Maximum principles for a class of semilinear parabolic equations and ETD schemes

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Outline

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Allen-Cahn equation

(Local) Allen-Cahn equation:

$$u_t - \varepsilon^2 \Delta u + u^3 - u = 0. \tag{LAC}$$

As an L^2 gradient flow w.r.t. the free energy functional

$$E_{\text{local}}(u) = \int \Big(\frac{1}{4}(u(\boldsymbol{x})^2 - 1)^2 + \frac{\varepsilon^2}{2} |\nabla u(\boldsymbol{x})|^2 \Big) \, \mathrm{d}\boldsymbol{x}, \tag{1}$$

- energy stability:

$$E_{\text{local}}(u(t_2)) \leq E_{\text{local}}(u(t_1)), \quad \forall\, t_2 \geq t_1 \geq 0. \tag{2}$$

As a second order reaction-diffusion equation,

- maximum principle:

$$\|u(\cdot, 0)\|_{L^\infty} \leq 1 \quad \Rightarrow \quad \|u(\cdot, t)\|_{L^\infty} \leq 1, \quad \forall\, t > 0. \tag{3}$$

Allen-Cahn equation (continued)

Energy stable schemes:

- *Stabilized semi-implicit (SSI) scheme* [Shen-Yang, 2010]: find u^{n+1} such that

$$\frac{u^{n+1}-u^n}{\tau} - \varepsilon^2 \Delta_h u^{n+1} + (u^n)^3 - u^n + \kappa(u^{n+1} - u^n) = 0. \quad (4)$$

- *Exponential time differencing (ETD) scheme* [Ju et al., 2015]: find $u^{n+1} = w(\tau)$ with $w(t)$ subject to

$$\begin{cases} \frac{\mathrm{d}w}{\mathrm{d}t} + (\kappa - \varepsilon^2 \Delta_h)w + (u^n)^3 - u^n - \kappa u^n = 0, \ t \in (0, \tau], \\ w(0) = u^n. \end{cases} \quad (5)$$

Both schemes are easy to implement and conditionally energy stable.

Allen-Cahn equation (continued)

$$F(u) = \frac{1}{4}(u^2 - 1)^2, \quad f(u) := F'(u) = u^3 - u.$$

What is the condition for energy stability?

$$\kappa \geq \frac{1}{2}\|f'(u)\|_{L^\infty}. \tag{6}$$

However,

$$f'(u) = 3u^2 - 1, \quad \text{unbounded in } L^\infty!$$

Allen-Cahn equation (continued)

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However,

$$f'(u) = 3u^2 - 1, \quad \text{unbounded in } L^\infty!$$

If we have that u is bounded in L^∞, then so does $f'(u)$.

Discrete maximum principle (DMP) insures the L^∞ boundness of u.

Allen-Cahn equation (continued)

Maximum principle preserving schemes:

- *first order semi-implicit scheme* [Tang-Yang, 2016]:

$$\frac{u^{n+1}-u^n}{\tau} - \varepsilon^2 \Delta_h u^{n+1} + (u^n)^3 - u^n + \kappa(u^{n+1}-u^n) = 0 \quad (7)$$

  condition for DMP: $\frac{1}{\tau} + \kappa \geq 2.$

- *Crank-Nicolson scheme* [Hou-Tang-Yang, 2017]:

$$\frac{u^{n+1}-u^n}{\tau} - \varepsilon^2 \Delta_h \frac{u^{n+1}+u^n}{2} + \frac{(u^{n+1})^3+(u^n)^3}{2} - \frac{u^{n+1}+u^n}{2} = 0 \quad (8)$$

  condition for DMP: $\tau \leq \frac{1}{2} \min\left\{1, \frac{h^2}{\varepsilon^2}\right\}.$

Cahn-Hilliard equation

(Local) Cahn-Hilliard equation:

$$u_t + \varepsilon^2 \Delta^2 u + \Delta(u^3 - u) = 0. \tag{LCH}$$

No maximum principle!

Li-Qiao-Tang, SINUM, 2016
Li-Qiao, JSC, 2017 (IMEX Frouier Spectral)
Song-Shu, JSC, 2018 (IMEX LDG)

A clean description on the size of the constant κ, in the sense that κ is independent of the L^∞ bound on the numerical solution.

