Part I. Efficient and Accurate Numerical Schemes for Gradient Flows

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Outline

Energy Stable Schemes for Gradient Flows:

- Motivation
- A brief review of energy stable methods for gradient flows
- The scalar auxiliary variable (SAV) approach
- Numerical examples
- Convergence and error analysis
- Several applications
- Concluding remarks

Part I. Gradient flows

- Many physical problems can be modeled by PDEs that take the form of gradient flows. Examples include heat equation, Allen-Cahn equation, Cahn-Hilliard equation, PNP equations, Erickssen-Leslie liquid crystal models, phase-field models, ...
- Gradient flows are dynamics driven by a free energy, e.g.,
  - heat equation: $E(\phi) = \int_\Omega \frac{1}{2}|\nabla\phi|^2$
  - Allen-Cahn and Cahn-Hilliard equation: $E(\phi) = \int_\Omega (\frac{1}{2}|\nabla\phi|^2 + F(\phi))$

  and satisfy a dissipative energy law:

$$\frac{d}{dt}E(\phi) = -\|\frac{\delta E(\phi)}{\delta\phi}\|_X^2.$$

- It is important that numerical schemes preserve the energy dissipation while being as efficient and accurate as possible.

Gradient flows

Given a free energy functional $E(\phi)$, the gradient flow in L^2:

$$\frac{\partial \phi}{\partial t} = -\frac{\partial E(\phi)}{\partial \phi};$$

or the gradient flow in H^{-1}:

$$\frac{\partial \phi}{\partial t} = \Delta \frac{\delta E(\phi)}{\delta \phi}.$$

If $E(\phi) = \int_\Omega [\frac{1}{2}|\nabla \phi|^2 + F(\phi)]dx$ with $F(\phi)$ being a double-well type potential, then the gradient flow in L^2 is the so called Allen-Cahn equation (Allen & Cahn '79):

$$\frac{\partial \phi}{\partial t} = \Delta \phi - F'(\phi),$$

and the gradient flow in H^{-1} is the so called Cahn-Hilliard equation (Cahn & Hilliard '58):

$$\frac{\partial \phi}{\partial t} = -\Delta(\Delta \phi - F'(\phi)).$$

Examples: Allen-Cahn and Cahn-Hillard equations

If $E(\phi) = \int_\Omega [\frac{1}{2}|\nabla\phi|^2 + F(\phi)]dx$ with $F(\phi)$ being a double-well type potential, then the gradient flow in L^2 is the so called Allen-Cahn equation (Allen & Cahn '79):

$$\frac{\partial\phi}{\partial t} = \Delta\phi - F'(\phi),$$

subjected to either periodic boundary conditions or the Neumann boundary condition $\frac{\partial\phi}{\partial n}|_\Omega = 0$;
and the gradient flow in H^{-1} is the so called Cahn-Hilliard equation (Cahn & Hilliard '58):

$$\frac{\partial\phi}{\partial t} = -\Delta(\Delta\phi - F'(\phi)),$$

subjected to either periodic boundary conditions or the Neumann boundary conditions $\frac{\partial\phi}{\partial n}|_\Omega = \frac{\partial\Delta\phi}{\partial n}|_\Omega = 0$.
Both equations play very important roles in materials science and fluid dynamics.

To fix the idea, we let $E(\phi)=\int_\Omega[\frac{1}{2}|\nabla\phi|^2+\frac{1}{\eta^2}F(\phi)]dx$, where $F(\phi)$ is a general nonlinear free energy, η may be a small parameter, and consider the gradient flow in H^{-1}:

$$\phi_t=\nabla\cdot\nabla\frac{\delta E}{\delta\phi},\qquad \partial_n w|_{\partial\Omega}=0;$$
$$w=\frac{\delta E}{\delta\phi}=-\Delta\phi+\frac{1}{\eta^2}F'(\phi),\qquad \partial_n\phi|_{\partial\Omega}=0,$$

which satisfies the energy law:

$$\frac{\partial}{\partial t}\int_\Omega\left(\frac{1}{2}|\nabla\phi|^2+\frac{1}{\eta^2}F(\phi)\right)=-\int_\Omega|\nabla(-\Delta\phi+\frac{1}{\eta^2}F'(\phi))|^2.$$

Goal: Design simple, efficient and accurate numerical schemes that satisfy a discrete energy law.

Linearly implicit with explicit treatment of nonlinear terms:

$$\frac{1}{\delta t}(\phi^{n+1} - \phi^n) = \Delta w^{n+1},$$
$$w^{n+1} = -\Delta\phi^{n+1} + \frac{1}{\eta^2} F'(\phi^n).$$

• Need $\delta t \leq C\eta^4$ to have energy stability $E(\phi^{n+1}) \leq E(\phi^n)$.
Full implicit schemes. many results available, including:
• Du & Nicolaides (1991) proposed a nonlinear implicit scheme which is unconditionally energy stable, but still need a severe time step restriction for the solution to be unique.
• Feng & Prohl (2003-2005) carried out a sequence of work on the error analysis of Allen-Cahn and Cahn-Hilliard equations, and derived error estimates with polynomial growth in η.

Convex splitting

The convex splitting was perhaps originally proposed Elliott and Stewart '93 (see also Eyre '98).
Assume that we can write $F(\phi) = F_c(\phi) - F_e(\phi)$ where $F_c(\phi)$ and $F_e(\phi)$ are both convex functions, the convex splitting scheme is:

$$\frac{1}{\delta t}(\phi^{n+1} - \phi^n) = \Delta w^{n+1},$$
$$w^{n+1} = -\Delta\phi^{n+1} + \frac{1}{\eta^2}(F_c'(\phi^{n+1}) - F_e'(\phi^n)).$$

(Example: For GL potential, we write $F(\phi) = \frac{1}{4}(\phi^4 + 1) - \frac{1}{2}\phi^2$.)
It is easy to show that the above scheme enjoys the following properties:

- It is unconditionally stable;
- It is uniquely solvable;
- At each time step, it can be interpreted as a minimization of a strictly convex functional.

- The convex splitting idea has been generalized to many other situations, cf. Hu, Wise, Wang, Lowengrub (2009), S., Wang, Wang, Wise (2012), W. Chen, C. Wang, X. Wang, S. Wise (2014), ...
- Second-order convex-splitting schemes for some special cases can be constructed.

Main disadvantages:

- A nonlinear equation has to be solved at each time step.
- It is very difficult, or even impossible, to construct second- or higher-order convex-splitting schemes with complicated free energies.

