Exponential time differencing methods for phase field equations

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Outline

1. ETD schemes for an MBE equation
   - Energy stability of ETD schemes
   - Numerical experiments
2. ETD schemes for nonlocal Allen-Cahn Equation
   - Maximum principle and energy stability of ETD schemes
   - Error estimates and asymptotic compatibility
   - Numerical experiments
3. Further discussions

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MBE models

We are considering two macroscopic coarsening processes for epitaxial thin film growth, which are gradient flows of two popular choices for the Ehrlich-Schwoebel energy:

• the case without slope selection,

$$E(u) = \iint_{\Omega} \left(-\frac{1}{2} \ln(1 + |\nabla u|^2) + \frac{\varepsilon^2}{2} |\Delta u|^2 \right) dxdy \tag{1}$$

• the case with slope selection,

$$E(u) = \iint_{\Omega} \left(\frac{1}{4} (|\nabla u|^2 - 1)^2 + \frac{\varepsilon^2}{2} |\Delta u|^2 \right) dxdy. \tag{2}$$

The gradient flow of (1) gives MBE equation without slope selection:

$$\frac{\partial u}{\partial t} + \varepsilon^2 \Delta^2 u + \nabla \cdot \left(\frac{\nabla u}{1 + |\nabla u|^2} \right) = 0, \quad (x, y) \in \Omega, 0 < t \leq T. \quad (3)$$

The gradient flow of (2) gives MBE equation with slope selection:

$$\frac{\partial u}{\partial t} + \varepsilon^2 \Delta^2 u + \nabla \cdot [(1 - |\nabla u|^2) \nabla u] = 0, \quad (x, y) \in \Omega, 0 < t \leq T. \quad (4)$$

Here $0 < \varepsilon \ll 1$.

With the initial condition

$$u(x, y, 0) = u_0(x, y), \quad (x, y) \in \bar{\Omega},$$

and the periodic boundary conditions, the following energy identity holds:

$$\frac{d}{dt}E(u) + \|u_t\|^2 = 0. \tag{5}$$

Existing numerical methods

- Stabilized methods:

C. Xu and T. Tang, *SIAM J. Numer. Anal.*, 2006.
D. Li, Z. Qiao and T. Tang, *SIAM J. Numer. Anal.*, 2016.

L. Ju, X. Li, Z. Qiao, H. Zhang, *Math. Comp.*, 2018

- Convex splitting methods:

C. Wang, X.M. Wang and S. Wise, *Disc. Cont. Dyn. Sys. A*, 2010.
J. Shen, C. Wang, X.M. Wang and S. Wise, *SIAM J. Numer. Anal.*, 2012.
W.B. Chen, C. Wang, X.M. Wang, S. Wise, *J. Sci. Comput.*, 2014.

W.B. Chen, S. Conde, C. Wang, X.M. Wang and S. Wise, *J. Sci. Comput.*, 2012.

- SAV method:

Q. Cheng, J. Shen and X.F. Yang, *J. Sci. Comput.*, 2018.

- Discrete Gradient schemes:

Z. Qiao, Z. Zhang and T. Tang, *SIAM J. Sci. Comput.*, 2011.
Z. Qiao, Z. Sun and Z. Zhang, *Math. Comp.*, 2015.

Z. Qiao, T. Tang and H. Xie, *SIAM J. Numer. Anal.*, 2015.

A stabilized first-order scheme of MBE model without slope selection

The classical first-order semi-implicit scheme:

$$\frac{u^{n+1}-u^n}{\Delta t} = -\varepsilon^2\Delta^2 u^{n+1} - \nabla\cdot\left(\frac{\nabla u^n}{1+|\nabla u^n|^2}\right).$$

The stabilized first-order semi-implicit scheme ($A>0$):

$$\frac{u^{n+1}-u^n}{\Delta t} = -\varepsilon^2\Delta^2 u^{n+1} + A\Delta(u^{n+1}-u^n) - \nabla\cdot\left(\frac{\nabla u^n}{1+|\nabla u^n|^2}\right). \qquad (6)$$

Theorem 1.

If $A \geq \frac{1}{8}$, then the numerical solutions of (6) satisfy

$$E(u^{n+1}) \leq E(u^n)$$

for any time step $\Delta t > 0$.

