Phase field models and their numerical methods

2. Energy stable numerical methods

August 14, 2019

Outline

Outline

Allen-Cahn equation

Allen-Cahn equation:

$$u_t - \Delta u + \frac{1}{\varepsilon^2} f(u) = 0, \quad f(u) = F'(u) = u^3 - u. \tag{1}$$

L^2 gradient flow of the energy functional:

$$E(u) = \int_\Omega \left(\frac{1}{2} |\nabla u|^2 + \frac{1}{\varepsilon^2} F(u) \right) \mathrm{d}x, \quad F(u) = \frac{1}{4}(u^2 - 1)^2. \tag{2}$$

Energy dissipation law (under suitable BCs):

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -\|u_t\|^2. \tag{3}$$

Outline

1. Classic implicit-explicit methods
   - Fully implicit schemes
   - Convex splitting schemes
   - Stabilization schemes
2. Energy quadratization methods
   - Invariant energy quadratization (IEQ) schemes
   - Scalar auxiliary variable (SAV) schemes
3. Exponential time differencing (ETD) methods
   - General theory for ODE systems
   - Example 1. Allen-Cahn equation
   - Example 2. No-slope-selection epitaxial growth model

First order scheme

Backward Euler (BE) scheme:

$$\frac{u_{n+1} - u_n}{\Delta t} - \Delta u_{n+1} + \frac{1}{\varepsilon^2} f(u_{n+1}) = 0. \tag{BE}$$

Theorem: Unique solvability and energy stability of (BE)

For $\Delta t \le \varepsilon^2$, the BE scheme admits a unique solution and is energy stable:

$$E_{n+1} - E_n \le -\left(\frac{1}{\Delta t} - \frac{1}{2\varepsilon^2}\right) \|u_{n+1} - u_n\|^2,$$

where $E_n = E(u_n) = \frac{1}{2}\|\nabla u_n\|^2 + \frac{1}{4\varepsilon^2}\|u_n^2 - 1\|^2.$

See [Feng-Prohl, 2003] for the unique solvability.
We just show the energy stability.

First order scheme (continued)

Energy stability of (BE)

For $\Delta t \leq \varepsilon^2$, the BE scheme is energy stable:

$$E_{n+1} - E_n \leq -\Big(\frac{1}{\Delta t} - \frac{1}{2\varepsilon^2}\Big)\|u_{n+1} - u_n\|^2,$$

where $E_n = E(u_n) = \frac{1}{2}\|\nabla u_n\|^2 + \frac{1}{4\varepsilon^2}\|u_n^2 - 1\|^2.$

Proof. Take the inner product of (BE) with $u_{n+1} - u_n$:

$$\frac{1}{\Delta t}\|u_{n+1}-u_n\|^2+(\nabla u_{n+1}, \nabla u_{n+1}-\nabla u_n)+\frac{1}{\varepsilon^2}(f(u_{n+1}), u_{n+1}-u_n) = 0.$$

Since $2a(a-b) = a^2 - b^2 + (a-b)^2$, we have

$$(\nabla u_{n+1}, \nabla u_{n+1}-\nabla u_n) = \frac{1}{2}\|\nabla u_{n+1}\|^2 - \frac{1}{2}\|\nabla u_n\|^2+\frac{1}{2}\|\nabla u_{n+1}-\nabla u_n\|^2.$$

First order scheme (continued)

The nonlinear term could be derived as

$$
\begin{aligned}
&(f(u_{n+1}), u_{n+1} - u_n) \\
=\ &(u_{n+1}^2 - 1, u_{n+1}(u_{n+1} - u_n)) \\
=\ &\frac{1}{2}(u_{n+1}^2 - 1, u_{n+1}^2 - u_n^2 + (u_{n+1} - u_n)^2) \\
=\ &\frac{1}{2}(u_{n+1}^2 - 1, (u_{n+1}^2 - 1) - (u_n^2 - 1)) + \frac{1}{2}(u_{n+1}^2 - 1, (u_{n+1} - u_n)^2) \\
=\ &\frac{1}{4}\|u_{n+1}^2 - 1\|^2 - \frac{1}{4}\|u_n^2 - 1\|^2 + \frac{1}{4}\|u_{n+1}^2 - u_n^2\|^2 \\
&\qquad + \frac{1}{2}\|u_{n+1}(u_{n+1} - u_n)\|^2 - \frac{1}{2}\|u_{n+1} - u_n\|^2.
\end{aligned}
$$

Then,

$$
E_{n+1} - E_n \leq -\left(\frac{1}{\Delta t} - \frac{1}{2\varepsilon^2}\right)\|u_{n+1} - u_n\|^2 - \frac{1}{2}\|\nabla u_{n+1} - \nabla u_n\|^2. \quad \square
$$

Second order scheme

The modified Crank-Nicolson (MCN) scheme:

$$\frac{u_{n+1} - u_n}{\Delta t} - \frac{1}{2}\Delta(u_{n+1} + u_n) + \frac{1}{\varepsilon^2}\tilde{f}(u_{n+1}, u_n) = 0, \qquad \text{(MCN)}$$

where

$$\tilde{f}(v,w) = \begin{cases} \dfrac{F(v) - F(w)}{v - w}, & v \neq w, \\ F'(v), & v = w. \end{cases}$$

Theorem: Energy stability of (MCN)

For any $\Delta t > 0$, the MCN scheme is energy stable:

$$E_{n+1} - E_n = -\frac{1}{\Delta t}\|u_{n+1} - u_n\|^2,$$

where $E_n = E(u_n) = \dfrac{1}{2}\|\nabla u_n\|^2 + \dfrac{1}{4\varepsilon^2}\|u_n^2 - 1\|^2.$

Second order scheme (continued)

Energy stability of (MCN)

For any $\Delta t > 0$, the MCN scheme is energy stable:

$$E_{n+1} - E_n = -\frac{1}{\Delta t}\|u_{n+1} - u_n\|^2,$$

where $E_n = E(u_n) = \frac{1}{2}\|\nabla u_n\|^2 + \frac{1}{4\varepsilon^2}\|u_n^2 - 1\|^2$.

Proof. Take the inner product of (MCN) with $u_{n+1} - u_n$:

$$\frac{1}{\Delta t}\|u_{n+1}-u_n\|^2+\frac{1}{2}(\|\nabla u_{n+1}\|^2-\|\nabla u_n\|^2)+\frac{1}{\varepsilon^2}(\tilde{f}(u_{n+1},u_n),u_{n+1}-u_n) = 0.$$

Since

$$(\tilde{f}(u_{n+1},u_n),u_{n+1} - u_n) = (F(u_{n+1}) - F(u_n), 1),$$

we obtain

$$E_{n+1} - E_n = -\frac{1}{\Delta t}\|u_{n+1} - u_n\|^2. \quad \square$$

Remarks on the fully implicit schemes

Advantages:

- Easy to construct;
- Truncated error only comes from the approximation of u_t.

Disadvantages:

- $\Delta t \leq \varepsilon^2$ for unique solvability and energy stability;
- Nonlinearity leads to large amounts of computation.

References:

- Feng-Prohl, *Numer. Math.*, 2003.
- Du-Nicolaides, *SIAM J. Numer. Anal.*, 1991.

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Convex splitting form

Notice that

$$F(u) = F_+(u) - F_-(u),$$

where $F_+(u) = \dfrac{1}{4}(u^4 + 1)$ and $F_-(u) = \dfrac{1}{2}u^2$ are both convex.

Correspondingly,

$$E(u) = E_+(u) - E_-(u), \tag{4}$$

with $E_\pm(u) = \displaystyle\int_\Omega F_\pm(u)dx$.

The form (4) gives a *convex splitting* of the energy E.

First order scheme

The first order convex splitting scheme:

$$\frac{u_{n+1}-u_n}{\Delta t} - \Delta u_{n+1} + \frac{1}{\varepsilon^2}\left(f_+(u_{n+1}) - f_-(u_n)\right) = 0, \qquad \text{(CS1)}$$

where $f_+(u) = F'_+(u) = u^3$ and $f_-(u) = F'_-(u) = u$.

Theorem: Unique solvability and energy stability of (CS1)

For any $\Delta t > 0$, the CS1 scheme admits a unique solution and is energy stable:

$$E_{n+1} - E_n \leq -\frac{1}{\Delta t}\|u_{n+1}-u_n\|^2,$$

where $E_n = E(u_n) = \frac{1}{2}\|\nabla u_n\|^2 + \frac{1}{\varepsilon^2}(F(u_n), 1)$.

First order scheme (continued)

Proof. Unique solvability. Define

$$\mathcal{E}(u) = \int_\Omega \left(\frac{1}{2}|\nabla u|^2 + \frac{1}{4\varepsilon^2}u^4 - \frac{1}{\varepsilon^2}u_n u + \frac{1}{2\Delta t}(u-u_n)^2\right)dx.$$

First variational derivative of $\mathcal{E}$:

$$\frac{\delta\mathcal{E}(u)}{\delta u} = -\Delta u + \frac{1}{\varepsilon^2}(u^3 - u_n) + \frac{1}{\Delta t}(u-u_n).$$

Notice that (CS1) is equivalent to

$$\frac{\delta\mathcal{E}(u_{n+1})}{\delta u} = 0. \tag{5}$$

Second variational of $\mathcal{E}$:

$$\frac{\mathrm{d}^2\mathcal{E}(u+\lambda v)}{\mathrm{d}\lambda^2}\bigg|_{\lambda=0} = \int_\Omega \left(|\nabla v|^2 + \frac{3}{\varepsilon^2}u^2v^2 + \frac{1}{\Delta t}v^2\right)dx > 0, \quad \forall v \neq 0.$$

That is, $\mathcal{E}$ is strictly convex and (CS1) is equivalent to

$$u_{n+1} = \operatorname{argmin} \mathcal{E}(v), \quad v \in H^1(\Omega).$$

First order scheme (continued)

Energy stability. Take the inner product of (CS1) with $u_{n+1} - u_n$:

$$\frac{1}{\Delta t}\|u_{n+1}-u_n\|^2 + (\nabla u_{n+1}, \nabla u_{n+1} - \nabla u_n) + \frac{1}{\varepsilon^2}(f_+(u_{n+1}) - f_-(u_n), u_{n+1}-u_n) = 0,$$

where

$$(\nabla u_{n+1}, \nabla u_{n+1} - \nabla u_n) = \frac{1}{2}\|\nabla u_{n+1}\|^2 - \frac{1}{2}\|\nabla u_n\|^2 + \frac{1}{2}\|\nabla u_{n+1} - \nabla u_n\|^2.$$

Using the Taylor formula

$$F_+(u_n) = F_+(u_{n+1}) - f_+(u_{n+1})(u_{n+1}-u_n) + \frac{1}{2}F_+''(\xi_1)(u_{n+1}-u_n)^2,$$

$$F_-(u_{n+1}) = F_-(u_n) + f_-(u_n)(u_{n+1}-u_n) + \frac{1}{2}F_-''(\xi_2)(u_{n+1}-u_n)^2,$$

we have

$$f_+(u_{n+1})(u_{n+1}-u_n) = F_+(u_{n+1}) - F_+(u_n) + \frac{1}{2}F_+''(\xi_1)(u_{n+1}-u_n)^2 \geq F_+(u_{n+1}) - F_+(u_n),$$

$$f_-(u_n)(u_{n+1}-u_n) = F_-(u_{n+1}) - F_-(u_n) - \frac{1}{2}F_-''(\xi_2)(u_{n+1}-u_n)^2 \leq F_-(u_{n+1}) - F_-(u_n).$$

Then,

$$E_{n+1} - E_n \leq -\frac{1}{\Delta t}\|u_{n+1}-u_n\|^2 - \frac{1}{2}\|\nabla u_{n+1} - \nabla u_n\|^2. \quad \square$$

Relation between the BE and CS1 schemes

The CS1 scheme can be rewritten as the fully implicit scheme

$$\frac{u_{n+1} - u_n}{\Delta t'} - \Delta u_{n+1} + \frac{1}{\varepsilon^2} f(u_{n+1}) = 0, \tag{6}$$

with different time step size $\Delta t' = \dfrac{\Delta t \varepsilon^2}{\Delta t + \varepsilon^2}$.

