Maximum principle preserving ETD schemes for the nonlocal Allen-Cahn equation

Xiao Li

Beijing Computational Science Research Center

Joint work with

Qiang Du (COLUMBIA), Lili Ju (USC), Zhonghua Qiao (HKPU)

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Outline

1. Introduction and motivation
2. Numerical schemes and numerical analysis
   - Exponential time differencing (ETD) schemes
   - Discrete maximum principle
   - Error estimates and asymptotic compatibility
   - Discrete energy stability
3. Numerical experiments

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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

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

- energy stability:

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

As a second order reaction-diffusion equation,

- maximum principle:

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

Allen-Cahn equation (continued)

Energy stable schemes:

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

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

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

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

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?

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

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]:

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

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

- *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: $\tau \leq \frac{1}{2}\min\{\varepsilon^2, h^2\}$.

- *ETD scheme* (in space-continuous version) [Du-Zhu, 2005].

Nonlocal diffusion operator

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

$$\mathcal{L}_\delta u(\boldsymbol{x}) = \frac{1}{2} \int_{B_\delta(\mathbf{0})} \rho_\delta(|\boldsymbol{s}|) \big(u(\boldsymbol{x}+\boldsymbol{s}) + u(\boldsymbol{x}-\boldsymbol{s}) - 2u(\boldsymbol{x}) \big) \, \mathrm{d}\boldsymbol{s}. \tag{9}$$

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

$$\frac{1}{2} \int_{B_\delta(\mathbf{0})} |\boldsymbol{s}|^2 \rho_\delta(|\boldsymbol{s}|) \, \mathrm{d}\boldsymbol{s} = d. \tag{10}$$

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

$$\max_{\boldsymbol{x}} |\mathcal{L}_\delta u(\boldsymbol{x}) - \mathcal{L}_0 u(\boldsymbol{x})| \leq C\delta^2 \|u\|_{C^4}. \tag{11}$$

In particular, in 1-D case,

$$\mathcal{L}_\delta u(x) = \frac{1}{2} \int_{-\delta}^{\delta} |s|^2 \rho_\delta(|s|) \cdot \frac{u(x+s) + u(x-s) - 2u(x)}{|s|^2} \, \mathrm{d}s. \tag{12}$$

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

$$E(u) = \int \left(\frac{1}{4}(u(\boldsymbol{x})^2 - 1)^2 - \frac{\varepsilon^2}{2} u(\boldsymbol{x}) \mathcal{L}_\delta u(\boldsymbol{x}) \right) \mathrm{d}\boldsymbol{x}, \tag{13}$$

- energy stability:

$$E(u(t_2)) \le E(u(t_1)), \quad \forall\, t_2 \ge t_1 \ge 0. \tag{14}$$

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

- maximum principle:

$$\|u(\cdot, 0)\|_{L^\infty} \le 1 \quad \Rightarrow \quad \|u(\cdot, t)\|_{L^\infty} \le 1, \quad \forall\, t > 0. \tag{15}$$

Nonlocal Allen-Cahn equation (continued)

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 $\mathbb{R}^d$.

Purpose:

- establish the 1st and 2nd order ETD schemes for (NAC).

Main theoretical results:

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

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Quadrature-based finite difference discretization

Setting

- $h = X/N$: uniform mesh size (N is a given positive integer);
- $\boldsymbol{x_i} = h\boldsymbol{i}$: nodes in the mesh ($\boldsymbol{i} \in \mathbb{Z}^d$ is a multi-index).

At any node $\boldsymbol{x_i} = h\boldsymbol{i}$, we have

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

where

- $|\cdot|_1$: the vector 1-norm in $\mathbb{R}^d$;
- $|\cdot|$: the standard Euclidean norm.