Stabilized schemes

Given a stabilization parameter S, we solve:

$$\frac{1}{\delta t}(\phi^{n+1} - \phi^n) = \Delta w^{n+1},$$
$$w^{n+1} + \frac{S}{\eta^2}(\phi^{n+1} - \phi^n) = -\Delta\phi^{n+1} + \frac{1}{\eta^2}F'(\phi^n).$$

(Similar idea has been used in Zhu, Chen & S. '99; Tang & Xu '06; S. & Yang '10,...)

• One can determine constants c_1, c_2 such that the above system becomes (Yue, Feng, Liu & S. '04):

$$c_1\psi^{n+1} - \Delta\psi^{n+1} = g^n,$$
$$c_2\phi^{n+1} - \Delta\phi^{n+1} = \psi^{n+1}.$$

Fast solvers can be used.

• An extra consistent error introduced by the stabilization term is of the same order as the linearized (or convex splitting) approach.

Remarks:

- Under the assumption $\|F''\|_{L^\infty} \le L$, it is shown that the scheme is unconditionally energy stable with a suitable choice of S.
- The condition $\|F''\|_{L^\infty} \le L$ is not "directly satisfied" by the Ginzburg-Landau potential $F(\phi) = \frac{1}{4}(\phi^2 - 1)^2$. However, it is shown by Caffarelli and Muler (1995) that, with the modified GL potential, the L^∞-norm of the solution is bounded. Hence, we can modify the potential to quadratic growth at infinity.
- It can be interpreted as a special convex splitting scheme.
- In general, direct second-order extensions are not unconditionally stable; but is possible with additional stabilization terms involving higher-order derivatives, cf. recent work by Z. Qiao & D. Li, and L. Wang & H. Yu.
- Another class of energy stable schemes related to stabilized schemes, can be constructed by using the exponential time differentiation (ETD) scheme (see recent work by Q. Du, L. Ju, J. Zhang, etc.)

The method with a Lagrange multiplier (Badia et al. '11, Tiera & Guillen-Gonzalez '13)

If $F(\phi) = \frac{1}{4}(\phi^2 - 1)^2$ so $F'(\phi) = (\phi^2 - 1)\phi$. Introduce a Lagrange multiplier (auxiliary function) $q = \phi^2 - 1$, and rewrite the Allen-Cahn equation $\frac{\partial \phi}{\partial t} = \Delta\phi - F'(\phi)$ as

$$\begin{aligned} \frac{\partial \phi}{\partial t} &= \Delta\phi - q\phi, \\ \frac{\partial q}{\partial t} &= 2\phi\frac{\partial \phi}{\partial t}. \end{aligned}$$

Taking the inner products of the above with ϕ_t and $\frac{1}{2}q$, we obtain the energy law:

$$\frac{d}{dt}\left(\frac{1}{2}\|\nabla\phi\|^2 + \frac{1}{4}\|q\|^2\right) = -\|\phi_t\|^2.$$

• One can then construct linear, unconditionally energy stable schemes for the above modified system:

$$\begin{aligned}\frac{\phi^{n+1}-\phi^n}{\Delta t} &= \Delta\phi^{n+1} - q^{n+1}\phi^n,\\ \frac{q^{n+1}-q^n}{\Delta t} &= 2\phi^n\frac{\phi^{n+1}-\phi^n}{\Delta t}\end{aligned}$$

Taking the inner products of the above with $\frac{\phi^{n+1}-\phi^n}{\Delta t}$ and $\frac{1}{2}q^{n+1}$, respectively, one obtains immediately:

$$\begin{aligned}&\frac{1}{\Delta t}\Big[\frac{1}{2}\|\nabla\phi^{n+1}\|^2 + \frac{1}{4}\int_\Omega (q^{n+1})^2 - \frac{1}{2}\|\nabla\phi^n\|^2 - \frac{1}{4}\int_\Omega (q^n)^2\\ &\quad + \frac{1}{2}\|\nabla(\phi^{n+1}-\phi^n)\|^2 + \frac{1}{4}\int_\Omega (q^{n+1}-q^n)^2\Big] = -\|\frac{\phi^{n+1}-\phi^n}{\Delta t}\|^2.\end{aligned}$$

• However, this approach only works with very special $F(\phi)$ such that $q'(\phi) = c\phi$, so its applicability is very limited; and it requires solving **coupled equations with variable coefficients**.

Invariant Energy Quadratization (IEQ) Method (X. Yang, Q. Wang, ...)

Assuming that $F(\phi)$ is bounded from below, i.e., $F(\phi) > -C_0$, and introducing two auxiliary functions

$$\bar{u}(t,x;\phi) = \nabla\phi, \quad v(t,x;\phi) = \sqrt{F(\phi)+C_0},$$

so the free energy becomes

$$E(\bar{u},v;\phi) = \int_\Omega (\frac{1}{2}\bar{u}^2 + v^2 - C_0)dx,$$

and the original gradient flow can be recast as:

$$\begin{aligned}
&\frac{\partial\phi}{\partial t} = \Delta w \\
&w = -\nabla\cdot\nabla\phi + 2v\frac{\delta v}{\delta\phi}, \\
&\frac{\partial v}{\partial t} = \frac{\delta v}{\delta\phi}\frac{\partial\phi}{\partial t}, \\
&\frac{\partial\bar{u}}{\partial t} = \nabla\frac{\partial\phi}{\partial t}.
\end{aligned}$$

Unconditionally stable schemes

Consider the following first-order scheme:

$$
\begin{aligned}
\frac{\phi^{n+1}-\phi^n}{\Delta t} =&\Delta w^{n+1}, \\
w^{n+1} =& -\nabla\cdot\nabla\phi^{n+1} + 2v^{n+1}\frac{\delta v}{\delta\phi}|_{\phi=\phi^n}, \\
\frac{v^{n+1}-v^n}{\Delta t} =& \frac{\delta v}{\delta\phi}|_{\phi=\phi^n}\frac{\phi^{n+1}-\phi^n}{\Delta t}, \\
\frac{\bar{u}^{n+1}-\bar{u}^n}{\Delta t} =& \nabla\frac{\phi^{n+1}-\phi^n}{\Delta t}.
\end{aligned}
$$

Taking the inner products of the above with w^{n+1}, $\frac{\phi^{n+1}-\phi^n}{\Delta t}$, $2v^{n+1}$ and $\bar{u}^{n+1}$, respectively, one obtains immediately:

$$
\begin{aligned}
&\frac{1}{\Delta t}\Big[\int_\Omega \big(\frac12|\bar{u}^{n+1}|^2+(v^{n+1})^2\big) - \int_\Omega \big(\frac12|\bar{u}^{n}|^2+(v^{n})^2\big) \\
&\quad + \frac12\int_\Omega \big(|\bar{u}^{n+1}-\bar{u}^n|^2 + (v^{n+1}-v^n)^2\big)\Big] = -\|\nabla w^{n+1}\|^2.
\end{aligned}
$$

Main advantages of the IEQ approach

This approach leads to efficient and flexible numerical schemes:

- It can be efficiently implemented: one can eliminate q^{n+1}, $\bar{u}^{n+1}$ and w^{n+1} from the coupled system, leading to a fourth-order equation for ϕ^{n+1} with variable coefficients at each time step;
- It can be easily extended to higher-order with the BDFk scheme, with BDF2 being unconditionally stable.
- It allows us to deal with a large class of gradient flows (cf. X. Yang, Q. Wang, L. Ju, J. Zhao, S., etc, 2016, 2017).

