



The Scalar Auxiliary Variable Approach for gradient flows

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Phase Field Recap

SAV Approach

Main Idea

Numerical Schemes

Numerical Experiments

Finite Difference Schemes for Cahn-Hilliard Equation

SAV with Fourier Transform for Allen-Cahn Equation

Code



Given a free energy functional $\mathcal{E}(\phi(x))$

$$\begin{cases} \phi_t = \mathcal{G}\mu \\ \mu = \frac{\delta \mathcal{E}}{\delta \phi} \end{cases}$$

In the above, operator \mathcal{G} gives the dissipation mechanism:

- L^2 gradient flows when $\mathcal{G} = -I$ (Allen-Cahn)
- H^{-1} gradient flow when $\mathcal{G} = \Delta$ (Cahn-Hilliard)
- $H^{-\alpha}$ gradient flow when $\mathcal{G} = -(-\Delta)^\alpha$ with $0 < \alpha < 1$

In this talk, we choose periodic boundary conditions or homogeneous Neumann boundary conditions.



As long as \mathcal{G} is non-positive, the free energy is non-increasing:

$$\frac{d\mathcal{E}(\phi)}{dt} = \frac{\delta\mathcal{E}}{\delta\phi} \cdot \frac{\partial\phi}{\partial t} = (\mu, \mathcal{G}\mu) \leq 0$$

In this talk, we consider \mathcal{G} is non-positive, linear and independent of ϕ .



Usually, the free energy functional contains a quadratic term, which we write explicitly as

$$\mathcal{E}(\phi) = \frac{1}{2}(\phi, \mathcal{L}\phi) + \mathcal{E}_1(\phi)$$

where \mathcal{L} is a symmetric non-negative linear operator (independent of ϕ), and $\mathcal{E}_1(\phi)$ are nonlinear but with only lower-order derivatives than \mathcal{L} . We take $\mathcal{E}_1(\phi) = \int_{\Omega} F(\phi) dx$



- Convex Splitting Approach

Assume $F(\phi) = F_c(\phi) - F_e(\phi)$ with $F_c''(\phi), F_e''(\phi) \geq 0$.

$$\begin{cases} \frac{\phi^{n+1} - \phi^n}{\delta t} = \mathcal{G}\mu^{n+1} \\ \mu^{n+1} = \mathcal{L}\phi^{n+1} + (F_c'(\phi^{n+1}) - F_e'(\phi^n)) \end{cases}$$

- Stabilized Approach

Introduce stabilization term S to balance nonlinear term.

$$\begin{cases} \frac{1}{\delta t} (\phi^{n+1} - \phi^n) = \mathcal{G}\mu^{n+1} \\ \mu^{n+1} = \mathcal{L}\phi^{n+1} + S(\phi^{n+1} - \phi^n) + F'(\phi^n) \end{cases}$$

- Invariant energy quadratization(IEQ)

Introduce a Lagrange multiplier $q(t, x; \phi) = \sqrt{F(\phi) + C_0}$.

$$\begin{cases} \phi_t = \mathcal{G}\mu \\ \mu = \mathcal{L}\phi + \frac{q}{\sqrt{F(\phi) + C_0}} F'(\phi) \\ q_t = \frac{F'(\phi)}{2\sqrt{F(\phi) + C_0}} \phi_t \end{cases}$$



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Assume $\mathcal{E}_1(\phi) = \int_{\Omega} F(\phi) dx$ is bounded from below, i.e., $\mathcal{E}_1(\phi) \geq -C_0$, introduce a scalar auxiliary variable $r(t) = \sqrt{\mathcal{E}_1(\phi) + C_0}$.

$$\begin{cases} \phi_t = \mathcal{G}\mu \\ \mu = \mathcal{L}\phi + \frac{r(t)}{\sqrt{\mathcal{E}_1[\phi] + C_0}} F'(\phi) \\ r_t = \frac{1}{2\sqrt{\mathcal{E}_1[\phi] + C_0}} \int_{\Omega} F'(\phi) \phi_t dx \end{cases}$$

Taking the inner products of the above with μ , ϕ_t and $2r$ respectively, one can obtain the modified energy dissipation law:

$$\frac{d}{dt} [(\phi, \mathcal{L}\phi) + r^2] = (\mu, \mathcal{G}\mu)$$



First-Order Scheme(1)

$$\left\{ \begin{array}{l} \frac{\phi^{n+1} - \phi^n}{\Delta t} = \mathcal{G}\mu^{n+1} \\ \mu^{n+1} = \mathcal{L}\phi^{n+1} + \frac{r^{n+1}}{\sqrt{\mathcal{E}_1(\phi^n) + C_0}} F'(\phi) \\ \frac{r^{n+1} - r^n}{\Delta t} = \frac{1}{2\sqrt{\mathcal{E}_1(\phi^n) + C_0}} \int_{\Omega} F'(\phi) \frac{\phi^{n+1} - \phi^n}{\Delta t} dx \end{array} \right.$$