Quadrature-based finite difference discretization (continued)

At any node $\boldsymbol{x_i} = h\boldsymbol{i}$:

$$\mathcal{L}_\delta u(\boldsymbol{x_i}) = \frac{1}{2}\int_{B_\delta(\mathbf{0})} \frac{u(\boldsymbol{x_i}+\boldsymbol{s}) + u(\boldsymbol{x_i}-\boldsymbol{s}) - 2u(\boldsymbol{x_i})}{|\boldsymbol{s}|^2}|\boldsymbol{s}|_1 \cdot \frac{|\boldsymbol{s}|^2}{|\boldsymbol{s}|_1}\rho_\delta(|\boldsymbol{s}|)\,\mathrm{d}\boldsymbol{s}. \tag{17}$$

Define the discrete version of $\mathcal{L}_\delta$ by [Du-Tao-Tian-Yang, 2018]

$$\mathcal{L}_{\delta,h} u(\boldsymbol{x_i}) = \frac{1}{2}\int_{B_\delta(\mathbf{0})} \mathcal{I}_h\left(\frac{u(\boldsymbol{x_i}+\boldsymbol{s}) + u(\boldsymbol{x_i}-\boldsymbol{s}) - 2u(\boldsymbol{x_i})}{|\boldsymbol{s}|^2}|\boldsymbol{s}|_1\right) \frac{|\boldsymbol{s}|^2}{|\boldsymbol{s}|_1}\rho_\delta(|\boldsymbol{s}|)\,\mathrm{d}\boldsymbol{s}. \tag{18}$$

For a function $v(\boldsymbol{s})$, the interpolation $\mathcal{I}_h v(\boldsymbol{s})$ is *piecewise linear w.r.t. each component of* $\boldsymbol{s}$ and

$$\mathcal{I}_h v(\boldsymbol{s}) = \sum_{\boldsymbol{s_j}} v(\boldsymbol{s_j})\psi_{\boldsymbol{j}}(\boldsymbol{s}),$$

where $\psi_{\boldsymbol{j}}$ is the piecewise d-multi-linear standard basis function.

Quadrature-based finite difference discretization (continued)

Finite difference discretization of $\mathcal{L}_\delta$ reads

$$\mathcal{L}_{\delta,h} u(\boldsymbol{x_i}) = \sum_{\boldsymbol{0} \neq \boldsymbol{s_j} \in B_\delta(\boldsymbol{0})} \frac{u(\boldsymbol{x_i} + \boldsymbol{s_j}) + u(\boldsymbol{x_i} - \boldsymbol{s_j}) - 2u(\boldsymbol{x_i})}{|\boldsymbol{s_j}|^2} |\boldsymbol{s_j}|_1 \beta_\delta(\boldsymbol{s_j}), \tag{19}$$

where

$$\beta_\delta(\boldsymbol{s_j}) = \frac{1}{2} \int_{B_\delta(\boldsymbol{0})} \psi_{\boldsymbol{j}}(\boldsymbol{s}) \frac{|\boldsymbol{s}|^2}{|\boldsymbol{s}|_1} \rho_\delta(|\boldsymbol{s}|)\, \mathrm{d}\boldsymbol{s}. \tag{20}$$

We have that $\mathcal{L}_{\delta,h}$ is self-adjoint and negative semi-definite.

Lemma (Uniform consistency of $\mathcal{L}_{\delta,h}$ [Du-Tao-Tian-Yang, 2018])

$$\max_{\boldsymbol{x_i} \in \Omega} |\mathcal{L}_{\delta,h} u(\boldsymbol{x_i}) - \mathcal{L}_\delta u(\boldsymbol{x_i})| \leq Ch^2 \|u\|_{C^4}, \tag{21}$$

where $C > 0$ is a constant independent of δ and h.

Quadrature-based finite difference discretization (continued)

We

- order the nodes lexicographically,
- denote by $D_h \in \mathbb{R}^{dN\times dN}$ the matrix associated with $\mathcal{L}_{\delta,h}$.