Observations:

The scheme (6) is corresponding to the split energy

$$E(u) = \int_\Omega \left(\frac{A}{2}|\nabla u|^2 + \frac{\varepsilon^2}{2}|\Delta u|^2\right) \mathrm{d}\boldsymbol{x} - \int_\Omega \left(\frac{A}{2}|\nabla u|^2 + \frac{1}{2}\ln(1+|\nabla u|^2)\right) \mathrm{d}\boldsymbol{x}$$

- $A \geq \frac{1}{8}$: a convex splitting scheme;
- $A = 1$: [Chen-Conde-Wang-Wang-Wise, *JSC*, 2012].

Key point of the proof:

Define

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

The function $G(a,b)$ is convex in $\mathbb{R}^2$ if and only if $A\geq\dfrac{1}{8}$.
Simple calculations give us the Hessian matrix

$$\nabla^2G(a,b)=\frac{1}{(1+a^2+b^2)^2}\begin{pmatrix} d_{11}(a^2,b^2) & -2ab \\ -2ab & d_{22}(a^2,b^2)\end{pmatrix}$$

with

$$d_{11}(p,q)=A(p+q)^2+(2A-1)p+(2A+1)q+A+1,$$
$$d_{22}(p,q)=A(p+q)^2+(2A+1)p+(2A-1)q+A+1.$$

The convexity of G is thus equivalent to the positive semi-definiteness of the matrix ∇^2G.

Expression of the exact solution

Rewrite the equation as:

$$u_t = -Lu - f(u),$$

where

$$L = \varepsilon^2 \Delta^2 - \frac{1}{8}\Delta, \quad f(u) = \nabla \cdot \left(\frac{\nabla u}{1 + |\nabla u|^2} \right) + \frac{1}{8}\Delta u.$$

Exact solution:

$$u(t_{n+1}) = \mathrm{e}^{-L\Delta t} u(t_n) - \int_0^{\Delta t} \mathrm{e}^{-L(\Delta t - \tau)} f(u(t_n + \tau))\, \mathrm{d}\tau. \tag{7}$$

For the numerical simulation, we need to approximate:

- the spatial differential operator L;
- the time integration term.

Energy stability

The energy functional

$$E(u)=\int_\Omega\Big(F(\nabla u)+\frac{\varepsilon^2}{2}|\Delta u|^2\Big)\,\mathrm{d}\boldsymbol{x},\ \ F(\boldsymbol{y})=-\frac{1}{2}\ln(1+|\boldsymbol{y}|^2).$$

Note:

- $f(u)=-\nabla_{\boldsymbol{x}}\cdot\nabla_{\boldsymbol{y}}F(\nabla u)+\frac{1}{2}\Delta u$, $L=\varepsilon^2\Delta^2-\frac{1}{2}\Delta$;
- L is positive definite.

Lemma 2.
For any $v,w\in H^2(\Omega)$, we always have

$$E(v)-E(w)\leq\big(f(w)+Lv,v-w\big)-\frac{\varepsilon^2}{2}\|\Delta(v-w)\|^2.$$

Energy stability for ETD1 scheme

The ETD1 scheme for computing $u(t_{n+1})$ is as follows:

$$
\begin{aligned}
u^{n+1} &= \mathrm{e}^{-L\Delta t} u^n - \int_0^{\Delta t} \mathrm{e}^{-L(\Delta t - \tau)} f(u^n)\, \mathrm{d}\tau \\
&= \mathrm{e}^{-L\Delta t} u^n - L^{-1} B f(u^n),
\end{aligned} \tag{8}
$$

where $B := I - \mathrm{e}^{-L\Delta t}$.

Theorem 2.
For any time step $\Delta t > 0$, the numerical solutions of (8) satisfy the energy inequality

$$
E(u^{n+1}) \leq E(u^n). \tag{9}
$$

In other words, the scheme (8) is unconditionally energy stable.

Definition.

The function g is said to be defined on the spectrum of $M \in \mathbb{C}^{d\times d}$ if the values

$$g^{(j)}(\lambda_i), \quad 0 \le j \le n_i, \quad 1 \le i \le d$$

exist, where n_i is the order of the largest Jordan block where λ_i appears.

Lemma 3.

Let g be defined on the spectrum of $M \in \mathbb{C}^{d\times d}$. Then
(1) $g(M)$ commutes with M;
(2) $g(M^T) = g(M)^T$;
(3) the eigenvalues of $g(M)$ are $g(\lambda_i)$, where the λ_i are the eigenvalues of M.