Nonlocal Allen-Cahn equation

Nonlocal Allen-Cahn (NAC) equation:

$$u_t - \varepsilon^2 \mathcal{L}_\delta u + u^3 - u = 0. \tag{NAC}$$

As an L^2 gradient flow w.r.t. the free energy functional

$$E(u) = \int \Big(\frac{1}{4}(u(\boldsymbol{x})^2 - 1)^2 - \frac{\varepsilon^2}{2} u(\boldsymbol{x}) \mathcal{L}_\delta u(\boldsymbol{x}) \Big) \, \mathrm{d}\boldsymbol{x}, \tag{9}$$

- energy stability:

$$E(u(t_2)) \leq E(u(t_1)), \quad \forall\, t_2 \geq t_1 \geq 0. \tag{10}$$

Similar to the case of local Allen-Cahn equation, we can prove

- maximum principle:

$$\|u(\cdot, 0)\|_{L^\infty} \leq 1 \quad \Rightarrow \quad \|u(\cdot, t)\|_{L^\infty} \leq 1, \quad \forall\, t > 0. \tag{11}$$

Nonlocal Allen-Cahn equation (continued)

Nonlocal diffusion operator ($\boldsymbol{x} \in \mathbb{R}^d$):

$$\mathcal{L}_\delta u(\boldsymbol{x}) = \frac{1}{2} \int_{B_\delta(\mathbf{0})} \rho_\delta(|\boldsymbol{s}|) \big(u(\boldsymbol{x}+\boldsymbol{s}) + u(\boldsymbol{x}-\boldsymbol{s}) - 2u(\boldsymbol{x}) \big) \, \mathrm{d}\boldsymbol{s}. \quad (12)$$

Kernel $\rho_\delta : [0, \delta] \to \mathbb{R}$ is nonnegative and

$$\frac{1}{2} \int_{B_\delta(\mathbf{0})} |\boldsymbol{s}|^2 \rho_\delta(|\boldsymbol{s}|) \, \mathrm{d}\boldsymbol{s} = d. \quad (13)$$

Consistency of $\mathcal{L}_\delta$ with $\mathcal{L}_0 := \Delta$ via [Du et al., 2012]

$$\max_{\boldsymbol{x}} |\mathcal{L}_\delta u(\boldsymbol{x}) - \mathcal{L}_0 u(\boldsymbol{x})| \leq C\delta^2 \|u\|_{C^4}. \quad (14)$$

In particular, in 1-D case,

$$\mathcal{L}_\delta u(x) = \frac{1}{2} \int_{-\delta}^{\delta} |s|^2 \rho_\delta(|s|) \cdot \frac{u(x+s) + u(x-s) - 2u(x)}{|s|^2} \, \mathrm{d}s. \quad (15)$$

Nonlocal Allen-Cahn equation (continued)

Our work:

- Du-Ju-Li-Qiao, *SIAM J. Numer. Anal.*, 2019.

Consider the initial-boundary-value problem of the NAC equation

$$\begin{aligned} u_t - \varepsilon^2 \mathcal{L}_\delta u + u^3 - u = 0, &\quad \boldsymbol{x} \in \Omega,\ t \in (0,T], \\ u(\cdot,t) \text{ is } \Omega\text{-periodic}, &\quad t \in [0,T], \\ u(\boldsymbol{x},0) = u_0(\boldsymbol{x}), &\quad \boldsymbol{x} \in \overline{\Omega}, \end{aligned}$$

where $\Omega = (0,X)^d$ is a hypercube domain in $\mathbb{R}^d$.

Main theoretical results:

- discrete maximum principle;
- maximum-norm error estimates;
- discrete energy stability.

Quadrature-based finite difference discretization

Uniform spatial mesh with the nodes $\{\boldsymbol{x_i}\}$.

The discretization of $\mathcal{L}_\delta$ is defined by [Du-Tao-Tian-Yang, 2018]

$$\mathcal{L}_{\delta,h}u(\boldsymbol{x_i}) = \frac{1}{2}\int_{B_\delta(\boldsymbol{0})} \mathcal{I}_h\left(\frac{u(\boldsymbol{x_i}+\boldsymbol{s})+u(\boldsymbol{x_i}-\boldsymbol{s})-2u(\boldsymbol{x_i})}{|\boldsymbol{s}|^2}|\boldsymbol{s}|_1\right)\frac{|\boldsymbol{s}|^2}{|\boldsymbol{s}|_1}\rho_\delta(|\boldsymbol{s}|)\,\mathrm{d}\boldsymbol{s}. \tag{16}$$

where $\mathcal{I}_h$ is the piecewise d-multi-linear interpolation.

The matrix $\mathcal{L}_{\delta,h}$ is

- symmetric and negative semi-definite;
- weakly diagonally dominant with all negative diagonal entries.

