi}^{n+1} = 0;
\]

\[
\Delta(p^{n+1} - p^n) = \frac{3\rho_0}{2\delta t} \nabla \cdot \bar{u}^{n+1}, \quad \partial_n(p^{n+1} - p^n)|_{\partial \Omega} = 0;
\]

\[
u^n + 1 = \bar{u}^{n+1} - \frac{2\delta t}{3\rho_0} \nabla(p^{n+1} - p^n).
\]
Several remarks:

- The pressure is decoupled from the rest by a pressure-correction projection method.

  If we take $\hat{u}^{n+1} = \tilde{u}^{n+1}$, the scheme is unconditionally stable, linear and 2nd-order, but weakly coupled between $(\phi^{n+1}, w^{n+1}, \tilde{u}^{n+1})$ by the term $u^{n+1} \cdot \nabla \tilde{\phi}^{n+1}$. The weakly coupled linear system is positive definite.

- If we take $\hat{u}^{n+1} = 2u^n - u^{n-1}$, the scheme is linear, decoupled and 2nd-order, only requires solving a sequence of Poisson type equations at each time step, but not unconditionally energy stable.

- One can use the decoupled scheme with $\hat{u}^{n+1} = 2u^n - u^{n-1}$ as a preconditioner for the coupled scheme if large time step is used.
variable density: using pressure-stabilized scheme

For problems with variable density, the projection type scheme leads to a pressure equation of the form:

\[ \nabla \cdot \left( \frac{1}{\rho^n} \nabla (p^{n+1} - p^n) \right) = \frac{1}{\delta t} \nabla \cdot u^{n+1}, \quad \partial_n(p^{n+1} - p^n)|_{\partial \Omega} = 0. \]

Difficult to solve when the density ratio is large. We adopt a pressure-stabilization (Rannacher '91, S. '92, etc.) which is based on relaxing \( \nabla \cdot u = 0 \) to

\[ \epsilon \Delta p_t - \rho \nabla \cdot u = 0; \quad \frac{\partial p_t}{\partial n}|_{\partial \Omega} = 0. \]

A decoupled pressure-stabilized scheme for the Navier-Stokes equations with \( \epsilon = (\delta t)^2 \):

\[
\frac{\rho}{2\delta t} \left( 3u^{n+1} - 4u^n + u^{n-1} \right) + \text{NLT} - \mu \Delta u^{n+1} + \nabla (2p^n - p^{n-1}) = 0, \quad u^{n+1}|_{\partial \Omega} = 0;
\]

\[
\delta t^2 \Delta \frac{p^{n+1} - p^n}{\delta t} = \rho \nabla \cdot u^{n+1}, \quad \partial_n(p^{n+1} - p^n)|_{\partial \Omega} = 0.
\]
A decoupled, linear, energy stable scheme for variable density

\[
\frac{1}{\delta t} (\phi^{n+1} - \phi^n) + (u^n - \delta t \frac{w^{n+1} \nabla \phi^n}{\rho^n}) \cdot \nabla \phi^n + M \Delta w^{n+1} = 0,
\]

\[
w^{n+1} + \frac{\lambda}{\eta^2} (\phi^{n+1} - \phi^n) - \lambda (\Delta \phi^{n+1} - f(\phi^n)) = 0,
\]

\[
\rho^{n+1} = \frac{\rho_1 - \rho_2}{2} \hat{\phi}^{n+1} + \frac{\rho_1 + \rho_2}{2}, \quad \mu^{n+1} = \frac{\mu_1 - \mu_2}{2} \hat{\phi}^{n+1} + \frac{\mu_1 + \mu_2}{2}.
\]

\[
\rho^n \frac{u^{n+1} - u^n}{\delta t} - \nabla \cdot \mu^n D(u^{n+1}) + \nabla (2p^n - p^{n-1})
\]
\[
+ \rho^n (u^n \cdot \nabla) u^{n+1} + J^n \cdot \nabla u^{n+1} + w^{n+1} \nabla \phi^n
\]
\[
+ \frac{1}{2} u^{n+1} \frac{\rho^{n+1} - \rho^n}{\delta t} + \frac{1}{2} \nabla \cdot (\rho^n u^n) u^{n+1} + \frac{1}{2} \nabla \cdot J^n u^{n+1} = 0,
\]

with \( J^n = -\frac{\rho_1 - \rho_2}{2} \nabla w^n; \)
The last three terms in the above is a first-order approximation of the term

$$\left( \frac{1}{2}(\rho_t + \nabla \cdot (\rho u + J), u) = (0, u) \right) \text{ at } t_{n+1}. $$

\[ \Delta(p^{n+1} - p^n) = \frac{\chi}{\delta t} \nabla \cdot u^{n+1}, \]
\[ \partial_n p^{n+1} |_{\partial \Omega} = 0; \]

with \( \chi = \frac{1}{2} \min(\rho_1, \rho_2). \)