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

$$\begin{cases} \dfrac{\mathrm{d}U}{\mathrm{d}t} = \varepsilon^2 D_h U + U - U^{\cdot 3}, \quad t \in (0,T], \\ U(0) = U_0. \end{cases} \tag{22}$$

We know D_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 $S > 0$ and define

$$L_h := -\varepsilon^2 D_h + SI, \qquad f(U) := SU + U - U^{\cdot 3}. \tag{23}$$

Then, we reach

$$\frac{\mathrm{d}U}{\mathrm{d}t} + L_h U = f(U), \tag{24}$$

whose solution satisfies

$$U(t+\tau) = \mathrm{e}^{-L_h \tau} U(t) + \int_0^\tau \mathrm{e}^{-L_h(\tau - s)} f(U(t+s))\,\mathrm{d}s. \tag{25}$$

We know L_h is

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

ETD methods for the temporal integration

Setting

- $\tau = T/N_t$: uniform time step (N_t is a given positive integer);
- $t_n = n\tau$: nodes in the time interval $[0, T]$.

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

$$U(t_{n+1}) = \mathrm{e}^{-L_h\tau} U(t_n) + \int_0^\tau \mathrm{e}^{-L_h(\tau-s)} f(U(t_n + s))\,\mathrm{d}s. \tag{26}$$

By

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

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

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

ETD methods for the temporal integration (continued)

At the time level $t = t_n$:

$$U(t_{n+1}) = \mathrm{e}^{-L_h\tau}U(t_n) + \int_0^\tau \mathrm{e}^{-L_h(\tau-s)} f(U(t_n+s))\,\mathrm{d}s. \tag{27}$$

By

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

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

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

Discrete maximum principle (DMP)

For both (ETD1) and (ETDRK2), we prove the DMP by induction:

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

For the ETD1 scheme, we have

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

We can prove

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

Then,

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

Discrete maximum principle (continued)

- $\|e^{-L_h\tau}\|_\infty \leq e^{-S\tau}$ for any $S > 0$ and $\tau > 0$.

Proof. We know L_h is strictly diagonally dominant with all positive diagonal entries, that is, $L_h = (\ell_{ij})$ has $\ell_{ii} > 0$, $\forall\, i$ and

$$|\ell_{ii}| \geq \sum_j |\ell_{ij}| + S, \quad \forall\, i.$$

For any $\theta(0) = \theta_0$, the solutions to $\dfrac{\mathrm{d}\theta}{\mathrm{d}t} = -L_h\theta$ satisfy [Lazer, 1971]

$$\|\theta(t_2)\|_\infty \leq e^{-S(t_2-t_1)}\|\theta(t_1)\|_\infty, \quad \forall\, t_2 \geq t_1 \geq 0.$$

In particular, noting that $\theta(t) = e^{-L_h t}\theta_0$, we have

$$\|e^{-L_h\tau}\theta_0\|_\infty = \|\theta(\tau)\|_\infty \leq e^{-S\tau}\|\theta_0\|_\infty, \quad \tau > 0.$$

Discrete maximum principle (continued)

- $\|f(U^k)\|_\infty \leq S$ when $S \geq 2$.

$$f(U) = SU + U - U^{.3}$$

Proof. Obviously,

$$f(-1) = -S, \quad f(1) = S.$$

For any $\xi \in [-1, 1]$, we have

$$f'(\xi) = S + 1 - 3\xi^2 \geq S - 2 \geq 0.$$

Therefore,

$$\max_{\xi \in [-1,1]} |f(\xi)| = S.$$

Discrete maximum principle (continued)

For the ETDRK2 scheme, we have

$$\begin{aligned}\|U^{k+1}\|_\infty \leq \|\mathrm{e}^{-L_h\tau}\|_\infty \|U^k\|_\infty \\ + \int_0^\tau \|\mathrm{e}^{-L_h(\tau-s)}\|_\infty \Big\| \Big(1-\frac{s}{\tau}\Big) f(U^k) + \frac{s}{\tau} f(\widetilde{U}^{k+1}) \Big\|_\infty \,\mathrm{d}s.\end{aligned}$$

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

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

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

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

Then,

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

Error estimates

Error estimates of ETD1 scheme

For a fixed $\delta > 0$, *if* $\|u_0\|_{L^\infty} \leq 1$ *and* $S \geq 2$, *then we have*

$$\|U^n - u(t_n)\|_\infty \leq C\mathrm{e}^{t_n}(h^2 + \tau), \quad t_n \leq T, \tag{28}$$

where $C > 0$ *depends on the* $C^1([0,T]; C^4_{\mathrm{per}}(\overline{\Omega}))$ *norm of* u.