From the above we have

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \mathcal{G} \left[\mathcal{L}\phi^{n+1} + \frac{F'(\phi)}{\sqrt{\mathcal{E}_1(\phi^n) + C_0}} \left(r^n + \int_{\Omega} \frac{F'(\phi)}{2\sqrt{\mathcal{E}_1(\phi^n) + C_0}} (\phi^{n+1} - \phi^n) dx \right) \right]$$



First-Order Scheme(2)

$$\text{denote } b^n = \frac{F'(\phi^n)}{\sqrt{\mathcal{E}_1(\phi^n) + C_0}},$$

$$\Rightarrow (I - \Delta t \mathcal{G}\mathcal{L})\phi^{n+1} - \frac{\Delta t}{2} \mathcal{G}b^n (b^n, \phi^{n+1}) = \phi^n + r^n \mathcal{G}b^n - \frac{\Delta t}{2} (b^n, \phi^n) \mathcal{G}b^n \triangleq c^n$$

Multiply it with $(I - \Delta t \mathcal{G}\mathcal{L})^{-1}$ and then take inner product with b^n

$$\Rightarrow (b^n, \phi^{n+1}) + \frac{\Delta t}{2} \gamma^n (b^n, \phi^{n+1}) = (b^n, (I - \Delta t \mathcal{G}\mathcal{L})^{-1} c^n)$$

$$\text{where } \gamma^n = - (b^n, (I - \Delta t \mathcal{G}\mathcal{L})^{-1} \mathcal{G}b^n) = (b^n, (-\mathcal{G}^{-1} + \Delta t \mathcal{L})^{-1} b^n) > 0$$

$$\text{hence } (b^n, \phi^{n+1}) = \frac{(b^n, (I - \Delta t \mathcal{G}\mathcal{L})^{-1} c^n)}{1 + \Delta t \gamma^n / 2}$$



To summarize, one can implement the first order SAV with following steps:

1. compute b^n and c^n
2. compute (b^n, ϕ^{n+1})
3. compute ϕ^{n+1}

Note that in 2 and 3 of the above procedure, one only need to solve, twice, a linear equation with constant coefficients of the form

$$(I - \Delta t \mathcal{GL})x = b$$



$$\left\{ \begin{array}{l} \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\Delta t} = \mathcal{G}\mu^{n+1}, \\ \mu^{n+1} = \mathcal{L}\phi^{n+1} + \frac{r^{n+1}}{\sqrt{\mathcal{E}_1(\bar{\phi}^{n+1}) + C_0}} F'(\phi) \\ 3r^{n+1} - 4r^n + r^{n-1} = \int_{\Omega} \frac{F'(\phi)}{2\sqrt{\mathcal{E}_1(\bar{\phi}^{n+1}) + C_0}} (3\phi^{n+1} - 4\phi^n + \phi^{n-1}) dx \end{array} \right.$$

Here $\bar{\phi}^{n+1}$ can be any explicit approximation of ϕ^{n+1} with an error of $\mathcal{O}(\Delta t^2)$.

With similar procedure as first order scheme, one can obtain the iteration format. Each iteration requires solving two linear equations with constant coefficients of the form of

$$(I - \Delta t \mathcal{G}\mathcal{L})x = b$$



The semi-implicit BDF2 can be replaced by semi-implicit Crank–Nicolson scheme.



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Consider free energy functional $\mathcal{E}(\phi) = \int_{\Omega} \left[\frac{\varepsilon^2}{2} |\nabla \phi|^2 + \frac{\phi^2(1-\phi^2)}{4} \right] dx$

One can obtain Cahn-Hilliard Equation from it

$$\begin{cases} \phi_t = \Delta \mu \\ \mu = -\varepsilon^2 \nabla^2 \phi + \phi^3 - \phi \end{cases}$$

I chose Neumann boundary conditions $\frac{\partial c}{\partial n} = 0 = \frac{\partial \omega}{\partial n}$.



For the first equation I used implicit Euler scheme

$$\phi^n - \frac{\Delta t}{h^2} D \mu^n - \phi^{n-1} = 0$$

where the matrix D is the central-difference Laplacian with Neumann boundary conditions.

