Asymptotic Analysis of Implicit Time Stepping for Allen Cahn and Cahn Hilliard Dynamics

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Institute of Applied Mathematics

University of British Columbia

- Faculty participation from many departments.
- Interdisciplinary graduate programme.

Overview

- Allen Cahn Dynamics
- Time Stepping for AC:
  - Fully Implicit and Energy Stable Schemes
  - Consistency
  - Adaptive Time Stepping
  - Solving the Implicit Problems
  - Benchmark Results
- Asymptotic Analysis of Fully Implicit Scheme and PCG for AC
- Cahn Hilliard Dynamics Accuracy and Benchmarks

Time Stepping Analysis: Cheng, Li, and Promislow. Including some results by Xu, shown in green.

Numerical Framework: Christlieb, Jones, Promislow, Willoughby, in JCP **257** 193-215 (2014)

Benchmark Project: Church, Guo, Jimack, Madzvamuse, Promislow, Wise, Yang, ongoing work.

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 slow 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

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

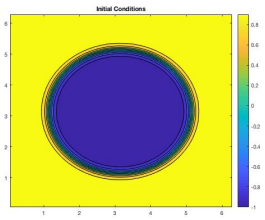
- This equation is gradient flow on the energy

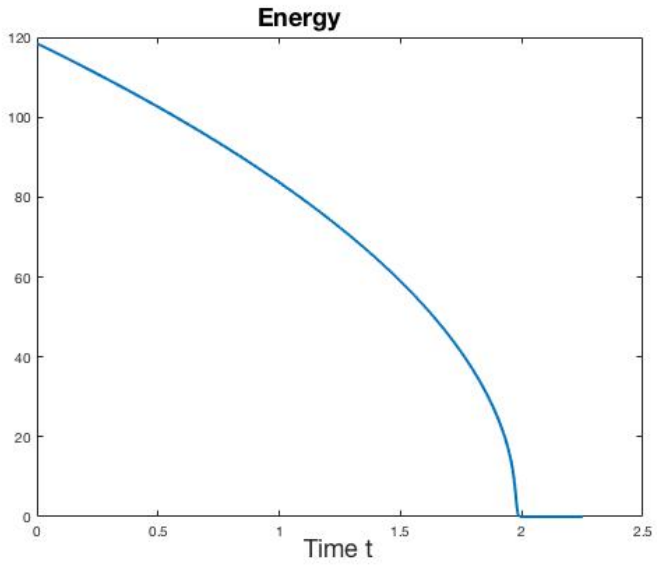
$$\mathcal{E} = \int_0^{2\pi} \left(|\nabla u|^2/2 + W(u)/\epsilon^2 \right) dx$$

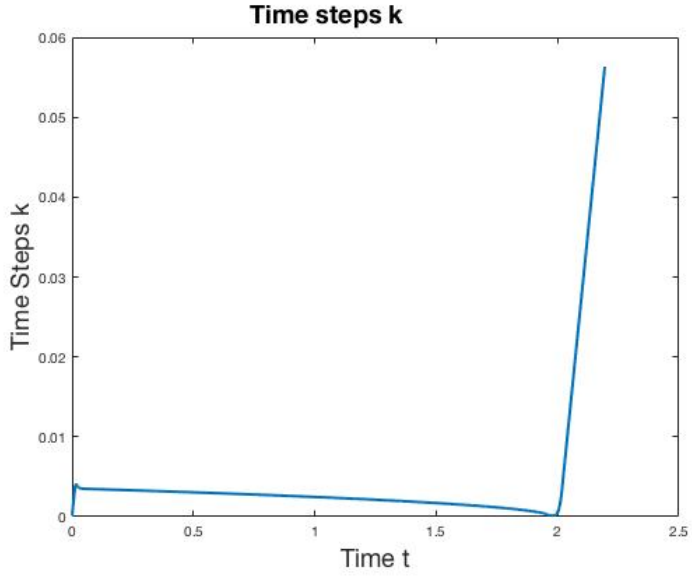
- This leads to a symmetric Jacobian matrix for the implicit time steps of the discretization
- Movie

Allen Cahn Dynamics

Details of Computational Results







The benchmark is the time the centre value changes sign.

Fully Implicit and Energy Stable Schemes

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

Consider Spatially Continuous Semi-Discretization

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 that ES.
- FI schemes are overall more efficient.

Consistency – I

Asymptotic Solution:

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

FI local error

$$\frac{1}{2}k^2 u_{tt} = kO(k/\epsilon^2) \text{ consistent } k = o(\epsilon^2).$$

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

$$k^2 u_t/\epsilon^2 = kO(k/\epsilon^3) \text{ consistent } k = o(\epsilon^3).$$

ES is asymptotically less accurate than FI.

