

Introduction of the scalar auxiliary variable (SAV) approach method

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Existence, Uniqueness, Convergence and Error of solution

- ▶ Linear equation:
Lax Theorem: Stability = Convergence
when Compatibility;
- ▶ Nonlinear equation: Gradient Flow[1];

Other necessary property

- ▶ Dissipation: Energy analysis method;
- ▶ Boundary limitation: Dangerous Extrapolation Method;
- ▶ Direction of propagation: Characteristic line/Upwind scheme

Computational overhead

- ▶ linear?
- ▶ Constant/variable coefficients?
Constant preconditioner;
- ▶ Parallelism?
Local/Global computation: Inner product/convolution;

Introduction of Gradient flows

A gradient flow is determined not only by the driving free energy, but also the dissipation mechanism. Given a free energy functional $E[\phi(x)]$ bounded from below. Denote its variational derivative as $\mu = \delta E / \delta \phi$. The general form of the gradient flow can be written as

$$\frac{\partial \phi}{\partial t} = G\mu, \quad (1)$$

supplemented with suitable boundary conditions. To simplify the presentation, we assume throughout the paper that the boundary conditions are chosen such that all boundary terms will vanish when integrating by parts are performed. This is true with periodic boundary conditions or homogeneous Neumann boundary conditions.

Example of Gradient Flow

- ▶ Allen–Cahn Equation
- ▶ Cahn–Hilliard Equation
- ▶ Phase Field Crystal Equation

Convex splitting approach

A very popular approach for gradient flow is the so called convex splitting method which appears to be introduced by [2] and popularized by [3]. Assuming the free energy density $F(\phi)$ can be split as the difference of two convex functions, namely, $F(\phi) = F_c(\phi) - F_e(\phi)$ with $F_c''(\phi), F_e''(\phi) \geq 0$.

Then, the first-order convex splitting scheme reads:

$$\begin{aligned} \frac{\phi^{n+1} - \phi^n}{\delta t} &= \Delta \mu^{n+1}, \\ \mu^{n+1} &= -\Delta \phi^{n+1} + (F'_c(\phi^{n+1}) - F'_e(\phi^n)). \end{aligned} \tag{2}$$

Convex splitting approach

$$F_c(\phi^{n+1}) - F_c(\phi^n) \leq (\phi^{n+1} - \phi^n)F'_c(\phi^{n+1}),$$

$$F_e(\phi^{n+1}) - F_e(\phi^n) \geq (\phi^{n+1} - \phi^n)F'_e(\phi^n),$$

One can easily show that the above scheme is unconditionally energy stable in the sense that

$$E(\phi^{n+1}) - E(\phi^n) \leq -\delta t \|\nabla \mu^{n+1}\|^2.$$

Stabilized approach

Another widely used approach is the stabilized scheme, introduced in [4] (see also [5]). The main idea is to introduce an artificial stabilization term to balance the explicit treatment of the nonlinear term. A first-order stabilized scheme for 1 reads:

$$\begin{aligned}\frac{1}{\delta t}(\phi^{n+1} - \phi^n) &= \Delta \mu^{n+1}, \\ \mu^{n+1} &= -\Delta \phi^{n+1} + S(\phi^{n+1} - \phi^n) + F\end{aligned}\tag{3}$$

where S is a suitable stabilization parameter. It is shown in [18] that, under the assumption $\|F''(\phi)\|_\infty \leq L$, the above scheme is unconditionally stable for all $S \geq \frac{L}{2}$.

Invariant energy quadratization (IEQ) approaches

The approach is proposed in [6] for dealing with Allen-Cahn and Cahn-Hilliard equations with double well free energy. It is based on a Lagrange multiplier approach introduced in [7].

Very recently, X. Yang and his collaborators [8], [9], [10], [11], [12], [13], [14] made a big leap in generalizing the Lagrange multiplier approach to the so called invariant energy quadratization (IEQ) approach which is applicable to a large class of free energies.

Assuming that there exists $C_0 \geq 0$ such that $F(\phi) \geq -C_0$, one then introduces a Lagrange multiplier (auxiliary variable) $q(t, x; \phi) = \sqrt{F(\phi) + C_0}$, and rewrite the equation as

Invariant energy quadratization (IEQ) approaches

$$\begin{aligned}\phi_t &= \Delta\mu, \\ \mu &= -\Delta\phi + \frac{q}{\sqrt{F(\phi) + C_0}} F'(\phi), \\ q_t &= \frac{F'(\phi)}{2\sqrt{F(\phi) + C_0}} \phi_t.\end{aligned}\tag{4}$$