[Nicholas J. Higham, *Functions of matrices: Theory and computation*, SIAM, Philadelphia, PA, 2008]

Proof of Theorem 2

Since $B = I - \mathrm{e}^{-L\Delta t}$, then $LB = BL$. (Lemma 3 (1))

From the ETD1 scheme

$$u^{n+1} = \mathrm{e}^{-L\Delta t} u^n - L^{-1} B f(u^n),$$

we obtain (using $LB = BL$)

$$f(u^n) = -B^{-1} L(u^{n+1} - u^n) - Lu^n.$$

Using Lemma 2, we have

$$\begin{aligned} E(u^{n+1}) - E(u^n) &\le \big(f(u^n) + Lu^{n+1}, u^{n+1} - u^n\big) \\ &= -\big(B^{-1} L(u^{n+1} - u^n), u^{n+1} - u^n\big) + \big(L(u^{n+1} - u^n), u^{n+1} - u^n\big) \\ &= -\big((B^{-1} - I)L(u^{n+1} - u^n), u^{n+1} - u^n\big). \end{aligned}$$

The energy stability results from the positive definiteness of $(B^{-1} - I)L$.

Proof of Theorem 2

Let

$$g(a) = \big((1 - \mathrm{e}^{-a\Delta t})^{-1} - 1\big)a, \quad a \in \mathbb{R},$$

then

$$g'(a) = -2(a\Delta t)\mathrm{e}^{-a\Delta t}(1 - \mathrm{e}^{-a\Delta t})^{-2} + (1 - \mathrm{e}^{-a\Delta t})^{-1} - 1,$$

so g is defined on the spectrum of L, and $(B^{-1} - I)L = g(L)$.

Since L is symmetry, $(B^{-1} - I)L$ is symmetry. (Lemma 3 (2))

Since L is positive definite, the eigenvalues of L are all positive.

For any $a > 0$, it is obvious that $g(a) > 0$, therefore, all the eigenvalues of $g(L)$ are positive (Lemma 3 (3)), which implies the positive definiteness of $(B^{-1} - I)L$.

Coarsening dynamics

$\Omega = (0, 12.8) \times (0, 12.8)$, $u_0(x_i, y_j) \sim U(-0.001, 0.001)$.

$$\Delta t = \begin{cases} 0.001, & t \in [0, 400), \\ 0.01, & t \in [400, 6000), \\ 0.1, & t \in [6000, T]. \end{cases}$$

- energy: $E(t) = \int_\Omega \left(-\frac{1}{2} \ln(1 + |\nabla u|^2) + \frac{\varepsilon^2}{2} |\Delta u|^2 \right) \mathrm{d}\boldsymbol{x}$;
- roughness: $r(t) = \sqrt{\frac{1}{|\Omega|} \int_\Omega |u(\boldsymbol{x}, t) - \bar{u}(t)|^2 \, \mathrm{d}\boldsymbol{x}}$,

  $\bar{u}(t) = \frac{1}{|\Omega|} \int_\Omega u(\boldsymbol{x}, t) \, \mathrm{d}\boldsymbol{x}$;
- width: $w(t) = \sqrt{\frac{1}{|\Omega|} \int_\Omega |\nabla u(\boldsymbol{x}, t)|^2 \, \mathrm{d}\boldsymbol{x}}$.

Coefficients of the linear fits

The theoretical results:

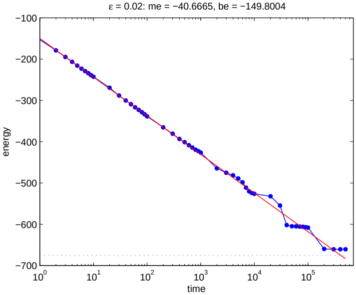
$$E(t) \sim \mathcal{O}(-\ln t), \quad r(t) \sim \mathcal{O}(t^{1/2}), \quad w(t) \sim \mathcal{O}(t^{1/4}).$$

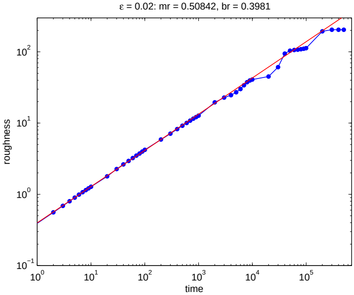
The results of linear fits (using the data up to $t = 400$):

