The scalar auxiliary variable (SAV) approach for Gradient Flows

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Motivation

- 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, thin film epitaxy, PNP equations, quasi-crystal models, phase-field models, ...

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- Gradient flows are dynamically driven by a free energy $E(\phi)$, and takes the form:

$$\frac{\partial \phi}{\partial t} = -\mathcal{L}\frac{\delta E(\phi)}{\delta \phi},$$

where $\mathcal{L}$ is a positive operator, and satisfy a dissipative energy law:

$$\frac{d}{dt}E(\phi) = -(\mathcal{L}\frac{\delta E(\phi)}{\delta \phi}, \frac{\delta E(\phi)}{\delta \phi}).$$

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Examples:

- heat equation: $E(\phi) = \int_\Omega \frac{1}{2}|\nabla \phi|^2$
- Allen-Cahn and Cahn-Hilliard equation: $E(\phi) = \int_\Omega (\frac{1}{2}|\nabla \phi|^2 + F(\phi))$

Gradient flows

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

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

or the gradient flow in H^{-1} ($\mathcal{L} = -\Delta$):

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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):

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

Time discretizations of gradient flows

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:

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

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

Existing approaches for time discretization

- Full implicit schemes: Du & Nicolaides '91, Feng & Prohl '03-'05, ...
- Linearly implicit and stabilized schemes: Chen & S. '98, Xu & Tang '06, S. & Yang '10, Li, Qiao & Tang '16, ...
- Convex splitting: Elliott and Stewart '93 (see also Eyre '98), ...
- The method with a Lagrange multiplier: Badia et al. '11, Tiera & Guillen-Gonzalez '13

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Desired properties:

- Second-order unconditionally energy stable;
- Only requiring solving decoupled, linear, positive definite system with constant coefficients, even for multi-component systems;
- Applicable to a large class of gradient flows;
- Amenable to error analysis without resorting to a Lipschitz condition.

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:

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

$$w^{n+1} = -\nabla\cdot\nabla\phi^{n+1} + 2v^{n+1}\frac{\delta v}{\delta\phi}|_{\phi=\phi^n},$$

$$\frac{v^{n+1}-v^n}{\Delta t} = \frac{\delta v}{\delta\phi}|_{\phi=\phi^n}\frac{\phi^{n+1}-\phi^n}{\Delta t},$$

$$\frac{\bar{u}^{n+1}-\bar{u}^n}{\Delta t} = \nabla\frac{\phi^{n+1}-\phi^n}{\Delta t}.$$

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

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:

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

Main advantages of the IEQ approach

This approach leads to efficient and flexible numerical schemes:

- It can be efficiently implemented: one can eliminate v^{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;

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- It can be easily extended to higher-order with the BDFk scheme, with BDF2 being unconditionally stable.

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- 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.

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Q. Can we do better?

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Q. Can we do better?

Yes, if the free energy takes the following form:

$$E(\phi) = \int_\Omega \{\frac{1}{2}(\mathcal{L}\phi, \phi) + F(\phi)\} dx,$$

where $\mathcal{L}$ is linear and positive definite, $F(\phi)$ includes only "lower-order" nonlinear terms.

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:

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

Unconditionally stable, linear and decoupled schemes

First-order scheme:

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

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

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:

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

Efficient implementation

We can write the schemes as a matrix system

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

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

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

which, under Neumann conditions for ϕ and w, can be further reduced to a set of decoupled equations:

$$\alpha\psi - \Delta\psi = \bar{f}, \beta\phi - \Delta\phi = -\psi.$$

Second-order BDF scheme:

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

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

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

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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.

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.

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- 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

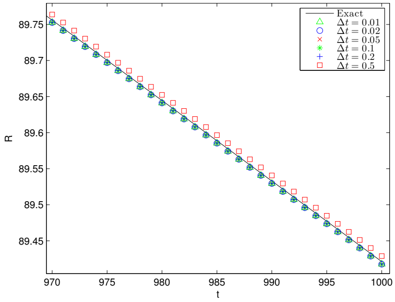

FIG. 3. *(Example 3) The evolution of radius with different time step.*

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.