Proof. Note that

$$u_{n+1}^3 - u_n = u_{n+1}^3 - u_{n+1} + (u_{n+1} - u_n) = f(u_{n+1}) + (u_{n+1} - u_n).$$

Substitute the above identity into (CS1):

$$\left(\frac{1}{\Delta t} + \frac{1}{\varepsilon^2}\right)(u_{n+1} - u_n) - \Delta u_{n+1} + \frac{1}{\varepsilon^2} f(u_{n+1}) = 0.$$

This is (6) with the time step $\Delta t'$ defined by $\dfrac{1}{\Delta t'} = \dfrac{1}{\Delta t} + \dfrac{1}{\varepsilon^2}$. □

Relation between the BE and CS1 schemes (continued)

- *Why is the CS1 scheme always energy stable?*
  For any $\Delta t > 0$, since
  $$\Delta t' = \frac{\Delta t \varepsilon^2}{\Delta t + \varepsilon^2} < \varepsilon^2,$$
  the fully implicit scheme (6) is energy stable.

- *Existence of a time-delay.*
  Denote by $u^{\mathrm{BE}}(t_n)$ and $u^{\mathrm{CS}}(t_n)$ the solutions to (BE) and (CS1). Then,
  $$u^{\mathrm{CS}}(t_n) = u^{\mathrm{BE}}(\delta t_n), \quad \delta = \frac{\varepsilon^2}{\Delta t + \varepsilon^2} < 1.$$
  A larger time step size Δt, giving a smaller δ, leads to a more significant time-delay. Such a delay will diminish as $\Delta t \to 0$.

Second order scheme

The second order convex splitting (CS2) scheme:

$$\frac{u_{n+1}-u_n}{\Delta t}-\Delta\frac{u_{n+1}+u_n}{2}+\frac{1}{\varepsilon^2}\left(\tilde{f}_+(u_{n+1},u_n)-\left(\frac{3}{2}u_n-\frac{1}{2}u_{n-1}\right)\right)=0. \tag{CS2}$$

Theorem: Energy stability of (CS2)

For any $\Delta t>0$, *the CS2 scheme is energy stable:*

$$E_{n+1}-E_n\leq-\frac{1}{\Delta t}\|u_{n+1}-u_n\|^2,$$

where E_n *is a modification of* $E(u_n)$*:*

$$E_n=\frac{1}{2}\|\nabla u_n\|^2+\frac{1}{4\varepsilon^2}\|u_n^2-1\|^2+\frac{1}{4\varepsilon^2}\|u_n-u_{n-1}\|^2.$$

Second order scheme (continued)

Energy stability of (CS2)

For any $\Delta t > 0$, the CS2 scheme is energy stable:

$$E_{n+1} - E_n \leq -\frac{1}{\Delta t}\|u_{n+1} - u_n\|^2,$$

where $E_n = \frac{1}{2}\|\nabla u_n\|^2 + \frac{1}{4\varepsilon^2}\|u_n^2 - 1\|^2 + \frac{1}{4\varepsilon^2}\|u_n - u_{n-1}\|^2.$

Proof. Take the inner product of (CS2) with $u_{n+1} - u_n$:

$$\begin{aligned}\frac{1}{\Delta t}\|u_{n+1} - u_n\|^2 &+ \frac{1}{2}(\|\nabla u_{n+1}\|^2 - \|\nabla u_n\|^2) \\ &+ \frac{1}{\varepsilon^2}(\tilde{f}_+(u_{n+1}, u_n), u_{n+1} - u_n) - \frac{1}{\varepsilon^2}\left(\frac{3}{2}u_n - \frac{1}{2}u_{n-1}, u_{n+1} - u_n\right) = 0,\end{aligned}$$

where

$$(\tilde{f}_+(u_{n+1}, u_n), u_{n+1} - u_n) = (F_+(u_{n+1}) - F_+(u_n), 1).$$

Second order scheme (continued)

Since
$\left(\frac{3}{2}b-\frac{1}{2}c\right)(a-b)=\frac{1}{2}a^2-\frac{1}{2}b^2-\frac{1}{4}(a-b)^2+\frac{1}{4}(b-c)^2-\frac{1}{4}(a-2b+c)^2,$
we have

$$\begin{aligned}\left(\frac{3}{2}u_n-\frac{1}{2}u_{n-1},u_{n+1}-u_n\right)=&\frac{1}{2}\|u_{n+1}\|^2-\frac{1}{2}\|u_n\|^2-\frac{1}{4}\|u_{n+1}-u_n\|^2\\&+\frac{1}{4}\|u_n-u_{n-1}\|^2-\frac{1}{4}\|u_{n+1}-2u_n+u_{n-1}\|^2.\end{aligned}$$

Then, we obtain

$$\begin{aligned}&\frac{1}{\Delta t}\|u_{n+1}-u_n\|^2+\frac{1}{2}(\|\nabla u_{n+1}\|^2-\|\nabla u_n\|^2)\\&\quad+\frac{1}{4\varepsilon^2}(F_+(u_{n+1})-F_+(u_n),1)-\frac{1}{2\varepsilon^2}\|u_{n+1}\|^2+\frac{1}{2\varepsilon^2}\|u_n\|^2\\&\quad+\frac{1}{4\varepsilon^2}\|u_{n+1}-u_n\|^2-\frac{1}{4\varepsilon^2}\|u_n-u_{n-1}\|^2+\frac{1}{4\varepsilon^2}\|u_{n+1}-2u_n+u_{n-1}\|^2=0,\end{aligned}$$

that is,

$$E_{n+1}-E_n=-\frac{1}{\Delta t}\|u_{n+1}-u_n\|^2-\frac{1}{4\varepsilon^2}\|u_{n+1}-2u_n+u_{n-1}\|^2. \qquad \square$$

Remarks on the convex splitting schemes

Advantages:

- Easy to construct;
- Unconditional unique solvability and energy stability (1st order);
- Easy to prove the energy stability.

Disadvantages:

- Existence of the time-delay may cause more truncated errors;
- Nonlinearity leads to large amounts of computation;
- Hard to obtain the energy stability for higher order schemes.

References:

- David J. Eyre, a note, 1997.
- Shen-Wang-Wang-Wise, *SIAM J. Numer. Anal.*, 2012.
- Xu-Li-Wu, *arXiv:1604.05402v4*, 2017.

Outline

First order scheme

The first order stabilization (STAB1) scheme:

$$\frac{u_{n+1}-u_n}{\Delta t} - \Delta u_{n+1} + \frac{1}{\varepsilon^2} f(u_n) + \frac{S}{\varepsilon^2}(u_{n+1}-u_n) = 0, \qquad \text{(STAB1)}$$

where the constant $S \geq 0$ is called the stabilizer.

Rewrite the *linear* scheme (STAB1):

$$\left(\frac{1}{\Delta t} + \frac{S}{\varepsilon^2} - \Delta\right) u_{n+1} = \left(\frac{1}{\Delta t} + \frac{S}{\varepsilon^2}\right) u_n - \frac{1}{\varepsilon^2} f(u_n).$$

The operator of u_{n+1} is self-adjoint and positive definite, so the STAB1 scheme must admit a unique solution.

First order scheme (continued)

Theorem: Energy stability of (STAB1)

Denote $L = \|f'\|_{L^\infty}$ *and assume that* $L < \infty$.

(i) *For* $S = 0$ *and* $\Delta t \leq \dfrac{2\varepsilon^2}{L}$, *the STAB1 scheme is energy stable:*

$$E_{n+1} - E_n \leq -\left(\frac{1}{\Delta t} - \frac{L}{2\varepsilon^2}\right)\|u_{n+1} - u_n\|^2;$$

(ii) *For* $S \geq \dfrac{L}{2}$ *and* $\Delta t > 0$, *the STAB1 scheme is energy stable:*

$$E_{n+1} - E_n \leq -\frac{1}{\Delta t}\|u_{n+1} - u_n\|^2,$$

where $E_n = E(u_n) = \dfrac{1}{2}\|\nabla u_n\|^2 + \dfrac{1}{\varepsilon^2}(F(u_n), 1)$.

First order scheme (continued)

Proof. Take the inner product of (STAB1) with $u_{n+1} - u_n$:

$$\left(\frac{1}{\Delta t}+\frac{S}{\varepsilon^2}\right)\|u_{n+1}-u_n\|^2+(\nabla u_{n+1}, \nabla u_{n+1}-\nabla u_n)+\frac{1}{\varepsilon^2}(f(u_n), u_{n+1}-u_n) = 0,$$

where

$$(\nabla u_{n+1}, \nabla u_{n+1}-\nabla u_n) = \frac{1}{2}\|\nabla u_{n+1}\|^2 - \frac{1}{2}\|\nabla u_n\|^2+\frac{1}{2}\|\nabla u_{n+1}-\nabla u_n\|^2.$$

Using the Taylor formula

$$F(u_{n+1}) = F(u_n) + f(u_n)(u_{n+1} - u_n) + \frac{1}{2}f'(\xi)(u_{n+1} - u_n)^2,$$

we have

$$\begin{aligned} f(u_n)(u_{n+1} - u_n) &= F(u_{n+1}) - F(u_n) - \frac{1}{2}f'(\xi)(u_{n+1} - u_n)^2 \\ &\geq F(u_{n+1}) - F(u_n) - \frac{L}{2}(u_{n+1} - u_n)^2. \end{aligned}$$

Then, $$E_{n+1} - E_n \leq -\left(\frac{1}{\Delta t} + \frac{S}{\varepsilon^2} - \frac{L}{2\varepsilon^2}\right)\|u_{n+1} - u_n\|^2.$$

First order scheme (continued)

$$E_{n+1} - E_n \leq -\left(\frac{1}{\Delta t} + \frac{S}{\varepsilon^2} - \frac{L}{2\varepsilon^2}\right)\|u_{n+1} - u_n\|^2.$$

For (i), when $S = 0$, we have

$$E_{n+1} - E_n \leq -\left(\frac{1}{\Delta t} - \frac{L}{2\varepsilon^2}\right)\|u_{n+1} - u_n\|^2.$$

The condition $\Delta t \leq \frac{2\varepsilon^2}{L}$ leads to the energy stability.

For (ii), when $S \geq \frac{L}{2}$, we have

$$E_{n+1} - E_n \leq -\frac{1}{\Delta t}\|u_{n+1} - u_n\|^2.$$

Energy stability holds for any $\Delta t > 0$.

First order scheme (continued)

A question is whether $\|f'\|_{L^\infty}$ is finite.

In fact, we have the following result:

For the Allen-Cahn equation, if $u(0) \in [-1, 1]$ a.e., then $u(t) \in [-1, 1]$ a.e. for any $t > 0$.

For a large positive number $M \gg 1$, we modify the potential $F(u)$ as

$$\tilde{F}(u) = \begin{cases} \frac{1}{4}(u^2 - 1)^2, & |u| \le M, \\ au^2 + bu + c, & |u| > M, \end{cases}$$

where $a, b, c \in \mathbb{R}$ are chosen such that $\tilde{F} \in C^2(\mathbb{R})$, and define $\tilde{f}(u) = \tilde{F}'(u)$. If we denote $L = \|\tilde{f}'\|_{L^\infty}$, then L must be a finite number.

Relation between the STAB1 and CS1 schemes

Consider the splitting form $F(u) = F_+(u) - F_-(u)$ with

$$F_+(u) = \frac{S}{2}u^2 + \frac{1}{4}, \quad F_-(u) = \frac{S+1}{2}u^2 - \frac{1}{4}u^4, \quad S \geq 0.$$

Here,

- F_+ is always convex in $\mathbb{R}$;
- F_- is convex on $[-1, 1]$ when $S \geq 2$.

The corresponding convex splitting scheme reads

$$\frac{u_{n+1} - u_n}{\Delta t} - \Delta u_{n+1} + \frac{S}{\varepsilon^2} u_{n+1} - \frac{1}{\varepsilon^2}(Su_n - f(u_n)) = 0,$$

which is exactly the STAB1 scheme.

Second order scheme

Second order BDF-type stabilization (STAB-BDF2) scheme:

$$\frac{3u_{n+1}-4u_n+u_{n-1}}{2\Delta t}-\Delta u_{n+1}+\frac{1}{\varepsilon^2}(2f(u_n)-f(u_{n-1}))+\frac{S}{\varepsilon^2}(u_{n+1}-2u_n+u_{n-1}) \tag{STAB-BDF2}$$

Theorem: Energy stability of (STAB-BDF2)

Denote $L=\|f'\|_{L^\infty}$ and assume that $L<\infty$.

