A Second Look at Time Stepping for Phase Field Models

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Overview

Joint work with Xinyu Cheng and Keith Promislow

- Allen Cahn and Cahn Hilliard Dynamics
- Time Stepping:
  - Schemes
  - Adaptive Time Stepping
  - Numerical Validation
- Accuracy:
  - Asymptotic Consistency
  - Asymptotic Analysis of BE for AC

Allen Cahn Dynamics

$u(x,t)$, 2π-periodic in x solves

$$u_t = u_{xx} - (u^3 - u)/\epsilon^2$$

Allen and Cahn, Acta Metall 1979

- For discussion forget the diffusion term. AC is then an autonomous ODE with fixed points $u = \pm 1$ (stable) and $u = 0$ (unstable) at each space location
- solutions tend to $u = \pm 1$ in $O(1/\epsilon^2)$ time: spinodal evolution
- with $\epsilon > 0$ there is an interface of width $O(\epsilon)$ that is formed between the two phases

Allen Cahn Dynamics

Gamma Limit

$$u_t = \Delta u - (u^3 - u)/\epsilon^2$$

- 1D steady state solution

$$u = \tanh\left(\frac{x - x_0}{\epsilon\sqrt{2}}\right)$$

- in higher dimensions, x_0 is replaced by the curve between the phases $u = \pm 1$ and $x - x_0$ is replaced by a normal distance to the curve
- in this case, the solution is approximate and the interface will move in a slower time scale: ripening evolution
- higher order asymptotic terms can determine a motion law for the interface: gamma limit
- For 2D & 3D AC curves move with curvature motion as $\epsilon \to 0$ in an O(1) time scale.

Allen Cahn Dynamics

Energy Gradient Flow

$$\begin{aligned} u_t &= \Delta u - W'(u)/\epsilon^2 \\ W(u) &= \frac{1}{4}(u^2-1)^2 \end{aligned}$$

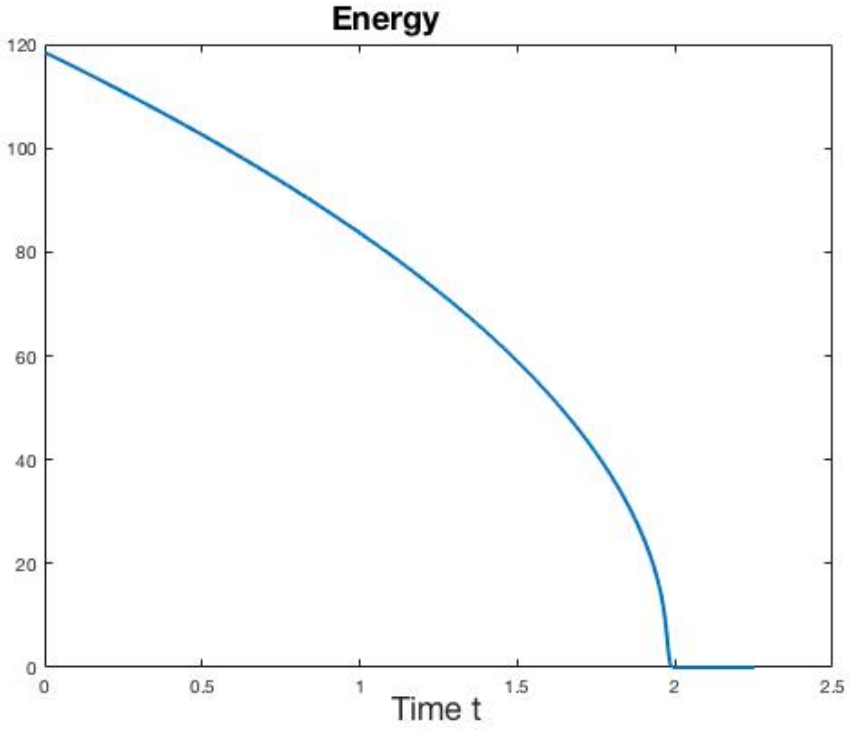
- This equation is gradient flow on the energy