Quadrature-based finite difference discretization (continued)

Introduce a stabilizing parameter $\kappa > 0$ and define

$$L_h := -\varepsilon^2 \mathcal{L}_{\delta,h} + \kappa I, \qquad N(U) := \kappa U + U - U^{.3}. \tag{17}$$

Then, we reach

$$\frac{\mathrm{d}U}{\mathrm{d}t} + L_h U = N(U), \tag{18}$$

whose solution satisfies

$$U(t+\tau) = \mathrm{e}^{-L_h \tau} U(t) + \int_0^\tau \mathrm{e}^{-L_h(\tau - s)} N(U(t+s)) \, \mathrm{d}s. \tag{19}$$

The matrix L_h is

- symmetric and positive definite;
- strictly diagonally dominant with all positive diagonal entries,

which implies that $\|\mathrm{e}^{-L_h \tau}\|_\infty \le \mathrm{e}^{-\kappa\tau}$ for any $\kappa, \tau > 0$.

ETD methods for the temporal integration

Uniform time step τ and the nodes $\{t_n = n\tau\}$.

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

$$U(t_{n+1}) = \mathrm{e}^{-L_h\tau} U(t_n) + \int_0^\tau \mathrm{e}^{-L_h(\tau-s)} N(U(t_n+s))\,\mathrm{d}s. \qquad (20)$$

By

- approximating $N(U(t_n+s))$ by $N(U(t_n))$ in $s \in [0,\tau]$,
- calculating the integral exactly,

we have the *first order ETD scheme* of (NAC):

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

ETD methods for the temporal integration (continued)

At the time level $t = t_n$:

$$U(t_{n+1}) = \mathrm{e}^{-L_h\tau}U(t_n) + \int_0^\tau \mathrm{e}^{-L_h(\tau-s)}N(U(t_n+s))\,\mathrm{d}s. \tag{21}$$

By

- approximating $N(U(t_n+s))$ by a linear interpolation based on $N(U(t_n))$ and $N(U(t_{n+1}))$,

we have the *second order ETD Runge-Kutta scheme* of (NAC):

$$\begin{cases} U^{n+1} = \mathrm{e}^{-L_h\tau}U^n + \displaystyle\int_0^\tau \mathrm{e}^{-L_h(\tau-s)}\left[\left(1-\frac{s}{\tau}\right)N(U^n) + \frac{s}{\tau}N(\widetilde{U}^{n+1})\right]\mathrm{d}s, \\ \widetilde{U}^{n+1} = \mathrm{e}^{-L_h\tau}U^n + \displaystyle\int_0^\tau \mathrm{e}^{-L_h(\tau-s)}N(U^n)\,\mathrm{d}s. \end{cases} \tag{ETDRK2}$$

Discrete maximum principle

For the ETD1 scheme, we prove it by induction:

- $\|U^0\|_\infty \le \|u_0\|_{L^\infty} \le 1$;
- assume $\|U^k\|_\infty \le 1$, prove $\|U^{k+1}\|_\infty \le 1$.

We have

$$\|U^{k+1}\|_\infty \le \|\mathrm{e}^{-L_h\tau}\|_\infty \|U^k\|_\infty + \int_0^\tau \|\mathrm{e}^{-L_h(\tau-s)}\|_\infty \,\mathrm{d}s \cdot \|N(U^k)\|_\infty.$$

We can prove

- $\|\mathrm{e}^{-L_h\tau}\|_\infty \le \mathrm{e}^{-\kappa\tau}$ for any $\kappa, \tau > 0$;
- $\|N(U^k)\|_\infty \le \kappa$ when $\kappa \ge 2$.

Then,

$$\|U^{k+1}\|_\infty \le \mathrm{e}^{-\kappa\tau} \cdot 1 + \frac{1-\mathrm{e}^{-\kappa\tau}}{\kappa} \cdot \kappa = 1.$$

Discrete maximum principle (continued)

For the ETDRK2 scheme, we have

$$\|U^{k+1}\|_\infty \le \|\mathrm{e}^{-L_h\tau}\|_\infty \|U^k\|_\infty + \int_0^\tau \|\mathrm{e}^{-L_h(\tau-s)}\|_\infty \left\| \left(1-\frac{s}{\tau}\right) f(U^k) + \frac{s}{\tau} f(\widetilde{U}^{k+1}) \right\|_\infty \mathrm{d}s.$$

Note that $\widetilde{U}^{k+1}$ is exactly the solution to ETD1 scheme, so

$$\|\widetilde{U}^{k+1}\|_\infty \le 1 \quad \Rightarrow \quad \|f(\widetilde{U}^{k+1})\|_\infty \le S.$$