Error estimates of ETDRK2 scheme

For a fixed $\delta > 0$, *if* $\|u_0\|_{L^\infty} \leq 1$ *and* $S \geq 2$, *then we have*

$$\|U^n - u(t_n)\|_\infty \leq C\mathrm{e}^{t_n}(h^2 + \tau^2), \quad t_n \leq T, \tag{29}$$

where $C > 0$ *depends on the* $C^2([0,T]; C^4_{\mathrm{per}}(\overline{\Omega}))$ *norm of* u.

Error estimates (continued)

Sketch of the proof for the ETD1 scheme:

$$U^{n+1} = \mathrm{e}^{-L_h\tau}U^n + \int_0^\tau \mathrm{e}^{-L_h(\tau-s)}f(U^n)\,\mathrm{d}s. \tag{ETD1}$$

For given U^n, the solution U^{n+1} is actually given by $U^{n+1} = W_1(\tau)$ with the function $W_1 : [0,\tau] \to \mathbb{R}^{dN}$ determined by

$$\begin{cases} \dfrac{\mathrm{d}W_1(s)}{\mathrm{d}s} = -SW_1(s) + \varepsilon^2 D_h W_1(s) + f(U^n), \quad s \in (0,\tau], \\ W_1(0) = U^n. \end{cases} \tag{30}$$

For given $u(\boldsymbol{x}, t_n)$, the solution $u(\boldsymbol{x}, t_{n+1})$ is determined by $u(\boldsymbol{x}, t_{n+1}) = w(\boldsymbol{x}, \tau)$ with the Ω-periodic function $w(\boldsymbol{x}, s)$ satisfying

$$\begin{cases} \dfrac{\partial w}{\partial s} = -Sw + \varepsilon^2\mathcal{L}_\delta w + f(w), \quad \boldsymbol{x} \in \Omega,\ s \in (0,\tau], \\ w(\boldsymbol{x}, 0) = u(\boldsymbol{x}, t_n), \quad \boldsymbol{x} \in \overline{\Omega}. \end{cases} \tag{31}$$

Error estimates (continued)

Let $e_1(s) = W_1(s) - w(s)$. Then,

$$\begin{cases} \dfrac{\mathrm{d}e_1}{\mathrm{d}s} = -L_h e_1 + f(U^n) - f(u(t_n)) + R_{h\tau}^{(1)}(s), \quad s \in (0, \tau], \\ e_1(0) = U^n - u(t_n) =: e^n, \end{cases} \tag{32}$$

with

$$\|R_{h\tau}^{(1)}(s)\|_\infty \leq C(h^2 + \tau), \quad \forall\, s \in (0, \tau],$$

where C depends on ε, S, and u. Then,

$$e_1(t) = \mathrm{e}^{-L_h t} e_1(0) + \int_0^t \mathrm{e}^{-L_h(t-s)} [f(U^n) - f(u(t_n)) + R_{h\tau}^{(1)}(s)]\, \mathrm{d}s, \quad t \in [0, \tau].$$

Setting $t = \tau$, we have

$$\begin{aligned} \|e_1^{n+1}\|_\infty &\leq \mathrm{e}^{-S\tau} \|e_1^n\|_\infty + \frac{1 - \mathrm{e}^{-S\tau}}{S} [(S+1)\|e_1^n\|_\infty + C(h^2 + \tau)] \\ &\leq (1 + \tau)\|e_1^n\|_\infty + C\tau(h^2 + \tau). \end{aligned}$$

An application of the Gronwall's inequality leads to the result.