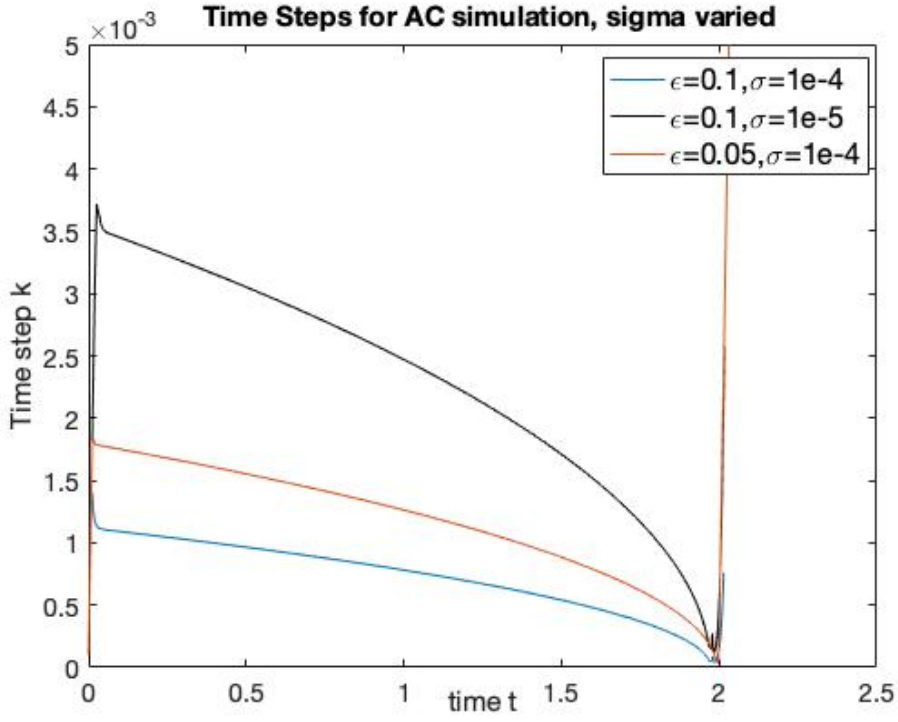
$$\mathcal{E} = \int_0^{2\pi} \left(|\nabla u|^2/2 + W(u)/\epsilon^2 \right) dx$$

- This leads to a symmetric Jacobian matrix for the implicit time steps of the discretization
- Movie

Allen Cahn Dynamics

Details of Computational Results





Cahn-Hilliard Dynamics

$$u_t = -\Delta \left(\epsilon \Delta u - (u^3 - u)/\epsilon \right)$$

Cahn and Hilliard, J Chem Phys 1958

- Gradient flow on the same energy a AC but in the H_{-1} norm that has inner product

$$(u, v)_{H_{-1}} := (u, \Delta^{-1} v)$$

- Conserves the mass of the two phases
- The gamma limit is nonlocal, Mullins-Sekerka flow, in $O(1)$ time scale.
- Movie

First Order Schemes for AC

$$u_t = \Delta u - (u^3 - u)/\epsilon^2$$

Consider Spatially Continuous Semi-Discretization (Map of Planes)

FI Fully Implicit (Backward Euler):

$$U^{n+1} = U^n + k\Delta U^{n+1} - k\left[(U^{n+1})^3 - U^{n+1}\right])/\epsilon^2$$

ES Energy Stable (Eyre, Convex/Concave Splitting):

$$U^{n+1} = U^n + k\Delta U^{n+1} - k\left[(U^{n+1})^3 - U^{n}\right])/\epsilon^2$$

- ES schemes have desirable properties.
- FI schemes are asymptotically more accurate than ES.