Consistency – II

Asymptotic Consistency

Asymptotic Consistency: Identify the minimum p such that the distinguished limit $k = O(\epsilon^p)$ of the numerical scheme is consistent with the Gamma limit.

- $p = 2$ for FI
- $p = 3$ for ES

Consistency – III

Large errors from splitting: second explanation

XLWB

Jinchao Xu, Li, Wu, Bousquet (arXiv preprint)

ES is equivalent to FI but with a decreased time step:

$$\tau = \frac{\epsilon^2 k}{\epsilon^2 + k}$$

ES is equivalent to FI but with a decreased time step:

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

Equivalent to FI with $1/\tau = 1/k + 1/\epsilon^2$.

Consistency – IV

Large errors from splitting: simple explanation

Consider the Dahlquist test problem for $u(t)$:

$$\dot{u} = -\gamma u$$

with $\gamma = O(1)$ and $\gamma = \alpha - \beta$ with α, β size $O(M)$, M large.
Consider handling the α term implicitly and the β term explicitly (IMEX scheme).
Now compare over one time step:

Exact: $e^{-\gamma k} \approx 1 - \gamma k + \frac{1}{2}\gamma^2 k^2$

BE: $1/(1+\gamma k) \approx 1 - \gamma k + \gamma^2 k^2$, error $\gamma^2 k^2/2$.

IMEX: $(1+\beta k)/(1+\alpha k) \approx 1 - \gamma k + \alpha\gamma k^2$, error $\gamma\alpha k^2$.

With $\gamma = O(1)$, and $\alpha = O(M)$, the IMEX scheme is much less accurate that the fully implicit scheme, although they are the same order.

Consistency – IV

Adaptive Time Stepping

Let σ be the allowable local error per time step.

FI:

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

ES:

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

ES takes more time steps and gives less accurate results.

PCG solution of the implicit system

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

- 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.

AC Numerical Results

Fully Implicit

$\epsilon = 0.2$, σ varied

σ	M	CG	transition
1e-4	717	5,348 [7.46]	1.924
1e-5	2,225 (3.10)	9,448 [4.24]	1.926
1e-6	7,010 (3.15)	23,017 [3.28]	1.926

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

ϵ varied, $\sigma = 1e-4$

ϵ	M	CG	transition
0.2	717	5,348 [7.46]	1.924
0.1	1,291 (1.80)	12,354 [9.57]	1.976
0.05	2,412 (1.87)	27,782 [11.52]	1.992
0.025	4,630 (1.92)	64,884 [14.01]	1.998

Validates $M = O(1/\epsilon)$ for constant σ. Consistent with condition number dependent (increasing) only on C when $k = C\epsilon^2$.

AC Numerical Results

Energy Stable

$\epsilon = 0.2$, σ varied

σ	M	CG	transition
1e-4	2,350	14,856 [6.32]	1.974
1e-5	7,351 (3.12)	28,263 [3.85]	1.941
1e-6	23,172 (3.15)	68,148 [2.94]	1.931

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]	1.974
0.1	6,463 (2.75)	44,717 [6.92]	2.046
0.05	18,218 (2.83)	143,416 [7.87]	2.092
0.025	52,595 (2.89)	497,846 [9.47]	2.139

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

FI Asymptotics and Energy Stability

Theorem

Under the scaling $k = C\epsilon^2$ with $C < 1$ there is an asymptotic solution to the FI problem, locally unique, that decreases energy.

XLWB

Theorem

Under the scaling $k = C\epsilon^2$ with $C < 1$ the FI problem is convex with unique solution that decreases the energy.

We have some preliminary ideas that extends this result to asymptotically larger time steps

Note that in this context, ES artificially decreases the time step so that it is equivalent to FI with $k < \epsilon^2$.

Asymptotic Solution - I

$$(U^{n+1} - U^n)/k = \Delta U^{n+1} - f(U^{n+1})/\epsilon^2$$

Assume that $k = C\epsilon^2$ and that U^n is a curve dressed with a homoclinic profile:

- There is a curve $\mathbf{x}(s)$ with normal $\hat{n}$ parametrized by arc length.
- Change coordinates to (s, z) : $\mathbf{x} = \mathbf{x}^{n+1}(s) + \epsilon z \hat{n}$
- $U^n \approx g(z)$ with $g(z) = \tanh(z/\sqrt{2})$

Under these assumptions it is asymptotically consistent that U^{n+1} has the same form. We write

$$U^n = g(z - \epsilon v(s)), \quad g \text{ based here at the } n+1 \text{ curve}$$

Asymptotic Solution - II

$$(U^{n+1} - U^n)/(C\epsilon^2) = \Delta U^{n+1} - f(U^{n+1})/\epsilon^2$$
$$U^{n+1} = g(z) \quad \text{and} \quad U^n = g(z - \epsilon v(s))$$
$$\Delta = \frac{1}{\epsilon^2}\frac{\partial^2}{\partial z^2} + \frac{\kappa}{\epsilon}\frac{\partial}{\partial z} \quad \text{to highest order}$$

- Highest order $O(1/\epsilon^2)$ terms cancel by choice of g.
- Next order terms are

$$\left(\frac{v}{C} - \kappa\right) g' = \quad \perp \text{ to } g'$$

- so $v = C\kappa$. Actual curve normal motion is v scaled by ϵ^2, since $k = C\epsilon^2$ we have an approximation of curvature motion.
- This discrete implicit curvature motion decreases curve length and to leading order this decreases Energy.
- C is not restricted to be less than 1 in this argument.