For $S\geq 0$ and $\Delta t\leq \frac{2\varepsilon^2}{3L}$, the STAB-BDF2 scheme is energy stable:

$$E_{n+1}\leq E_n,$$

where

$$E_n=\frac{1}{2}\|\nabla u_n\|^2+\frac{1}{\varepsilon^2}(F(u_n),1)+\left(\frac{1}{4\Delta t}+\frac{S+L}{2\varepsilon^2}\right)\|u_n-u_{n-1}\|^2.$$

Remarks on the stabilization schemes

Advantages:

- Easy to construct;
- Unconditional unique solvability and energy stability (1st order);
- Linear scheme with constant coefficient, so we can use FFT.

Disadvantages:

- Stabilization term introduces an extra truncated error;
- Theoretically, $\|f'(u)\|_{L^\infty} < \infty$ does not hold for general cases, unless we know $\|u\|_{L^\infty} \leq C$ for some certain C;
- Hard to obtain the energy stability for higher order schemes.

References:

- Shen-Yang, *Discrete Contin. Dyn. Syst.*, 2010.

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Gradient flow and energy functional

Gradient flow:

$$\frac{\partial u}{\partial t} = G\mu, \quad \mu = \frac{\delta E}{\delta u}. \tag{7}$$

Energy dissipation law:

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \left(\frac{\delta E}{\delta u}, \frac{\partial u}{\partial t}\right) = (\mu, G\mu) \leq 0.$$

Energy functional:

$$E(u) = \frac{1}{2}(u, Lu) + E_1(u), \tag{8}$$

- G is self-adjoint and *negative definite*;
- L is self-adjoint and *positive semi-definite*;
- E_1 is nonlinear but with lower order derivatives than L and *bounded from below*.

The gradient flow (7) equipped with the energy (8) reads

$$u_t = G\mu, \quad \mu = Lu + N(u), \quad N(u) = \frac{\delta E_1}{\delta u}. \tag{9}$$

Outline

Equivalent forms

We further assume that E_1 takes the form $E_1(u) = \int F(u)\,\mathrm{d}x$ with F *bounded from below*. Without loss of generality, we assume $F(u) > 0$. Introduce an auxiliary variable $q(x,t) = \sqrt{F(u(x,t))}$.

Equivalent form of the gradient flow:

$$u_t = G\mu, \tag{10a}$$

$$\mu = Lu + \frac{q}{\sqrt{F(u)}}N(u), \tag{10b}$$

$$q_t = \frac{N(u)}{2\sqrt{F(u)}}u_t. \tag{10c}$$

Equivalent form of the energy:

$$\widetilde{E}(u,q) = \frac{1}{2}(u, Lu) + \|q\|^2. \tag{11}$$

Equivalent forms (continued)

$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{E}(u,q) = (\mu, G\mu) \leq 0.$$

Proof. Take the inner product of (10a) with μ:

$$(\mu, u_t) = (\mu, G\mu).$$

Take the inner product of (10b) with u_t:

$$(\mu, u_t) = (Lu, u_t) + \left(\frac{N(u)}{\sqrt{F(u)}}q, u_t\right).$$

Take the inner product of (10c) with $2q$:

$$2(q, q_t) = \left(\frac{N(u)}{\sqrt{F(u)}}u_t, q\right).$$

Then, we obtain

$$(\mu, G\mu) = (Lu, u_t) + 2(q, q_t) = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{2}(u, Lu) + \|q\|^2\right). \quad \square$$

First order IEQ scheme

Gradient flow:

$$u_t = G\mu,$$
$$\mu = Lu + \frac{q}{\sqrt{F(u)}}N(u),$$
$$q_t = \frac{N(u)}{2\sqrt{F(u)}}u_t.$$

First order IEQ (IEQ1) scheme:

$$\frac{u_{n+1} - u_n}{\Delta t} = G\mu_{n+1}, \tag{12a}$$
$$\mu_{n+1} = Lu_{n+1} + \frac{q_{n+1}}{\sqrt{F(u_n)}}N(u_n), \tag{12b}$$
$$\frac{q_{n+1} - q_n}{\Delta t} = \frac{N(u_n)}{2\sqrt{F(u_n)}}\frac{u_{n+1} - u_n}{\Delta t}. \tag{12c}$$

IEQ1 scheme: Unique solvability (continued)

For any $\Delta t > 0$, the IEQ1 scheme admits a unique solution.

IEQ1 scheme (denote $b_n = \dfrac{N(u_n)}{\sqrt{F(u_n)}}$):

$$\frac{u_{n+1} - u_n}{\Delta t} = G\mu_{n+1},$$
$$\mu_{n+1} = Lu_{n+1} + q_{n+1}b_n,$$
$$q_{n+1} - q_n = \frac{1}{2}b_n(u_{n+1} - u_n).$$

Proof. Eliminate μ_{n+1} and q_{n+1}:

$$\frac{u_{n+1} - u_n}{\Delta t} = GLu_{n+1} + G(q_n b_n) + \frac{1}{2}G(b_n^2 u_{n+1}) - \frac{1}{2}G(b_n^2 u_n),$$

or equivalently,

$$u_{n+1} - \Delta t GLu_{n+1} - \frac{\Delta t}{2}G(b_n^2 u_{n+1}) = u_n + \Delta t G(q_n b_n) - \frac{\Delta t}{2}G(b_n^2 u_n) =: c_n.$$

IEQ1 scheme: Unique solvability (continued)

$$u_{n+1} - \Delta t G L u_{n+1} - \frac{\Delta t}{2} G(b_n^2 u_{n+1}) = c_n.$$

Act G^{-1} on both sides:

$$\left(G^{-1} - \Delta t L - \frac{\Delta t}{2} b_n^2 I\right) u_{n+1} = G^{-1} c_n.$$

Here, $G^{-1} - \Delta t L - \frac{\Delta t}{2} b_n^2 I$ is negative definite. $\square$

Algorithm: IEQ1 scheme

Given u_n, q_n, to compute u_{n+1}, q_{n+1} as follows:

1. Calculate b_n and c_n;
2. Solve $(I - \Delta t G L) u_{n+1} - \frac{\Delta t}{2} G(b_n^2 u_{n+1}) = c_n$ to obtain u_{n+1};
3. Calculate q_{n+1} by $q_{n+1} = q_n + \frac{1}{2} b_n (u_{n+1} - u_n)$.

IEQ1 scheme: Energy stability

For any $\Delta t > 0$, we have $E_{n+1} - E_n \leq \Delta t(\mu_{n+1}, G\mu_{n+1}) \leq 0$, where $E_n = \widetilde{E}(u_n, q_n) = \frac{1}{2}(u_n, Lu_n) + \|q_n\|^2$.

Proof. Take the inner product of (12a) with $\Delta t \mu_{n+1}$:

$$(\mu_{n+1}, u_{n+1} - u_n) = \Delta t(\mu_{n+1}, G\mu_{n+1}).$$

Take the inner product of (12b) with $u_{n+1} - u_n$:

$$(\mu_{n+1}, u_{n+1} - u_n) = (Lu_{n+1}, u_{n+1} - u_n) + (q_{n+1}b_n, u_{n+1} - u_n).$$

Take the inner product of (12c) with $2q_{n+1}$:

$$(2q_{n+1}, q_{n+1} - q_n) = (q_{n+1}b_n, u_{n+1} - u_n).$$

Then, we obtain

$$E_{n+1} - E_n + \frac{1}{2}(L(u_{n+1} - u_n), u_{n+1} - u_n) + \|q_{n+1} - q_n\|^2 = \Delta t(\mu_{n+1}, G\mu_{n+1}). \quad \square$$

Remark. Generally, $q_n \neq \sqrt{F(u_n)}$, so $E_n \neq E(u_n)$.

Second order IEQ scheme: IEQ-CN

$$
\begin{aligned}
u_t &= G\mu, \\
\mu &= Lu + \frac{q}{\sqrt{F(u)}} N(u), \\
q_t &= \frac{N(u)}{2\sqrt{F(u)}} u_t.
\end{aligned}
$$

Crank-Nicolson-type IEQ (IEQ-CN) scheme:

$$
\frac{u_{n+1} - u_n}{\Delta t} = G\mu_{n+\frac{1}{2}}, \tag{13a}
$$

$$
\mu_{n+\frac{1}{2}} = \frac{1}{2} L(u_{n+1} + u_n) + \frac{q_{n+1} + q_n}{2} \overline{b}_{n+\frac{1}{2}}, \tag{13b}
$$

$$
\frac{q_{n+1} - q_n}{\Delta t} = \frac{1}{2} \overline{b}_{n+\frac{1}{2}} \frac{u_{n+1} - u_n}{\Delta t}, \tag{13c}
$$

where $\overline{b}_{n+\frac{1}{2}} = \frac{3}{2} b_n - \frac{1}{2} b_{n-1}$ with $b_n = \frac{N(u_n)}{\sqrt{F(u_n)}}$.

Second order IEQ scheme: IEQ-CN (continued)

Unique solvability

For any $\Delta t > 0$, the IEQ-CN scheme admits a unique solution.

Energy stability

For any $\Delta t > 0$, the IEQ-CN scheme is energy stable:

$$E_{n+1} - E_n = \Delta t(\mu_{n+1}, G\mu_{n+1}) \leq 0,$$

where $E_n = \widetilde{E}(u_n, q_n) = \frac{1}{2}(u_n, Lu_n) + \|q_n\|^2$.

Proof. Taking the inner products of (13a), (13b), (13c) with $\Delta t \mu_{n+\frac{1}{2}}$, $-(u_{n+1} - u_n)$, $\Delta t(q_{n+1} + q_n)$, respectively, and adding the resulted three equalities yield the expected result. □

Second order IEQ scheme: IEQ-BDF2

$$
\begin{aligned}
u_t &= G\mu, \\
\mu &= Lu + \frac{q}{\sqrt{F(u)}}N(u), \\
q_t &= \frac{N(u)}{2\sqrt{F(u)}}u_t.
\end{aligned}
$$

Second order BDF-type IEQ (IEQ-BDF2) scheme:

$$
\frac{3u_{n+1} - 4u_n + u_{n-1}}{2\Delta t} = G\mu_{n+1}, \tag{14a}
$$

$$
\mu_{n+1} = Lu_{n+1} + q_{n+1}\bar{b}_{n+1}, \tag{14b}
$$

$$
\frac{3q_{n+1} - 4q_n + q_{n-1}}{2\Delta t} = \frac{1}{2}\bar{b}_{n+1}\frac{3u_{n+1} - 4u_n + u_{n-1}}{2\Delta t}, \tag{14c}
$$

where $\bar{b}_{n+1} = 2b_n - b_{n-1}$.

Second order IEQ scheme: IEQ-BDF2 (continued)

Unique solvability

For any $\Delta t > 0$, *the IEQ-BDF2 scheme admits a unique solution.*

Energy stability

For any $\Delta t > 0$, *the IEQ-BDF2 scheme is energy stable:*

$$E_{n+1} - E_n \leq \Delta t(\mu_{n+1}, G\mu_{n+1}) \leq 0,$$

where

$$E_n = \frac{1}{4}\big((u_n, Lu_n) + (2u_n - u_{n-1}, L(2u_n - u_{n-1}))\big) + \frac{1}{2}\big(\|q_n\|^2 + \|2q_n - q_{n-1}\|^2\big).$$

Hints:

$$a(3a-4b+c) = \frac{1}{2}(a^2+(2a-b)^2) - \frac{1}{2}(b^2+(2b-c)^2) + \frac{1}{2}(a-2b+c)^2.$$

Remarks on the IEQ schemes

Advantages:

- Linear scheme and unique solvability;
- Unconditional energy stability (w.r.t. a modified energy);
- Easy to construct higher order schemes;

Disadvantages:

- Linear system with variable coefficient, cannot use FFT;
- For some problems, $F(u)$ is not bounded from below.

References:

- XF Yang et al, *J. Comput. Phys.*, 2016-2017.

Example 1. Phase field crystal model

Phase field crystal (PFC) model:

$$u_t = \Delta\mu, \quad \mu = u^3 + (1-\varepsilon)u + 2\Delta u + \Delta^2 u.$$

Energy functional:

$$E(u) = \int \left(\frac{1}{4}u^4 + \frac{1-\varepsilon}{2}u^2 - |\nabla u|^2 + \frac{1}{2}|\Delta u|^2\right)dx.$$

Introduce an auxiliary variable $q = u^2$.