Although the IEQ approach has proven to be a very powerful way to construct energy stable schemes, it does leave somethings to be desired:

- It involves solving problems with complicated VARIABLE coefficients.
- It requires that the free energy density $F(\phi)$ is bounded from below.
- For gradient flows with multiple components, it leads to coupled system.

Q. Can we do better?

The SAV approach is inspired by the IEQ method. It preserves their advantages while overcomes most of its shortcomings.

Assuming that $E_1(\phi) := \int_\Omega F(\phi)dx$ is bounded from below, i.e., $E_1(\phi) > -C_0$ for some $C_0 > 0$, and introduce one scalar auxiliary variable (SAV):

$$r(t) = \sqrt{E_1(\phi) + C_0}.$$

Then, the original gradient flow can be recast as:

$$\begin{aligned} \frac{\partial \phi}{\partial t} &= \Delta w \\ w &= -\Delta\phi + \frac{r(t)}{\sqrt{E_1[\phi] + C_0}} F'(\phi) \\ r_t &= \frac{1}{2\sqrt{E_1[\phi] + C_0}} \int_\Omega F'(\phi)\phi_t dx. \end{aligned}$$

First-order scheme:

$$\frac{\phi^{n+1}-\phi^n}{\Delta t} = \Delta w^{n+1},$$
$$w^{n+1} = -\Delta\phi^{n+1} + \frac{r^{n+1}}{\sqrt{E_1[\phi^n]+C_0}} F'(\phi^n),$$
$$\frac{r^{n+1}-r^n}{\Delta t} = \frac{1}{2\sqrt{E_1[\phi^n]+C_0}} \int_\Omega F'(\phi^n)\frac{\phi^{n+1}-\phi^n}{\Delta t}\, dx.$$

Taking the inner products of the above with w^{n+1}, $\frac{\phi^{n+1}-\phi^n}{\Delta t}$ and $2r^{n+1}$, respectively, one obtains immediately:

$$\frac{1}{\Delta t}\Big[\frac{1}{2}\|\nabla\phi^{n+1}\|^2 + (r^{n+1})^2 - \frac{1}{2}\|\nabla\phi^n\|^2 - (r^n)^2 + \frac{1}{2}\|\nabla(\phi^{n+1}-\phi^n)\|^2 + (r^{n+1}-r^n)^2\Big] = -\|\nabla w^{n+1}\|^2.$$

Second-order BDF scheme:

$$\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\Delta t} = \Delta w^{n+1},$$

$$w^{n+1} = -\Delta\phi^{n+1} + \frac{r^{n+1}}{\sqrt{E_1[\tilde{\phi}^{n+1}] + C_0}} F'(\tilde{\phi}^{n+1}),$$

$$\frac{3r^{n+1} - 4r^n + r^{n-1}}{2\Delta t} = \int_\Omega \frac{F'(\tilde{\phi}^{n+1})}{2\sqrt{E_1[\tilde{\phi}^{n+1}] + C_0}} \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\Delta t}\, dx,$$

where $g(\tilde{\phi}^{n+1}) := 2g(\phi^n) - g(\phi^{n-1})$.

- Taking the inner products of the above with w^{n+1}, $\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\Delta t}$ and $2r^{n+1}$, respectively, one can also derive that the scheme is unconditionally stable.
- One can also construct k-th order scheme based on BDF-k and Adam-Bashforth, while they are not unconditionally stable, but they do have very good stability property as high-order schemes.

Efficient implementation

We can write the schemes as a matrix system

$$\begin{pmatrix} c_1 I & -\Delta & 0 \\ \Delta & c_2 I & * \\ * & 0 & c_3 \end{pmatrix} \begin{pmatrix} \phi^{n+1} \\ w^{n+1} \\ r^{n+1} \end{pmatrix} = \bar{b}^n,$$

So we can solve r^{n+1} with a block Gaussian elimination, which requires solving a system with constant coefficients of the form

$$\begin{pmatrix} c_1 I & -\Delta \\ \Delta & c_2 I \end{pmatrix} \begin{pmatrix} \phi \\ w \end{pmatrix} = \bar{b}.$$

With r^{n+1} known, we can obtain (ϕ^{n+1}, w^{n+1}) by solving one more equation in the above form.

Main advantages of the SAV approach

- The SAV schemes, up to second-order, are unconditionally energy stable, and can be easily extended to higher-order with the BDFk schemes.
- It only requires solving decoupled, linear system with CONSTANT coefficients.
- It only requires $E_1(\phi) := \int_\Omega F(\phi)dx$, instead of $F(\phi)$, be bounded from below, so it applies to a larger class of gradient flows.
- For gradient flows with multiple components, the scheme will lead to decoupled equations with constant coefficients to solve at each time step.

Some numerical examples

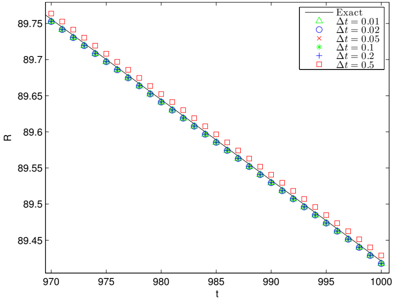


FIG. 3. *(Example 3) The evolution of radius with different time step.*

Scheme		Δt=1.6e-4	Δt=8e-5	Δt=4e-5	Δt=2e-5	Δt=1e-5
SAVT/CN	Error	1.74e-7	4.54e-8	1.17e-8	2.94e-9	2.01e-10
	Rate	-	1.93	1.96	1.99	2.01
SAVT/BDF	Error	1.38e-6	3.72e-7	9.63e-8	2.43e-8	5.98e-9
	Rate	-	1.89	1.95	1.99	2.02

TABLE 1

(Example 4) Errors and convergence rates of SAVT/CN and SAVT/BDF for the Cahn–Hilliard equation.

The proposed schemes are unconditionally energy stable with a modified energy. How about the dissipation of original energy?