Condition Number of $\mathcal{Q}^{-1}\mathcal{J}$

XLWB

Theorem

Under the scaling $k = C\epsilon^2$ with $C < 1$ the operator $\mathcal{Q}^{-1}\mathcal{J}$ has condition number bounded by

$$\kappa < \frac{1+2C}{1-C}$$

(increasing function of C as observed in the numerical benchmark).

In the computations, $C > 1$ also exhibit good PCG convergence when the adaptive time steps direct the size of k.

Cahn-Hilliard Dynamics

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

Cahn and Hilliard, J Chem Phys 1958

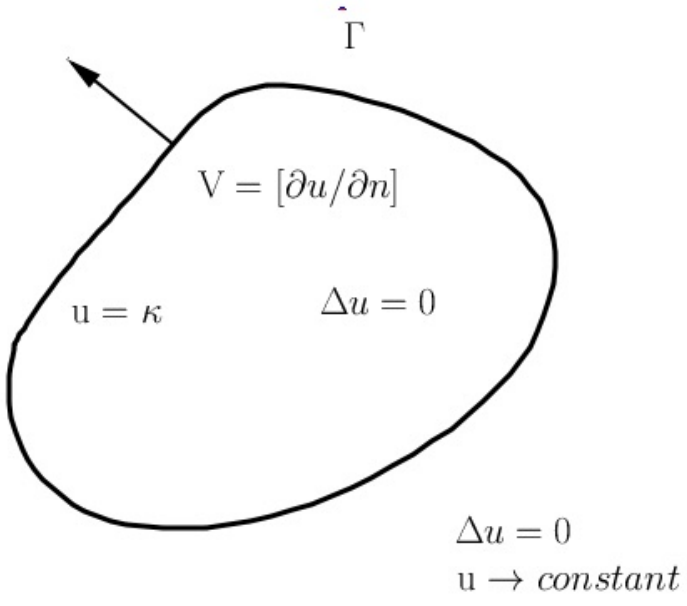
- Gradient flow on the same energy a AC but in the H_{-1} norm that has inner product

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

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

Cahn Hilliard Dynamics

Mullins-Sekerka Flow



- Mullins and Sekerka 1963
- Sharp interface limit of Cahn Hilliard equations, Pego 1989 and Alikakos, Bates, and Chen 1994

Consistency and Stability

2D Cahn Hilliard

Asymptotic Consistency: Identify the minimum p such that the distinguished limit $k = O(\epsilon^p)$ of the numerical scheme is consistent with the Gamma limit.

- $p = 2$, $M = O(1/(\sqrt{\sigma}\epsilon))$, error $O(\sqrt{\sigma}/\epsilon)$ for FI
- $p = 4$, $M = O(1/(\sqrt{\sigma}\epsilon^2))$, error $O(\sqrt{\sigma}/\epsilon^2)$ for ES

XLWB

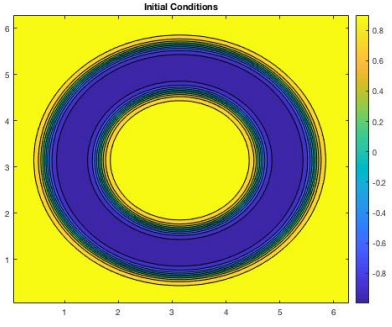
Theorem

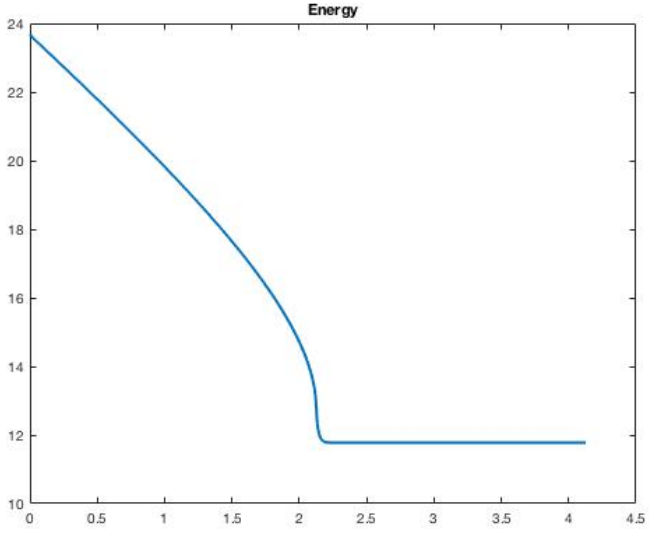
Under the scaling $k = C\epsilon^3$ with $C < 4$ the FI problem is convex with unique solution that decreases the energy.

