Energy Stable Schemes for Two-phase Viscous Fluid Flows

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Joint work with
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2 Structure-preserving spatial discretization

3 Full-discrete energy stable scheme

4 Numerical experiments
Mathematical Model

Consider the hydrodynamic phase field model

\[
\begin{aligned}
\rho (\partial_t v + v \cdot \nabla v) &= -\nabla p + \nabla \cdot (\sigma^d + \sigma^e), \\
\nabla \cdot v &= 0, \\
\partial_t \phi + \nabla \cdot (\phi v - \Gamma \nabla \mu) &= 0,
\end{aligned}
\]  

(1)

where \(v\) is the mass averaged velocity, \(\phi\) is the volume fraction of one fluid, \(p\) is the hydrostatic pressure, \(\mu = \frac{\delta f}{\delta \phi}\) is the chemical potential, \(f\) is the free energy density function, \(\Gamma\) is the mobility coefficient that is a function of phase variable \(\phi\),

\[
\sigma^d = 2\eta D,
\]  

(2)

is the viscous stress tensor, \(D = \frac{1}{2}(\nabla v + \nabla v^T)\) is the rate of strain tensor, and

\[
\sigma^e_{\alpha\beta} = (f - \mu \phi)\delta_{\alpha\beta} - \frac{\partial f}{\partial (\partial_\beta \phi)} \partial_\alpha \phi,
\]  

(3)

is the Ericksen stress tensor.
The total energy functional of the system is

\[ E = \int_{\Omega} \left( \rho |\mathbf{v}|^2 / 2 + f \right) d\mathbf{x}. \] (4)

**Energy identity**

\[ \frac{d}{dt} E + \int_{\Omega} \left[ 2\eta \mathbf{D} : \mathbf{D} + \Gamma |\nabla \mu|^2 \right] d\mathbf{x} = 0. \] (5)
The drop problem

\[ f = \gamma \left( \frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{\varepsilon} \phi^2 (1 - \phi)^2 \right), \]  

where \( \gamma \) is a surface tension coefficient.

The Flory-Huggins free energy

\[ f = \gamma_1 |\nabla \phi|^2 + \gamma_2 \left( \frac{\phi}{N_1} \ln \phi + \frac{1 - \phi}{N_2} \ln (1 - \phi) + \chi \phi (1 - \phi) \right), \]  

where \( N_1 \) and \( N_2 \) are the polymerization index of polymer 1 and 2, respectively, \( \gamma_1 \) is the strength of the conformational entropy and \( \gamma_2 \) is the strength of the bulk mixing energy.

General free energy

\[ f = c |\nabla \phi|^2 + g(\phi), \]  

where \( g \) is a function of \( \phi \).
Equivalent system

\[
\begin{aligned}
\rho \left( \partial_t \mathbf{v} + \frac{1}{2} (\mathbf{v} \cdot \nabla \mathbf{v} + \nabla \cdot (\mathbf{v} \mathbf{v})) \right) &= -\nabla p + \eta \Delta \mathbf{v} - \phi \nabla \mu, \\
\nabla \cdot \mathbf{v} &= 0, \\
\partial_t \phi + \nabla \cdot (\phi \mathbf{v} - \Gamma \nabla \mu) &= 0,
\end{aligned}
\]

(8)

where \( \mu = g'(\phi) - 2c \Delta \phi \).

The corresponding energy identity

\[
\frac{dE}{dt} + \eta \| \nabla \mathbf{v} \|^2 + \Gamma \| \nabla \mu \|^2 = 0.
\]

(9)
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Three semi-discrete energy stable schemes

**Scheme I**

$$\begin{align}
\rho \left( \frac{d}{dt} v_{j,k} + \frac{1}{2} (v_{j,k} \cdot \nabla_h^+ v_{j,k} + \nabla_h^- \cdot (v_{j,k} v_{j,k})) \right) &= -\nabla_h^+ p_{j,k} + \eta \Delta_h v_{j,k} - \phi_{j,k} \nabla_h^+ \mu_{j,k}, \\
\nabla_h^- \cdot v_{j,k} &= 0, \\
\frac{d}{dt} \phi_{j,k} + \nabla_h^- \cdot (\phi_{j,k} v_{j,k}) - \Gamma \Delta_h \mu_{j,k} &= 0.
\end{align}$$