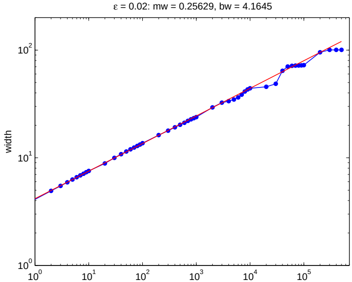
$$E(t) \sim m_e \ln t + b_e, \quad r(t) \sim b_r t^{m_r}, \quad w(t) \sim b_w t^{m_w}.$$

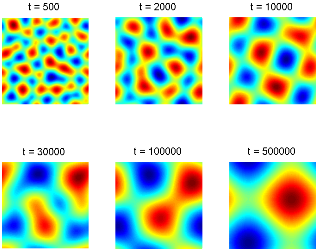
ε	0.08	0.07	0.06	0.05	0.04	0.03	0.02
m_e	-40.039	-38.231	-38.786	-40.178	-39.680	-40.155	-40.667
b_e	-43.127	-57.311	-67.685	-76.282	-95.028	-118.309	-149.800
m_r	0.536	0.512	0.514	0.522	0.511	0.509	0.508
b_r	0.351	0.374	0.377	0.362	0.378	0.391	0.398
m_w	0.275	0.264	0.264	0.267	0.260	0.257	0.256
b_w	1.890	2.094	2.281	2.468	2.837	3.359	4.164

$\varepsilon = 0.02, N = 1024, T = 5 \times 10^5$









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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

$$E_{\text{local}}(u) = \int \left(\frac{1}{4} (u(\boldsymbol{x})^2 - 1)^2 + \frac{\varepsilon^2}{2} |\nabla u(\boldsymbol{x})|^2 \right) \mathrm{d}\boldsymbol{x}, \tag{10}$$

- energy stability:

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

As a second order reaction-diffusion equation,

- maximum principle:

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

Stabilization methods

Energy stable schemes:

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

$$\frac{u^{n+1} - u^n}{\tau} - \varepsilon^2 \Delta_h u^{n+1} + (u^n)^3 - u^n + S(u^{n+1} - u^n) = 0. \quad (11)$$

This scheme is easy to implement and conditionally energy stable.

Stabilization methods

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

What is the condition for energy stability?

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

However,

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

Stabilization methods

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However,

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

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

Stabilization methods

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

$$\frac{u^{n+1}-u^n}{\tau}-\varepsilon^2\Delta_h u^{n+1}+(u^n)^3-u^n+S(u^{n+1}-u^n)=0 \quad (12)$$

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

Stabilization methods

(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 S, in the sense that S is independent of the L^∞ bound on the numerical solution.

Nonlocal Allen-Cahn equation

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

$$\mathcal{L}_\delta u(\boldsymbol{x}) = \frac{1}{2} \int_{B_\delta(\mathbf{0})} \rho_\delta(|\boldsymbol{s}|) \big(u(\boldsymbol{x}+\boldsymbol{s}) + u(\boldsymbol{x}-\boldsymbol{s}) - 2u(\boldsymbol{x}) \big) \, \mathrm{d}\boldsymbol{s}. \tag{13}$$

Kernel function $\rho_\delta : [0, \delta] \to \mathbb{R}$:

- nonnegative function;
- has a finite second order moment:

$$\int_{B_\delta(\mathbf{0})} |\boldsymbol{s}|^2 \rho_\delta(|\boldsymbol{s}|) \, \mathrm{d}\boldsymbol{s} = 2d. \tag{14}$$

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

$$\max_{\boldsymbol{x}} |\mathcal{L}_\delta u(\boldsymbol{x}) - \mathcal{L}_0 u(\boldsymbol{x})| \le C\delta^2 \|u\|_{C^4}. \tag{15}$$

Nonlocal Allen-Cahn equation (continued)

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

$$E(u) = \int \left(\frac{1}{4}(u(\boldsymbol{x})^2 - 1)^2 - \frac{\varepsilon^2}{2} u(\boldsymbol{x}) \mathcal{L}_\delta u(\boldsymbol{x}) \right) \mathrm{d}\boldsymbol{x}, \tag{16}$$

- energy stability:

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

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

- maximum principle:

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

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

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

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

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 $\boldsymbol{x_i} = h\boldsymbol{i}$:

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

Define the discrete version of $\mathcal{L}_\delta$ by [Du-Tao-Tian-Yang, 2017]

$$\mathcal{L}_{\delta,h} u(\boldsymbol{x_i}) = \frac{1}{2}\int_{B_\delta(\mathbf{0})} \mathcal{I}_h\left(\frac{u(\boldsymbol{x_i}+\boldsymbol{s}) + u(\boldsymbol{x_i}-\boldsymbol{s}) - 2u(\boldsymbol{x_i})}{|\boldsymbol{s}|^2}|\boldsymbol{s}|_1\right) \frac{|\boldsymbol{s}|^2}{|\boldsymbol{s}|_1}\rho_\delta(|\boldsymbol{s}|)\,\mathrm{d}\boldsymbol{s}. \tag{19}$$

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

$$\mathcal{L}_{\delta,h}u(\boldsymbol{x_i}) = \sum_{\boldsymbol{0}\neq \boldsymbol{s_j}\in B_\delta(\boldsymbol{0})} \frac{u(\boldsymbol{x_i}+\boldsymbol{s_j}) + u(\boldsymbol{x_i}-\boldsymbol{s_j}) - 2u(\boldsymbol{x_i})}{|\boldsymbol{s_j}|^2} |\boldsymbol{s_j}|_1 \beta_\delta(\boldsymbol{s_j}), \tag{20}$$

where

$$\beta_\delta(\boldsymbol{s_j}) = \frac{1}{2}\int_{B_\delta(\boldsymbol{0})} \psi_{\boldsymbol{j}}(\boldsymbol{s}) \frac{|\boldsymbol{s}|^2}{|\boldsymbol{s}|_1} \rho_\delta(|\boldsymbol{s}|)\,\mathrm{d}\boldsymbol{s}. \tag{21}$$

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, 2017])

$$\max_{\boldsymbol{x_i}\in\Omega} |\mathcal{L}_{\delta,h}u(\boldsymbol{x_i}) - \mathcal{L}_\delta u(\boldsymbol{x_i})| \le Ch^2\|u\|_{C^4}, \tag{22}$$

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

Quadrature-based finite difference discretization (continued)

- 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

$$\begin{cases} \dfrac{\mathrm{d}U}{\mathrm{d}t} = \varepsilon^2 D_h U + U - U^{.3}, \quad t \in (0,T], \\ U(0) = U_0. \end{cases} \tag{23}$$

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

$$L_h := -\varepsilon^2 D_h + SI, \qquad f(U) := (S+1)U - U^{\cdot 3}. \tag{24}$$

Then, we reach

$$\frac{\mathrm{d}U}{\mathrm{d}t} + L_h U = f(U), \tag{25}$$

whose solution satisfies

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

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

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

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 $t = t_n$:

$$U(t_{n+1}) = \mathrm{e}^{-L_h\tau} U(t_n) + \int_0^\tau \mathrm{e}^{-L_h(\tau-s)} f(U(t_n+s))\,\mathrm{d}s. \tag{28}$$

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):

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

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)

- $\|e^{-L_h\tau}\|_\infty \le e^{-S\tau}$ 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

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

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

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

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

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

Discrete maximum principle (continued)

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

$$f(U) = (S+1)U - U^{.3}$$

Proof. Define

$$f_0(\xi) = (S+1)\xi - \xi^3, \quad \xi \in \mathbb{R}.$$

Obviously,

$$f_0(-1) = -S, \quad f_0(1) = S.$$

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

$$f_0'(\xi) = S + 1 - 3\xi^2 \geq S - 2 \geq 0.$$

Therefore,

$$\max_{\xi \in [-1,1]} |f_0(\xi)| = S.$$

Discrete maximum principle (continued)

For the ETDRK2 scheme, we have

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

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

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

Then,

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

Energy stability

We define the discretized energy E_h:

$$E_h(U) = \frac{1}{4}\sum_{i=1}^{dN} F(U_i) - \frac{\varepsilon^2}{2} U^T D_h U, \quad F(s) = \frac{1}{4}(s^2-1)^2. \tag{29}$$

Energy stability of ETD1 and ETDRK2 schemes

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

- ETD1: $E_h(U^{n+1}) + (S-1)\|U^{n+1} - U^n\|_2^2 \leq E_h(U^n)$;
- ETDRK2: $E_h(U^{n+1}) \leq E_h(U^n) + \mathcal{O}(\tau^2)$.

For the ETD1 scheme, the proof includes two steps.