For $s \in [0,\tau]$,

$$\left\| \left(1-\frac{s}{\tau}\right) f(U^k) + \frac{s}{\tau} f(\widetilde{U}^{k+1}) \right\|_\infty \le \left(1-\frac{s}{\tau}\right) \|f(U^k)\|_\infty + \frac{s}{\tau} \|f(\widetilde{U}^{k+1})\|_\infty \le S.$$

Then,

$$\|U^{k+1}\|_\infty \le \mathrm{e}^{-S\tau} \cdot 1 + \frac{1-\mathrm{e}^{-S\tau}}{S} \cdot S = 1.$$

Discrete energy stability

We define the discretized energy E_h:

$$E_h(U) = \sum_{i=1}^{dN} F(U_i) - \frac{\varepsilon^2}{2} U^T \mathcal{L}_{\delta,h} U, \quad F(s) = \frac{1}{4}(s^2 - 1)^2. \qquad (22)$$

Discrete energy stability of the ETD1 scheme

Under the condition $\kappa \geq 2$, for any $\tau > 0$, we have

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

Energy stability for ETD1

Step 1. We have

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

where $\|f'(\xi)\|_\infty = \|3\xi^2 - 1\|_\infty \leq 2$ since $\|\xi\|_\infty \leq 1$ due to DMP. Then, we obtain

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

Step 2. Solve $N(U^n)$ from (ETD1) to get

$$N(U^n) = (I - \mathrm{e}^{-L_h\tau})^{-1}L_h(U^{n+1} - U^n) + L_h U^n,$$

and then,

$$L_h U^{n+1} - N(U^n) = B_1(U^{n+1} - U^n)$$

with $B_1 = L_h - (I - \mathrm{e}^{-L_h\tau})^{-1}L_h$ symmetric and negative definite. So,

$$E_h(U^{n+1}) - E_h(U^n) \leq (U^{n+1} - U^n)^T B_1(U^{n+1} - U^n) \leq 0.$$

Numerical experiments

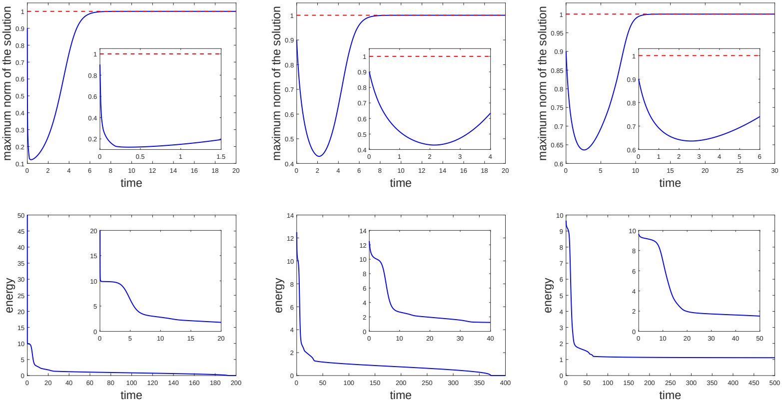
We consider the 2-D case.

Setting

- $\Omega = (0, 2\pi) \times (0, 2\pi)$, $\varepsilon = 0.1$;
- kernel: $\rho_\delta(r) = \dfrac{6}{\pi\delta^3 r}$, $r > 0$;
- $N = 512$, $\tau = 0.01$;
- random initial data ranging from -0.9 to 0.9 uniformly;
- $\delta = 0$, $\delta = 3\varepsilon$, $\delta = 4\varepsilon$.

Numerical experiments (continued)

From left to right: $\delta = 0$ (local), $\delta = 3\varepsilon$, $\delta = 4\varepsilon$.
Top: maximum norms; bottom: energies.



Recall the proof of the discrete maximum principle

The crucial results are

- $\|e^{-L_h\tau}\|_\infty \leq e^{-\kappa\tau}$ for any $\kappa, \tau > 0$,

(This is the result of the strictly diagonal dominance of L_h.)

and

- $\|N(U)\|_\infty \leq \kappa$ when $\kappa \geq 2$, for any U such that $\|U\|_\infty \leq 1$.

(This comes from the property of the function $f(u) = u - u^3$.)

Outline

Domain Ω and Banach space X

Consider the domain $\Omega \subset \mathbb{R}^d$ in the following two situations:

(D1) Ω is an open connected and bounded set with boundary $\partial\Omega$;
(D2) Ω consists of all nodes in a mesh dividing a set defined as (D1).