**Scheme II**

$$\begin{align}
\rho \left( \frac{d}{dt} v_{j,k} + \frac{1}{2} (v_{j,k} \cdot \nabla_h^- v_{j,k} + \nabla_h^+ \cdot (v_{j,k} v_{j,k})) \right) &= -\nabla_h^- p_{j,k} + \eta \Delta_h v_{j,k} - \phi_{j,k} \nabla_h^- \mu_{j,k}, \\
\nabla_h^+ \cdot v_{j,k} &= 0, \\
\frac{d}{dt} \phi_{j,k} + \nabla_h^+ \cdot (\phi_{j,k} v_{j,k}) - \Gamma \Delta_h \mu_{j,k} &= 0.
\end{align}$$
Scheme III

\[
\begin{cases}
\rho \left( \frac{d}{dt} v_{j,k} + \frac{1}{2} (v_{j,k} \cdot \nabla_h v_{j,k} + \nabla_h \cdot (v_{j,k} v_{j,k})) \right) = -\nabla_h p_{j,k} + \eta \Delta_h v_{j,k} - \phi_{j,k} \nabla_h \mu_{j,k}, \\
\nabla_h \cdot v_{j,k} = 0, \\
\frac{d}{dt} \phi_{j,k} + \nabla_h \cdot (\phi_{j,k} v_{j,k}) - \Gamma \Delta_h \mu_{j,k} = 0.
\end{cases}
\]

(12)

For all the above schemes, \( j = 0, 1, \ldots, N_x - 1, \ k = 0, 1, \ldots, N_y - 1 \) and

\[ \mu_{j,k} = g'(\phi_{j,k}) - 2c \Delta_h \phi_{j,k}. \]

Theorem

All schemes I–III preserve the same discrete form of the energy identity (9)

\[
\frac{dE_h}{dt} + \eta \| \nabla_h^+ v \|^2_h + \Gamma \| \nabla_h^+ \mu \|^2_h = 0,
\]

(13)

where \( E_h \) is the discrete energy functional defined as

\[ E_h = \frac{\rho}{2} \| v \|^2_h + c \| \nabla_h^+ \phi \|^2_h + (g(\phi), 1)_h. \]
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Fully discretized scheme

\[
\begin{cases}
\delta_t^+ \mathbf{v}^n_{j,k} + \frac{1}{2} (\nabla \mathbf{v}^n_{j,k} \cdot \nabla \mathbf{v}^n_{j,k} + \nabla \cdot (\mathbf{v}^n_{j,k} \mathbf{v}^n_{j,k})) \\
\quad = -\nabla \mathbf{p}^{n+1/2}_{j,k} + \eta \Delta_h \mathbf{v}^{n+1/2}_{j,k} - \phi^{n+1/2}_{j,k} \nabla \mu^{n,n+1}_{j,k}, \\
\nabla_h \cdot \mathbf{v}^n_{j,k} = 0, \\
\delta_t^+ \phi^n_{j,k} + \nabla_h \cdot (\phi^{n+1/2}_{j,k} \mathbf{v}^{n+1/2}_{j,k}) - \Gamma \Delta_h \mu^{n,n+1}_{j,k} = 0,
\end{cases}
\]  

(14)

where

\[
\mu^{n,n+1}_{j,k} = \begin{cases}
g(\phi^{n+1}_{j,k}) - g(\phi^n_{j,k}) & -2c \Delta_h \phi^{n+1/2}_{j,k}, \quad \text{if } \phi^{n+1}_{j,k} \neq \phi^n_{j,k}, \\
g'(\phi^n_{j,k}) - 2c \Delta_h \phi^{n+1/2}_{j,k}, & \text{if } \phi^{n+1}_{j,k} = \phi^n_{j,k}.
\end{cases}
\]

Remark

When \(g\) is a polynomial of \(\phi\), \(\mu^{n,n+1}_{j,k}\) can be simplified. In particular, for the drop problem,

\[
\mu^{n,n+1}_{j,k} = \frac{\gamma}{\varepsilon} (\phi^n_{j,k} (1 - \phi^n_{j,k}) + \phi^{n+1}_{j,k} (1 - \phi^{n+1}_{j,k})) (1 - \phi^n_{j,k} - \phi^{n+1}_{j,k}) - \gamma \varepsilon \Delta_h \phi^{n+1/2}_{j,k}.
\]
Theorem

