Efficient 2nd order schemes for phase-field fluid equations

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Cahn-Hilliard-Navier-Stokes equation with matched density

Hohenberg & Halperin’77 (Model H), Gurtin et al. ’96

\[
\begin{align*}
\mathbf{u}_t - \nu \Delta \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p &= -\frac{\gamma}{\epsilon} \phi \nabla \mu, \\
\phi_t + \nabla \cdot (\phi \mathbf{u}) &= \nabla \cdot (M \nabla \mu), \\
\mu &= f'_0(\phi) - \epsilon^2 \Delta \phi, \\
f_0(\phi) &= \frac{1}{4}(\phi^2 - 1)^2 \\
\nabla \cdot \mathbf{u} &= 0.
\end{align*}
\]

- \(\mathbf{u}\): velocity; \(p\): pressure; \(\mu\): chemical potential
- \(\nu\): viscosity; \(M\): mobility
- Well-posedness: Starovoitov’97, Boyer’ 99, Abels’ 09, ...
- Long-time behavior: Abels’09, Zhao& Wu & Huang’09, Gal & Grasselli’10, ...
- Sharp interface limit: Abels & Roger’09, Abels& Lengeler’12
Initial boundary conditions

\[ u|_{\partial \Omega} = 0, \]
\[ \partial_n \phi|_{\partial \Omega} = \partial_n \mu|_{\partial \Omega} = 0, \]
\[ (u, \phi)|_{t=0} = (u_0, \phi_0). \]

Energy law

\[ \frac{d}{dt} E_{\text{tot}}(u, \phi) = - \int_{\Omega} \nu |\nabla u|^2 \, dx - \frac{\gamma}{\epsilon} \int_{\Omega} M |\nabla \mu|^2 \, dx, \]

where \( E_{\text{tot}} \) is the total energy

\[ E_{\text{tot}}(u, \phi) = \int_{\Omega} \frac{1}{2} |u|^2 \, dx + \int_{\Omega} \gamma \left( \frac{1}{\epsilon} f_0(\phi) + \frac{\epsilon}{2} |\nabla \phi|^2 \right) \, dx. \]
Numerical Challenges

- stability issue: stiffness associated with the interfacial width
  - fully explicit: $\delta t \approx \epsilon^4$
  - semi-explicit: $\delta t \approx \epsilon^2$

  Key: energy-law preserving scheme, unconditional stability

- Long time behavior

  Key: high order scheme

- Navier-Stokes equation: coupling of velocity and pressure

  Key: pressure projection scheme
Existing Work

- Cahn-Hilliard-Navier-Stokes:
  - Kim & Kang & Lowengrub’04, 2nd order, FD, but fully implicit
  - Feng’06, 1st order, finite element in space
  - Kay & Styles & Welford’08, first order, finite element in space, decoupled, but conditionally stable
  - Minjeaud 13: 1st order decoupled CH and NS but not velocity and pressure
  - Dong&Shen: BDF based highly efficient but conditionally stable
  - Liu&Shen, Qian&Shen&Wang, ...


- Phase field crystal equation: Hu & Wise & C. Wang & Lowengrubi’09, 2nd order, convex-splitting


- Cahn-Hilliard-Brinkman: Collins & Shen & Wise’ 13

- Cahn-Hilliard-Darcy-Stokes: Diegel & Feng & Wise’ 14
Our Scheme

Notations:

\[ \phi^{k+\frac{1}{2}} = \frac{1}{2}(\phi^{k+1} + \phi^k), \quad \tilde{\phi}^{k+\frac{1}{2}} = \frac{3\phi^k - \phi^{k-1}}{2}, \]

\[ \bar{u}^{k+\frac{1}{2}} = \frac{u^{k+1} + u^k}{2}, \quad \tilde{u}^{k+\frac{1}{2}} = \frac{3u^k - u^{k-1}}{2}, \]

\[ B(u, v) := (u \cdot \nabla)v + \frac{1}{2}(\nabla \cdot u)v. \]