Example 1. Phase field crystal model (continued)

Equivalent energy:

$$\widetilde{E}(u,q) = \int \left(\frac{1}{4}q^2 + \frac{1-\varepsilon}{2}u^2 - |\nabla u|^2 + \frac{1}{2}|\Delta u|^2 \right) dx.$$

Equivalent equation:

$$\begin{aligned} u_t &= \Delta \mu, \\ \mu &= qu + (1-\varepsilon)u + 2\Delta u + \Delta^2 u, \\ q_t &= 2uu_t. \end{aligned}$$

IEQ1 scheme:

$$\frac{u_{n+1} - u_n}{\Delta t} = \Delta \mu_{n+1}, \tag{15a}$$

$$\mu_{n+1} = q_{n+1}u_n + (1-\varepsilon)u_{n+1} + 2\Delta u_n + \Delta^2 u_{n+1}, \tag{15b}$$

$$q_{n+1} - q_n = 2u_n(u_{n+1} - u_n). \tag{15c}$$

Example 1. Phase field crystal model (continued)

Energy stability (Note that $q_n \neq u_n^2$, so $E_n \neq E(u_n)$.)

For any $\Delta t > 0$, we have $E_{n+1} - E_n \le -\Delta t \|\nabla \mu_{n+1}\|^2 \le 0$,
where $E_n = \widetilde{E}(u_n, q_n) = \frac{1}{4}\|q_n\|^2 + \frac{1-\varepsilon}{2}\|u_n\|^2 - \|\nabla u_n\|^2 + \frac{1}{2}\|\Delta u_n\|^2$.

Proof. Take the inner product of (15a) with $\Delta t \mu_{n+1}$:

$$(\mu_{n+1}, u_{n+1} - u_n) = \Delta t(\mu_{n+1}, \Delta\mu_{n+1}) = -\Delta t\|\nabla \mu_{n+1}\|^2.$$

Take the inner product of (15b) with $u_{n+1} - u_n$:

$$(\mu_{n+1}, u_{n+1} - u_n) = (q_{n+1}u_n, u_{n+1} - u_n) + (1-\varepsilon)(u_{n+1}, u_{n+1} - u_n) \\ - 2(\nabla u_n, \nabla u_{n+1} - \nabla u_n) + (\Delta u_{n+1}, \Delta u_{n+1} - \Delta u_n).$$

Take the inner product of (15c) with $\frac{1}{2}q_{n+1}$:

$$\frac{1}{2}(q_{n+1}, q_{n+1} - q_n) = (q_{n+1}u_n, u_{n+1} - u_n).$$

Just use the identities $a(a-b) = \cdots$ and $b(a-b) = \cdots$. □

Example 2. No-slope-selection epitaxial growth

Epitaxial growth model without slope selection:

$$u_t = -\nabla \cdot \left(\frac{\nabla u}{1 + |\nabla u|^2} \right) - \varepsilon^2 \Delta^2 u, \tag{16}$$

Energy functional:

$$E(u) = \int \left(-\frac{1}{2} \ln(1 + |\nabla u|^2) + \frac{\varepsilon^2}{2} |\Delta u|^2 \right) dx. \tag{17}$$

Strictly speaking, the IEQ method cannot be applied on this model since $-\frac{1}{2} \ln(1 + |\nabla u|^2)$ is *unbounded from below*. However, the basic idea could be used to construct an IEQ-like scheme.

Example 2. No-slope-selection epitaxial growth (continued)

Introduce an auxiliary variable $q = \sqrt{\ln(1+|\nabla u|^2)+A}$, $\forall A > 0$.

Equivalent equation:

$$u_t = -\varepsilon^2 \Delta^2 u - \nabla \cdot (q\boldsymbol{v}), \tag{18a}$$

$$q_t = \boldsymbol{v} \cdot \nabla u_t, \tag{18b}$$

where

$$\boldsymbol{v} = \frac{\nabla u}{(1+|\nabla u|^2)\sqrt{\ln(1+|\nabla u|^2)+A}}.$$

Equivalent energy:

$$\widetilde{E}(u,q) = \int_\Omega \left(\frac{\varepsilon^2}{2}|\Delta u|^2 - \frac{1}{2}q^2 + \frac{1}{2}A \right) dx.$$

Taking the inner products of (18a) and (18b) with u_t and $-q$, and adding the resulted two equalities yield the energy dissipation law:

$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{E}(u,q) = -\|u_t\|^2 \leq 0.$$

Example 2. No-slope-selection epitaxial growth (continued)

Equivalent equation:

$$
\begin{aligned}
u_t &= -\varepsilon^2 \Delta^2 u - \nabla \cdot (q\boldsymbol{v}), \\
q_t &= \boldsymbol{v} \cdot \nabla u_t,
\end{aligned}
$$

where

$$
\boldsymbol{v} = \frac{\nabla u}{(1 + |\nabla u|^2)\sqrt{\ln(1 + |\nabla u|^2) + A}}.
$$

First order scheme:

$$
\frac{u_{n+1} - u_n}{\Delta t} = -\varepsilon^2 \Delta^2 u_{n+1} - \nabla \cdot (q_n \boldsymbol{v}_n), \tag{19a}
$$

$$
q_{n+1} - q_n = \boldsymbol{v}_n \cdot (\nabla u_{n+1} - \nabla u_n), \tag{19b}
$$

where

$$
\boldsymbol{v}_n = \frac{\nabla u_n}{(1 + |\nabla u_n|^2)\sqrt{\ln(1 + |\nabla u_n|^2) + A}}.
$$

Example 2. No-slope-selection epitaxial growth (continued)

Energy stability

For any $\Delta t > 0$, we have $E_{n+1} - E_n \le -\frac{1}{\Delta t}\|u_{n+1} - u_n\|^2$,
where $E_n = \widetilde{E}(u_n, q_n) = \frac{\varepsilon^2}{2}\|\Delta u_n\|^2 - \frac{1}{2}\|q_n\|^2 + \frac{1}{2}A|\Omega|$.

Proof. Take the inner product of (19a) with $u_{n+1} - u_n$:

$$\frac{1}{\Delta t}\|u_{n+1}-u_n\|^2 = -\varepsilon^2(\Delta u_{n+1}, \Delta u_{n+1}-\Delta u_n)+(q_n\boldsymbol{v}_n, \nabla u_{n+1}-\nabla u_n).$$

Take the inner product of (19b) with q_n:

$$(q_n, q_{n+1} - q_n) = (q_n\boldsymbol{v}_n, \nabla u_{n+1} - \nabla u_n).$$

Then, we obtain

$$E_{n+1}-E_n+\frac{\varepsilon^2}{2}\|\Delta u_{n+1}-\Delta u_n\|^2+\frac{1}{2}\|q_{n+1}-q_n\|^2 = -\frac{1}{\Delta t}\|u_{n+1}-u_n\|^2. \quad \square$$

Remark. Generally, $q_n \neq \sqrt{\ln(1 + |\nabla u_n|^2) + A}$, so $E_n \neq E(u_n)$.

Outline

Equivalent forms

Without loss of generality, we assume $E_1(u) > 0$.
Introduce a Scalar Auxiliary Variable $r(t) = \sqrt{E_1(u(t))}$.

Equivalent form of the gradient flow:

$$u_t = G\mu, \tag{20a}$$

$$\mu = Lu + \frac{r}{\sqrt{E_1(u)}} N(u), \tag{20b}$$

$$r_t = \frac{1}{2\sqrt{E_1(u)}} \int N(u) u_t \, \mathrm{d}x. \tag{20c}$$

Equivalent form of the energy:

$$\widetilde{E}(u, r) = \frac{1}{2}(u, Lu) + r^2. \tag{21}$$

Equivalent forms (continued)

$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{E}(u,r) = (\mu, G\mu) \leq 0.$$

Proof. Take the inner product of (20a) with μ:

$$(\mu, u_t) = (\mu, G\mu).$$

Take the inner product of (20b) with u_t:

$$(\mu, u_t) = (Lu, u_t) + \frac{r}{\sqrt{E_1(u)}}(N(u), u_t).$$

Multiply (20c) by $2r$:

$$2rr_t = \frac{r}{\sqrt{E_1(u)}}\int N(u)u_t\,\mathrm{d}x.$$

Then, we obtain

$$(\mu, G\mu) = (Lu, u_t) + 2rr_t = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{2}(u, Lu) + r^2\right) = \frac{\mathrm{d}}{\mathrm{d}t}\widetilde{E}(u,r). \quad \square$$

First order SAV scheme

Gradient flow:

$$
\begin{aligned}
u_t &= G\mu, \\
\mu &= Lu + \frac{r}{\sqrt{E_1(u)}} N(u), \\
r_t &= \frac{1}{2\sqrt{E_1(u)}} \int N(u) u_t \,\mathrm{d}x.
\end{aligned}
$$

First order SAV (SAV1) scheme:

$$\frac{u_{n+1} - u_n}{\Delta t} = G\mu_{n+1}, \tag{22a}$$

$$\mu_{n+1} = Lu_{n+1} + \frac{r_{n+1}}{\sqrt{E_1(u_n)}} N(u_n), \tag{22b}$$

$$\frac{r_{n+1} - r_n}{\Delta t} = \frac{1}{2\sqrt{E_1(u_n)}} \int N(u_n) \frac{u_{n+1} - u_n}{\Delta t} \,\mathrm{d}x. \tag{22c}$$

SAV1 scheme: Unique solvability

For any $\Delta t > 0$, the SAV1 scheme admits a unique solution.

SAV1 scheme (denote $b_n = \dfrac{N(u_n)}{\sqrt{E_1(u_n)}}$):

$$\frac{u_{n+1}-u_n}{\Delta t} = G\mu_{n+1},$$
$$\mu_{n+1} = Lu_{n+1} + r_{n+1}b_n,$$
$$r_{n+1} - r_n = \frac{1}{2}(b_n, u_{n+1}-u_n).$$

Proof. Eliminate μ_{n+1} and r_{n+1}:

$$\frac{u_{n+1}-u_n}{\Delta t} = GLu_{n+1} + r_nGb_n + \frac{1}{2}(b_n, u_{n+1})Gb_n - \frac{1}{2}(b_n, u_n)Gb_n,$$

or equivalently,

$$u_{n+1} - \Delta tGLu_{n+1} - \frac{\Delta t}{2}(b_n, u_{n+1})Gb_n = u_n + \Delta tr_nGb_n - \frac{\Delta t}{2}(b_n, u_n)Gb_n =: c_n.$$

SAV1 scheme: Unique solvability (continued)

$$u_{n+1} - \Delta t G L u_{n+1} - \frac{\Delta t}{2}(b_n, u_{n+1}) G b_n = c_n.$$

Act $(I - \Delta t G L)^{-1}$ on both sides:

$$u_{n+1} - \frac{\Delta t}{2}(b_n, u_{n+1})(I - \Delta t G L)^{-1} G b_n = (I - \Delta t G L)^{-1} c_n.$$

Take the inner product with b_n:

$$(b_n, u_{n+1}) - \frac{\Delta t}{2}(b_n, u_{n+1})(b_n, (I - \Delta t G L)^{-1} G b_n) = (b_n, (I - \Delta t G L)^{-1} c_n),$$

or equivalently,

$$\left[1 - \frac{\Delta t}{2}(b_n, (I - \Delta t G L)^{-1} G b_n)\right](b_n, u_{n+1}) = (b_n, (I - \Delta t G L)^{-1} c_n).$$

Here, $(I - \Delta t G L)^{-1} G = (G^{-1} - \Delta t L)^{-1}$ is negative definite. $\square$

SAV1 scheme: Algorithm

Algorithm: SAV1 scheme

Given u_n, r_n, to compute u_{n+1}, r_{n+1} as follows:

1. Calculate b_n, (b_n, u_n), Gb_n, and c_n;
2. Solve $(I - \Delta t GL)\theta_1 = Gb_n$ and $(I - \Delta t GL)\theta_2 = c_n$ to get θ_1, θ_2;
3. Calculate (b_n, u_{n+1}) by $(b_n, u_{n+1}) = \dfrac{(b_n, \theta_2)}{1 - \frac{\Delta t}{2}(b_n, \theta_1)}$;
4. Calculate u_{n+1} by $u_{n+1} = \dfrac{\Delta t}{2}(b_n, u_{n+1})\theta_1 + \theta_2$;
5. Calculate r_{n+1} by $r_{n+1} = r_n + \dfrac{1}{2}(b_n, u_{n+1}) - \dfrac{1}{2}(b_n, u_n)$.