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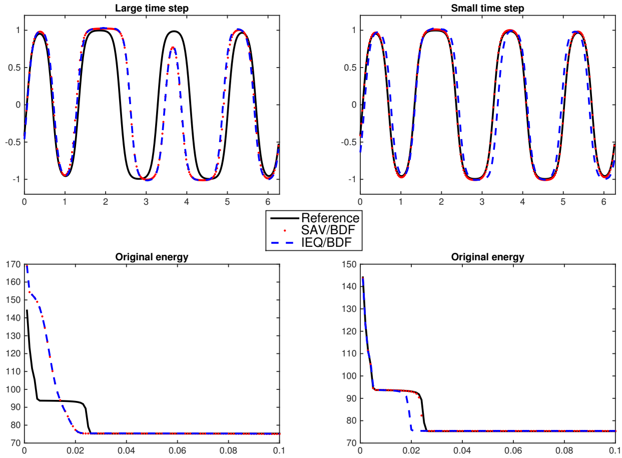


Figure: Solid line: current method; dash line: another method

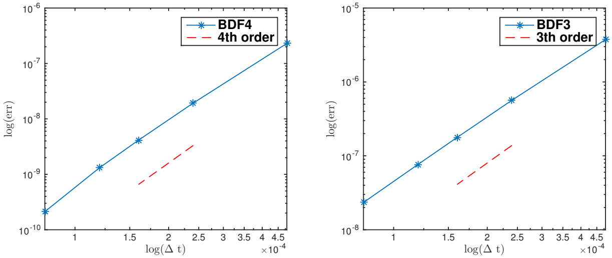


FIG. 8. *(Example 7) Numerical convergences of BDF3 and BDF4.*

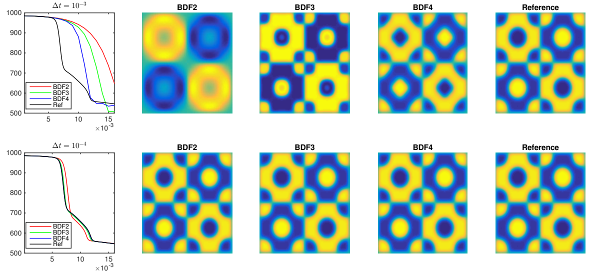


FIG. 9. *(Example 7) Numerical comparison among BDF2, BDF3 and BDF4.*

Adaptive time stepping

Thanks to its unconditionally energy stability, one can (and should) couple the scheme with an adaptive time stepping strategy.

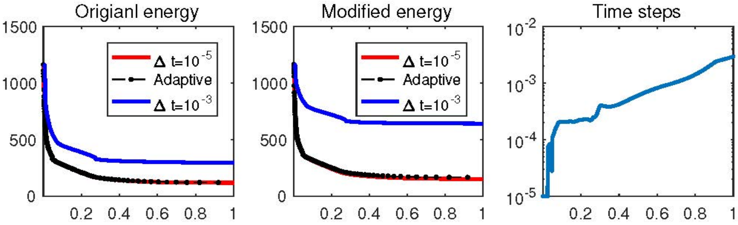
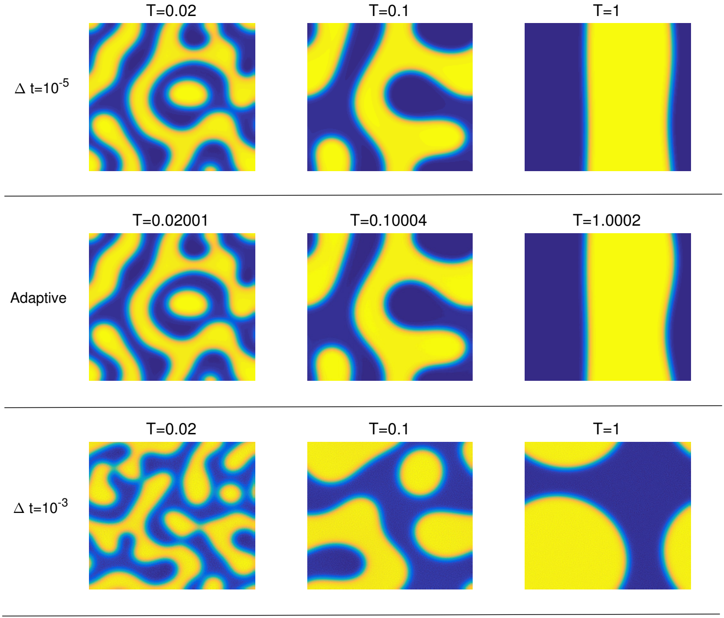