Once again, the systems for \((\phi^{n+1}, w^{n+1}), u^{n+1} \text{ and } p^{n+1} \) are decoupled and **linear**!
Theorem. (S. & Yang ’15) The above scheme is energy stable for any $\delta t$. More precisely:

$$
\|\sigma^{n+1}u^{n+1}\|_{L^2}^2 + \frac{\delta t^2}{\chi} \|\nabla p^{n+1}\|_{L^2}^2 + \lambda \|\nabla \phi^{n+1}\|_{L^2}^2 + 2\lambda (F(\phi^{n+1}), 1) \\
+ \delta t \left( 2M \|\nabla w^{n+1}\|_{L^2}^2 + \|\sqrt{\mu^n}D(u^{n+1})\|_{L^2}^2 \right) \\
\leq \|\sigma^n u^n\|_{L^2}^2 + \frac{\delta t^2}{\chi} \|\nabla p^n\|_{L^2}^2 + \lambda \|\nabla \phi^n\|_{L^2}^2 + 2\lambda (F(\phi^n), 1),
$$

where $\sigma^k = \sqrt{\rho^k}$.
Let $G(d) = \frac{1}{4\delta^2}(|d|^2 - 1)^2$ and $g(d) = \nabla G(d)$. Given $(d^n, \phi^n, \mu^n, u^n, p^n)$, compute $(d^{n+1}, \phi^{n+1}, \mu^{n+1}, u^{n+1}, p^{n+1})$ as follows:

$$C_1^n(d^{n+1} - d^n) + \frac{1}{M_1} \dot{d}^{n+1} = K \nabla \cdot (\frac{1+\phi^n}{2})^2 \nabla d^{n+1} - K(\frac{1+\phi^n}{2})^2 g(d^n),$$

$$\frac{\partial d^{n+1}}{\partial n} |_{\partial \Omega} = 0$$

with

$$\dot{d}^{n+1} = \frac{d^{n+1} - d^n}{\delta t} + (u^n_\star \cdot \nabla) d^n, \quad u^n_\star = \frac{u^n - \frac{d^{n+1} - d^n}{M_1} \nabla d^n}{1 + \delta t \frac{\nabla d^n}{M_1}^2}.$$
\begin{align*}
\dot{\phi}^{n+1} &= -\Delta \mu^{n+1}, \\
C_2^n(\phi^{n+1} - \phi^n) + \frac{1}{M_2} \mu^{n+1} &= \lambda(\Delta \phi^{n+1} - f(\phi^n)) - K\left(\frac{1+\phi^{n+1}}{2}\right)W(d^{n+1}), \\
\frac{\partial \mu^{n+1}}{\partial n}|_{\partial \Omega} &= 0, \quad \frac{\partial \phi^{n+1}}{\partial n}|_{\partial \Omega} = 0
\end{align*}

with

\begin{align*}
W(d^{n+1}) &= \left(\frac{\left|\nabla d^{n+1}\right|^2}{2} + G(d^{n+1})\right), \\
\dot{\phi}^{n+1} &= \frac{\phi^{n+1} - \phi^n}{\delta t} + (u_\star \star \cdot \nabla) \phi^n, \quad u_\star \star = \frac{u^n - \frac{\phi^{n+1} - \phi^n}{M_2} \nabla \phi^n}{1 + \delta t \left|\nabla \phi^n\right|^2}.
\end{align*}
\[
\frac{\tilde{u}^{n+1} - u^n}{\delta t} + (u^n \cdot \nabla)\tilde{u}^{n+1} - \nu \Delta \tilde{u}^{n+1} + \nabla p^n + \frac{\dot{d}^{n+1}}{M_1} \nabla d^n + \frac{\mu^{n+1}}{M_2} \nabla \phi^n = 0,
\]
\[
\tilde{u}^{n+1}|_{\partial \Omega} = 0.
\]

\[
\Delta(p^{n+1} - p^n) = \frac{1}{\delta t} \nabla \cdot \tilde{u}^{n+1}, \quad \partial_n(p^{n+1} - p^n)|_{\partial \Omega} = 0;
\]
\[
u^{n+1} = \tilde{u}^{n+1} - \delta t(p^{n+1} - p^n).
\]

- The above scheme is **totally decoupled and linear**!
- At each time step, one only has to solve a sequence of elliptic equations.
Theorem.

(S. & Yang '14) Assuming

\[ \max_{|d| \in \mathbb{R}} |H(d)| \leq L_1, \quad \max_{|\phi| \in \mathbb{R}} |F''(\phi)| \leq L_2, \]

where \( H(d) \) is the Hessian matrix of \( G(d) \). Then, if \( C_1^n \geq KL_1 \|(\frac{1+\phi^n}{2})^2\|_{\infty} \) and \( C_2^n = C_2 \geq \lambda L_2 \), the above scheme admits a unique solution satisfying the following discrete energy dissipation law:

\[
\frac{1}{2} \|u^{n+1}\|^2 + F^{n+1} + \frac{\delta t^2}{2} \|\nabla p^{n+1}\|^2 \\
+ \{ \nu \delta t \|\tilde{u}^{n+1}\|^2 + \delta t \left( \frac{\|\nabla \mu^{n+1}\|^2}{M_2} + \frac{\|\dot{d}^{n+1}\|^2}{M_1} \right) \} \\
\leq \frac{1}{2} \|u^n\|^2 + F^n + \frac{\delta t^2}{2} \|\nabla p^n\|^2.
\]
Effect of spatial accuracy