Taking the inner products of the above with μ , ϕ_t and $2q$, respectively, we see that the above system satisfies a modified energy dissipation law:

$$\frac{d}{dt} \left(\frac{1}{2} \|\nabla\phi\|^2 + \int_{\Omega} q^2 dx \right) = -\|\nabla\mu\|^2.$$

Invariant energy quadratization (IEQ) approaches

The above formulation is amenable to simple and efficient numerical schemes. Consider for instance,

$$\begin{aligned}\frac{\phi^{n+1} - \phi^n}{\delta t} &= \Delta \mu^{n+1}, \\ \mu^{n+1} &= -\Delta \phi^{n+1} + \frac{q^{n+1}}{\sqrt{F(\phi^n) + C_0}} F'(\phi^n), \\ \frac{q^{n+1} - q^n}{\delta t} &= \frac{F'(\phi^n)}{2\sqrt{F(\phi^n) + C_0}} \frac{\phi^{n+1} - \phi^n}{\delta t}.\end{aligned}\tag{5}$$

Invariant energy quadratization (IEQ) approaches

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

$$\begin{aligned} \frac{1}{\delta t} \left[\frac{1}{2} \|\nabla \phi^{n+1}\|^2 + \int_{\Omega} (q^{n+1})^2 dx - \frac{1}{2} \|\nabla \phi^n\|^2 - \int_{\Omega} (q^n)^2 dx \right. \\ \left. + \frac{1}{2} \|\nabla(\phi^{n+1} - \phi^n)\|^2 + \int_{\Omega} (q^{n+1} - q^n)^2 dx \right] = -\|\nabla \mu^{n+1}\|^2, \end{aligned} \quad (6)$$

which indicates that the above scheme is unconditionally stable with respect to the modified energy.

The scalar auxiliary variable (SAV) approach

we now only assume $E_1(\phi) := \int_{\Omega} F(\phi) dx$ is bounded from below, i.e., $E_1(\phi) \geq C_0$, which is necessary for the free energy to be physically sound, and introduce a scalar auxiliary variable (SAV):

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

Then, (1) can be rewritten as:

$$\begin{aligned}\phi_t &= \Delta \mu, \\ \mu &= -\Delta \phi + \frac{r}{\sqrt{E_1[\phi] + C_0}} F'(\phi), \\ r_t &= \frac{1}{2\sqrt{E_1[\phi] + C_0}} \int_{\Omega} F'(\phi) \phi_t dx.\end{aligned}\tag{7}$$

The scalar auxiliary variable (SAV) approach

Taking the inner products of the above with μ , $\frac{\partial \phi}{\partial t}$ and $2r$, respectively, we obtain the modified energy dissipation law:

$$\frac{d}{dt} \left(\frac{1}{2} \|\nabla \phi\|^2 + r^2(t) \right) = -\|\nabla \mu\|^2.$$

We now construct a semi-implicit second-order BDF scheme for the above system.

The scalar auxiliary variable (SAV) approach

$$\begin{aligned}\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\delta t} &= \Delta\mu^{n+1}, \\ \mu^{n+1} &= -\Delta\phi^{n+1} + \frac{r^{n+1}}{\sqrt{E_1[\bar{\phi}^{n+1}] + C_0}} F'(\bar{\phi}^{n+1}), \\ \frac{3r^{n+1} - 4r^n + r^{n-1}}{2\delta t} &= \int_{\Omega} \frac{F'(\bar{\phi}^{n+1})}{2\sqrt{E_1[\bar{\phi}^{n+1}] + C_0}} \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\delta t} dx.\end{aligned}\tag{8}$$

where $\bar{\phi}^{n+1}$ is any explicit $O(\delta t^2)$ approximation for $\phi(t^{n+1})$, which can be flexible according to the problem, and which we will specify in our numerical results.

The scalar auxiliary variable (SAV) approach

We can eliminate μ^{n+1} and r^{n+1} from (8) to obtain

$$\begin{aligned} \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\delta t} = & -\Delta^2 \phi^{n+1} + \frac{\Delta F'(\bar{\phi}^{n+1})}{3\sqrt{E_1[\bar{\phi}^{n+1}] + C_0}}(4r^n \\ & - r^{n-1} + \int_{\Omega} \frac{F'(\bar{\phi}^{n+1})}{2\sqrt{E_1[\bar{\phi}^{n+1}] + C_0}}(3\phi^{n+1} - 4\phi^n + \phi^{n-1})dx). \end{aligned} \quad (9)$$

The scalar auxiliary variable (SAV) approach

Denote

$$\begin{aligned} b^n &= \frac{F'(\bar{\phi}^{n+1})}{\sqrt{E_1[\bar{\phi}^{n+1}] + C_0}}, \\ A &= I + (2\delta t/3)\Delta^2 \\ g^n &= \frac{1}{3}(4\phi^n - 3\phi^{n-1}) \\ &\quad + \frac{2\delta t}{9}[4r^n - r^{n-1} - \frac{1}{2}(b^n, 4\phi^n - \phi^{n-1})]\Delta b^n \end{aligned} \tag{10}$$