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

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

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,

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

Error estimates

Error estimates of ETD1 scheme

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

$$\|U^n - I^h u(t_n)\|_\infty \le C e^{t_n}(h^2 + \tau), \quad t_n \le T, \tag{30}$$

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

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

Error estimates (continued)

ETDRK2 scheme:

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

Error estimates of ETDRK2 scheme

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

$$\|U^n - I^h u(t_n)\|_\infty \le C\mathrm{e}^{t_n}(h^2+\tau^2), \quad t_n \le T, \tag{31}$$

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

Asymptotic compatibility

$$
\begin{tikzcd}
u_h^\delta \arrow[r, "\delta \to 0"] \arrow[d, "h \to 0"'] \arrow[dr, "(\delta \to 0,\ h \to 0)" description] & u_h^0 \arrow[d, "h \to 0"] \\
u^\delta \arrow[r, "\delta \to 0"] & u^0
\end{tikzcd}
$$

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

Then,

$$\max_{\boldsymbol{x_i}\in\Omega} |\mathcal{L}_{\delta,h}u(\boldsymbol{x_i}) - \mathcal{L}_0 u(\boldsymbol{x_i})| \le C(\delta^2 + h^2)\|u\|_{C^4}. \tag{32}$$

Fractional power kernel

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

Fractional power kernel:

$$\rho_\delta(r) = \frac{2(4-\alpha)}{\pi\delta^{4-\alpha}r^\alpha}, \quad r > 0,\ \alpha \in [0,4), \tag{33}$$

which satisfies

$$\int_{B_\delta(\mathbf{0})} |\boldsymbol{s}|^2 \rho_\delta(|\boldsymbol{s}|)\,\mathrm{d}\boldsymbol{s} = 2d = 4. \tag{34}$$

- $\alpha \in [0,2)$: 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

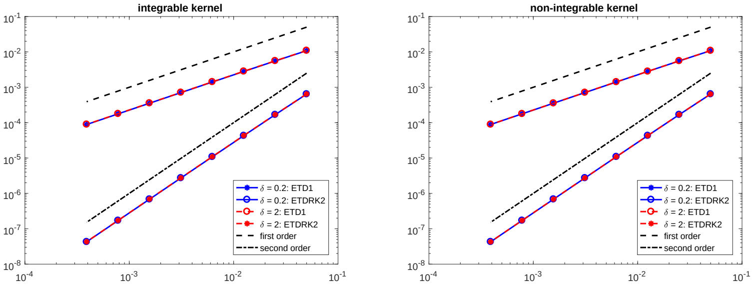
1. temporal convergence rate, i.e., $\tau \to 0$;
2. spatial convergence rate, i.e., $h \to 0$;
3. convergence to the local limit, i.e., $\delta \to 0$.

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 $\tau = 10^{-6}$.



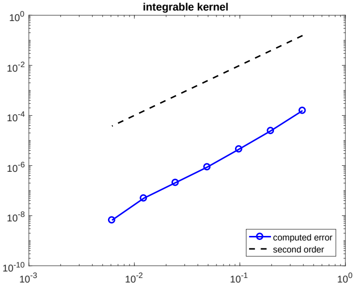
The computed errors are almost independent on choices of δ and α.

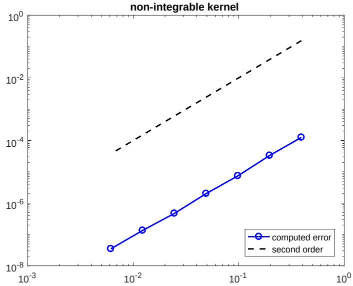
Convergence tests (continued)

2. Spatial convergence rate.

Setting

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





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

Stability tests

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

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

[Du-Yang, 2016]

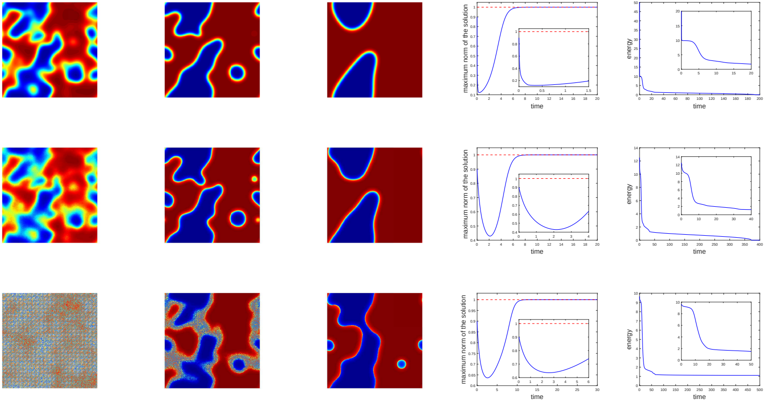
The steady state solution u^* to (NAC) is continuous if $\varepsilon^2 C_\delta \geq 1$.