Local Truncation Error

Asymptotic solution in metastable dynamics:

$$u(x,t) \approx \tanh\left(\frac{\mathrm{dist}(x,\Gamma)}{\epsilon\sqrt{2}}\right), \text{ so } \quad \frac{\partial^n u}{\partial t^n} = O(\epsilon^{-n})$$

FI local error

$$\frac{1}{2}k^2 u_{tt} = O(k^2/\epsilon^2)$$

ES

$$U^{n+1} = U^n + k\Delta U^{n+1} - k\left[(U^{n+1})^3 - U^n\right])/\epsilon^2 = \text{FI} - k(U^{n+1} - U^n)/\epsilon^2$$

ES dominant local error term

$$k^2 u_t/\epsilon^2 = O(k^2/\epsilon^3)$$

ES is asymptotically less accurate than FI.

Adaptive Time Stepping

Let σ be the allowable local error per time step.

FI (local error $O(k^2/\epsilon^2)$)

- $k = O(\sqrt{\sigma}\epsilon)$
- $M = O(1/k) = O(1/(\sqrt{\sigma}\epsilon))$

ES (local error $O(k^2/\epsilon^3)$)

- $k = O(\sqrt{\sigma}\epsilon^{3/2})$
- $M = O(1/k) = O(1/(\sqrt{\sigma}\epsilon^{3/2}))$

First Goal: Identify how M behaves with ϵ for fixed σ for different schemes and problems

Spatial Discretization and Discrete Solution

$$\mathbf{G}(U) := U - k\left[\Delta U - (U^3 - U)/\epsilon^2\right] - U^n = 0$$

- Newton's method with symmetric Frechet derivative

$$\mathcal{J} = I - k(\Delta - \Lambda_2/\epsilon^2 + I/\epsilon^2)$$

  where Λ_2 is pointwise multiplication by $3U^2$.
- Symmetric preconditioner (Scott Maclachlan and Zhengfu Xu)

$$\mathcal{Q} = I - k(\Delta - 2/\epsilon^2)$$

- $\mathcal{J}$ and $\mathcal{Q}^{-1}$ can be implemented easily in a PCG solve of a Newton step with a spectral spatial discretization.
- Solver properties are independent of the spatial resolution.

Error Estimation

- Perform two time steps of the same size k
- Compute the predictor U^p for U^{n+2}

$$U^p = U^n + \frac{k}{3}\left(\mathcal{F}(U^n) + 4\mathcal{F}(U^{n+1}) + \mathcal{F}(U^{n+2})\right)$$

  where $\mathcal{F}(u) = \Delta u - f(u)/\epsilon^2$ for AC.
- Time step sizes are adjusted so that

$$\|U^{n+2} - U^p\|_\infty \leq \sigma.$$

- U^p is one order more accurate than U^{n+2}, up to fifth order
- U^p has an inherent dominant local error $k^5 u_{ttttt}/90$

AC Numerical Results

Fully Implicit $M = O(1/(\sqrt{\sigma}\epsilon))$

$\epsilon = 0.2$, σ varied

σ	M	CG	E
1e-4	717	5,348 [7.46]	0.003
1e-5	2,225 (3.10)	9,448 [4.24]	0.001
1e-6	7,010 (3.15)	23,017 [3.28]	0.001

Validates $M = O(\sqrt{\sigma})$ for constant ϵ. $(\sqrt{10} \approx 3.16)$.

ϵ varied, $\sigma = 1e-4$

ϵ	M	CG	E
0.2	717	5,348 [7.46]	0.003
0.1	1,291 (1.80)	12,354 [9.57]	0.001
0.05	2,412 (1.87)	27,782 [11.52]	0.001
0.025	4,630 (1.92)	64,884 [14.01]	*

Validates $M = O(1/\epsilon)$ for constant σ.

AC Numerical Results

Energy Stable $M = O(1/(\sqrt{\sigma}\epsilon^{3/2}))$

$\epsilon = 0.2$, σ varied

σ	M	CG	E
1e-4	2,350	14,856 [6.32]	0.047
1e-5	7,351 (3.12)	28,263 [3.85]	0.014
1e-6	23,172 (3.15)	68,148 [2.94]	0.004

Validates $M = O(\sqrt{\sigma})$ for constant ϵ, ($\sqrt{10} \approx 3.16$).

