Asymptotic Behaviour of Time Stepping Methods for Phase Field Models

Brian Wetton

Mathematics Department
University of British Columbia
www.math.ubc.ca/∼wetton

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Overview

Joint work with Xinyu Cheng, Dong Li, and Keith Promislow
JSC (2021)

- Allen Cahn and Cahn Hilliard Meta-Stable Dynamics
- Adaptive Time Stepping:
  - Schemes
  - Predictions (Profile Fidelity)
  - Numerical Validation
- Rigorous Result for Backward Euler for AC

High Accuracy Benchmark Problems for Allen-Cahn and Cahn-Hilliard Dynamics, CiCP (2019).

Allen Cahn Dynamics

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

Allen and Cahn, Acta Metall 1979

- 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.
- Interfaces move approximately with curvature motion as $\epsilon \to 0$ in an $O(1)$ time scale (meta-stable dynamics).
- This equation is gradient flow on the energy

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

  with $W(u) = \frac{1}{4}(u^2 - 1)^2$.
- This leads to a symmetric Jacobian matrix for the implicit time steps of the spatial discretization.

Cahn-Hilliard Dynamics

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

Cahn and Hilliard, J Chem Phys 1958

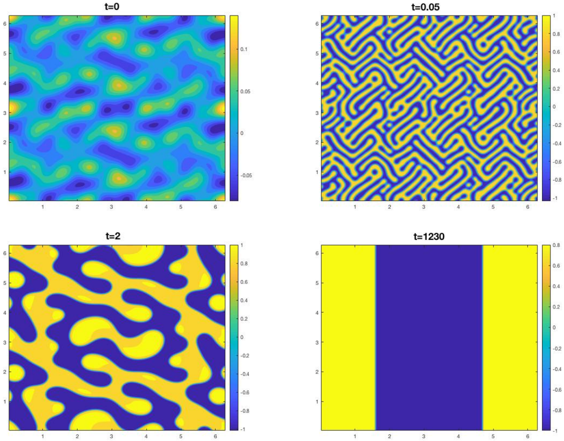
- Gradient flow on the same energy a AC but in the H_{-1} norm that has inner product

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

- Conserves the mass of the two phases
- The meta-stable interface motion is nonlocal, Mullins-Sekerka flow, in $O(1)$ time scale.

Cahn-Hilliard Dynamics

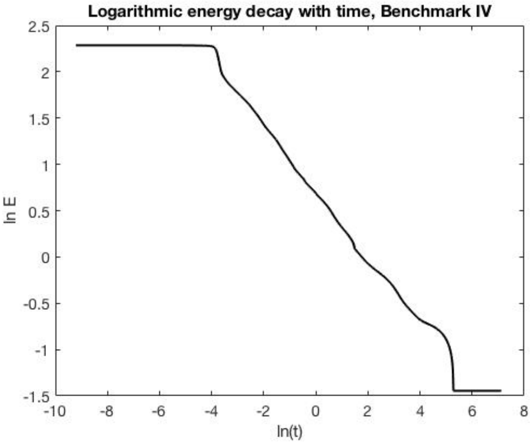
Computational Results



YouTube: https://youtu.be/MovUu2DwWvI

Cahn-Hilliard Dynamics

Computational Results



Two Wisdoms for Time Stepping

Wisdom #1:

- It is a problem with two equally stiff terms and dynamics of widely varying time scales
- Use implicit stiff solvers with variable time steps (local error tolerance σ)
- Choke down the extra effort to solve the nonlinear problem at every time step

Wisdom #2:

- It is a gradient flow
- Use fixed time steps and Energy Stable time stepping schemes for efficiency
- Choke down the loss of accuracy when time steps cannot capture fast dynamics

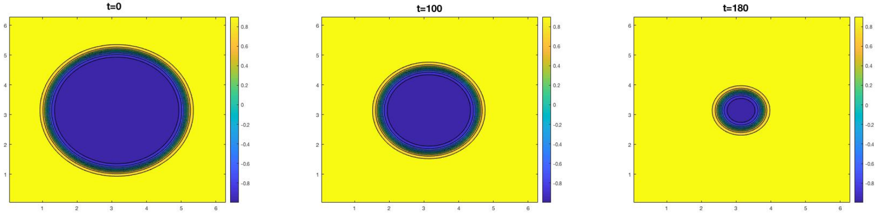
Accuracy more important in FCH: Jae Hyun Park talk tomorrow

Honest Message

- Goal is to compare the efficiency between time stepping strategies to achieve a result with a given accuracy.
- No reason to use fixed time steps, adapt with a local error tolerance σ.
- Clear story when we consider the comparison of time step size k dependence on σ and $\epsilon \to 0$.
- But that is not the whole story (solver efficiency).

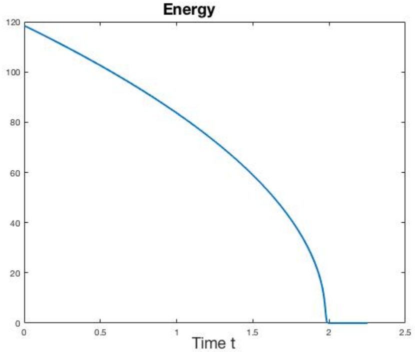
Allen Cahn Dynamics

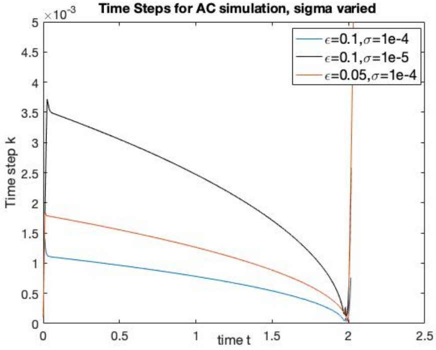
Computational Results



Allen Cahn Dynamics

Details of Computational Results





Next Step: Get a formal understanding of how time steps k depend on ϵ and σ.

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

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

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 $O(k^2/\epsilon^3)$) also SDBF1 and SAV1

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

This formal argument relies on the fact that the schemes with these time steps retain the layer profile structure: profile fidelity

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 $M = O(\sqrt{1/\sigma})$ 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.

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

Local truncation error (also SBDF2, SAV2, Secant)

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 (SBDF2, SAV2) have truncation errors that involve the reaction term individually, hence the amplification in size.

Surprises:

- No time step accepted for accuracy by the adaptive time stepping strategy for any scheme for any of the computations exhibited an energy increase.
- With adaptive time stepping, SBDF and SAV schemes behave identically.

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. A formal asymptotic analysis shows that the dominant truncation error term is strongly damped at each time step.

Rigorous analysis of BE for AC (radial case) has been done: in meta-stable dynamics, BE has profile fidelity and energy stability with $k = o(\epsilon)$ (appropriate for accuracy).

Another Surprise: $f(u) = u^3 - u \to f(u) = u^5 - u^3$
BE performance is unchanged but Eyre time steps change dramatically

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

due to a loss of profile fidelity.

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 (fewer time steps) than those that do not. BE and BDF2 have this desirable property.
3. We observe better accuracy for BE applied to AC than expected. A formal asymptotic argument can explain the behaviour.
4. Rigorous proof for large energy stable time steps with BE.