Let X be the Banach space consisting of real scalar-valued continuous functions defined on $\overline{\Omega} = \Omega \cup \partial\Omega$ associated with the norm

$$\|u\| = \max_{\boldsymbol{x}\in\overline{\Omega}} |u(\boldsymbol{x})|, \quad u \in X.$$

In particular, we consider the following two cases:

(C1) $X = C_0(\overline{\Omega}; \mathbb{R})$ (continuous on $\overline{\Omega}$ and vanishing on $\partial\Omega$);
(C2) $X = C_{\mathrm{per}}(\overline{\Omega}; \mathbb{R})$ (continuous in $\mathbb{R}^d$ and periodic w.r.t. Ω).

Model equation

Let

- $f : X \to X$ be a nonlinear operator;
- $\mathcal{L} : D(\mathcal{L}) \to X$ be a linear operator, where the domain $D(\mathcal{L})$ is a linear subspace of X.

The model equation is a class of semilinear parabolic equations:

$$u_t = \mathcal{L}u + f[u], \quad t > 0, \tag{23}$$

where $u : [0, \infty) \to X$ is the unknown function subject to the initial condition

$$u(0) = u_0, \quad \text{in } \overline{\Omega} \tag{24}$$

and the homogenous Dirichlet boundary condition for Case (C1) or the periodic boundary condition for Case (C2).

Linear operator $\mathcal{L}$

Main idea: $\mathcal{L}$ should be a generalization of Δ.

Assumption 1

The linear operator $\mathcal{L}$ satisfies the followings:
(a) $\mathcal{L} : D(\mathcal{L}) \to X$ is closed and the domain $D(\mathcal{L})$ is dense in X;
(b) there exists $\lambda_0 > 0$ such that $\lambda_0 \mathcal{I} - \mathcal{L} : D(\mathcal{L}) \to X$ is surjective;
(c) it always holds that $\mathcal{L}w(\boldsymbol{x}_0) \leq 0$ for any $w \in D(\mathcal{L})$ and $\boldsymbol{x}_0 \in \Omega$ such that

$$\begin{aligned} & w(\boldsymbol{x}_0) = \max_{\boldsymbol{x}\in\Omega} w(\boldsymbol{x}) \text{ for Case (C1)} \\ \text{or} \quad & w(\boldsymbol{x}_0) = \max_{\boldsymbol{x}\in\overline{\Omega}} w(\boldsymbol{x}) \text{ for Case (C2).} \end{aligned}$$

Linear operator $\mathcal{L}$ (continued)

Lemma 1

Under Assumption 1, it holds that
(i) $\mathcal{L}$ is dissipative, i.e., for any $\lambda > 0$ and any $w \in D(\mathcal{L})$,

$$\|(\lambda\mathcal{I} - \mathcal{L})w\| \geq \lambda\|w\|; \tag{25}$$

(ii) $\mathcal{L}$ is the generator of a contraction semigroup $\{S_{\mathcal{L}}(t)\}_{t\geq 0}$, i.e.,

$$\|S_{\mathcal{L}}(t)\|_{\mathcal{B}(X)} \leq 1.$$

Nonlinear operator f

Main idea: f should be a generalization of $f(u) = u - u^3$.

Assumption 2

The nonlinear operator f acts as a composite function induced by a given one-variable continuously differentiable function $f_0 : \mathbb{R} \to \mathbb{R}$, that is,

$$f[w](\boldsymbol{x}) = f_0(w(\boldsymbol{x})), \quad \forall\, w \in X,\ \forall\, \boldsymbol{x} \in \overline{\Omega}, \tag{26}$$

and there exists $\beta > 0$ such that

$$f_0(\beta) \leq 0 \leq f_0(-\beta). \tag{27}$$

If f_0 satisfies $f_0(a) \geq 0 \geq f_0(b)$ for some $a < b$, one can carry out an affine transform to u.

Nonlinear operator f (continued)

Introduce a stabilizing constant $\kappa \geq 0$, and then we obtain

$$u_t + \kappa u = \mathcal{L}u + \mathcal{N}[u], \tag{28}$$

where $\mathcal{N} := \kappa\mathcal{I} + f$. The solution to (28) satisfies

$$u(t+\tau) = \mathrm{e}^{-\kappa\tau} S_{\mathcal{L}}(\tau)u(t) + \int_0^\tau \mathrm{e}^{-\kappa(\tau-s)} S_{\mathcal{L}}(\tau-s)\mathcal{N}[u(t+s)]\,\mathrm{d}s. \tag{29}$$

Requirement on the selection of the stabilizing constant:

$$\kappa \geq \max_{|\xi|\leq\beta} |f_0'(\xi)|. \tag{$*$}$$

Lemma 2

Denote $X_\beta = \{w \in X : \|w\| \leq \beta\}$. Under Assumption 2 and the condition $(*)$, it holds that
(i) $\|\mathcal{N}[w]\| \leq \kappa\beta$ for any $w \in X_\beta$;
(ii) $\|\mathcal{N}[w_1] - \mathcal{N}[w_2]\| \leq 2\kappa\|w_1 - w_2\|$ for any $w_1, w_2 \in X_\beta$.