SAV1 scheme: Energy stability

For any $\Delta t > 0$, we have $E_{n+1} - E_n \leq \Delta t(\mu_{n+1}, G\mu_{n+1}) \leq 0$, where $E_n = \widetilde{E}(u_n, r_n) = \frac{1}{2}(u_n, Lu_n) + r_n^2$.

Proof. Take the inner product of (22a) with $\Delta t \mu_{n+1}$:

$$(\mu_{n+1}, u_{n+1} - u_n) = \Delta t(\mu_{n+1}, G\mu_{n+1}).$$

Take the inner product of (22b) with $u_{n+1} - u_n$:

$$(\mu_{n+1}, u_{n+1} - u_n) = (Lu_{n+1}, u_{n+1} - u_n) + r_{n+1}(b_n, u_{n+1} - u_n).$$

Multiply (22c) by $2r_{n+1}$:

$$2r_{n+1}(r_{n+1} - r_n) = r_{n+1}(b_n, u_{n+1} - u_n).$$

Then, we obtain

$$E_{n+1} - E_n + \frac{1}{2}(L(u_{n+1} - u_n), u_{n+1} - u_n) + (r_{n+1} - r_n)^2 = \Delta t(\mu_{n+1}, G\mu_{n+1}). \qquad \square$$

Second order SAV scheme: SAV-CN

$$
\begin{aligned}
u_t &= G\mu,\\
\mu &= Lu + \frac{r}{\sqrt{E_1(u)}}N(u),\\
r_t &= \frac{1}{2\sqrt{E_1(u)}}\int N(u)u_t\,\mathrm{d}x.
\end{aligned}
$$

Crank-Nicolson-type SAV (SAV-CN) scheme:

$$
\frac{u_{n+1}-u_n}{\Delta t} = G\mu_{n+\frac{1}{2}}, \tag{23a}
$$

$$
\mu_{n+\frac{1}{2}} = \frac{1}{2}L(u_{n+1}+u_n) + \frac{r_{n+1}+r_n}{2\sqrt{E_1(\bar{u}_{n+\frac{1}{2}})}}N(\bar{u}_{n+\frac{1}{2}}), \tag{23b}
$$

$$
\frac{r_{n+1}-r_n}{\Delta t} = \frac{1}{2\sqrt{E_1(\bar{u}_{n+\frac{1}{2}})}}\int N(\bar{u}_{n+\frac{1}{2}})\frac{u_{n+1}-u_n}{\Delta t}\,\mathrm{d}x, \tag{23c}
$$

where $\bar{u}_{n+\frac{1}{2}}$ is an approximation of $u(t_{n+\frac{1}{2}})$ with error $\mathcal{O}(\Delta t^2)$.

Second order SAV scheme: SAV-CN (continued)

Unique solvability

For any $\Delta t > 0$, the SAV-CN scheme admits a unique solution.

Energy stability

For any $\Delta t > 0$, the SAV-CN scheme is energy stable:

$$E_{n+1} - E_n = \Delta t(\mu_{n+1}, G\mu_{n+1}) \leq 0,$$

where $E_n = \widetilde{E}(u_n, q_n) = \frac{1}{2}(u_n, Lu_n) + r_n^2$.

Second order SAV scheme: SAV-BDF2

$$
\begin{aligned}
u_t &= G\mu, \\
\mu &= Lu + \frac{r}{\sqrt{E_1(u)}} N(u), \\
r_t &= \frac{1}{2\sqrt{E_1(u)}} \int N(u) u_t \, \mathrm{d}x.
\end{aligned}
$$

Second order BDF-type SAV (SAV-BDF2) scheme:

$$
\frac{3u_{n+1} - 4u_n + u_{n-1}}{2\Delta t} = G\mu_{n+1}, \tag{24a}
$$

$$
\mu_{n+1} = Lu_{n+1} + \frac{r_{n+1}}{\sqrt{E_1(\bar{u}_{n+1})}} N(\bar{u}_{n+1}), \tag{24b}
$$

$$
\frac{3r_{n+1} - 4r_n + r_{n-1}}{2\Delta t} = \frac{1}{2\sqrt{E_1(\bar{u}_{n+1})}} \int N(\bar{u}_{n+1}) \frac{3u_{n+1} - 4u_n + u_{n-1}}{2\Delta t} \, \mathrm{d}x, \tag{24c}
$$

where $\bar{u}_{n+1}$ is an approximation of $u(t_{n+1})$ with error $\mathcal{O}(\Delta t^2)$.

Second order SAV scheme: SAV-BDF2 (continued)

Unique solvability

For any $\Delta t > 0$*, the SAV-BDF2 scheme admits a unique solution.*

Energy stability

For any $\Delta t > 0$*, the SAV-BDF2 scheme is energy stable:*

$$E_{n+1} - E_n \leq \Delta t(\mu_{n+1}, G\mu_{n+1}) \leq 0,$$

where

$$E_n = \frac{1}{4}\big((u_n, Lu_n) + (2u_n - u_{n-1}, L(2u_n - u_{n-1}))\big) + \frac{1}{2}\big(r_n^2 + (2r_n - r_{n-1})^2\big).$$

References for SAV schemes:

- Shen-Xu-Yang, *J. Comput. Phys.*, 2017.
- Shen-Xu-Yang, *arXiv:1710.01331v1*, 2017.

Example 1. Fractional Cahn-Hilliard equation

Consider the fractional Cahn-Hilliard equation

$$u_t = -(-\Delta)^\alpha\left(-\Delta u + \frac{1}{\varepsilon^2}(u^3 - u)\right), \quad 0 \le \alpha \le 1, \tag{25}$$

which is the $H^{-\alpha}$ gradient flow of the energy

$$E(u) = \int \left(\frac{1}{2}|\nabla u|^2 + \frac{1}{4\varepsilon^2}(u^2 - 1)^2\right) \mathrm{d}x. \tag{26}$$

We write the energy (26) in the form (8) by specifying

$$G = -(-\Delta)^\alpha, \quad L = -\Delta + \frac{S}{\varepsilon^2}, \quad E_1(u) = \frac{1}{4\varepsilon^2}\int (u^2 - 1 - S)^2 \,\mathrm{d}x,$$

where $S > 0$ is a constant. Then, we have

$$N(u) = \frac{\delta E_1}{\delta u} = \frac{1}{\varepsilon^2} u(u^2 - 1 - S).$$

Example 2. No-slope-selection epitaxial growth

Consider the L^2 gradient flow of the energy

$$E(u) = \int \left(-\frac{1}{2}\ln(1+|\nabla u|^2) + \frac{\varepsilon^2}{2}|\Delta u|^2 \right) \mathrm{d}x. \tag{27}$$

- IEQ method cannot be used.
- $\forall \alpha_0 > 0$, $\exists C_0 > 0$ s.t. $\forall \alpha \geq \alpha_0$, it holds

$$\int \left(-\frac{1}{2}\ln(1+|\nabla u|^2) + \frac{\alpha}{2}|\Delta u|^2 \right) \mathrm{d}x \geq -C_0.$$

Choosing $\alpha \in (\alpha_0, \varepsilon^2)$, we write the energy (27) in the form (8) by specifying $G = -I$, $L = (\varepsilon^2 - \alpha)\Delta^2$, and

$$E_1(u) = \int \left(-\frac{1}{2}\ln(1+|\nabla u|^2) + \frac{\alpha}{2}|\Delta u|^2 \right) \mathrm{d}x.$$

Outline

Outline

From PDE to ODE system

Consider the PDE for a scalar function $u : \overline{\Omega} \times [0, \infty) \to \mathbb{R}$ as

$$u_t = \mathcal{L}u + \mathcal{N}(u), \tag{28}$$

where

- $\mathcal{L}$ is a linear, self-adjoint, and negative definite operator;
- $\mathcal{N}$ denotes a generic nonlinear term.

Discretizing the PDE (28) in spatial variables (for instance, by spectral or finite difference approximations) often leads to a system of ODEs:

$$u_t + \boldsymbol{L}u = \boldsymbol{N}(u). \tag{29}$$

Note that $\boldsymbol{L}$ is symmetric, so could be diagonalized.

A single ODE: Exponential integration

The model ODE is

$$u' + cu = F(u). \tag{30}$$

Multiply (30) by the integrating factor e^{ct}:

$$(\mathrm{e}^{ct}u)' = \mathrm{e}^{ct}F(u).$$

Integrate the above from t_n to $t_{n+1} = t_n + \Delta t$:

$$\begin{aligned}\mathrm{e}^{ct_{n+1}}u(t_{n+1}) &= \mathrm{e}^{ct_n}u(t_n) + \int_{t_n}^{t_{n+1}} \mathrm{e}^{ct}F(u(t))\,\mathrm{d}t \\ &= \mathrm{e}^{ct_n}u(t_n) + \mathrm{e}^{ct_n}\int_0^{\Delta t} \mathrm{e}^{cs}F(u(t_n+s))\,\mathrm{d}s.\end{aligned}$$

Multiply $\mathrm{e}^{-ct_{n+1}}$ on both sides:

$$u(t_{n+1}) = \mathrm{e}^{-c\Delta t}u(t_n) + \mathrm{e}^{-c\Delta t}\int_0^{\Delta t} \mathrm{e}^{cs}F(u(t_n+s))\,\mathrm{d}s. \tag{31}$$

First order ETD scheme

$$u(t_{n+1}) = \mathrm{e}^{-c\Delta t} u(t_n) + \mathrm{e}^{-c\Delta t} \int_0^{\Delta t} \mathrm{e}^{cs} F(u(t_n + s))\, \mathrm{d}s. \tag{31}$$

This formula is exact.

The essence of the ETD methods is *to approximate the integral*.

First order ETD scheme

$$u(t_{n+1}) = \mathrm{e}^{-c\Delta t} u(t_n) + \mathrm{e}^{-c\Delta t} \int_0^{\Delta t} \mathrm{e}^{cs} F(u(t_n + s))\, \mathrm{d}s. \tag{31}$$

This formula is exact.

The essence of the ETD methods is *to approximate the integral.*

We denote by u_n the approximation to $u(t_n)$ and write $F_n = F(u_n)$.

First order ETD (ETD1) scheme

Using the first order approximation of F, that is, assuming that F is constant, $F = F_n + \mathcal{O}(\Delta t)$, *in* $[t_n, t_{n+1}]$, *we obtain the ETD1 scheme*

$$u_{n+1} = \mathrm{e}^{-c\Delta t} u_n + \Delta t \phi_0(c\Delta t) F_n,$$

where $\phi_0(a) = \frac{1-\mathrm{e}^{-a}}{a}$.