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)

$\delta = 0, \delta = 3\varepsilon, \delta = 4\varepsilon.$



Solutions at times $t = 6, 14, 50$, maximum-norms, 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

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

[Du-Yang, 2016]

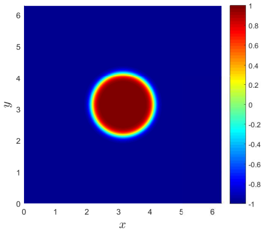
Under certain assumptions, if $\varepsilon^2 C_\delta < 1$, the locally increasing u^* has a discontinuity at x_* with the jump

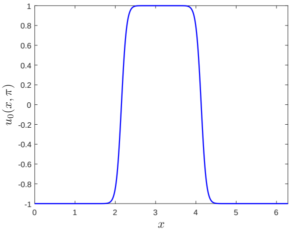
$$[\![u^*]\!](x_*) = 2\sqrt{1-\varepsilon^2 C_\delta}. \tag{35}$$

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)

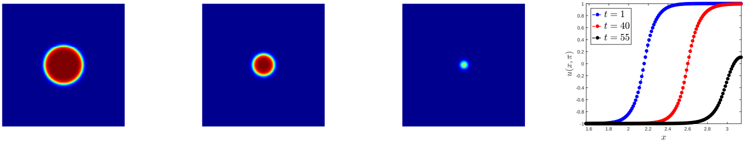




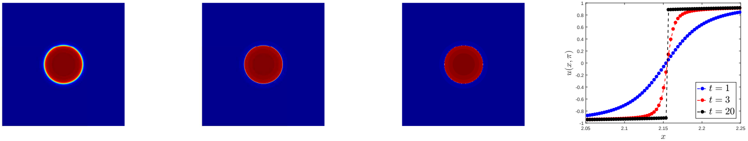
$$\text{theoretical jump} = 2\sqrt{1-\frac{0.12}{\delta^2}}, \quad \delta > \delta_0 = \sqrt{0.12} \approx 0.3464.$$

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

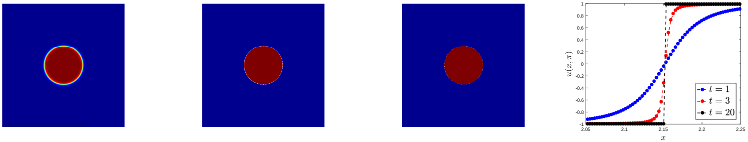
Discontinuity in the steady state solution (continued)



(a) $\delta = 0.2$: solutions at $t = 1, 40, 55$, cross-sections with $y = \pi$ and $x \in [\frac{\pi}{2}, \pi]$



(b) $\delta = 0.8$: solutions at $t = 1, 3, 20$, cross-sections with $y = \pi$ and $x \in [2.05, 2.35]$



(c) $\delta = 3.2$: solutions at $t = 1, 3, 20$, cross-sections with $y = \pi$ and $x \in [2.05, 2.35]$

Outline

1. ETD schemes for an MBE equation
   - Energy stability of ETD schemes
   - Numerical experiments
2. ETD schemes for nonlocal Allen-Cahn Equation
   - Maximum principle and energy stability of ETD schemes
   - Error estimates and asymptotic compatibility
   - Numerical experiments
3. Further discussions

Abstract framework

Let us consider Ω as either a connected set or a collection of isolated points in $\mathbb{R}^d$. More precisely, we consider the following two situations:

(D1) Ω is an open connected and bounded set with its boundary denoted by $\partial\Omega$;

(D2) $\widetilde{\Omega}$ is a set described as (D1) and Σ consists of all the nodes in a mesh triangulating $\widetilde{\Omega}$, uniformly or not, then set $\Omega = \widetilde{\Omega} \cap \Sigma$ and $\partial\Omega = \partial\widetilde{\Omega} \cap \Sigma$.