The fully discrete scheme (14) preserves the discrete energy identity

\[
\frac{E^n_{h,n+1} - E^n_{h,n}}{\Delta t} + \eta \| \nabla_h v^{n+1/2} \|^2_h + \Gamma \| \nabla_h \mu^{n,n+1} \|^2_h = 0, \tag{15}
\]

where

\[
E^n_{h,n} = \frac{1}{2} \| v^n \|^2_h + c \| \nabla_h \phi^n \|^2_h + (g(\phi^n), 1)_h.
\]
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We consider the system (8) in a rectangular domain $\Omega = [0, 1]^2$ with the free energy defined as in (6). With suitable forcing functions, the exact solution is given by

\[
\begin{align*}
    u(x, y, t) &= \frac{\pi}{2} \sin(\pi x) \sin(2\pi y) \sin(t), \\
    v(x, y, t) &= -\frac{\pi}{2} \sin(2\pi x) \sin^2(\pi y) \sin(t), \\
    \phi(x, y, t) &= \cos(2\pi x) \cos(2\pi y) \cos(t), \\
    p(x, y, t) &= \cos(2\pi x) \sin(2\pi y) \sin(t).
\end{align*}
\] (16)

The parameters are taken as $\eta = 1, \gamma = 1, \varepsilon = 0.01, \Gamma = 1.0e - 7$. 

**Table:** Accuracy test of the scheme (14) for $u$ (or $v$) at $t = 1$.

<table>
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<tr>
<th>$\tau$</th>
<th>$N$</th>
<th>Error</th>
<th>Order</th>
<th>CPU(s)</th>
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<td>$L^2$</td>
<td>$L^\infty$</td>
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<td>32</td>
<td>8.5421e-03</td>
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**Table:** Accuracy test of the scheme (14) for $\phi$ at $t = 1$.

<table>
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<th>$\tau$</th>
<th>$N$</th>
<th>Error</th>
<th>Order</th>
<th>CPU(s)</th>
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</table>
Drop dynamics

In this example, we consider the system (8) with the free energy defined as in (6) to study two drops merging process. The initial condition is given by

\[ u(x, y, 0) = v(x, y, 0) = 0, \quad (x, y) \in [0, 1]^2, \]

\[ \phi(x, y, 0) = \begin{cases} 
1, & r_1 \leq 0.2 - \delta \text{ or } r_2 \leq 0.2 - \delta, \\
\tanh \left( (0.2 + \delta - r_1) / \delta \right), & 0.2 - \delta < r_1 < 0.2 + \delta, \\
\tanh \left( (0.2 + \delta - r_2) / \delta \right), & 0.2 - \delta < r_2 < 0.2 + \delta, \\
0, & \text{other},
\end{cases} \quad (x, y) \in [0, 1]^2, \]

where \( r_1 = \sqrt{(x - 0.3 + \delta)^2 + (y - 0.5)^2} \), \( r_2 = \sqrt{(x - 0.7 - \delta)^2 + (y - 0.5)^2} \) and \( \delta = 0.01 \). The parameters are taken as \( \eta = 1, \gamma = 1, \varepsilon = 0.01, \Gamma = 1.0e - 7 \).
Figure: Coalescence of two drops simulated using ESM with $N = 128$, $\tau = 0.01$. 
Figure: Compare between ESM with $N = 128$, $\tau = 0.01$ and IFM with $N = 128$, $\tau = 0.0001$. 

(a) The evolution of energy
(b) The rate of energy dissipation
(c) The residual of energy identity
(d) The evolution of $\nabla \cdot \mathbf{v}$
In this example, we consider the system (8) with the free energy defined as in (7) to study phase separation process. The initial condition is given by

\[ u(x, y, 0) = v(x, y, 0) = 0, \]

\[ \phi(x, y, 0) = 0.5 + 0.45 \sin(4\pi x) \sin(4\pi y). \]

The parameters are taken as \( \eta = 1, \gamma_1 = 0.0001, \gamma_2 = 1, N_1 = 1, N_2 = 2, \chi = 2, \Gamma = 1.0e - 4. \)
Figure: Phase separation and coarsening dynamics simulated using ESM with $N = 128$, $\tau = 0.01$. 
(a) The evolution of energy

(b) The rate of energy dissipation

(c) The residual of energy identity

(d) The evolution of $\nabla \cdot \mathbf{v}$

Figure: Compare with $N = 128, \tau = 0.01$. 
• D. Furihata, Finite difference schemes for $\frac{\partial u}{\partial t} = (\frac{\partial}{\partial x})^\alpha \frac{\delta G}{\delta u}$ that inherit energy conservation or dissipation property, J. Comput. Phys., 156 (1999), 181-205.


Thanks for your attention!