We propose the semi-implicit, semi-discrete scheme as follows

\[ \frac{\phi^{k+1} - \phi^k}{\delta t} = \nabla \cdot \left( M \nabla \mu^{k+\frac{1}{2}} - \tilde{\phi}^{k+\frac{1}{2}} \bar{u}^{k+\frac{1}{2}} \right), \]

\[ \mu^{k+\frac{1}{2}} = \frac{1}{2} \left( (\phi^{k+1})^2 + (\phi^k)^2 \right) \phi^{k+\frac{1}{2}} - \tilde{\phi}^{k+\frac{1}{2}} - \epsilon^2 \Delta \phi^{k+\frac{1}{2}}, \]

\[ \frac{\bar{u}^{k+1} - u^k}{\delta t} - \nu \Delta \bar{u}^{k+\frac{1}{2}} + B(\tilde{u}^{k+\frac{1}{2}}, \bar{u}^{k+\frac{1}{2}}) = -\nabla p^k - \frac{\gamma}{\epsilon} \tilde{\phi}^{k+\frac{1}{2}} \nabla \mu^{k+\frac{1}{2}}, \]

\[ \left\{ \begin{array}{l} \frac{u^{k+1} - \bar{u}^{k+1}}{\delta t} + \frac{1}{2} \nabla (p^{k+1} - p^k) = 0, \\ \nabla \cdot u^{k+1} = 0, \end{array} \right. \]
Features:

- Cahn-Hilliard: second order convex splitting $\Rightarrow$ unconditional stability and solvability

- Navier-Stokes:
  - van Kan kind of second order pressure projection $\Rightarrow$ decoupling
  - Crank-Nicolson with linear extrapolation for nonlinear advection

- phase-field-velocity coupling is weak for large Weber number: through $\vec{u}^{k+\frac{1}{2}}$ or $\mu^{k+\frac{1}{2}}$

- weak nonlinearity

Boundary conditions:

$$\nabla \phi^{k+1} \cdot n|_{\partial \Omega} = 0, \quad \nabla \mu^{k+\frac{1}{2}} \cdot n|_{\partial \Omega} = 0, \quad \vec{u}^{k+\frac{1}{2}}|_{\partial \Omega} = 0, \quad u^{k+1} \cdot n|_{\partial \Omega} = 0.$$
Recall $E_{tot}(u, \phi) = \int_{\Omega} \frac{1}{2} |u|^2 \, dx + \int_{\Omega} \gamma \left( \frac{1}{\epsilon} f_0(\phi) + \frac{\epsilon}{2} |\nabla \phi|^2 \right) \, dx$.

**Theorem (Han & Wang, JCP 2015)**

*The scheme satisfies the modified energy law*

\[
\begin{align*}
\left\{ E_{tot}(u^{k+1}, \phi^{k+1}) + \frac{\gamma}{4\epsilon} \|\phi^{k+1} - \phi^k\|^2 + \frac{\delta t^2}{8} \|\nabla p^{k+1}\|^2 \right\} \\
- \left\{ E_{tot}(u^k, \phi^k) + \frac{\gamma}{4\epsilon} \|\phi^k - \phi^k\|^2 + \frac{\delta t^2}{8} \|\nabla p^k\|^2 \right\}
= -\delta t \frac{\gamma}{\epsilon} \|\sqrt{\mu} \nabla \mu^{k+\frac{1}{2}}\|^2 - \delta t \nu \|\nabla u^{k+\frac{1}{2}}\|^2 - \frac{\gamma}{4\epsilon} \|\phi^{k+1} - 2\phi^k + \phi^{k-1}\|^2.
\end{align*}
\]

Thus it is *unconditionally stable*. 

Unconditional Stability
Unique Solvability

Theorem (Han & Wang, JCP 2015)

The scheme is unconditionally uniquely solvable in the weak sense.

- unknowns $\phi^{k+1}$, $\mu^{k+\frac{1}{2}}$, $\overline{u}^{k+\frac{1}{2}}$ (omit the superscripts from now on)

- Keys: to explore the weak coupling through $\mu^{k+\frac{1}{2}}$ and monotonicity associated with convex-splitting
Mixed finite element in space

- $\mathcal{T}_h$: a quasi-uniform triangulation of the domain $\Omega$ of mesh size $h$.
- $P_r(K)$: the space of polynomials of degree less than or equal to $r$ on $K$.
- Introduce

\[
Y_h = \{ \phi_h \in C^0(\bar{\Omega}); \phi_h|_K \in P_1(K) \},
\]

\[
X_h = \{ v_h \in C^0(\bar{\Omega}) \cap H^1_0(\Omega); v_h|_K \in P_2(K), \},
\]

\[
M_h = \{ q_h \in C^0(\bar{\Omega}) \cap H^1(\Omega); q_h|_K \in P_1(K) \}.
\]

- $Y_h \times Y_h$: a stable pair for the biharmonic operator.
- $X_h \times M_h$: a stable pair for Navier-Stokes equation.
find \((\phi_h^{k+1}, \mu_h^{k+\frac{1}{2}}, \overline{u}_h^{k+\frac{1}{2}}, \rho_h^{k+1}, u_h^{k+1}) \in Y_h \times Y_h \times X_h \times M_h \times X_h\) such that