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

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

Note that the continuity of functions mentioned above is defined as follows:

$$f \text{ is continuous at } \boldsymbol{x}^* \in \overline{\Omega} \iff \forall \boldsymbol{x}_n \to \boldsymbol{x}^* \text{ in } \overline{\Omega} \text{ implies } f(\boldsymbol{x}_n) \to f(\boldsymbol{x}^*),$$

thus the definition of X makes sense whenever Ω is a open connected set or a collection of isolated points. In particular, the following two cases are considered in this work:

(C1) $X = C_0(\overline{\Omega};\mathbb{R})$, the set of functions continuous on $\overline{\Omega}$ and vanishing on $\partial\Omega$;

(C2) $X = C_{\text{per}}(\overline{\Omega};\mathbb{R})$, the set of functions continuous in $\mathbb{R}^d$ and periodic with respect to Ω.

Let $f : X \to X$ be a nonlinear operator, and $\mathcal{L} : D(\mathcal{L}) \to X$ be a linear operator where the domain $D(\mathcal{L})$ is a linear subspace of X. The model equation we consider in this paper is a semilinear parabolic equation taking the following form

$$u_t = \mathcal{L}u + f[u], \quad t > 0, \tag{36}$$

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

$$u(0) = u_0, \quad \text{in } \overline{\Omega} \tag{37}$$

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

Regarding the operators $\mathcal{L}$ and f, we make the following specific assumptions.

Assumption 1.

The linear operator $\mathcal{L}$ satisfies the followings:

(a) $\mathcal{L} : D(\mathcal{L}) \to X$ is a closed operator 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, where $\mathcal{I}$ is the identity opereator;

(c) it always holds that $\mathcal{L}w(\boldsymbol{x}_0) \le 0$ for any $w \in D(\mathcal{L})$ and $\boldsymbol{x}_0 \in \Omega$ such that

$$w(\boldsymbol{x}_0) = \max_{\boldsymbol{x}\in\Omega} w(\boldsymbol{x}) \text{ for Case (C1)}$$

or

$$w(\boldsymbol{x}_0) = \max_{\boldsymbol{x}\in\overline{\Omega}} w(\boldsymbol{x}) \text{ for Case (C2).}$$

Assumption 2.
The nonlinear operator f acts as a composite function induced by a given one-variable smooth function $f_0 : \mathbb{R} \to \mathbb{R}$, that is,

$$f[w](\boldsymbol{x}) = f_0(w(\boldsymbol{x})), \quad \forall\, w \in X,\ \forall\, \boldsymbol{x} \in \overline{\Omega}, \tag{38}$$

and there exists $\beta > 0$ such that

$$f_0(\beta) \le 0 \le f_0(-\beta). \tag{39}$$

Theorem

Given a constant $T > 0$. *Under Assumptions 1 and 2,, if the initial condition* (37) *satisfies* $\|u_0\| \le \beta$, *then the equation* (36) *has a unique solution* $u \in C([0,T];X)$ *and satisfies* $\|u(t)\| \le \beta$ *for any* $t \in (0,T]$.

Let us introduce a stabilizing constant $\kappa \geq 0$ and rewrite the equation (36) in the following equivalent form:

$$u_t + \kappa u = \mathcal{L}u + \mathcal{N}[u], \tag{40}$$

where $\mathcal{N} := \kappa\mathcal{I} + f$. According to (38) in Assumption 2, we know

$$\mathcal{N}[w](\boldsymbol{x}) = N_0(w(\boldsymbol{x})), \quad \forall\, w \in X,\ \forall\, \boldsymbol{x} \in \overline{\Omega}, \tag{41}$$

where

$$N_0(\xi) := \kappa\xi + f_0(\xi), \quad \xi \in \mathbb{R}. \tag{42}$$

The solution to the differential equation (40) satisfies the following integrating formula:

$$u(t+\tau) = \mathrm{e}^{-\kappa\tau} S_{\mathcal{L}}(\tau) u(t) + \int_0^{\tau} \mathrm{e}^{-\kappa(\tau-s)} S_{\mathcal{L}}(\tau-s) \mathcal{N}[u(t+s)] \, \mathrm{d}s, \quad \forall\, t, \tau \geq 0. \tag{43}$$

To show the maximum principle holds for both the model equation (36) and its discretiztions proposed later, we impose a requirement on the selection of the stabilizing constant κ such that

$$\kappa \geq \max_{|\xi| \leq \beta} |f_0'(\xi)| \tag{44}$$

holds. Note that the condition (44) can always be reached since f_0 is a smooth function.

Thanks for your attention!