Remark. In the limit $c \to 0$,

$$\text{the ETD1 scheme} \quad \longrightarrow \quad u_{n+1} = u_n + \Delta t F_n.$$

Second order ETD multistep scheme

$$u(t_{n+1}) = \mathrm{e}^{-c\Delta t} u(t_n) + \mathrm{e}^{-c\Delta t} \int_0^{\Delta t} \mathrm{e}^{cs} F(u(t_n + s))\,\mathrm{d}s. \qquad (31)$$

Second order ETD multistep (ETDMs2) scheme

Assuming that F *is linear,* $F = F_n + \frac{F_n - F_{n-1}}{\Delta t}(t - t_n) + \mathcal{O}(\Delta t^2)$, *we obtain the ETDMs2 scheme*

$$u_{n+1} = \mathrm{e}^{-c\Delta t} u_n + \frac{(1 - c\Delta t)\mathrm{e}^{-c\Delta t} - 1 + 2c\Delta t}{c^2 \Delta t} F_n + \frac{-\mathrm{e}^{-c\Delta t} + 1 - c\Delta t}{c^2 \Delta t} F_{n-1}.$$

Remark. In the limit $c \to 0$,

the ETDMs2 scheme $\longrightarrow$ $u_{n+1} = u_n + \Delta t\left(\frac{3}{2}F_n - \frac{1}{2}F_{n-1}\right).$

Second order ETD Runge-Kutta scheme

$$u(t_{n+1}) = \mathrm{e}^{-c\Delta t}u(t_n) + \mathrm{e}^{-c\Delta t}\int_0^{\Delta t} \mathrm{e}^{cs}F(u(t_n+s))\,\mathrm{d}s. \tag{31}$$

Second order ETD Runge-Kutta (ETDRK2) scheme

First, use the ETD1 scheme to generate

$$\tilde{u}_{n+1} = \mathrm{e}^{-c\Delta t}u_n + \frac{1-\mathrm{e}^{-c\Delta t}}{c}F_n.$$

Assuming that F is linear, $F = F_n + \dfrac{F(\tilde{u}_{n+1}) - F_n}{\Delta t}(t-t_n) + \mathcal{O}(\Delta t^2)$, *we obtain the ETDRK2 scheme*

$$u_{n+1} = \tilde{u}_{n+1} + \frac{\mathrm{e}^{-c\Delta t} - 1 + c\Delta t}{c^2\Delta t}(F(\tilde{u}_{n+1}) - F_n).$$

A system of ODEs: Exponential integration

The model system of ODEs:

$$u_t + \boldsymbol{L}u = \boldsymbol{N}(u). \tag{29}$$

Pre-multiply (29) by the integrating factor $\mathrm{e}^{\boldsymbol{L}t}$:

$$(\mathrm{e}^{\boldsymbol{L}t}u)' = \mathrm{e}^{\boldsymbol{L}t}\boldsymbol{N}(u).$$

Integrate the above from t_n to $t_{n+1} = t_n + \Delta t$:

$$\begin{aligned} \mathrm{e}^{\boldsymbol{L}t_{n+1}}u(t_{n+1}) &= \mathrm{e}^{\boldsymbol{L}t_n}u(t_n) + \int_{t_n}^{t_{n+1}} \mathrm{e}^{\boldsymbol{L}t}\boldsymbol{N}(u(t))\,\mathrm{d}t \\ &= \mathrm{e}^{\boldsymbol{L}t_n}u(t_n) + \mathrm{e}^{\boldsymbol{L}t_n}\int_0^{\Delta t} \mathrm{e}^{\boldsymbol{L}s}\boldsymbol{N}(u(t_n+s))\,\mathrm{d}s. \end{aligned}$$

Pre-multiply $\mathrm{e}^{-\boldsymbol{L}t_{n+1}}$ on both sides:

$$u(t_{n+1}) = \mathrm{e}^{-\boldsymbol{L}\Delta t}u(t_n) + \mathrm{e}^{-\boldsymbol{L}\Delta t}\int_0^{\Delta t} \mathrm{e}^{\boldsymbol{L}s}\boldsymbol{N}(u(t_n+s))\,\mathrm{d}s. \tag{32}$$

First order ETD scheme

$$u(t_{n+1}) = \mathrm{e}^{-\boldsymbol{L}\Delta t}u(t_n) + \int_0^{\Delta t} \mathrm{e}^{-\boldsymbol{L}(\Delta t - s)}\boldsymbol{N}(u(t_n+s))\,\mathrm{d}s. \tag{32}$$

The essence of the ETD methods is *to approximate the integral*.

We denote by u_n the approximation of $u(t_n)$.

- approximate $\boldsymbol{N}(u(t_n+s)) \approx \boldsymbol{N}(u(t_n))$ in $s \in [0, \Delta t]$;
- calculate the integral exactly.

ETD1 scheme

$$u_{n+1} = \mathrm{e}^{-\boldsymbol{L}\Delta t}u_n + \Delta t\phi_0(\boldsymbol{L}\Delta t)\boldsymbol{N}(u_n),$$

where

$$\phi_0(\boldsymbol{L}\Delta t) = \int_0^{\Delta t} \mathrm{e}^{-\boldsymbol{L}(\Delta t - s)}\,\mathrm{d}s = (\boldsymbol{L}\Delta t)^{-1}(\boldsymbol{I} - \mathrm{e}^{-\boldsymbol{L}\Delta t}).$$

First order ETD scheme (continued)

ETD1 scheme

$$u_{n+1} = \mathrm{e}^{-\boldsymbol{L}\Delta t} u_n + \Delta t (\boldsymbol{L}\Delta t)^{-1} (\boldsymbol{I} - \mathrm{e}^{-\boldsymbol{L}\Delta t}) \boldsymbol{N}(u_n).$$

Act $\mathrm{e}^{\boldsymbol{L}\Delta t}$ on both sides of ETD1:

$$\mathrm{e}^{\boldsymbol{L}\Delta t} u_{n+1} = u_n + \Delta t (\boldsymbol{L}\Delta t)^{-1} (\mathrm{e}^{\boldsymbol{L}\Delta t} - \boldsymbol{I}) \boldsymbol{N}(u_n).$$

If we approximate $\mathrm{e}^{\boldsymbol{L}\Delta t} \approx \boldsymbol{I} + \boldsymbol{L}\Delta t$, then we obtain

$$(\boldsymbol{I} + \boldsymbol{L}\Delta t) u_{n+1} = u_n + \Delta t \boldsymbol{N}(u_n),$$

that is, the first order semi-implicit scheme of (29):

$$\frac{u_{n+1} - u_n}{\Delta t} + \boldsymbol{L} u_{n+1} = \boldsymbol{N}(u_n).$$

Second order ETD multistep scheme

$$u(t_{n+1}) = \mathrm{e}^{-\boldsymbol{L}\Delta t} u(t_n) + \int_0^{\Delta t} \mathrm{e}^{-\boldsymbol{L}(\Delta t - s)} \boldsymbol{N}(u(t_n + s))\, \mathrm{d}s. \tag{32}$$

We denote by u_n the approximation of $u(t_n)$.

- approximate $\boldsymbol{N}(u(t_n + s)) \approx \left(1 + \frac{s}{\Delta t}\right)\boldsymbol{N}(u(t_n)) - \frac{s}{\Delta t}\boldsymbol{N}(u(t_{n-1}))$, $s \in [-\Delta t, \Delta t]$;
- calculate the integral exactly.

ETDMs2 scheme

$$\begin{aligned} u_{n+1} &= \mathrm{e}^{-\boldsymbol{L}\Delta t} u_n + \Delta t[(\phi_0 + \phi_1)(\boldsymbol{L}\Delta t)\boldsymbol{N}(u_n) - \phi_1(\boldsymbol{L}\Delta t)\boldsymbol{N}(u_{n-1})] \\ &= \mathrm{e}^{-\boldsymbol{L}\Delta t} u_n + \Delta t\{\phi_0(\boldsymbol{L}\Delta t)\boldsymbol{N}(u_n) + \phi_1(\boldsymbol{L}\Delta t)[\boldsymbol{N}(u_n) - \boldsymbol{N}(u_{n-1})]\}, \end{aligned}$$

where

$$\phi_1(\boldsymbol{L}\Delta t) = \int_0^{\Delta t} \frac{s}{\Delta t} \mathrm{e}^{-\boldsymbol{L}(\Delta t - s)}\, \mathrm{d}s = (\boldsymbol{L}\Delta t)^{-2}(\boldsymbol{L}\Delta t - \boldsymbol{I} + \mathrm{e}^{-\boldsymbol{L}\Delta t}).$$

Second order ETD Runge-Kutta scheme

$$u(t_{n+1}) = \mathrm{e}^{-L\Delta t}u(t_n) + \int_0^{\Delta t} \mathrm{e}^{-L(\Delta t - s)} N(u(t_n + s))\,\mathrm{d}s. \tag{32}$$

We denote by u_n the approximation of $u(t_n)$.

- approximate
  $N(u(t_n + s)) \approx \left(1 - \frac{s}{\Delta t}\right) N(u(t_n)) + \frac{s}{\Delta t} N(u(t_{n+1}))$, $s \in [0, \Delta t]$,
  where $u(t_{n+1})$ is approximated by the ETD1 method;
- calculate the integral exactly.

ETDRK2 scheme

$$\begin{aligned}
\tilde{u}_{n+1} &= \mathrm{e}^{-L\Delta t}u_n + \Delta t \phi_0(L\Delta t) N(u_n),\\
u_{n+1} &= \mathrm{e}^{-L\Delta t}u_n + \Delta t[(\phi_0 - \phi_1)(L\Delta t)N(u_n) + \phi_1(L\Delta t)N(\tilde{u}_{n+1})]\\
&= \mathrm{e}^{-L\Delta t}u_n + \Delta t\{\phi_0(L\Delta t)N(u_n) + \phi_1(L\Delta t)[N(\tilde{u}_{n+1}) - N(u_n)]\}.
\end{aligned}$$

Outline

Allen-Cahn equation

Initial-boundary-value problem of the Allen-Cahn equation:

$$\begin{aligned} u_t - \varepsilon^2 u_{xx} + u^3 - u = 0, &\quad x \in (0, X),\ t \in (0, T], \\ u(\cdot, t) \text{ is } X\text{-periodic}, &\quad t \in [0, T], \\ u(x, 0) = u_0(x), &\quad x \in [0, X]. \end{aligned}$$

Energy functional:

$$E(u) = \int_{(0,X)} \left(\frac{\varepsilon^2}{2} u_x^2 + \frac{1}{4}(u^2 - 1)^2 \right) \mathrm{d}x.$$

We consider

- finite difference method for spatial discretization;
- ETD1 and ETDRK2 methods for temporal integration;
- energy stability for the fully discrete ETD1 scheme.

Spatial discretization: Finite difference method

We use the *central finite difference* to approximate the Laplacian.

- $h = X/N_x$: uniform mesh size;
- $\{x_j = jh : 0 \leq j \leq N_x\}$: nodes on $[0, X]$;
- D_h: the discrete matrix of the Laplacian operator.

Under the periodic boundary conditions, the matrix D_h is given by

$$D_h = \frac{1}{h^2} \begin{pmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ 1 & & & 1 & -2 \end{pmatrix} \in \mathbb{R}^{N_x \times N_x}.$$

The discrete matrix D_h is symmetric and negative semi-definite.

Spatial discretization: Finite difference method (continued)

The space-discrete scheme: find $v : [0, T] \to \mathbb{R}^{N_x}$ such that

$$\begin{cases} \dfrac{\mathrm{d}v}{\mathrm{d}t} = \varepsilon^2 D_h v + v - v^{.3}, & t \in (0, T], \\ v(0) = v_0. \end{cases}$$

Introduce a stabilizing parameter $S > 0$ and define

$$L_h := -\varepsilon^2 D_h + SI, \qquad f(v) := Sv + v - v^{.3}.$$

Then, we obtain

$$\frac{\mathrm{d}v}{\mathrm{d}t} + L_h v = f(v),$$

whose solution satisfies

$$v(t + \Delta t) = \mathrm{e}^{-L_h \Delta t} v(t) + \int_0^{\Delta t} \mathrm{e}^{-L_h(\Delta t - s)} f(v(t + s))\, \mathrm{d}s.$$

We know L_h is symmetric and positive definite.

ETD methods for the temporal integration

Setting

- $\Delta t = T/N_t$: uniform time step;
- $t_n = n\Delta t$: nodes in the time interval $[0, T]$.

At the time level $t = t_n$, we have

$$v(t_{n+1}) = \mathrm{e}^{-L_h\Delta t} v(t_n) + \int_0^{\Delta t} \mathrm{e}^{-L_h(\Delta t - s)} f(v(t_n + s))\,\mathrm{d}s. \tag{33}$$

- approximate $f(v(t_n + s))$ by $f(v(t_n))$ in $s \in [0, \Delta t]$,
- calculate the integral exactly.