- **Cahn-Hilliard part**

\[
(\phi_h^{k+1} - \phi_h^k, v_h) + \delta t (M \nabla \mu_h^{k+\frac{1}{2}}, \nabla v_h) - \delta t (\overline{\phi}_h^{k+\frac{1}{2}} \overline{u}_h^{k+\frac{1}{2}}, \nabla v_h) = 0, \quad \forall v_h \in Y_h
\]

\[
(\mu_h^{k+\frac{1}{2}}, \varphi_h) = \frac{1}{4} \left( [(\phi_h^{k+1})^2 + (\phi_h^k)^2](\phi_h^{k+1} + \phi_h^k), \varphi_h \right) - (\overline{\phi}_h^{k+\frac{1}{2}}, \varphi_h)
\]

\[
+ \frac{\epsilon^2}{2} (\nabla (\phi_h^{k+1} + \phi_h^k), \nabla \varphi_h), \quad \forall \varphi_h \in Y_h,
\]
Elliptic equation for intermediate velocity

\[
(2\overline{u}_h^{k+\frac{1}{2}}, \mathbf{v}_h) + \delta t (\nabla \overline{u}_h^{k+\frac{1}{2}}, \nabla \mathbf{v}_h) + \delta t b(\tilde{\mathbf{u}}_h^{k+\frac{1}{2}}, \overline{\mathbf{u}}_h^{k+\frac{1}{2}}, \mathbf{v}_h) = \delta t (\nabla p_h^k, \mathbf{v}_h) \\
+ (2\mathbf{u}_h^k, \mathbf{v}_h) - \delta t \gamma (\tilde{\phi}_h^{k+\frac{1}{2}} \nabla \mu_h^{k+\frac{1}{2}}, \mathbf{v}_h), \quad \forall \mathbf{v}_h \in \mathbf{X}_h,
\]

where

\[
b(\mathbf{u}, \mathbf{v}, \mathbf{w}) = \frac{1}{2} ((\mathbf{u} \cdot \nabla \mathbf{v}, \mathbf{w}) - (\mathbf{u} \cdot \nabla \mathbf{w}, \mathbf{v})),
\]

Poisson equation for pressure increment

\[
(\nabla (p_h^{k+1} - p_h^k), \nabla q_h) = \frac{2}{\delta t} (\overline{\mathbf{u}}_h^{k+1}, \nabla q_h), \quad \forall q_h \in \mathbf{M}_h,
\]

Projection for end-of-step velocity

\[
\int_{\Omega} \mathbf{u}_h^{k+1} \cdot \mathbf{v}_h \, dx = \int_{\Omega} [\overline{\mathbf{u}}_h^{k+1} - \frac{\delta t}{2} \nabla (p_h^{k+1} - p_h^k)] \cdot \mathbf{v}_h \, dx, \quad \forall \mathbf{v}_h \in \mathbf{X}_h.
\]
Remarks on projection step:

- $\mathbf{u}_{h}^{k+1} \in X_h$ satisfies essential boundary condition!!!
- algebraic update of end-of-step velocity renders poor stability!!!
- Alternatively, solve the projection step as a Darcy problem.

Decoupling the computation of Cahn-Hilliard equation and Navier-Stokes equation through Picard iteration

- Solve Cahn-Hilliard using velocity at previous iteration.
- Solve viscous step using current chemical potential.
- Iterate until the relative difference of the iteration is small.
Numerical convergence by manufactured solution

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<th>$\delta t, h$</th>
<th>$|e_\phi|_{L^2}$</th>
<th>rate</th>
<th>$|e_{u_1}|_{L^2}$</th>
<th>rate</th>
<th>$|e_p|_{L^2}$</th>
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**Table:** $L^2$ Convergence test by using FreeFem++. The final time is $T = 1.0$, and the refinement path is taken to be $\delta t = h$. The other parameters are $\epsilon = 1.0$, $\gamma = 1.0$, $\nu = 1.0$, $\Omega = (0, 1)^2$. $\|e_\phi\|_{L^2}$ is the relative error of order parameter $\phi$, analogous for $e_{u_1}$ and $e_p$. The error for $\phi$ and $u_1$ are expected to be $O(h^2)$, and $O(h)$ for $p$. 
Spinodal decomposition
Rising Bubble
Pinchoff–Rayleigh-Taylor Instability
Ongoing work

- exploring monotonicity in solving the system.
- parallel computing.
- efficient preconditioning.
- mesh refinement.
- local time stepping.
- rigorous error analysis.
- extending the methodology to case of large density contrast.
- Cahn-Hilliard-Darcy (Cahn-Hilliard-Hele-Shaw)
Thanks for your attention!