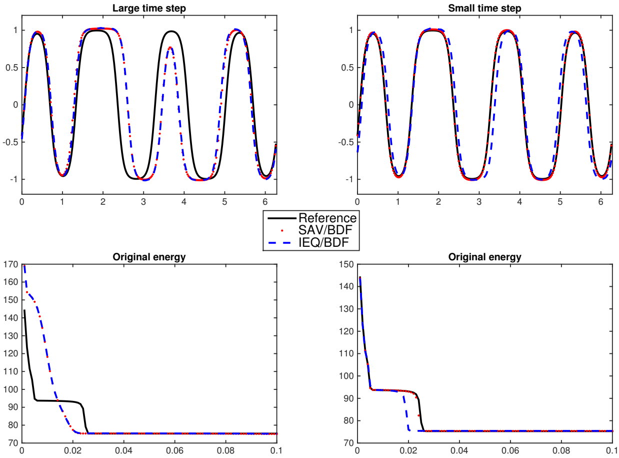


Figure: Solid line: current method; dash line: another method

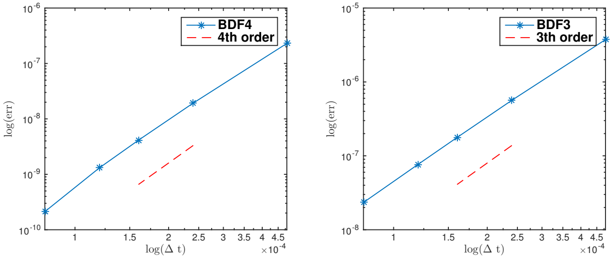


FIG. 8. *(Example 7) Numerical convergences of BDF3 and BDF4.*

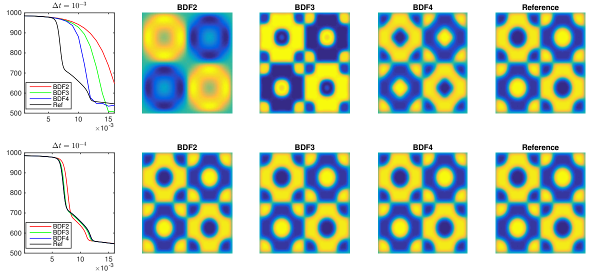


FIG. 9. *(Example 7) Numerical comparison among BDF2, BDF3 and BDF4.*

Adaptive time stepping

Thanks to its unconditionally energy stability, one can (and should) couple the scheme with an adaptive time stepping strategy.
A simple but effective strategy is to update the time step size by using the formula:

$$A_{dp}(e,\tau)=\rho\left(\frac{tol}{e}\right)^{\frac{1}{2}}\tau,$$

where e is a relative error, τ is the time step, tol is the error tolerance and ρ is a parameter.

Second-order daptive time stepping with CN-SAV

Given Solutions at time steps n and $n-1$; parameters tol, ρ, δt_{min} and δt_{max}.

Step 1 Compute $(\phi_1, U_1, V_1)^{n+1}$ by the first-order SAV scheme with δt.

Step 2 Compute $(\phi_2, U_2, V_2)^{n+1}$ by CN-SAV with δt.

Step 3 Calculate
$e_{n+1} = \max\{\frac{\|U_2^{n+1}-U_1^{n+1}\|}{\|U_2^{n+1}\|}, \frac{\|V_2^{n+1}-V_1^{n+1}\|}{\|V_2^{n+1}\|}, \frac{\|\phi_2^{n+1}-\phi_1^{n+1}\|}{\|\phi_2^{n+1}\|}\}$.

Step 4 **if** $e_{n+1} > tol$, **then**
Recalculate time step
$t \leftarrow \max\{\delta t_{min}, \min\{A_{dp}(e_{n+1}, \delta t), \delta t_{max}\}\}$.

Step 5 **goto** Step 1

Step 6 **else**
Update time step
$t_{n+1} \leftarrow \max\{\delta t_{min}, \min\{A_{dp}(e_{n+1}, \delta t), \delta t_{max}\}\}$.

Step 7 **endif**

Adaptive time stepping: numerical results

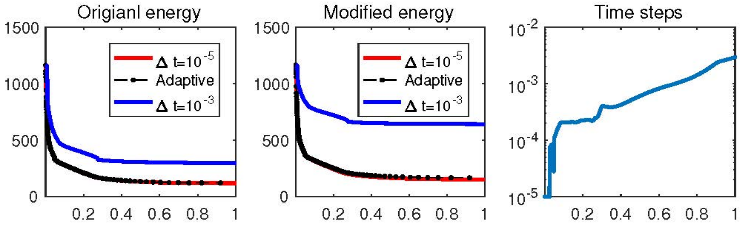
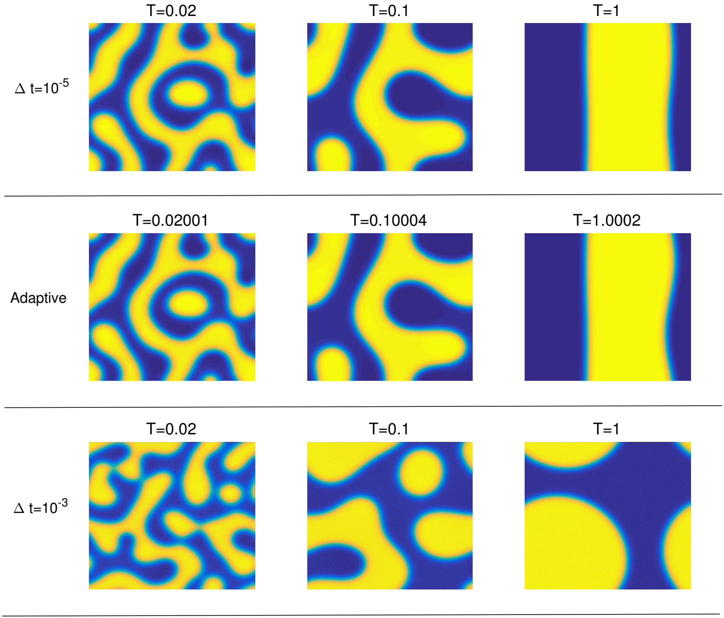


Figure: Numerical comparisons among small time steps, adaptive time steps, and large time steps


T=0.02
T=0.1
T=1
Δ t=10-5
T=0.02001
T=0.10004
T=1.0002
Adaptive
T=0.02
T=0.1
T=1
Δ t=10-3

Convergence and error analysis (S. & J. Xu)

- The SAV schemes are semi-implicit schemes. Previous stability and error analysis on semi-implicit schemes usually assume a Lipschitz condition on the derivative of the free energy, which is not satisfied by even the double-well potential.
- Thanks to the unconditional energy stability of the SAV schemes, we can derive H^2 bounds for the numerical solution under mild conditions on the free energy.
- The H^2 bounds on the numerical solution will enable us to establish the convergence, and with additional smoothness assumption, the error estimates.

H^2 bounds

Theorem.