For the second equation, I considered five different schemes of the form:

$$\mu^n + \frac{\epsilon^2}{h^2} D \phi^n - \Phi^n = 0$$

where Φ^n is a discretization of the free energy term $F'(\phi)$.



Depend sensitively on the discretization of the nonlinear term Φ^n , and so I considered the following possibilities:

$$\Phi^n = (\phi^{n-1})^2 \phi^n - \phi^{n-1}$$

$$\Phi^n = (\phi^{n-1})^3 - 3\phi^{n-1} + 2\phi^n$$

$$\Phi^n = 3(\phi^{n-1})^2 \phi^n - 2(\phi^{n-1})^2 \phi^{n-1} - \phi^n,$$

$$\Phi^n = (\phi^n)^3 - \phi^{n-1}$$

$$\Phi^n = (\phi^n)^3 - \phi^n$$



The first three schemes result in linear system of the form:

$$\begin{bmatrix} I & -\mu D \\ R_n & I \end{bmatrix} \begin{bmatrix} \phi^n \\ \mu^n \end{bmatrix} = \begin{bmatrix} \phi^{n-1} \\ b_n \end{bmatrix}$$

where

$$R_n = \begin{cases} \epsilon^2/h^2 D - \phi_{n-1}^2, \\ \epsilon^2/h^2 D - 2I, \\ \epsilon^2/h^2 D - 3\phi_{n-1}^2 + I \end{cases}$$
$$b_n = \begin{cases} -\phi^{n-1} \\ -3\phi^{n-1} + (\phi^{n-1})^3 \\ -2(\phi^{n-1})^3 \end{cases}$$



The last two schemes take the form of vector systems:

$$g_n = \begin{bmatrix} \phi^n - \frac{\Delta t}{h^2} D \mu^n - \phi^{n-1} \\ f(\phi^n, \phi^{n-1}) + \mu^n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

g_n has Jacobian J_n :

$$J_n = \begin{bmatrix} I & -\frac{\Delta t}{h^2} D \\ \partial f / \partial \phi^n & I \end{bmatrix}$$

where the partial derivative term for the two schemes is:

$$\frac{\partial f}{\partial c^n} = \begin{cases} \epsilon^2 / h^2 D - 3\phi_n^2 \\ \epsilon^2 / h^2 D - 3\phi_n^2 + I \end{cases}$$

When implementing Newton's method, at each time-step n I used the previous iterates ϕ^{n-1} and μ^{n-1} as starting guesses for the roots, and computed the Newton step s by solving the linear system

$$J_n s = -g_n$$



I ran the above five schemes on $[0, 1]^2 \times 200\Delta t$, with smooth initial conditions $\phi_0(x, y) = \cos(2\pi x)\cos(\pi y)$, and the mesh resolution was set 64×64 .

The animation gif files are in attachment.



- Let $\mathcal{G} = -1, \mathcal{L} = -\Delta$, one gets the Allen-Cahn Equation from previous discussion
- The complexity of SAV mainly locates in solving equation of the form

$$(I - \Delta t \mathcal{G} \mathcal{L})x = b$$

- I used Fourier Transform to solve the above equation in the frequency domain and then inverse transform the result back to the phase field



Numerical Results

- I ran the above five schemes on $[0, 1]^2 \times 20000\Delta t$, with smooth initial conditions $\phi_0(x, y) = 0.05\sin(2\pi x)\sin(2\pi y)$, and the mesh resolution was set 128×128 . The difference scheme was first order.
- The animation gif files are in attachment.
- The modified and raw free energy changes as follow

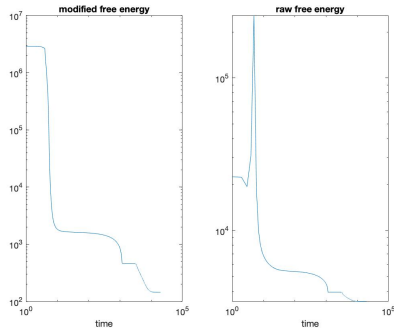


Figure 1: Modified and Raw Free Energy



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Code



Related code is uploaded to

<https://github.com/burning489/cahn-hiliard>

<https://github.com/burning489/sav>

Welcome further discussion :)



Thank you!



- [SXY17] Jie Shen, Jie Xu, and Jiang Yang, *A new class of efficient and robust energy stable schemes for gradient flows*, SIAM Review **61** (2017).
- [SXY18] Jie Shen, Jie Xu, and Jiang Yang, *The scalar auxiliary variable (sav) approach for gradient flows*, Journal of Computational Physics **353** (2018), 407–416.