Consider, for example, the stabilized scheme for the Allen-Cahn equation with a spectral-Galerkin discretization in space. Then, we have the following error estimate (S. & Yang ’10):

\[
\left\| u(t_k) - u^k_N \right\|_0 \leq C(\eta, T)(K_1(u, \eta)\delta t + K_2(u, \eta)N^{-m}), \quad \forall 0 \leq k \leq \frac{T}{\delta t},
\]

where

\[
K_1(u, \eta) = \| u_{tt} \|_{L^2(0, T; H^{-1})} + \frac{1}{\eta} \| u_t \|_{L^2(0, T; L^2)},
\]

\[
K_2(u, \eta) = \| u_0 \|_m + (\eta + \frac{\delta t}{\eta}) \| u_t \|_{L^2(0, T; H^m)} + \frac{1}{\eta} \| u \|_{C(0, T; H^m)}.
\]

For interface problems, it is reasonable to assume that

\[
\partial^m x u \sim \eta^{-m}, \quad \forall m \geq 0.
\]
Hence, the error estimate indicates that

$$\|u(t^n) - u_N^n\|_0 \lesssim C(\eta, T)(K_1(u, \eta)\delta t + N^{-m}\eta^{-1-m}).$$

• Since the solution is usually “smooth” around the interface, the above can be expected to be valid for all $m$. Hence, as soon as we have $N > \eta^{-1}$, the spatial error will decay exponentially fast.

• For lower-order methods, we have $h = 1/N$ and $m$ is fixed. For $m = 2$, one needs $h \ll \eta^{3/2}$ for the scheme to be convergent, and $h \sim \eta^3$ for the error to be $O(h)$. 

Jie Shen

Part II. Efficient and Accurate Numerical Schemes for Phase-Field Models for Two-Phase Incompressible Flows
A benchmark problem by Prosperetti ’81: The small-amplitude waves on the interface between two incompressible viscous fluids.

- The two fluids may have different densities and dynamic viscosities, but must have the same kinematic viscosity, with the lighter fluid on top;
- The interface is perturbed from the equilibrium position in the form of a sinusoidal wave;
- Then, Prosperetti derived the explicit exact form for the amplitude evolution of the interface wave.
Figure: Case of matched density
Figure 3: Capillary wave (different density ratios): Comparison of time histories of the capillary wave amplitude between simulation and Prosperetti’s exact solution [18] for density ratios (a) $\rho_2/\rho_1 = 10$, (b) $\rho_2/\rho_1 = 100$, (c) $\rho_2/\rho_1 = 1000$. Simulation results correspond to time step size $\Delta t = 2.5 \times 10^{-5}$, element order 14.
Two-phase Newtonian flow with large density ratios: air bubble in water (with S. Dong, JCP '12)

text=(loading movie)
Figure: inverted heart shape in experiment by Akers & Belmonte ’06: air bubble rising in a polymeric fluid
Air bubbles rising in a shampoo bottle

text=(loading movie)
Figure: A Newtonian bubble rising in a nematic fluid (Yue, Feng, Liu, S. & Zhou '07)

Jie Shen

Part II. Efficient and Accurate Numerical Schemes for Phase-Field Models for Two-Phase Incompressible Flows
Figure: Snapshots of the deformation of a nematic liquid crystal fluid filament that is immersed in a Newtonian fluid, with elastic bulk energy constant $K = 3$, anchoring constant $A = 0$. 
Figure: Qualitatively comparison between the experimental result (Basaran et al. 2010) and our simulation at $t = 1.8$. 
Phase-field models for two-phase flows with different density and for complex fluids are considered:

decoupled, linear, unconditionally energy stable schemes:
  - a pressure-stabilized scheme for the Navier-Stokes equations;
  - the SAV approach for the phase equation;
  - decoupled systems for \((\phi, w), u\) and \(p\);
  - a moving mesh spectral discretization in space.

The proposed numerical schemes are easy to implement: if we treat the nonlinear terms explicitly, it only requires elliptic solvers for the velocity with regular Poisson equation for the pressure and phase function.
The approach can be extended to deal with various types of interface problems:

- multiphase (> 2) flows by introducing multiple phase functions (e.g., Kim & Lowengrub ’05, Boyer ’06, S. Dong ’14, ...)
- multi-phase flows with moving contact lines (e.g., Qian, Wang & Sheng ’06, Yue, Zhou & Feng ’10, S., Yang & Yu ’15, ...)
- multi-phase flows with other non-Newtonian components, such as Oldroyd-B and other visco-elastic fluid (e.g., Yue, Feng, Liu & S. ’04, ...) ...
- vesicle membranes under elastic bending energy (e.g., Du, Liu & Wang ’04 & 06, ...)
- tumor growth (Cristini, Lowengrub et al.), solidification (Boettinger et al. ’02), ...
- Q-tensor hydrodynamic models for liquid crystal flows (Zhao & Wang ’15, Cai & S. ’16), ...
Thank you!