Figure: Numerical comparisons among small time steps, adaptive time steps, and large time steps


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.

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- 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

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

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- 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

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

Convergence results

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. $r_{\Delta t}(\cdot, t^n) = r^n$).

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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 $L^\infty(0, T)$.

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  - $r_{\Delta t} \to r = \sqrt{E_1}$ 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 $0 \leq n \leq T/\Delta t$, we have

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

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

- 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

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

Several applications

Molecular beam epitaxy (MBE)

Consider the energy functional for MBE without slope selection (SAV can be applied directly to the case with slope selection):

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

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:

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

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:

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

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

MBE (continued):

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

- 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.

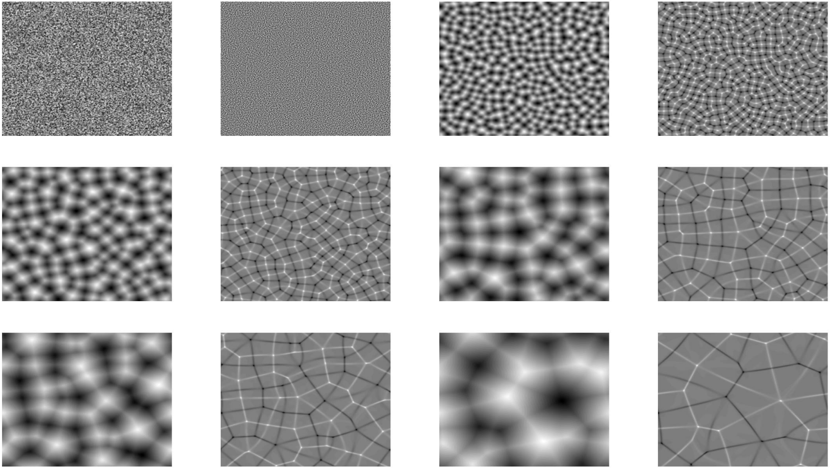

FIGURE 7. The isolines of the numerical solutions of the height function ϕ and its Laplacian $\Delta\phi$ for the slope model with random initial condition (4.6) using Scheme-1 and time step $\delta t = 10^{-4}$. For each subfigure, the left is ϕ and the right is $\Delta\phi$. Snapshots are taken at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

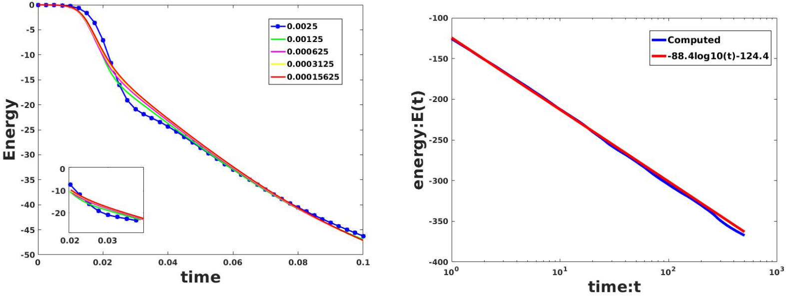

Figure: Simulation of MBE: Left, energy evolution; Right, log-log plot of the energy compared with $o(\log_{10} t)$.

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 $G(\phi) = F'(\phi)$.

Phase-field vesicle membrane model

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Volume and surface area of the vesicle:

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

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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.

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Note that $G(\phi) = F'(\phi) = (\phi^2 - 1)\phi$, we find

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

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

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

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

.