The scalar auxiliary variable (SAV) approach

We can get

$$A\phi^{n+1} - \frac{\delta t}{3}(b^n, \phi^{n+1})\Delta b^n = g^n, \quad (11)$$

Then

$$(b^n, \phi^{n+1}) + \frac{\delta t}{3}\gamma^n(b^n, \phi^{n+1}) = (b^n, A^{-1}g^n), \quad (12)$$

where $\gamma = -(b^n, A^{-1}\Delta b^n) \geq 0$, so

$$(b^n, \phi^{n+1}) = \frac{(b^n, A^{-1}g^n)}{1 + \delta t\gamma^n/3}. \quad (13)$$

Finally, we can solve ϕ^{n+1} from (11).

Unconditional energy stability of SAV/BDF2

The scheme (8) is second-order accurate, unconditionally energy stable in the sense that

$$\begin{aligned} & \frac{1}{\Delta t} \{ \tilde{E}[(\phi^{n+1}, r^{n+1}), (\phi^n, r^n)] - \tilde{E}[(\phi^n, r^n), (\phi^{n-1}, r^{n-1})] \} \\ & + \frac{1}{\Delta t} \left\{ \frac{1}{4} (\phi^{n+1} - 2\phi^n + \phi^{n-1}, -\Delta(\phi^{n+1} - 2\phi^n + \phi^{n-1})) \right. \\ & \left. + \frac{1}{2} (r^{n+1} - 2r^n + r^{n-1})^2 \right\} = (\mu, \Delta\mu), \end{aligned} \quad (14)$$

where the modified discrete energy is defined as

$$\begin{aligned} \tilde{E}[(\phi^{n+1}, r^{n+1}), (\phi^n, r^n)] &= \frac{1}{4} ((\phi^{n+1}, -\Delta\phi^{n+1}) \\ &+ (2\phi^{n+1} - \phi^n, -\Delta(2\phi^{n+1} - \phi^n))) + \frac{1}{2} ((r^{n+1})^2 + (2r^{n+1} - r^n)^2), \end{aligned} \quad (15)$$

SAV/Crank-Nicolson

A semi-implicit second-order SAV scheme based on CrankNicolson is as follows:

$$\begin{aligned}\frac{\phi^{n+1} - \phi^n}{\delta t} &= \Delta \mu^{n+1/2}, \\ \mu^{n+1/2} &= -\Delta \frac{1}{2}(\phi^{n+1} + \phi^n) + \frac{r^{n+1} + r^n}{2\sqrt{E_1[\bar{\phi}^{n+1/2}] + C_0}} F'(\bar{\phi}^{n+1/2}), \\ \frac{r^{n+1} - r^n}{\delta t} &= \int_{\Omega} \frac{F'(\bar{\phi}^{n+1/2})}{2\sqrt{E_1[\bar{\phi}^{n+1/2}] + C_0}} \frac{\phi^{n+1} - \phi^n}{\delta t} dx.\end{aligned}\tag{16}$$

where $\bar{\phi}^{n+1/2}$ is any explicit $O(\delta t^2)$ approximation for $\Phi^{n+1/2}$.

SAV/BDF3

$$\begin{aligned}
 11\phi^{n+1} - 18\phi^n + 9\phi^{n-1} - 2\phi^{n-2} &= 6\delta t \Delta \mu^{n+1}, \\
 \mu^{n+1} &= -\Delta \phi^{n+1} + \frac{r^{n+1}}{\sqrt{E_1[\bar{\phi}^{n+1}] + C_0}} F'(\bar{\phi}^{n+1}), \\
 11r^{n+1} - 18r^n + 9r^{n-1} - 2r^{n-2} &= \\
 \int_{\Omega} \frac{F'(\bar{\phi}^{n+1})}{2\sqrt{E_1[\bar{\phi}^{n+1}] + C_0}} (11\phi^{n+1} - 18\phi^n + 9\phi^{n-1} - 2\phi^{n-2}) dx.
 \end{aligned} \tag{17}$$

where $\bar{\phi}^{n+1}$ is any explicit $O(\delta t^2)$ approximation for Φ^{n+1} .

SAV/BDF3

To obtain $\bar{\phi}^{n+1}$ in BDF3, we can use the extrapolation (called BDF3A):

$$\bar{\phi}^{n+1} = 3\phi^n - 3\phi^{n-1} + \phi^{n-2},$$

or prediction by one BDF2 step (called BDF3B):

$$\bar{\phi}^{n+1} = \text{BDF2} \{ \phi^n, \phi^{n-1}, \Delta t \}.$$

It is noticed that using the prediction with a lower order BDF step will double the total computation cost.