We obtain the *first order ETD scheme*:

$$\begin{aligned} v^{n+1} &= \mathrm{e}^{-L_h\Delta t} v^n + \int_0^{\Delta t} \mathrm{e}^{-L_h(\Delta t - s)} f(v^n)\,\mathrm{d}s \\ &= \mathrm{e}^{-L_h\Delta t} v^n + \Delta t (L_h\Delta t)^{-1}(I - \mathrm{e}^{-L_h\Delta t}) f(v^n). \end{aligned} \tag{ETD1}$$

ETD methods for the temporal integration (continued)

At the time level $t = t_n$:

$$v(t_{n+1}) = \mathrm{e}^{-L_h \Delta t} v(t_n) + \int_0^{\Delta t} \mathrm{e}^{-L_h(\Delta t - s)} f(v(t_n + s))\, \mathrm{d}s. \tag{33}$$

- approximate $f(v(t_n + s))$ by a linear interpolation based on $f(v(t_n))$ and $f(v(t_{n+1}))$,

We obtain the *second order ETD Runge-Kutta scheme*:

$$\begin{cases} \widetilde{v}^{n+1} = \mathrm{e}^{-L_h \Delta t} v^n + \int_0^{\Delta t} \mathrm{e}^{-L_h(\Delta t - s)} f(v^n)\, \mathrm{d}s, \\ v^{n+1} = \mathrm{e}^{-L_h \Delta t} v^n + \int_0^{\Delta t} \mathrm{e}^{-L_h(\Delta t - s)} \left[\left(1 - \frac{s}{\Delta t}\right) f(v^n) + \frac{s}{\Delta t} f(\widetilde{v}^{n+1}) \right] \mathrm{d}s. \end{cases} \tag{ETDRK2}$$

Properties of matrix functions

Lemma: Properties of matrix functions

Given a symmetric matrix $M \in \mathbb{R}^{d\times d}$, let ϕ be defined on the spectrum of M, i.e., the values $\{\phi(\lambda_i) : 1 \leq i \leq d\}$ exist, where $\{\lambda_i\}_{i=1}^d$ are the eigenvalues of M. Then

1. *$\phi(M)$ commutes with M;*
2. *$\phi(M^T) = \phi(M)^T$;*
3. *the eigenvalues of $\phi(M)$ are $\phi(\lambda_i)$, $1 \leq i \leq d$;*
4. *$\phi(P^{-1}MP) = P^{-1}\phi(M)P$ for any nonsingular $P \in \mathbb{R}^{d\times d}$.*

Example

If $\phi(s) > 0$ for any $s \in \mathbb{R}$, then for any symmetric matrix $M \in \mathbb{R}^{d\times d}$, the matrix $\phi(M)$ is always symmetric and positive definite.

Implementations of matrix exponentials

Letting

$$\phi_{-1}(a) = \mathrm{e}^{-a}, \quad \phi_0(a) = \frac{1-\mathrm{e}^{-a}}{a}, \quad \phi_1(a) = \frac{\mathrm{e}^{-a}-1+a}{a^2},$$

we could write the ETD1 scheme as

$$v^{n+1} = \phi_{-1}(L_h\Delta t)v^n + \Delta t\phi_0(L_h\Delta t)f(v^n),$$

and the ETDRK2 scheme as

$$\begin{cases} \widetilde{v}^{n+1} = \phi_{-1}(L_h\Delta t)v^n + \Delta t\phi_0(L_h\Delta t)f(v^n), \\ v^{n+1} = \phi_{-1}(L_h\Delta t)v^n + \Delta t(\phi_0 - \phi_1)(L_h\Delta t)f(v^n) + \Delta t\phi_1(L_h\Delta t)f(\widetilde{v}^{n+1}). \end{cases}$$

The actions of exponentials $\phi_\gamma(L_h\Delta t)$ can be implemented efficiently.

Implementations of matrix exponentials (continued)

The exponentials $\phi_\gamma(L_h \Delta t)$ can be implemented by FFT.

Since $L_h = -\varepsilon^2 D_h + SI$ is self-adjoint and positive definite, we have $L_h = P^{-1}\widehat{L}_h P$, where

$$(\widehat{L}_h \hat{f})_k = \lambda_k \hat{f}_k,$$

where $\{\lambda_k\}$ are the eigenvalues of L_h, that is,

$$\lambda_k = \frac{4\varepsilon^2}{h^2} \sin^2 \frac{k\pi}{N_x} + S > 0.$$

Then, we have

$$\phi_\gamma(L_h \Delta t) = P^{-1} \phi_\gamma(\widehat{L}_h \Delta t) P, \quad (\phi_\gamma(\widehat{L}_h \Delta t)\hat{f})_k = \phi_\gamma(\lambda_k \Delta t)\hat{f}_k.$$

P and P^{-1} can be implemented by FFT and iFFT, respectively, so the computational complexity is $\mathcal{O}(N \log N)$ per time step.

Energy stability of the ETD1 scheme

Energy functional:

$$E(u)=\int_\Omega F(u)\,\mathrm{d}x-\frac{\varepsilon^2}{2}(u,u_{xx}),\quad F(u)=\frac{1}{4}(u^2-1)^2.$$

Define the discretized energy E_h:

$$E_h(v)=\sum_{i=1}^{N_x}F(v_i)-\frac{\varepsilon^2}{2}v^TD_hv. \tag{34}$$

Theorem: Energy stability of the ETD1 scheme

Assume that $K:=\|F''\|_{L^\infty}$ *and* $S\geq\frac{K}{2}$. *For any* $\Delta t>0$, *we have*

$$E_h(v^{n+1})\leq E_h(v^n).$$

Energy stability of the ETD1 scheme (continued)

$$E_h(v) = \sum_{i=1}^{N_x} F(v_i) - \frac{\varepsilon^2}{2} v^T D_h v, \qquad f(v) = Sv - F'(v), \quad L_h = S - \varepsilon^2 D_h.$$

Proof. **Step 1.** Direct calculations:

$$E_h(v^{n+1}) - E_h(v^n) = \sum_{i=1}^{N_x} [F(v_i^{n+1}) - F(v_i^n)] - \frac{\varepsilon^2}{2}[(v^{n+1})^T D_h v^{n+1} - (v^n)^T D_h v^n].$$

We have

$$F(v_i^{n+1}) - F(v_i^n) = F'(v_i^n)(v_i^{n+1} - v_i^n) + \frac{1}{2}F''(\xi)(v_i^{n+1} - v_i^n)^2,$$

then, since $S \geq \frac{1}{2}F''(\xi)$,

$$\sum_{i=1}^{N_x} [F(v_i^{n+1}) - F(v_i^n)] \leq (v^{n+1} - v^n)^T F'(v^n) + S(v^{n+1} - v^n)^T (v^{n+1} - v^n)$$

$$= S(v^{n+1} - v^n)^T v^{n+1} - (v^{n+1} - v^n)^T f(v^n).$$

Energy stability of the ETD1 scheme (continued)

$$E_h(v^{n+1}) - E_h(v^n) = \sum_{i=1}^{N_x}[F(v_i^{n+1}) - F(v_i^n)] - \frac{\varepsilon^2}{2}[(v^{n+1})^T D_h v^{n+1} - (v^n)^T D_h v^n].$$

$$\sum_{i=1}^{N_x}[F(v_i^{n+1}) - F(v_i^n)] \leq S(v^{n+1} - v^n)^T v^{n+1} - (v^{n+1} - v^n)^T f(v^n).$$

Direct calculations (using $2a(a-b) = a^2 - b^2 + (a-b)^2$):

$$\begin{aligned} & -\frac{\varepsilon^2}{2}[(v^{n+1})^T D_h v^{n+1} - (v^n)^T D_h v^n] \\ = & -\varepsilon^2 (v^{n+1} - v^n)^T D_h v^{n+1} + \frac{\varepsilon^2}{2}(v^{n+1} - v^n)^T D_h (v^{n+1} - v^n) \\ \leq & -\varepsilon^2 (v^{n+1} - v^n)^T D_h v^{n+1} \end{aligned}$$

Then,

$$E_h(v^{n+1}) - E_h(v^n) \leq (v^{n+1} - v^n)^T (L_h v^{n+1} - f(v^n)).$$

Energy stability of the ETD1 scheme (continued)

$$v^{n+1} = \mathrm{e}^{-L_h\Delta t}v^n + L_h^{-1}(I - \mathrm{e}^{-L_h\Delta t})f(v^n). \qquad \text{(ETD1)}$$

$$E_h(v^{n+1}) - E_h(v^n) \le (v^{n+1} - v^n)^T(L_h v^{n+1} - f(v^n)).$$

Step 2. Solve $f(v^n)$ from (ETD1):

$$\begin{aligned} f(v^n) &= (I - \mathrm{e}^{-L_h\Delta t})^{-1}L_h(v^{n+1} - \mathrm{e}^{-L_h\Delta t}v^n) \\ &= (I - \mathrm{e}^{-L_h\Delta t})^{-1}L_h(v^{n+1} - v^n + (I - \mathrm{e}^{-L_h\Delta t})v^n) \\ &= (I - \mathrm{e}^{-L_h\Delta t})^{-1}L_h(v^{n+1} - v^n) + L_h v^n, \end{aligned}$$

and then,

$$\begin{aligned} L_h v^{n+1} - f(v^n) &= L_h(v^{n+1} - v^n) - (I - \mathrm{e}^{-L_h\Delta t})^{-1}L_h(v^{n+1} - v^n) \\ &= \Delta t^{-1}B_1(v^{n+1} - v^n), \end{aligned}$$

where $B_1 := L_h\Delta t - (I - \mathrm{e}^{-L_h\Delta t})^{-1}L_h\Delta t$. Then, we obtain

$$E_h(v^{n+1}) - E_h(v^n) \le \Delta t^{-1}(v^{n+1} - v^n)^T B_1(v^{n+1} - v^n).$$

Energy stability of the ETD1 scheme (continued)

We have obtained

$$E_h(v^{n+1}) - E_h(v^n) \le \Delta t^{-1}(v^{n+1} - v^n)^T B_1(v^{n+1} - v^n),$$

where $B_1 = L_h\Delta t - (I - \mathrm{e}^{-L_h\Delta t})^{-1} L_h\Delta t$.

Define a function

$$g_1(a) := a - \frac{a}{1 - \mathrm{e}^{-a}}, \quad a \neq 0,$$

then $B_1 = g_1(L_h\Delta t)$. Since

- $g_1(a) < 0$ for any $a > 0$,
- $L_h\Delta t$ is symmetric and positive definite,

we know that B_1 is symmetric and negative definite. So,

$$E_h(v^{n+1}) - E_h(v^n) \le \Delta t^{-1}(v^{n+1} - v^n)^T B_1(v^{n+1} - v^n) \le 0. \quad \square$$

Remarks

Recall the condition for the energy stability:

$$\textit{Assume that } K := \|F''\|_{L^\infty} \textit{ and } S \geq \frac{K}{2}.$$

Theoretically, we need to check whether K exists and is finite or not.

- Another topic on the *maximum principle preserving* schemes;
- For some special model, S could be a genetic constant independent on the solution, see the next example.

Outline

No-slope-selection epitaxial growth model

Initial-boundary-value problem:

$$\begin{aligned} & u_t + \varepsilon^2 u_{xxxx} + \left(\frac{u_x}{1+u_x^2} \right)_x = 0, \quad (x,t) \in (0, 2\pi) \times (0, T], \\ & u(\cdot, t) \text{ is } 2\pi\text{-periodic}, \quad t \in [0, T], \\ & u(x, 0) = u_0(x), \quad x \in [0, 2\pi]. \end{aligned}$$

Energy functional:

$$E(u) = \int_{(0,2\pi)} \left(\frac{\varepsilon^2}{2} u_{xx}^2 - \frac{1}{2} \ln(1 + u_x^2) \right) \mathrm{d}x.$$

We consider

- pseudo-spectral method for spatial discretization;
- ETD1 and ETDMs2 methods for temporal integration;
- energy stability for the fully discrete ETD1 scheme.

Linear convex splitting of the energy functional

Consider a splitting of the form $E(u) = E_c(u) - E_e(u)$ as

$$E(u) = \int \left(\frac{A}{2}u_x^2 + \frac{\varepsilon^2}{2}u_{xx}^2\right) \mathrm{d}x - \int \left(\frac{A}{2}u_x^2 + \frac{1}{2}\ln(1+u_x^2)\right) \mathrm{d}x,$$

where $A > 0$ is expected to be as small as possible.

- The convexity of $E_c(u)$ is obvious when $A > 0$.
- The convexity of $E_e(u)$ comes from the convexity of

$$G(a) := \frac{A}{2}a^2 + \frac{1}{2}\ln(1+a^2), \quad a \in \mathbb{R}.$$

Existence of the linear convex splitting

The function $G(a)$ is convex in $\mathbb{R}$ if and only if $A \geq \frac{1}{8}$.

Linear convex splitting of the energy functional (continued)

Letting $A \geq \frac{1}{8}$ be the stabilizer.

Rewrite the model equation as the splitting form:

$$u_t + \varepsilon^2 u_{xxxx} - A u_{xx} = -\left(\frac{u_x}{1+u_x^2}\right)_x - A u_{xx}.$$

Due to the periodic boundary condition, we have

$$\int u(x,t)\,\mathrm{d}x = \int u_0(x)\,\mathrm{d}x, \quad t \in (0,T].$$

Without loss of generality, we assume that the mean of u is zero.

Spatial discretization: Pseudo-spectral method

Use the *pseudo-spectral method* to approximate spatial derivatives.