Asymptotic compatibility

$$
\begin{tikzcd}[column sep=huge, row sep=huge]
 & \text{(nonlocal)} & \text{(local)} \\
\text{(discrete)} & u_h^\delta \arrow[r, "\delta \to 0"] \arrow[d, "h \to 0"'] \arrow[dr, bend left, "{\delta \to 0,\ h \to 0}"] & u_h^0 \arrow[d, "h \to 0"] \\
\text{(continuous)} & u^\delta \arrow[r, "\delta \to 0"] & u^0
\end{tikzcd}
$$

- $\max\limits_{\boldsymbol{x_i} \in \Omega} |\mathcal{L}_{\delta,h} u(\boldsymbol{x_i}) - \mathcal{L}_\delta u(\boldsymbol{x_i})| \leq Ch^2 \|u\|_{C^4}$, C independent of δ;
- $\max\limits_{\boldsymbol{x} \in \Omega} |\mathcal{L}_\delta u(\boldsymbol{x}) - \mathcal{L}_0 u(\boldsymbol{x})| \leq C\delta^2 \|u\|_{C^4}$.

Then,

$$\max_{\boldsymbol{x_i} \in \Omega} |\mathcal{L}_{\delta,h} u(\boldsymbol{x_i}) - \mathcal{L}_0 u(\boldsymbol{x_i})| \leq C(\delta^2 + h^2) \|u\|_{C^4}. \tag{33}$$

Asymptotic compatibility (continued)

Let $\widehat{e}(s) = W_1(s) - \varphi(s)$, where $\varphi(\boldsymbol{x}, s)$ denotes the exact solution to the local Allen-Cahn equation. Then,

$$\begin{cases} \dfrac{\mathrm{d}\widehat{e}}{\mathrm{d}s} = -L_h\widehat{e} + f(U^n) - f(\varphi(t_n)) + \widehat{R}^{\delta}_{h\tau}(s), \quad s \in (0, \tau], \\ \widehat{e}(0) = U^n - \varphi(t_n) =: \widehat{e}^n, \end{cases} \tag{34}$$

where

$$\|\widehat{R}^{\delta}_{h\tau}(s)\|_\infty \le C(\delta^2 + h^2 + \tau), \quad \forall\, s \in (0, \tau],$$

where $C > 0$ depends on ε, S, and φ, but independent of δ, h and τ.

Asymptotic compatibility of ETD1 scheme

If $\|\varphi_0\|_{L^\infty} \le 1$ *and* $S \ge 2$, *then we have*

$$\|U^n - \varphi(t_n)\|_\infty \le C\mathrm{e}^{t_n}(\delta^2 + h^2 + \tau), \quad t_n \le T, \tag{35}$$

where $C > 0$ *depends on the* $C^1([0, T]; C^4_{\mathrm{per}}(\overline{\Omega}))$ *norm of* φ.

Discrete energy stability

We define the discretized energy E_h:

$$E_h(U) = \frac{1}{4}\sum_{i=1}^{dN} F(U_i) - \frac{\varepsilon^2}{2} U^T D_h U, \quad F(s) = \frac{1}{4}(s^2-1)^2. \tag{36}$$

Discrete energy stability of the ETD1 scheme

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

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

The proof includes two steps.

Discrete energy stability (continued)

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

$$E_h(U^{n+1}) - E_h(U^n) \leq (U^{n+1} - U^n)^T (L_h U^{n+1} - f(U^n)). \qquad (37)$$

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

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

and then,

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

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

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

Discrete energy stability (continued)

Discrete energy stability of the ETDRK2 scheme

Under the condition $S \geq 2$,

- for any $h > 0$ and $\tau \leq 1$, we have

$$E_h(U^{n+1}) \leq E_h(U^n) + \widetilde{C} h^{-\frac{1}{2}} (h^2 + \tau)^2,$$

  where $\widetilde{C}$ is independent of h and τ;

- if $h \leq 1$ and $\tau = \lambda\sqrt{h}$ for some constant $\lambda > 0$, we have

$$E_h(U^n) \leq E_h(U^0) + \widehat{C},$$

  where $\widehat{C}$ is independent of h and τ, i.e., the discrete energy is uniformly bounded.