- For the L^2 gradient flow, let $u^0 \in H^3$, and

  $$|F''(x)| < C(|x|^p+1), \quad p > 0 \text{ if } n = 1, 2; \quad 0 < p < 4 \text{ if } n = 3.$$

  Then

  $$\|\Delta u^n\|^2 + \frac{\Delta t}{2} \sum_{k=0}^{n} \|\nabla \Delta u^k\|^2 \le C(T+1) + \|\Delta u^0\|^2 + \Delta t \|\nabla \Delta u^0\|^2.$$

- For the H^{-1} gradient flow, let $u^0 \in H^4$, and additionally

  $$|F'''(x)| < C(|x|^{p'}+1), \quad p' > 0 \text{ if } n = 1, 2; \quad 0 < p' < 3 \text{ if } n = 3.$$

  Then

  $$\|\Delta u^n\|^2 + \frac{\Delta t}{2} \sum_{k=0}^{n} \|\Delta^2 u^k\|^2 \le C(T+1) + \|\Delta u^0\|^2 + \Delta t \|\Delta^2 u^0\|^2.$$

Let $u_{\Delta t}(\cdot, t)$ (resp. $r_{\Delta t}(\cdot, t)$) be a piece-wise linear function such that $u_{\Delta t}(\cdot, t^n) = u^n$ (resp. $r_{\Delta t}(\cdot, t^n) = r^n$).

Theorem. Under the same assumptions needed for the H^2 bounds, we have:

- For L^2 gradient flow: when $\Delta t \to 0$, we have
  - $u_{\Delta t} \to u$ strongly in $L^2(0, T; H^{3-\epsilon})\, \forall \epsilon > 0$, weakly in $L^2(0, T; H^3)$, weak-star in $L^\infty(0, T; H^2)$;
  - $r_{\Delta t} \to r = \sqrt{E_1}$ weak-star in $L^\infty(0, T)$.
- For H^{-1} gradient flow: when $\Delta t \to 0$, we have
  - $u_{\Delta t} \to u$ strongly in $L^2(0, T; H^{4-\epsilon})\, \forall \epsilon > 0$, weakly in $L^2(0, T; H^4)$, weak-star in $L^\infty(0, T; H^2)$;
  - $r_{\Delta t} \to r = \sqrt{E_1}$ weak-star in $L^\infty(0, T)$.

Theorem.

- For L^2 gradient flow, we assume additionally

$$u_t \in L^\infty(0,T;L^2)\cap L^2(0,T;L^4), \quad u_{tt}\in L^2(0,T;L^2).$$

Then, for all $0 \le n \le T/\Delta t$, we have

$$\frac{1}{2}\|\nabla(u^n - u(\cdot,t^n))\|^2 + (r^n - r(t^n))^2$$
$$\le C\exp\left((1-C\Delta t)^{-1}t^n\right)\Delta t^2\int_0^{t^n}(\|u_{tt}(s)\|^2 + \|u_t(s)\|^2_{L^4})ds.$$

- For H^{-1} gradient flow, we assume additionally

$$u_t \in L^\infty(0,T;H^{-1})\cap L^2(0,T;H^1), \quad u_{tt}\in L^2(0,T;H^{-1}).$$

Then, for all $0 \le n \le T/\Delta t$, we have

$$\frac{1}{2}\|\nabla(u^n - u(\cdot,t^n))\|^2 + (r^n - r(t^n))^2$$
$$\le C\exp\left((1-C\Delta t)^{-1}t^n\right)\Delta t^2\int_0^{t^n}(\|u_{tt}(s)\|^2_{H^{-1}} + \|u_t(s)\|^2_{H^1})ds.$$

Several applications

Gradient flows of several functions

Consider the energy functional

$$E(\phi) = \sum_{i=1}^{k} (\phi_i, \mathcal{L}_i \phi_i) + E_1[\phi_1, \ldots, \phi_k],$$

where $\mathcal{L}_i$ are non-negative linear operators, $E_1[\phi_1, \ldots, \phi_k] > -C_0$. Introduce $r(t) = \sqrt{E_1 + C_0}$. Then then gradient flow associated with $E(\phi)$ reads:

$$\begin{aligned}
\frac{\partial \phi_i}{\partial t} =& \Delta \mu_i, \quad i = 1, \cdots, k, \\
\mu_i =& \mathcal{L}_i \phi_i + \frac{r}{\sqrt{E_1 + C_0}} \frac{\delta E_1}{\delta \phi_i}, \quad i = 1, \cdots, k, \\
r_t =& \frac{1}{2\sqrt{E_1 + C_0}} \int_\Omega \sum_{i=1}^{k} \frac{\delta E_1}{\delta \phi_i} \frac{\partial \phi_i}{\partial t} dx.
\end{aligned}$$

Setting $U_i = \frac{\delta E_1}{\delta \phi_i}$, the 2nd-order scheme based on Crank-Nicolson:

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \Delta \mu_i^{n+1/2}, \quad i = 1, \cdots, k,$$

$$\mu_i^{n+1/2} = \mathcal{L}_i \frac{\phi_i^{n+1} + \phi_i^n}{2} + \frac{r^{n+1} + r^n}{2\sqrt{E_1[\bar{\phi}_j^{n+1/2}] + C_0}} U_i[\bar{\phi}_j^{n+1/2}], \quad i = 1, \cdots$$

$$r^{n+1} - r^n = \int_\Omega \sum_{i=1}^{k} \frac{U_i[\bar{\phi}^{n+1/2}]}{2\sqrt{E_1[\bar{\phi}_j^{n+1/2}] + C_0}} (\phi_i^{n+1} - \phi_i^n) dx.$$

- Multiplying the above three equations with $\Delta t \mu_i^{n+1/2}$, $\phi_i^{n+1} - \phi_i^n$, $r^{n+1} + r^n$ and taking the sum over i, we can show that the scheme is unconditionally energy stable.
- We can determine r^{n+1} explicitly which requires solving k decoupled equations with constant coefficients of the form:

$$(I - \lambda \Delta \mathcal{L}_i)\phi_i = f_i, \quad i = 1, \cdots, k;$$

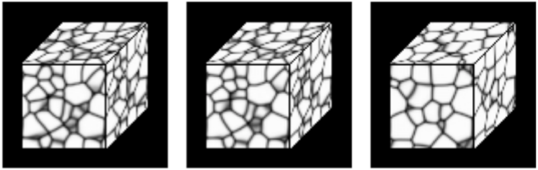
then obtain $\{\phi_j\}$ by solving another k decoupled equations in the above form.

