The Scalar Auxiliary Variable Approach for gradient flows

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Definition

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

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

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-Hiliard)
- $H^{-\alpha}$ gradient flow when $\mathcal{G} = -(-\Delta)^{\alpha}$ with $0 < \alpha < 1$

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

Dissipation

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

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

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

Free Energy Functional

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 $\mathcal{E}_1(\phi) = \int_\Omega F(\phi) dx$

Existing Approaches

- Convex Splitting Approach

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

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

- Stablized Approach

  Introduce stabilization term S to balance nonlinear term.

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

- Invariant energy quadratization(IEQ)

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

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

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SAV

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 $r(t) = \sqrt{\mathcal{E}_1(\phi) + C_0}$.

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

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

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

First-Order Scheme(1)

$$
\begin{cases}
\dfrac{\phi^{n+1}-\phi^n}{\Delta t} = \mathcal{G}\mu^{n+1} \\
\mu^{n+1} = \mathcal{L}\phi^{n+1} + \dfrac{r^{n+1}}{\sqrt{\mathcal{E}_1(\phi^n)+C_0}} F'(\phi) \\
\dfrac{r^{n+1}-r^n}{\Delta t} = \dfrac{1}{2\sqrt{\mathcal{E}_1(\phi^n)+C_0}} \displaystyle\int_\Omega F'(\phi) \dfrac{\phi^{n+1}-\phi^n}{\Delta t} dx
\end{cases}
$$

From the above we have

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

First-Order Scheme(2)

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

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

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

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

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

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

First-Order Scheme(3)

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

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

BDF2

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

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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Problem

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-Hiliard 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 $\frac{\partial c}{\partial n} = 0 = \frac{\partial \omega}{\partial n}$.

Finite Difference Scheme

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 $F'(\phi)$.

Five Finite Difference Schemes

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

$$
\begin{aligned}
&\Phi^n = \left(\phi^{n-1}\right)^2 \phi^n - \phi^{n-1} \\
&\Phi^n = \left(\phi^{n-1}\right)^3 - 3\phi^{n-1} + 2\phi^n \\
&\Phi^n = 3\left(\phi^{n-1}\right)^2 \phi^n - 2\left(\phi^{n-1}\right)^2 \phi^{n-1} - \phi^n, \\
&\Phi^n = \left(\phi^n\right)^3 - \phi^{n-1} \\
&\Phi^n = \left(\phi^n\right)^3 - \phi^n
\end{aligned}
$$

Linear Schemes

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

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

$$b_n = \begin{cases} -c^{n-1} \\ -3c^{n-1} + \left(c^{n-1}\right)^3 \\ -2\left(c^{n-1}\right)^3 \end{cases}$$

The last two schemes take the form of vector systems:

$$g_n = \left[\begin{array}{c} \phi^n - \frac{\Delta t}{h^2} D\mu^n - \phi^{n-1} \\ f\left(\phi^n, \phi^{n-1}\right) + \mu^n \end{array} \right] = \left[\begin{array}{c} 0 \\ 0 \end{array} \right]$$

g_n has Jacobian J_n:

$$J_n = \left[\begin{array}{cc} I & -\frac{\Delta t}{h^2} D \\ \partial f / \partial \phi^n & I \end{array} \right]$$

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

$$J_n s = -g_n$$

Numerical Results

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.

Configuration and Main Idea

- 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 Transfom to solve the above equation in the frequency domain and then inverse transform the result back to the phase field

- 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

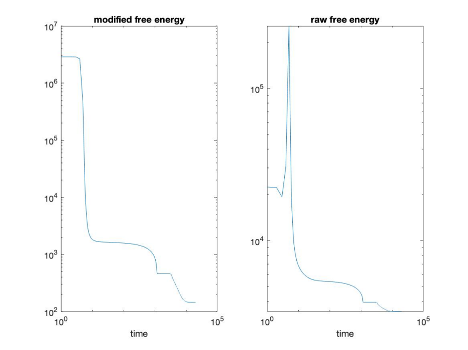

Figure 1: Modified and Raw Free Energy

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.