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   - Discrete energy stability
3. Numerical experiments

Fractional power kernel

We consider the 2-D case in all the experiments.

Fractional power kernel:

$$\rho_\delta(r) = \frac{2(4-\alpha)}{\pi\delta^{4-\alpha} r^\alpha}, \quad r > 0,\ \alpha \in [0,4), \tag{38}$$

which satisfies

$$\frac{1}{2}\int_{B_\delta(\mathbf{0})} |\boldsymbol{s}|^2 \rho_\delta(|\boldsymbol{s}|)\, \mathrm{d}\boldsymbol{s} = d = 2. \tag{39}$$

- $\alpha \in [0,2)$: integrable, $\rho_\delta(|\boldsymbol{s}|) \in L^1(B_\delta(\mathbf{0}))$, $\mathcal{L}_\delta$ is bounded;
- $\alpha \in [2,4)$: non-integrable.

Convergence tests

Setting

- $\Omega = (0, 2\pi) \times (0, 2\pi)$, $T = 0.5$, $\varepsilon = 0.1$;
- smooth initial data $u_0(x, y) = 0.5 \sin x \sin y$;
- kernel: $\alpha = 1$ (integrable) and $\alpha = 3$ (non-integrable).

We consider

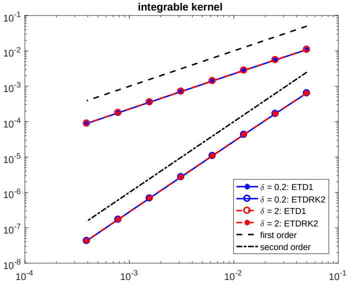
1. temporal convergence rate, i.e., $\tau \to 0$;
2. spatial convergence rate, i.e., $h \to 0$;
3. convergence to the local limit, i.e., $\delta \to 0$.

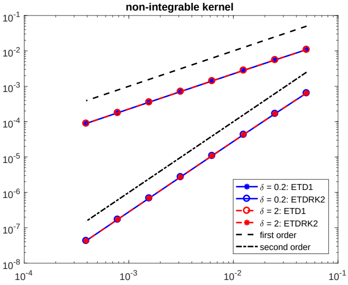
Convergence tests (continued)

1. Temporal convergence rate.

Setting

- $\delta = 0.2$ and $\delta = 2$, respectively;
- $N = 256$;
- $\tau = 0.05 \times 2^{-k}$ with $k = 0, 1, \ldots, 7$;
- benchmark: ETDRK2 scheme with $\tau = 10^{-6}$.





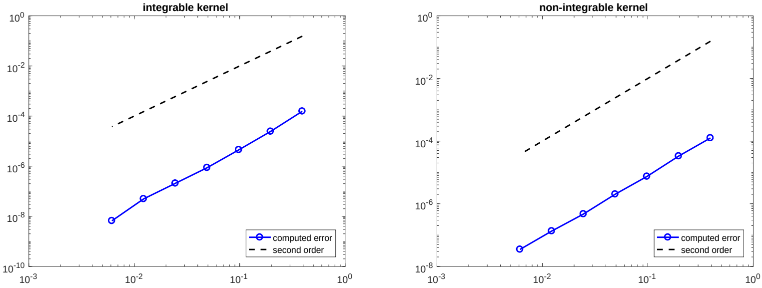
The computed errors are almost independent of choices of δ and α.

Convergence tests (continued)

2. Spatial convergence rate.

Setting

- $\delta = 2$ and $\tau = T$;
- $N = 2^k$ with $k = 4, 5, \ldots, 10$;
- benchmark: $N = 4096$.



The $\mathcal{O}(h^2)$ convergence rate is observed as $h \to 0$.

Convergence tests (continued)

3. Convergence to the local limit.

Setting

- $N = 4096$ and $\tau = T$;
- local solution: ETDRK2 scheme for LAC equation.