ϵ varied, $\sigma = 1e-4$

ϵ	M	CG	transition
0.2	2,350	14,856 [6.32]	0.047
0.1	6,463 (2.75)	44,717 [6.92]	0.069
0.05	18,218 (2.83)	143,416 [7.87]	0.099
0.025	52,595 (2.89)	497,846 [9.47]	0.141

Validates $M = O(1/\epsilon^{3/2})$ for constant σ, ($2^{3/2} \approx 2.83$), and reduced accuracy as $\epsilon \to 0$.

Cahn Hilliard Equation

Local Truncation Error

FI local error as before

$$\frac{1}{2}k^2 u_{tt} = O(k^2/\epsilon^2)$$

ES dominant local error term

$$k^2 \Delta u_t/\epsilon = O(k^2/\epsilon^4)$$

Gap in performance between FI and ES larger for CH than AC.

Adaptive Time Stepping for CH

Let σ be the allowable local error per time step.

FI (local error $O(k^2/\epsilon^2)$)

- $k = O(\sqrt{\sigma}\epsilon)$
- $M = O(1/k) = O(1/(\sqrt{\sigma}\epsilon))$

ES (local error $O(k^2/\epsilon^4)$)

- $k = O(\sqrt{\sigma}\epsilon^2)$
- $M = O(1/k) = O(1/(\sqrt{\sigma}\epsilon^2))$

Observed computationally.

Second Order L-stable Schemes

$$\text{BDF2: } \frac{3U}{2} - k\mathcal{F}(U) = 2U^n - U^{n-1}/2$$

Local truncation error $-k^3 u_{ttt}/3 = O(k^3/\epsilon^3)$ for both AC and CH.

$$\text{DIRK2: } U^* - \alpha k\mathcal{F}(U^*) = U^n$$
$$U - \alpha k\mathcal{F}(U) = U^n + (1-\alpha)k\mathcal{F}(U^*)$$

Local truncation error:

AC: $3\alpha^2(1-\alpha)uu_t^2/(2\epsilon^2) = O(k^3/\epsilon^4)$

CH: $-\Delta\left(3\alpha^2(1-\alpha)uu_t^2/(2\epsilon)\right) = O(k^3/\epsilon^5)$

Observed computationally.

Source of Increased Error

- In the metastable regimes of AC and CH, diffusion and nonlinear reaction are both large but approximately cancel to give the slow dynamics.
- FI(BE) and BDF2 dominant truncation errors that are pure time derivatives of the solution, which inherit this high order cancellation.
- ES and DIRK2 have truncation errors that involve the reaction term individually, hence the amplification in size.

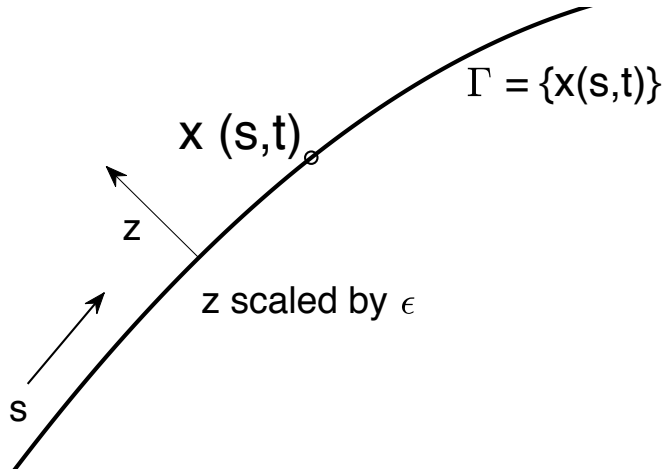
BE Accuracy for AC

A naïve prediction for the final accuracy of BE is $M\sigma = O(\sqrt{\sigma}/\epsilon)$, but we see computationally accuracy independent of ϵ for fixed σ.