Maximum principle

Theorem 1

Given a constant $T > 0$. Under Assumptions 1 and 2, if the initial data satisfies $\|u_0\| \leq \beta$, then the model equation has a unique solution $u \in C([0,T];X)$ and satisfies $\|u(t)\| \leq \beta$ for any $t \in (0,T]$.

Sketch of the proof. For any $t_1 > 0$,

$$u(\tau) = \mathrm{e}^{-\kappa\tau} S_{\mathcal{L}}(\tau) u_0 + \int_0^\tau \mathrm{e}^{-\kappa(\tau-s)} S_{\mathcal{L}}(\tau-s) \mathcal{N}[u(s)]\,\mathrm{d}s, \ \tau \in [0, t_1].$$

Given $v \in C([0,t_1];X_\beta)$, define a mapping $\mathcal{A}$ by setting

$$\mathcal{A}[v](\tau) = \mathrm{e}^{-\kappa\tau} S_{\mathcal{L}}(\tau) u_0 + \int_0^\tau \mathrm{e}^{-\kappa(\tau-s)} S_{\mathcal{L}}(\tau-s) \mathcal{N}[v(s)]\,\mathrm{d}s, \ \tau \in [0, t_1].$$

Step 1. Prove $\mathcal{A}[v] \in C([0,t_1];X_\beta)$.
Step 2. Prove $\mathcal{A}$ is a strict contraction if t_1 is sufficiently small.
Step 3. Repeat the same argument on $[t_1, 2t_1]$, $[2t_1, 3t_1]$, $\ldots$.

Examples of the nonlinear function f_0

Example 1. Consider the function

$$f_0(s) = \lambda s(1 - s^p), \tag{30}$$

where $\lambda > 0$ and $p \in \mathbb{N}_+$.

- f_0 satisfies $f_0(a) \geq 0 \geq f_0(b)$ with any $a \in [0, 1)$ and $b \geq 1$;
- for even p, one can choose $\beta \geq 1$ to meet Assumption 2.

Special cases:

- Case $p = 2$ with $\lambda = 1$ gives

$$f_0(s) = s - s^3, \tag{31}$$

  the derivative of $-F$ with $F(s) = \frac{1}{4}(s^2 - 1)^2$.

Examples of the nonlinear function f_0 (continued)

Example 2. Consider the Flory-Huggins free energy

$$F(s) = \frac{\theta}{2}[(1+s)\ln(1+s) + (1-s)\ln(1-s)] - \frac{\theta_c}{2}s^2,$$

where θ and θ_c are two constants satisfying $0 < \theta < \theta_c$, and

$$f_0(s) = -F'(s) = \frac{\theta}{2}\ln\frac{1-s}{1+s} + \theta_c s. \tag{32}$$

Denote by ρ the positive root of $f_0(\rho) = 0$, i.e.,

$$\frac{1}{2\rho}\ln\frac{1+\rho}{1-\rho} = \frac{\theta_c}{\theta}. \tag{33}$$

Then f_0 satisfies Assumption 2 with $\beta \in [\rho, 1)$.

Examples of the linear operator $\mathcal{L}$

1. Cases in the *infinite* dimensional space

Example 3. Second order elliptic differential operator

$$\mathcal{L}w(\boldsymbol{x}) = A(\boldsymbol{x}) : \nabla^2 w(\boldsymbol{x}) + q(\boldsymbol{x}) \cdot \nabla w(\boldsymbol{x}), \tag{34}$$

where $q \in C(\overline{\Omega}; \mathbb{R}^d)$ and $A \in C(\overline{\Omega}; \mathbb{R}^{d\times d})$ is symmetric and positive definite uniformly.

Example 4. Nonlocal diffusion operator

$$\mathcal{L}w(\boldsymbol{x}) = \int_{\Omega} \rho(\boldsymbol{x}, \boldsymbol{y})(w(\boldsymbol{y}) - w(\boldsymbol{x}))\, \mathrm{d}\boldsymbol{y}, \tag{35}$$

where $\rho : \Omega \times \Omega \to \mathbb{R}$ is a symmetric nonnegative kernel function, i.e., $\rho(\boldsymbol{x}, \boldsymbol{y}) = \rho(\boldsymbol{y}, \boldsymbol{x}) \geq 0$.