Preliminary results on grain growth (with Longqing Chen)

- Cahn-Hilliard system with $k = 100$ order parameters, and $E_1 = \int_\Omega f(\phi_1, \cdots, \phi_k)$ with

$$f(\phi_1, \cdots, \phi_k) = -\frac{\alpha}{2}\sum_{i=1}^{k}\phi_i^2 + \frac{\beta}{4}(\sum_{i=1}^{k}\phi_i^2)^2 + (\gamma - \frac{\beta}{2})\sum_{i=1}^{k}\sum_{j>i}\phi_i^2\phi_j^2.$$

- Existing schemes use explicit or semi-implicit discretization, requiring possible severe time step constraint.
- The SAV scheme is unconditionally stable and only required solving PDEs with constant-coefficients that can be solved fast by FFT.



Molecular beam epitaxial (MBE) without slope selection (with Qing Cheng and X. Yang)

Consider the energy function:

$$E(\phi) = \int_\Omega [-\frac{1}{2}\ln(1+|\nabla\phi|^2) + \frac{\eta^2}{2}|\Delta\phi|^2]dx.$$

Note that the first part of the energy density, $-\frac{1}{2}\ln(1+|\nabla\phi|^2)$, is unbounded from below, but one can show that

$$E_1(\phi) = \int_\Omega [-\frac{1}{2}\ln(1+|\Delta\phi|^2) + \frac{\alpha}{2}|\Delta\phi|^2]dx > -C_0, \quad \forall\alpha > 0.$$

Hence, we take $\alpha < \eta^2$ and split $E(\phi)$ as

$$E(\phi) = E_1(\phi) + \int_\Omega \frac{\eta^2-\alpha}{2}|\Delta\phi|^2 dx$$

and introduce

$$r(t) = \sqrt{\int_\Omega \frac{\alpha}{2}|\Delta\phi|^2 - \frac{1}{2}\ln(1+|\nabla\phi|^2)dx + C_0}.$$

MBE (continued)

We can then rewrite the original system as

$$\phi_t + (\eta^2 - \alpha)\Delta^2\phi + \frac{r(t)}{G(\phi)}\frac{\delta E_1(\phi)}{\delta\phi} = 0,$$
$$r_t = \frac{1}{2G(\phi)}\int_\Omega \frac{\delta E_1(\phi)}{\delta\phi}\phi_t dx,$$

where

$$G(\phi) = \sqrt{\int_\Omega \frac{\alpha}{2}|\Delta\phi|^2 - \frac{1}{2}\log(1+|\nabla\phi|^2)dx + C_0}.$$

- Taking the inner product of the above equations with ϕ_t and $2r(t)$, respectively, we obtain:

$$\frac{d}{dt}[\int_\Omega \frac{\eta^2-\alpha}{2}|\Delta\phi|^2 dx + r^2(t)] = -\|\phi_t\|^2.$$

MBE (continued):

Let $\bar{\phi}^{n+1/2} = \frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}$. A second-order, unconditionally energy stable scheme for the modified system is:

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + (\eta^2 - \alpha)\Delta^2 \frac{\phi_i^{n+1} + \phi_i^n}{2} + \frac{r^{n+1} + r^n}{2G(\bar{\phi}^{n+1/2})} \frac{\delta E_1}{\delta \phi}[\bar{\phi}^{n+1/2})] = 0,$$

$$r^{n+1} - r^n = \frac{1}{2G(\bar{\phi}^{n+1/2})} \int_\Omega \frac{\delta E_1}{\delta \phi}[\bar{\phi}^{n+1/2})](\phi_i^{n+1} - \phi_i^n) dx.$$

- It is easy to show that the above scheme is unconditionally energy stable.
- One can solve r^{n+1} explicitly, and then obtain ϕ^{n+1} by solving a fourth-order equation with constant coefficients.

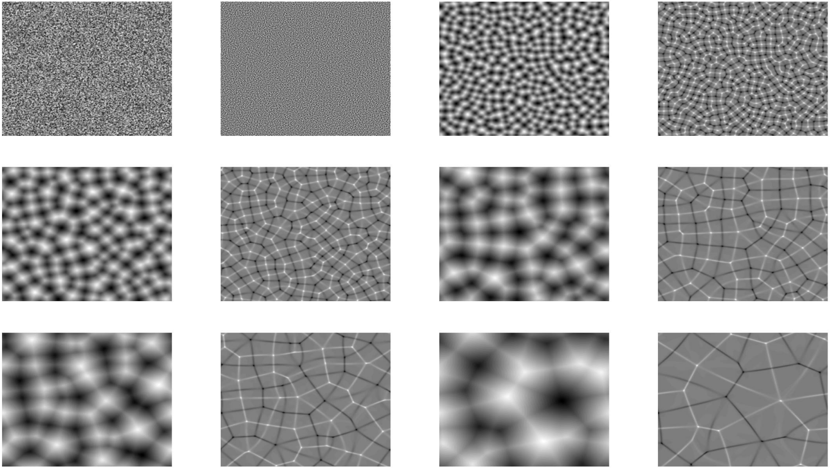


FIGURE 7. The isolines of the numerical solutions of the height function ϕ and its Laplacian $\Delta\phi$ for the slope model with random initial condition (4.6) using Scheme-1 and time step $\delta t = 10^{-4}$. For each subfigure, the left is ϕ and the right is $\Delta\phi$. Snapshots are taken at $t = 0, 1, 10, 50, 100, 500$, respectively.

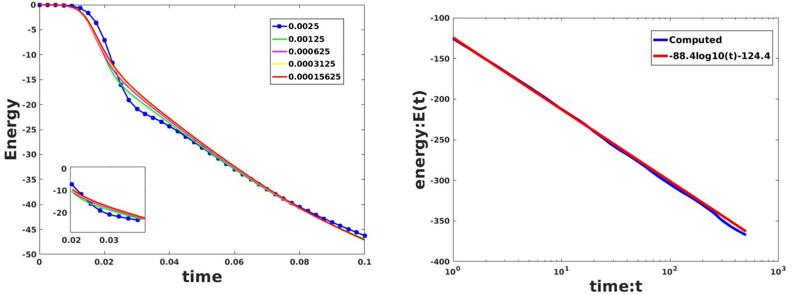


Figure: Simulation of MBE: Left, energy evolution; Right, semi-log fit of the energy.

Gradient flows with non-local terms

Consider, e.g., phase field crystal model with free energy:

$$E(\phi) = \int_\Omega \left\{ \frac{1}{4}\phi^4 + \frac{1-\epsilon}{2}\phi^2 + \phi\mathcal{L}_\delta\phi + \frac{1}{2}(\mathcal{L}_\delta\phi)^2 \right\} dx,$$

where $\mathcal{L}_\delta$ is a non-local diffusion operator, e.g., $(-\Delta)^{1-\delta}$ or:

$$\mathcal{L}_\delta\phi(x) = \int_{\mathcal{B}(x,\delta)} \rho_\delta(|y-x|)\big(\phi(y) - \phi(x)\big)\,dy.$$

Its gradient flow is given by

$$\frac{\partial\phi}{\partial t} = \mathcal{L}_\delta(\mathcal{L}_\delta^2\phi + 2\mathcal{L}_\delta\phi + (1-\epsilon)\phi + \phi^3).$$

Due to the non-local terms, the above equation is very challenging if the discretized system is nonlinear or involves variable coefficients.