Therefore, we introduce

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

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

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

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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.

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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

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

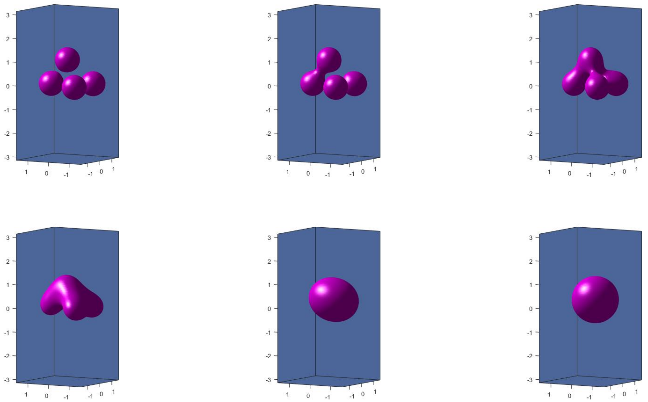


Figure: The dynamical behaviors of four spherical vesicles without the volume and surface area constraints using the **Scheme 2** with the time step size $\delta t = 0.0001$. Snapshots of the numerical approximation of the isosurfaces of $\phi = 0$ are taken at t = 0, 0.005, 0.002, 0.1, 0.5, 2.

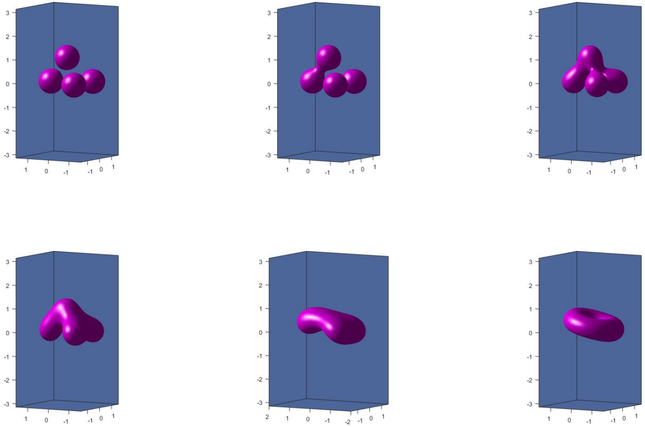


Figure: Collision of four spherical vesicles with the volume and surface area constraints (i.e., $\eta = \gamma = 0.001$). Snapshots of the iso-surfaces of $\phi = 0$ at t $=$ 0, 0.005,0.002, 0.1, 0.5,2

Multi-component gradient flows

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.
- As before, we can determine r^{n+1} by solving k decoupled equations with constant coefficients of the form:

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

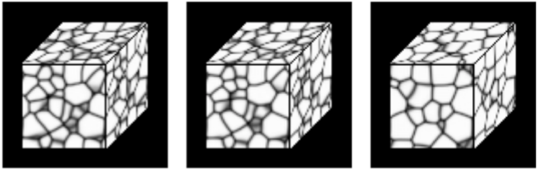
then obtain $\{\phi_j\}$ by solving another k decoupled equations in the above form.

Preliminary results on grain growth (with Longqing Chen)

- Allen-Cahn 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.



Phase separation of diblock co-polymers (with Y. Nishiura)

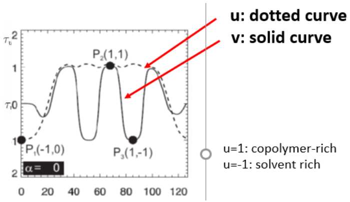
Consider the free energy of Ohta-Kawasaki type (Nishiura et al. '16):

$$E(u,v) = \int_\Omega \{\frac{\epsilon_u}{2}|\nabla u|^2 + \frac{\epsilon_v}{2}|\nabla v|^2 + W(u,v) + \frac{\sigma}{2}|(-\Delta)^{-1/2}(v-\bar{v})|^2\},$$

where $\bar{v} = \frac{1}{|\Omega|}\int_\Omega v$ and

$$W(u,v) = \frac{1}{4}(u^2-1)^2 + \frac{1}{4}(v^2-1)^2 + b_1 uv + b_2\frac{uv^2}{2}.$$

- u: volume fraction of constrained co-polymers, $u = \pm 1$: co-polymers or solvant.
- v: micro-phase separation variable: $v = \pm 1$ A-polymer rich or B-polymer rich.
- b_1: incompatibility; b_2 bounds of co-polymer rich domain.