Examples of the linear operator $\mathcal{L}$ (continued)

1. Cases in the *infinite* dimensional space (continued)

Example 5. Fractional Laplace operator

$$\mathcal{L}w(\boldsymbol{x}) = \frac{1}{2}\pi^{-\frac{d}{2}-2s}\frac{\Gamma(\frac{d}{2}+s)}{\Gamma(-s)}\int_{\mathbb{R}^d}\frac{w(\boldsymbol{x}+\boldsymbol{y})+w(\boldsymbol{x}-\boldsymbol{y})-2w(\boldsymbol{x})}{|\boldsymbol{y}|^{d+2\alpha}}\,\mathrm{d}\boldsymbol{y}. \tag{36}$$

Example 6. Riesz fractional derivative operator

$$\mathcal{L}w(\boldsymbol{x}) = -\frac{1}{2\cos\frac{\pi\alpha}{2}}\frac{1}{\Gamma(2-\alpha)}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\int_a^b\frac{w(\xi)}{|x-\xi|^{\alpha-1}}\,\mathrm{d}\xi,\ x\in(a,b). \tag{37}$$

Examples of the linear operator $\mathcal{L}$ (continued)

2. Cases in the *finite* dimensional space

Example 7. Central difference operator for Laplacian

$$\mathcal{L}_h w(x_i) = \frac{1}{h^2}\big(w(x_{i-1}) - 2w(x_i) + w(x_{i+1})\big). \tag{38}$$

Example 8. Quadrature-based difference operator

$$\mathcal{L}_h w(\boldsymbol{x_i}) = \sum_{\boldsymbol{0}\neq \boldsymbol{s_j}\in B_\delta(\boldsymbol{0})} \frac{w(\boldsymbol{x_i}+\boldsymbol{s_j}) + w(\boldsymbol{x_i}-\boldsymbol{s_j}) - 2w(\boldsymbol{x_i})}{|\boldsymbol{s_j}|^2} |\boldsymbol{s_j}|_1 \beta_\delta(\boldsymbol{s_j}), \tag{39}$$

where

$$\beta_\delta(\boldsymbol{s_j}) = \frac{1}{2}\int_{B_\delta(\boldsymbol{0})} \psi_{\boldsymbol{j}}(\boldsymbol{s}) \frac{|\boldsymbol{s}|^2}{|\boldsymbol{s}|_1} \rho_\delta(|\boldsymbol{s}|)\, \mathrm{d}\boldsymbol{s},$$

Example 9. Fractional difference operator (discretization of (36)).

Example 10. Mass-lumping finite element approximation for Δ.

Outline

ETD1 scheme and the DMP

Uniform time step τ and the nodes $\{t_n = n\tau\}$. At $t = t_n$, we have

$$u(t_{n+1}) = \mathrm{e}^{-\kappa\tau} S_{\mathcal{L}}(\tau) u(t_n) + \int_0^\tau \mathrm{e}^{-\kappa(\tau-s)} S_{\mathcal{L}}(\tau - s) \mathcal{N}[u(t_n + s)]\,\mathrm{d}s. \tag{40}$$

By

- approximating $\mathcal{N}[u(t_n + s)] \approx \mathcal{N}[u(t_n)]$ in $s \in [0, \tau]$,
- calculating the integral exactly,

we obtain the *first order ETD scheme*:

$$v^{n+1} = \mathrm{e}^{-\kappa\tau} S_{\mathcal{L}}(\tau) v^n + \left(\int_0^\tau \mathrm{e}^{-\kappa(\tau-s)} S_{\mathcal{L}}(\tau - s)\,\mathrm{d}s \right) \mathcal{N}[v^n]. \tag{ETD1}$$

Theorem 2 (Maximum principle of the ETD1 scheme)

Under Assumptions 1–2 and the condition $(*)$, the ETD1 scheme preserves the maximum principle unconditionally, namely, if $\|u_0\| \leq \beta$, the solution to (ETD1) satisfies $\|v^n\| \leq \beta$ for any $\tau > 0$.

Higher order ETDRK schemes and the DMPs

Let $P_r(s)$ be an interpolation of $\mathcal{N}[u(t_n+s)]$ on $\{s_k := \frac{k}{r}\tau\}_{k=0}^{r}$:

$$P_r(s) = \sum_{k=0}^{r} \ell_{r,k}(s)\mathcal{N}[\tilde{v}^{n+\frac{k}{r}}], \quad s \in [0,\tau],$$

where $\tilde{v}^{n+\frac{k}{r}}$ is an approximated value of $u(t_n+s_k)$.