The SAV approach

We split the free energy as

$$E(\phi) = \int_\Omega [\frac{1}{4}\phi^4 + \frac{1-\epsilon}{2}\phi^2] + [\phi\mathcal{L}_\delta\phi + \frac{1}{2}(\mathcal{L}_\delta\phi)^2] dx = E_1(\phi) + E_2(\phi).$$

Denote $r(t) = \sqrt{E_1(\phi) + \epsilon}$. We rewrite the original gradient flow as:

$$\frac{\partial\phi}{\partial t} = \mathcal{L}_\delta w,$$
$$w = \mathcal{L}_\delta^2\phi + 2\mathcal{L}_\delta\phi + \frac{r(t)}{\sqrt{E_1(\phi)+\epsilon}}\frac{\delta E_1(\phi)}{\delta\phi},$$
$$r_t = \frac{1}{2\sqrt{E_1(\phi)+\epsilon}}\int_\Omega \frac{\delta E_1(\phi)}{\delta\phi}\phi_t dx.$$

As before, we can construct unconditionally stable, 2nd-order SAV schemes which only require solving decoupled, linear systems with constant coefficients.

Phase-field vesicle membrane model

Bending energy:

$$E_b(\phi) = \frac{\epsilon}{2}\int_\Omega \Big(-\Delta\phi + \frac{1}{\epsilon^2} G(\phi)\Big)^2 dx,$$

where $G(\phi) = F'(\phi)$.
Volume and surface area of the vesicle:

$$A(\phi) = \frac{1}{2}\int_\Omega (\phi+1)dx \quad and \quad B(\phi) = \int_\Omega \Big(\frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{\epsilon}F(\phi)\Big)dx.$$

Total energy:

$$E_{tot}(\phi) = E_b(\phi) + \frac{1}{2\gamma}\Big(A(\phi)-\alpha\Big)^2 + \frac{1}{2\eta}\Big(B(\phi)-\beta\Big)^2,$$

where γ and η are two small parameters, and α, β represent the initial volume and surface area.

To apply the SAV approach, we need to fist split the free energy into two parts: one with (high-order) linear terms and the other with nonlinear terms.
Note that $G(\phi) = F'(\phi) = (\phi^2 - 1)\phi$, we find

$$E_b(\phi) = \frac{\epsilon}{2}\int_\Omega \Big(-\Delta\phi + \frac{1}{\epsilon^2}G(\phi)\Big)^2 dx$$
$$= \frac{\epsilon}{2}\int_\Omega \Big(|\Delta\phi|^2 - \frac{2}{\epsilon^2}|\nabla\phi|^2 + \frac{6}{\epsilon^2}\phi^2|\nabla\phi|^2 + \frac{1}{\epsilon^4}(G(\phi))^2 \Big) dx.$$

So the first two terms should be in the first part, and for the remaining terms, we introduce a SAV:

$$r(t) = \sqrt{\int_\Omega \frac{\epsilon}{2}\Big(\frac{6}{\epsilon^2}\phi^2|\nabla\phi|^2 + \frac{1}{\epsilon^4}(G(\phi))^2\Big) + \frac{1}{2\gamma}(A(\phi)-\alpha)^2 + \frac{1}{2\eta}(B(\phi)-\beta)^2 +}$$

However, the nonlinear terms in E_{tot} behave very differently so a single SAV does not lead to accurate numerical results

.

Therefore, we introduce

$$U = B(\phi) - \beta, \qquad V = \sqrt{\int_\Omega \Big(\frac{6}{\epsilon^2}\phi^2|\nabla\phi|^2 + \frac{1}{\epsilon^4}(G(\phi))^2\Big)dx + C},$$

where C is a positive constant, so the total energy becomes

$$E_{tot} = \frac{\epsilon}{2}\int_\Omega \big(|\Delta\phi|^2 - \frac{2}{\epsilon^2}|\nabla\phi|^2\big)dx + \frac{1}{2\gamma}(A(\phi)-\alpha)^2 + \frac{U^2}{2\eta} + \frac{\epsilon}{2}(V^2 - C).$$

Then, the L^2 gradient flow can be written as:

$$\begin{aligned}
\phi_t &= -M\mu,\\
\mu &= \frac{\delta E_{tot}}{\delta\phi} = \epsilon\Delta^2\phi + \frac{2}{\epsilon}\Delta\phi + \frac{1}{\gamma}(A(\phi)-\alpha) + \frac{1}{\eta}U\frac{\delta U}{\delta\phi} + \epsilon V\frac{\delta V}{\delta\phi},\\
U_t &= \int_\Omega \frac{\delta U}{\delta\phi}\phi_t dx, , \quad V_t = \int_\Omega \frac{\delta V}{\delta\phi}\phi_t dx,
\end{aligned}$$

Second-order MSAV-CN scheme

$$\frac{\phi^{n+1}-\phi^n}{\delta t} = -M\mu^{n+\frac{1}{2}},$$

$$\mu^{n+\frac{1}{2}} = \epsilon\Delta^2\phi^{n+\frac{1}{2}} + \frac{2}{\epsilon}\Delta\phi^{\star,n+\frac{1}{2}}$$

$$+\frac{1}{\gamma}(A(\phi^{n+\frac{1}{2}})-\alpha) + \frac{1}{\eta}U^{n+\frac{1}{2}}\frac{\delta U}{\delta\phi}(\phi^{\star,n+\frac{1}{2}}) + \epsilon V^{n+\frac{1}{2}}\frac{\delta V}{\delta\phi}(\phi^{\star,n+\frac{1}{2}}),$$

$$U^{n+1}-U^n = \int_\Omega \frac{\delta U}{\delta\phi}(\phi^{\star,n+\frac{1}{2}})(\phi^{n+1}-\phi^n)dx,$$

$$V^{n+1}-V^n = \int_\Omega \frac{\delta V}{\delta\phi}(\phi^{\star,n+\frac{1}{2}})(\phi^{n+1}-\phi^n)dx,$$

where $\phi^{\star,n+\frac{1}{2}} = \frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}$ is a second-order extrapolation for $\phi^{n+\frac{1}{2}}$.

- One can first solve U^{n+1} and V^{n+1} by bock Gaussian elimination which leads to a 2×2 linear system.
- Then, one can determine (ϕ^{n+1}, μ^{n+1}) as in previous models.