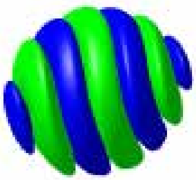


Figure: (a) sketch of typical profile for u, v; (b) a case with $b_1 = 0$: morphology does not change; (b) a case with $b_1 \neq 0$: different morphology appears.

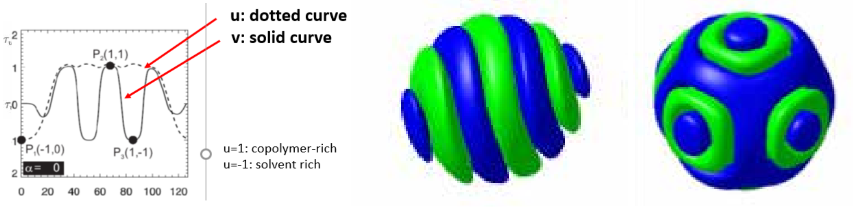


Figure: (a) sketch of typical profile for u, v; (b) a case with $b_1 = 0$: morphology does not change; (b) a case with $b_1 \neq 0$: different morphology appears.

- The non-local term can be treated implicitly along with the linear term.
- By using the Young's inequality, it can be easily shown that $W(u, v) > C_0$.

Hence, one can introduce $r(t) = \sqrt{\int_\Omega W(u, v) + \frac{C_0}{|\Omega|}}$ and apply the standard SAV approach.

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:

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

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- Cahn-Hilliard phase-field equation:

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

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- 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:

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

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Energy dissipation law:

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

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

by

$$w=-\lambda\Delta\phi+\lambda\frac{r(t)}{\sqrt{E_1(\phi)+\delta}}F'(\phi),$$

$$r_t=\frac{1}{2\sqrt{E_1(\phi)+\delta}}\int_\Omega(F'(\phi)\frac{d\phi}{dt})dx.$$

Second-order SAV scheme

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 $\tilde{u}^{n+1}$.

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

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

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

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

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

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

$$\rho_0 \{ \frac{3\tilde{u}^{n+1} - 4u^n + u^{n-1}}{2\delta t} + \bar{u}^{n+1} \cdot \nabla \tilde{u}^{n+1} \} - \nu \Delta \tilde{u}^{n+1} + \nabla p^n - w^{n+1} \nabla \bar{\phi}^{n+1} = 0;$$

Second-order SAV scheme

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 $\tilde{u}^{n+1}$.

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

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

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

$$\rho_0 \{ \frac{3\tilde{u}^{n+1} - 4u^n + u^{n-1}}{2\delta t} + \bar{u}^{n+1} \cdot \nabla \tilde{u}^{n+1} \} - \nu \Delta \tilde{u}^{n+1} + \nabla p^n - w^{n+1} \nabla \bar{\phi}^{n+1} = 0;$$

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

$$u^{n+1} = \tilde{u}^{n+1} - \frac{2\delta t}{3\rho_0} \nabla (p^{n+1} - p^n).$$

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- 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.

Concluding remarks

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

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- 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.

References:

- "The scalar auxiliary variable (SAV) approach for gradient flows", by J. S., Jie Xu and Jiang Yang, *J. Comput. Phys.*, 2018.
- "A new class of efficient and robust energy stable schemes for gradient flows", by J. S., Jie Xu and Jiang Yang, Submitted to *SIAM Reviews*.
- "Convergence and error analysis for the scalar auxiliary variable (SAV) schemes to gradient flows", by Jie Shen and Jie Xu, in revision, *SIAM J. Numer. Anal.*

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Thank you!