We consider the scaling $k = c\epsilon$ with c small and fixed. We write

$$U^n(\mathbf{x}) = u(\mathbf{x}, nk) + e^n$$

where $e^n(s, z)$ is the error.



Error Analysis for BE applied to AC – I

$$U^n(\mathbf{x}) = u(\mathbf{x}, nk) + e^n$$

Insert into the discrete equation

$$U^{n+1} = U^n + k\Delta U^{n+1} + kf(U^{n+1})$$

linearize around the exact solution keeping only dominant terms:

$$e^{n+1} + \frac{k}{\epsilon^2}\mathcal{L}e^{n+1} \approx e^n + \tau^{n+1}$$

where $\mathcal{L} := -\partial^2/\partial z^2 + f'(g)$, $g(z) = \tanh(z/\sqrt{2})$, and τ^n is the local truncation error:

$$\tau^n = k^2 u_{tt}/2 = \frac{k^2}{2}\left(-g'(z)V_t/\epsilon + g''V^2/\epsilon^2\right)$$

The error is approximately due to the linearized problem forced by the truncation error.

Error Analysis for BE applied to AC – II

$$e^{n+1} + \frac{k}{\epsilon^2}\mathcal{L}e^{n+1} \approx e^n + \tau^{n+1}$$

At each s we make an L_2 (in z) orthogonal decomposition of e^n:

$$e^n = r^n + w^n,\ r^n(s,z) \in \mathrm{span}\{g'(z)\} := G \text{ and } w^n \in G^\perp$$

$\mathcal{L}$ has G as its kernel and is positive with bounded inverse on $G^\perp$.

$$\tau^n = \frac{k^2}{2}\left(-g'(z)V_t/\epsilon + g''V^2/\epsilon^2\right)$$

Note that $g'' \in G^\perp$.

$$r^{n+1} = r^n + \frac{k^2}{2\epsilon}|V_t| \tag{1}$$

$$\|w^{n+1}\| \le \frac{1}{1 + kK/\epsilon^2}\left(\|w^n\| + k^2V^2\|g''\|/\epsilon^2\right) \tag{2}$$

to dominant order (as $\epsilon \to 0$).

Error Analysis for BE applied to AC – III

$$r_{n+1} = r_n + \frac{k^2}{2\epsilon}|V_t| \tag{3}$$

$$\|w_{n+1}\| \leq \frac{1}{1 + kK/\epsilon^2}\left(\|w_n\| + k^2 V^2 \|g''\|/\epsilon^2\right) \tag{4}$$

- Recall $k = c\epsilon$.
- We can sum the first equation over $O(1/k)$ time steps to find $r = O(c)$.
- Consider the second equation to see that $w = O(k)$.
- Error is $O(c)$ independent of ϵ.

Because the dominant truncation error is in $G^{\perp}$, it is heavily damped every time step and only a lower order term accumulates in the global temporal error. No other time stepping method we considered has this property.

Asymptotic Consistency

Definition

Consider a family of solutions $u(\epsilon)$ and a family of schemes $U(k, \epsilon)$ to approximate $u(\epsilon)$ with numerical parameter k. A map $k(\epsilon)$ is said to be *asymptotically consistent* of order p if

$$\lim_{\epsilon \to 0} \| U(ck(\epsilon), \epsilon) - u(\epsilon) \| \leq Kc^p$$

with K independent of ϵ.

We can convincingly conjecture that BE for AC in metastable dynamics is first order asymptotically consistent with $k = \epsilon$.

Summary

1. Behaviour of time steps for different schemes for AC and CH with σ and ϵ is predicted and validated with numerical experiments.
2. It is seen that methods with a dominant local truncation error that is a pure time derivative behave asymptotically better than those that do not. BE and BDF2 have this desirable property.
3. We observe better accuracy for BE applied to AC than expected and show a formal asymptotic argument that explains the behaviour.
4. The asymptotic consistency of higher order methods is left as an open question.
5. Accurate local error estimation is another open question.