- $h = 2\pi/N_x$: uniform mesh size;
- $\Omega_h = \{x_j = jh : 0 \le j \le N_x\}$: nodes on $[0, 2\pi]$;
- $\mathcal{M} = \{f : \Omega_h \to \mathbb{R}\}$: set of all grid functions;
- $\mathcal{M}_0 = \{f \in \mathcal{M} : \sum_i f_i = 0\}$;
- D_h: the discrete differentiation operator;
- $\Delta_h = D_h^2$: the discrete Laplacian operator.

Recall that

$$\mathcal{F}[u_x](k) = \mathrm{i}k\mathcal{F}[u](k), \quad \mathcal{F}\text{: Fourier transform.}$$

Spatial discretization: Pseudo-spectral method (continued)

For $f \in \mathcal{M}_0$, define the discrete Fourier transform $\hat{f} = Pf$ by

$$\hat{f}_k = \frac{1}{N_x} \sum_{i=1}^{N_x} f_i \mathrm{e}^{-\mathrm{i}kx_i}, \quad -\frac{N_x}{2} + 1 \le k \le \frac{N_x}{2},$$

and f can be reconstructed via $f = P^{-1}\hat{f}$ given by

$$f_i = \sum_{k=-\frac{N_x}{2}+1}^{\frac{N_x}{2}} \hat{f}_k \mathrm{e}^{\mathrm{i}kx_i}, \quad 1 \le i \le N_x.$$

For the discrete version, we can define the operator D_h by

$$D_h v = P^{-1}\widehat{D}_h P v, \quad v \in \mathcal{M},$$

where P denotes the discrete Fourier transform, and

$$(\widehat{D}_h \hat{v})_k = \mathrm{i}k\hat{v}_k, \quad \hat{v} = Pv.$$

Spatial discretization: Pseudo-spectral method (continued)

Note that

- $\mathcal{M}_0 = \{f \in \mathcal{M} : \hat{f}_0 = 0\}$.
- $D_h v = 0$ for $v \in \mathcal{M}$ with $v_i = 1$ $(1 \leq i \leq N_x)$.

In fact, for (i),

$$\hat{f}_0 = \frac{1}{N_x} \sum_{i=1}^{N_x} f_i.$$

For (ii), we have $\hat{v}_0 = 1$ and for $k \neq 0$,

$$\hat{v}_k = \frac{1}{N_x} \sum_{j=1}^{N_x} (\mathrm{e}^{-\mathrm{i}jh})^k = \frac{1}{N_x} \cdot \frac{\mathrm{e}^{-\mathrm{i}jh}(1 - (\mathrm{e}^{-\mathrm{i}jh})^{N_x})}{1 - \mathrm{e}^{-\mathrm{i}jh}} = 0.$$

So, $(\widehat{D}_h \hat{v})_k = 0$ for any k, and then $D_h v = 0$.

Spatial discretization: Pseudo-spectral method (continued)

The space-discrete scheme: find $v : [0, T] \to \mathbb{R}^{N_x}$ such that

$$\begin{cases} \dfrac{\mathrm{d}v}{\mathrm{d}t} + \varepsilon^2 \Delta_h^2 v - A\Delta_h v = -D_h\left(\dfrac{D_h v}{1 + |D_h v|^2}\right) - A\Delta_h v, \quad t \in (0, T], \\ v(0) = v_0. \end{cases}$$

Define

$$L_h := \varepsilon^2 \Delta_h^2 - A\Delta_h, \qquad f(v) := D_h\left(\frac{D_h v}{1 + |D_h v|^2}\right) + A\Delta_h v.$$

Then, we obtain

$$\frac{\mathrm{d}v}{\mathrm{d}t} + L_h v = -f(v),$$

whose solution satisfies

$$v(t + \Delta t) = \mathrm{e}^{-L_h \Delta t} v(t) - \int_0^{\Delta t} \mathrm{e}^{-L_h(\Delta t - s)} f(v(t + s))\,\mathrm{d}s.$$

We know L_h is symmetric and positive definite since v is mean-zero.

ETD methods for the temporal integration

Setting

- $\Delta t = T/N_t$: uniform time step;
- $t_n = n\Delta t$: nodes in the time interval $[0, T]$.

At the time level $t = t_n$, we have

$$v(t_{n+1}) = \mathrm{e}^{-L_h \Delta t} v(t_n) - \int_0^{\Delta t} \mathrm{e}^{-L_h(\Delta t - \tau)} f(v(t_n + s))\, \mathrm{d}s.$$

We need to approximate the time integration.

ETD methods for the temporal integration (continued)

At the time level $t = t_n$, we have

$$v(t_{n+1}) = \mathrm{e}^{-L_h \Delta t} v(t_n) - \int_0^{\Delta t} \mathrm{e}^{-L_h(\Delta t - s)} f(v(t_n + s))\, \mathrm{d}s.$$

- approximating $f(v(t_n + s))$ by $f(v(t_n))$ in $s \in [0, \Delta t]$,
- calculating the integral exactly.

We obtain the *first order ETD scheme*:

$$\begin{aligned} u^{n+1} &= \mathrm{e}^{-L_h \Delta t} u^n - \int_0^{\Delta t} \mathrm{e}^{-L_h(\Delta t - s)} f(u^n)\, \mathrm{d}s \\ &= \mathrm{e}^{-L_h \Delta t} u^n - L_h^{-1}(I - \mathrm{e}^{-L_h \Delta t}) f(u^n). \end{aligned} \qquad \text{(ETD1)}$$

Mean-zero conservation: $\sum_i u_i^{n+1} = \sum_i u_i^n$.

ETD methods for the temporal integration (continued)

ETD1 scheme: $u^{n+1} = \mathrm{e}^{-L_h \Delta t} u^n - L_h^{-1}(I - \mathrm{e}^{-L_h \Delta t}) f(u^n)$.

Mean-zero conservation: $\sum_i u_i^{n+1} = \sum_i u_i^n$.

Proof. We obtain from (ETD1) that

$$\begin{aligned} u^{n+1} - u^n &= -(I - \mathrm{e}^{-L_h \Delta t}) u^n - L_h^{-1}(I - \mathrm{e}^{-L_h \Delta t}) f(u^n) \\ &= -(I - \mathrm{e}^{-L_h \Delta t})(u^n + L_h^{-1} f(u^n)). \end{aligned}$$

Denote $v \in \mathcal{M}$ with $v_i = 1$ $(1 \le i \le N_x)$, so $L_h v = 0$. Then,

$$\begin{aligned} \sum_{i=1}^{N_x} (u_i^{n+1} - u_i^n) = v^T (u^{n+1} - u^n) &= -v^T (I - \mathrm{e}^{-L_h \Delta t})(u^n + L_h^{-1} f(u^n)) \\ &= -(u^n + L_h^{-1} f(u^n))^T (I - \mathrm{e}^{-L_h \Delta t}) v. \end{aligned}$$

Note that $I - \mathrm{e}^{-L_h \Delta t} = L_h \Delta t - \dfrac{1}{2}(L_h \Delta t)^2 + \cdots$, so $(I - \mathrm{e}^{-L_h \Delta t}) v = 0$.

ETD methods for the temporal integration (continued)

At the time level $t = t_n$, we have

$$v(t_{n+1}) = \mathrm{e}^{-L_h\Delta t} v(t_n) - \int_0^{\Delta t} \mathrm{e}^{-L_h(\Delta t - s)} f(v(t_n + s))\, \mathrm{d}s.$$

- approximating $f(v(t_n + s))$ by a linear *extrapolation* based on $f(v(t_n))$ and $f(v(t_{n-1}))$.

We obtain the *second order ETD multistep scheme*:

$$u^{n+1} = \mathrm{e}^{-L_h\Delta t} u^n - \int_0^{\Delta t} \mathrm{e}^{-L_h(\Delta t - s)} \left[\left(1 + \frac{s}{\Delta t}\right) f(u^n) - \frac{s}{\Delta t} f(u^{n-1}) \right] \mathrm{d}s. \tag{ETDMs2}$$

Mean-zero conservation: $\sum_i u_i^{n+1} = \sum_i u_i^n$.

Implementations of matrix exponentials

Letting

$$\phi_{-1}(a) = \mathrm{e}^{-a}, \quad \phi_0(a) = \frac{1 - \mathrm{e}^{-a}}{a}, \quad \phi_1(a) = \frac{\mathrm{e}^{-a} - 1 + a}{a^2},$$

we could write the ETD1 scheme as

$$u^{n+1} = \phi_{-1}(L_h \Delta t) u^n - \Delta t \phi_0(L_h \Delta t) f(u^n),$$

and the ETDMs2 scheme as

$$u^{n+1} = \phi_{-1}(L_h \Delta t) u^n - \Delta t (\phi_0 + \phi_1)(L_h \Delta t) f(u^n) - \Delta t \phi_1(L_h \Delta t) f(u^{n-1}).$$

The actions of exponentials $\phi_\gamma(L_h \Delta t)$ can be implemented efficiently.

Implementations of matrix exponentials (continued)

The exponentials $\phi_\gamma(L_h\Delta t)$ can be implemented by FFT.

Since $L_h = \varepsilon^2\Delta_h^2 - A\Delta_h$ is self-adjoint and positive definite, we have $L_h = P^{-1}\widehat{L}_h P$, where

$$(\widehat{L}_h\hat{f})_k = \lambda_k \hat{f}_k, \quad \hat{f} = Pf,\, f \in \mathcal{M}_0,$$

where $\{\lambda_k\}$ are the eigenvalues of L_h, that is,

$$\lambda_k = \varepsilon^2 k^4 + Ak^2 > 0, \quad k \neq 0.$$

Then, we have

$$\phi_\gamma(L_h\Delta t) = P^{-1}\phi_\gamma(\widehat{L}_h\Delta t)P, \quad (\phi_\gamma(\widehat{L}_h\Delta t)\hat{f})_k = \phi_\gamma(\lambda_k\Delta t)\hat{f}_k.$$

P and P^{-1} can be implemented by FFT and iFFT, respectively, so the computational complexity is $\mathcal{O}(N\log N)$ per time step.

Energy stability of the ETD1 scheme

We always assume that $A \geq \dfrac{1}{8}$.

The discrete energy functional is defined as

$$E_h(u) = \frac{\varepsilon^2}{2}\|\Delta_h u\|_2^2 - \frac{1}{2}\sum_{i=1}^{N_x} \ln(1 + (D_h u)_i^2).$$

ETD1 scheme: $u^{n+1} = \mathrm{e}^{-L_h\Delta t}u^n - L_h^{-1}(I - \mathrm{e}^{-L_h\Delta t})f(u^n)$.

Theorem: Energy stability of the ETD1 scheme

For any $\Delta t > 0$, we have $E_h(u^{n+1}) \leq E_h(u^n)$.

Basic idea of the proof (similar to Allen-Cahn equation):

- $f(u^n) = -(I - \mathrm{e}^{-L_h\Delta t})^{-1}L_h(u^{n+1} - u^n) - L_h u^n$;
- $$\begin{aligned} E_h(u^{n+1}) - E_h(u^n) &\leq (u^{n+1} - u^n)^T(L_h u^{n+1} + f(u^n)) \\ &= -(u^{n+1} - u^n)^T((I - \mathrm{e}^{-L_h\Delta t})^{-1} - I)L_h(u^{n+1} - u^n); \end{aligned}$$
- positive definiteness of $((I - \mathrm{e}^{-L_h\Delta t})^{-1} - I)L_h$.

Energy stability of the ETD1 scheme (continued)

$$E_h(u) = \frac{\varepsilon^2}{2}\|\Delta_h u\|_2^2 - \frac{1}{2}\sum_{i=1}^{N_x} \ln(1 + (D_h u)_i^2).$$

Corollary: Uniform H^2 stability of the ETD1 scheme

For any $\Delta t > 0$, we have

$$\max_{1\le n\le N_t} \|\Delta_h u^n\|_2 \le \frac{2}{\varepsilon}\sqrt{E_h(u^0) + C},$$

where the constant C depends only on ε.

Basic idea of the proof:

- $\ln(1+y) \le \alpha y - \ln\alpha + \alpha - 1$ for any $y \ge 0$, $\alpha \ge 0$;
- discrete Poincaré inequality: $\|D_h u^n\|_2^2 \le C'\|\Delta_h u^n\|_2^2$;
- $\frac{\varepsilon^2}{4}\|\Delta_h u^n\|_2^2 - C \le E_h(u^n) \le E_h(u^{n-1}) \le \cdots \le E_h(u^0)$.

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