Numerical result I

Example.1: Evolutions of coarsening process and of energy[15]

In this example, we simulate the Cahn-Hilliard equation on $[0, 2\pi)^2$, starting from

$$\phi(x, y, 0) = 0.25 + 0.4\mathbf{Rand}(x, y) \quad (18)$$

We choose $\beta = 4$, $C_0 = 0$ and discretize the space by the Fourier spectral method with 256×256 modes.

We investigate the coarsening process with $\epsilon^2 = 0.01$ and $\delta t = 2 \times 10^{-5}$. The reference solution and the results of SAV/BDF2 are shown in Fig.1, no visible difference is observed.

Numerical result II

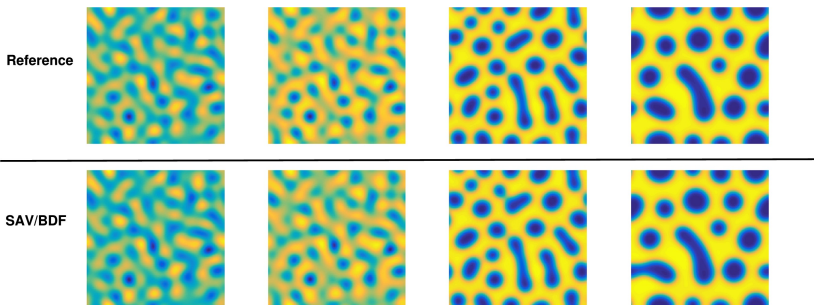


Figure: Coarsening process with SAV/BDF2.

Example.2: Energy evolutions for BDF3 and BDF4 schemes.[16]

We take Cahn–Hilliard equation as an example to demonstrate the numerical performances of SAV/BDF3 and SAV/BDF4 schemes. We fix the computational domain as $[0, 2\pi)^2$ and $\epsilon = 0.1$.

Numerical result III

We use the Fourier Galerkin method for spatial discretization with $N = 2^7$. The initial data is $u_0(x, y) = 0.05 \sin(x) \sin(y)$.

The numerical results are shown in Fig.2.

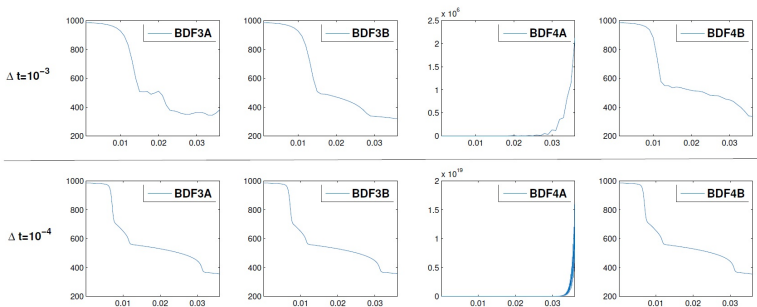


Figure: Energy evolutions for BDF3 and BDF4 schemes.

Numerical result IV

Next, we compare the numerical results of BDF2, BDF3 and BDF4. The energy evolution and the configuration at $t = 0.016$ are shown in FIG.3 (for the first row $\Delta t = 10^3$, and for the second row $\Delta t = 10^4$).

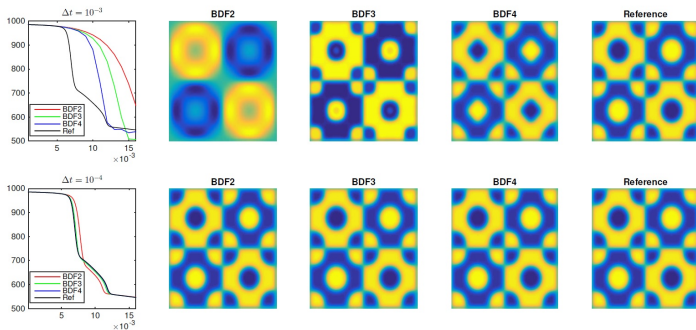


Figure: Comparison of BDF2, BDF3 and BDF4.

Advantage of SAV

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

Advantage of SAV

- ▶ 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.[1]

Disadvantage of SAV

- ▶ Restrictions on the free energy;
- ▶ Extrapolation scheme of nonlinear part;
- ▶ Restrictions on convergence and error analysis[1];

Possible improvement of SAV

- ▶ More relaxed restrictions on the free energy;
e.g. $r(t) = \sqrt{\int_{\Omega} |F(\phi)| dx}$
- ▶ BDF4C, BDF4D? or implicit scheme of nonlinear part;
- ▶ More work in convergence and error analysis of SAV;

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