The above scheme satisfies the following energy law:

$$E_{cn}^{n+1,n} - E_{cn}^{n,n-1} \le -\delta t M \|\mu^{n+\frac{1}{2}}\|^2,$$

where

$$E_{cn}^{n+1,n} = \frac{\epsilon}{2}\|\Delta\phi^{n+1}\|^2 - \frac{1}{\epsilon}\|\nabla\phi^{n+1}\|^2 + \frac{1}{2\epsilon}\|\nabla\phi^{n+1} - \nabla\phi^n\|^2 + \frac{1}{2\eta}(U^{n+1})^2 + \frac{\epsilon}{2}(V^{n+1})^2 + \frac{1}{2\gamma}(A(\phi^{n+1}) - \alpha)^2,$$

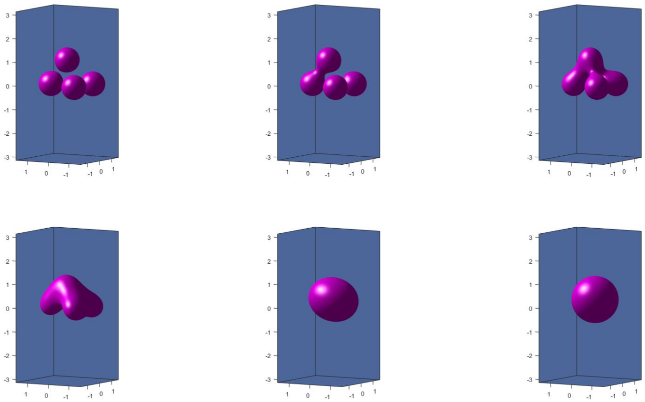


Figure: The dynamical behaviors of four spherical vesicles without the volume and surface area constraints using the **Scheme 2** with the time step size $\delta t = 0.0001$. Snapshots of the numerical approximation of the isosurfaces of $\phi = 0$ are taken at t = 0, 0.005, 0.002, 0.1, 0.5, 2.

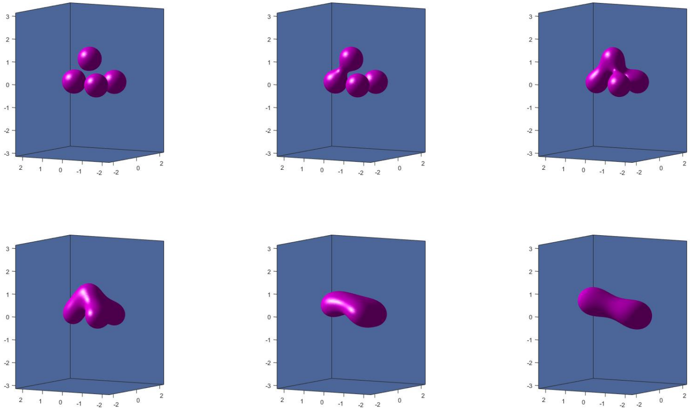


Figure: Collision of four spherical vesicles with the volume and surface area constraints (i.e., $\eta = \gamma = 0.02$). Snapshots of the iso-surfaces of $\phi = 0$ at t = 0, 0.005, 0.002, 0.1, 0.5, 2.

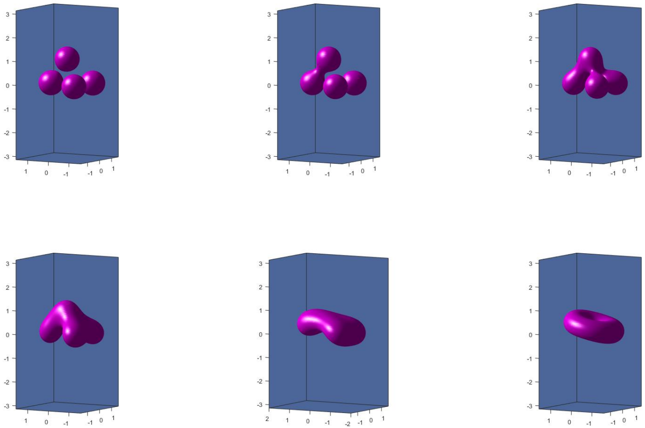


Figure: Collision of four spherical vesicles with the volume and surface area constraints (i.e., $\eta = \gamma = 0.001$). Snapshots of the iso-surfaces of $\phi = 0$ at t = 0, 0.005,0.002, 0.1, 0.5,2

Phase-field model for two-phase incompressible flows

Let $F(\phi) = \frac{1}{4\eta^2}(\phi^2 - 1)^2$. Consider the mixing free energy:

$$E_{mix}(\phi) = \lambda \int_\Omega (\frac{1}{2}|\nabla\phi|^2 + F(\phi))\, dx = \lambda \int_\Omega \frac{1}{2}|\nabla\phi|^2\, dx + E_1(\phi).$$

- Cahn-Hilliard phase-field equation:

$$\phi_t + (u \cdot \nabla)\phi = \nabla \cdot (\gamma \nabla w),$$
$$w = \frac{\delta E_{mix}}{\delta \phi} = -\lambda \Delta\phi + \lambda F'(\phi).$$

- Momentum equation:

$$\rho_0(u_t + (u \cdot \nabla)u) = \nu \Delta u - \nabla p + w \nabla \phi.$$

- Incompressibility:

$$\nabla \cdot u = 0.$$

Energy dissipation law:

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

As before, we introduce $r(t) = \sqrt{E_1(\phi) + \delta}$, and replace

$$w = -\lambda\Delta\phi + \lambda F'(\phi)$$

by

$$w = -\lambda\Delta\phi + \lambda\frac{r(t)}{\sqrt{E_1(\phi)+\delta}}F'(\phi),$$
$$r_t = \frac{1}{2\sqrt{E_1(\phi)+\delta}}\int_\Omega (F'(\phi)\frac{d\phi}{dt})dx.$$

We presented the SAV approach for gradient flows, which is inspired by the Lagrange multiplier/IEQ methods. It preserves all their advantages, plus:

- It leads to linear, decoupled equations with CONSTANT coefficients. So fast direct solvers are often available!
- It only requires the nonlinear energy functional, instead of nonlinear energy density, be bounded from below, so it applies to a larger class of gradient flows.
- For gradient flows with multiple components, the scheme will lead to decoupled equations with constant coefficients to solve at each time step.

- A particular advantage of unconditionally energy stable scheme is that it can be coupled with an adaptive time stepping strategy.
- The proofs are based on variational formulation with simple test functions, so that they can be extended to full discrete discretization with Galerkin approximation in space.
- We have performed rigorous error analysis to show that, under mild conditions, the solution of proposed schemes converge to the solution of the original problem.

Thank you!