$\delta = 0.2$	$\alpha = 1$		$\alpha = 3$	
	error	rate	error	rate
δ	1.076e-5	$*$	5.371e-6	$*$
$\delta/2$	2.703e-6	1.9927	1.344e-6	1.9991
$\delta/4$	6.250e-7	2.1124	3.153e-7	2.0912
$\delta/8$	1.580e-7	1.9835	6.373e-8	2.3068

The $\mathcal{O}(\delta^2)$ convergence rate is observed as $\delta \to 0$.

Stability tests

For the case $\rho_\delta(|\boldsymbol{s}|) \in L^1(B_\delta(\boldsymbol{0}))$, i.e., $\alpha \in [0, 2)$, denote

$$C_\delta = \int_{B_\delta(\boldsymbol{0})} \rho_\delta(|\boldsymbol{s}|)\,\mathrm{d}\boldsymbol{s} = \frac{4(4-\alpha)}{(2-\alpha)\delta^2}.$$

Theorem [Du-Yang, 2016]

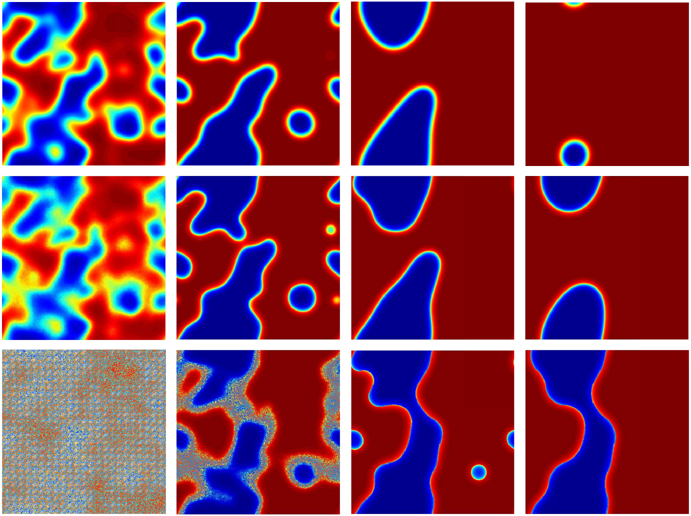
The steady state solution u^* to (NAC) is continuous if $\varepsilon^2 C_\delta \geq 1$.

Setting

- $\Omega = (0, 2\pi) \times (0, 2\pi)$, $\varepsilon = 0.1$;
- $N = 512$, $\tau = 0.01$;
- random initial data ranging from -0.9 to 0.9 uniformly;
- integrable kernel: $\alpha = 1$ (now $\varepsilon^2 C_\delta \geq 1$ leads to $\delta \leq 2\sqrt{3}\varepsilon$);
- $\delta = 0$, $\delta = 3\varepsilon$, $\delta = 4\varepsilon$.

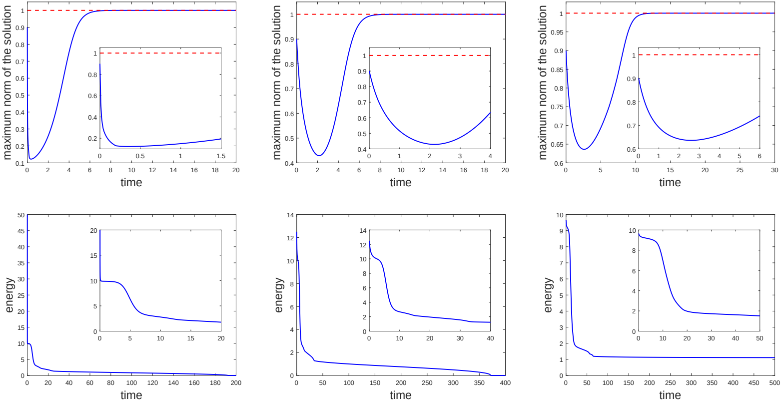
Stability tests (continued)

From top to bottom: $\delta = 0, 3\varepsilon, 4\varepsilon$.
From left to right: $t = 6, 14, 50, 180$.