Higher order ETD Runge-Kutta scheme:

$$v^{n+1} = \mathrm{e}^{-\kappa\tau} S_{\mathcal{L}}(\tau) v^n + \int_0^{\tau} \mathrm{e}^{-\kappa(\tau-s)} S_{\mathcal{L}}(\tau-s) P_r(s)\,\mathrm{d}s.$$

Could the higher order schemes preserve the maximum principle?

Higher order ETDRK schemes and the DMPs (continued)

In the proof of the DMP, we meet

$$\|v^{k+1}\| \leq \mathrm{e}^{-\kappa\tau}\|S_{\mathcal{L}}(\tau)\|\|v^k\| + \int_0^\tau \mathrm{e}^{-\kappa(\tau-s)}\|S_{\mathcal{L}}(\tau-s)\|\|P_r(s)\|\,\mathrm{d}s.$$

The maximum principle would be preserved as long as

$$\|P_r(s)\| \leq \max\{\|\mathcal{N}[\tilde{v}^{n+\frac{k}{r}}]\| : 0 \leq k \leq r\}, \quad \forall\, s \in [0,\tau], \tag{41}$$

with $\|\tilde{v}^{n+\frac{k}{r}}\| \leq \beta$ for all $k = 0, 1, \ldots, r$, which leads to $\|P_r(s)\| \leq \kappa\beta$.

The unique interpolation satisfying (41) corresponds to the case $r = 1$, that is, the linear interpolation

$$P_1(s) = \Big(1 - \frac{s}{\tau}\Big)\mathcal{N}[\tilde{v}^n] + \frac{s}{\tau}\mathcal{N}[\tilde{v}^{n+1}], \quad s \in [0,\tau].$$

ETDRK2 scheme and the DMP

By

- approximating $\mathcal{N}[u(t_n+s)] \approx P_1(s)$ in $s \in [0,\tau]$,
- calculating the integral exactly,

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

$$\tilde{v}^{n+1} = \mathrm{e}^{-\kappa\tau} S_{\mathcal{L}}(\tau) v^n + \Big(\int_0^\tau \mathrm{e}^{-\kappa(\tau-s)} S_{\mathcal{L}}(\tau-s)\,\mathrm{d}s \Big) \mathcal{N}[v^n],$$

$$v^{n+1} = \mathrm{e}^{-\kappa\tau} S_{\mathcal{L}}(\tau) v^n + \int_0^\tau \mathrm{e}^{-\kappa(\tau-s)} S_{\mathcal{L}}(\tau-s) \Big[\Big(1-\frac{s}{\tau}\Big) \mathcal{N}[v^n] + \frac{s}{\tau} \mathcal{N}[\tilde{v}^{n+1}]$$

Theorem 3 (Maximum principle of the ETDRK2 scheme)

Under Assumptions 1–2 and the condition $(*)$, *the ETDRK2 scheme preserves the maximum principle unconditionally, namely, if* $\|u_0\| \le \beta$, *the solution to (ETDRK2) satisfies* $\|v^n\| \le \beta$ *for any* $\tau > 0$.

Energy stability of ETD schemes for phase field models

Phase field models are derived as the gradient flows w.r.t. the energy

$$E[u] = -\frac{1}{2}(u, \mathcal{L}u)_{L^2(\Omega)} + \int_\Omega F(u(\boldsymbol{x}))\,\mathrm{d}\boldsymbol{x},$$

with $F : \mathbb{R} \to \mathbb{R}$ subject to $f_0 = -F'$. We have the energy law:

$$E[u(t_2)] \le E[u(t_1)], \quad \forall\, t_2 \ge t_1 \ge 0.$$

Proposition (Energy stability of ETD1 and ETDRK2 schemes)

(i) The solution $\{v^n\}_{n\ge 0}$ to the ETD1 scheme satisfies

$$E[v^{n+1}] \le E[v^n], \quad \forall\, \tau > 0;$$

(ii) Under the assumptions of Theorem 5, the solution $\{v^n\}_{n\ge 0}$ to the ETDRK2 scheme satisfies

$$E[v^n] \le E[v^0] + \widehat{C}(|\Omega|, T, \kappa), \quad \tau \in (0, 1].$$

Conclusion

Model equation:

$$u_t = \mathcal{L}u + f[u]. \qquad (**)$$

Main results:

$$\left.\begin{array}{c} \text{maximum} \\ \text{principle} \\ \text{of } (**) \end{array} \left\{ \begin{array}{l} \text{assumption on } \mathcal{L} \\ \\ \text{assumption on } f \end{array} \right. \atop \text{requirement on } \kappa \right\} \begin{array}{c} \text{maximum principle} \\ \text{preserving ETD} \\ \text{schemes for } (**) \end{array}$$

Thanks for your attention!