Stability tests (continued)

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



Discontinuity in the steady state solution

For the case $\rho_\delta(|\mathbf{s}|) \in L^1(B_\delta(\mathbf{0}))$, i.e., $\alpha \in [0,2)$, denote

$$C_\delta = \int_{B_\delta(\mathbf{0})} \rho_\delta(|\mathbf{s}|)\,\mathrm{d}\mathbf{s} = \frac{4(4-\alpha)}{(2-\alpha)\delta^2}.$$

Theorem [Du-Yang, 2016]

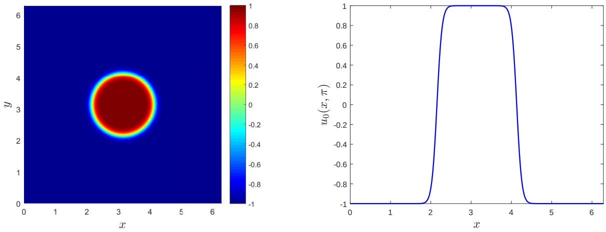
Under certain assumptions, if $\varepsilon^2 C_\delta < 1$, the locally increasing u^* has a discontinuity at x_* with the jump

$$[\![u^*]\!](x_*) = 2\sqrt{1-\varepsilon^2 C_\delta}. \tag{40}$$

Setting

- $\Omega = (0,2\pi)\times(0,2\pi)$, $\varepsilon = 0.1$;
- $N = 2048$, $\tau = 0.01$;
- smooth initial data;
- integrable kernel: $\alpha = 1$.

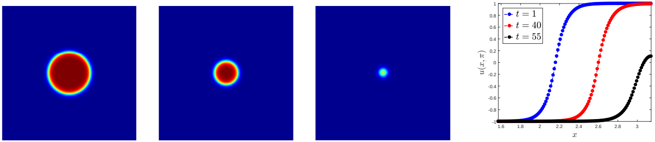
Discontinuity in the steady state solution (continued)



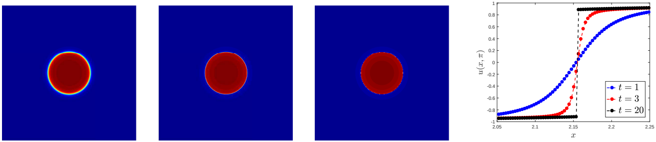
$$\text{theoretical jump} = 2\sqrt{1 - \frac{0.12}{\delta^2}}, \quad \delta > \delta_0 = \sqrt{0.12} \approx 0.3464.$$

	$\delta = 0.2$	$\delta = 0.8$	$\delta = 1.6$	$\delta = 3.2$
theoretical jumps	0	1.802776	1.952562	1.988247
numerical jumps	0	1.804496	1.952713	1.988242

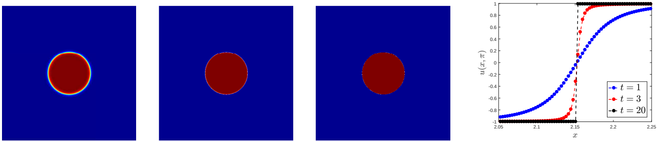
Discontinuity in the steady state solution (continued)



(a) $\delta = 0.2$: solutions at $t = 1, 40, 55$, cross-sections with $y = \pi$



(b) $\delta = 0.8$: solutions at $t = 1, 3, 20$, cross-sections with $y = \pi$



(c) $\delta = 3.2$: solutions at $t = 1, 3, 20$, cross-sections with $y = \pi$

Conclusion

For the NAC equation

$$u_t - \varepsilon^2 \mathcal{L}_\delta u + u^3 - u = 0, \qquad \text{(NAC)}$$

we present the first and second order ETD schemes by using

- quadrature-based difference method for spatial discretization,
- exponential time differencing methods for temporal integration,

and obtain

- discrete maximum principle,
- error estimates and asymptotic compatibility,
- discrete energy stability.

Conclusion (continued)

Something to consider further:

- high-order and other schemes preserving the maximum principle;
- not DMP, but L^∞ stable schemes for high-order PDE;
- asymptotic compatibility for nonlocal C-H equation or others.

Thanks for your attention!