We observe $k = O(\epsilon^2)$ computations in the meta-stable regime.

Cahn-Hilliard Dynamics

2D Benchmark Problem





Benchmark is the time at which the values at (π, π) changes sign.

CH 2D Benchmark Numerical Results

ϵ varied, $\sigma = 1e-4$

FI:

ϵ	M	CG	T
0.1	1,156	24,871 [21.5]	2.13
0.05	2,044 (1.77)	66,559 [32.6]	2.34
0.025	3,754 (1.84)	200,067 [53.3]	2.44

Validates $M = O(1/\epsilon)$ for constant σ. Evidence that condition number increases with ϵ.

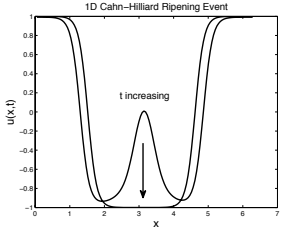
ES:

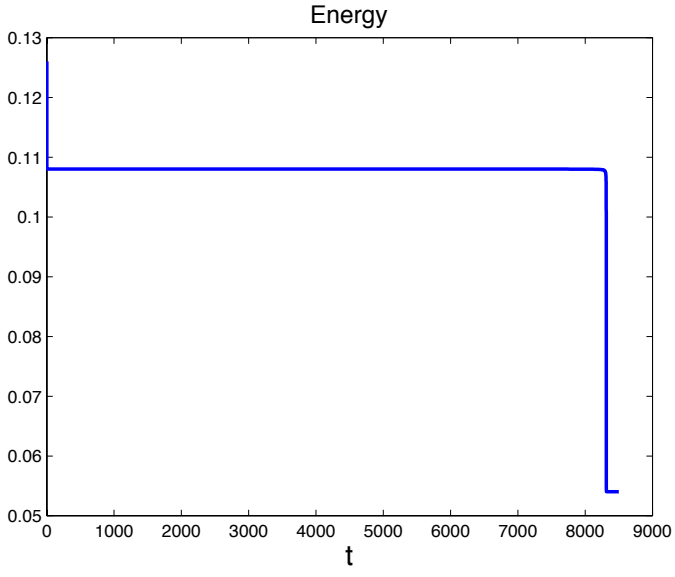
ϵ	M	CG	T
0.1	12,781	190,864 [14.9]	2.15
0.05	52,783 (4.13)	938,548 [17.7]	2.36
0.015	217,465 (4.11)	4,540,748 [20.1]	2.47

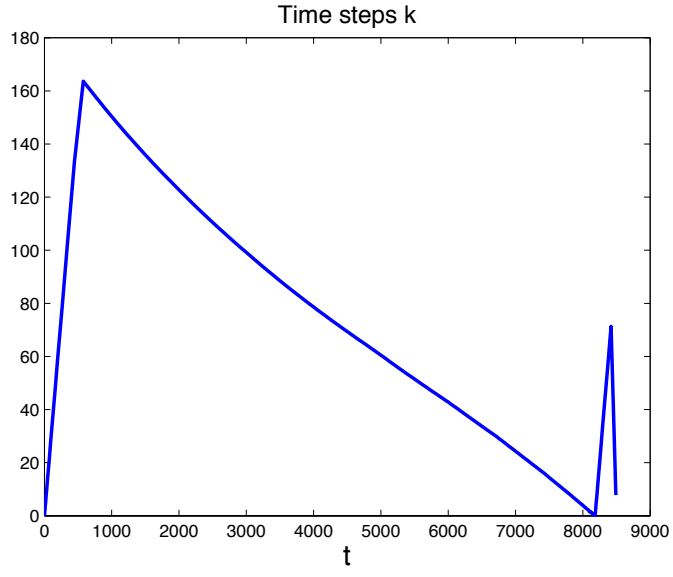
Evidence of rapid loss of accuracy and efficiency as $\epsilon \to 0$.
Validates $M = O(1/\epsilon^2)$.

Cahn-Hilliard Dynamics

1D Benchmark Problem







Benchmark is the time the centre value changes sign.

Carr and Pego (1989) In 1D, the dynamics of a ripening state with M transition layers is exponentially slow (in ϵ).

CH 1D Benchmark Problem

Performance Comparison $\epsilon = 0.18$

FI – Asymptotics show condition number $O(k/\epsilon)$:

σ	time steps	ripening time	total CG
1e-4	848	8180	19,105
1e-5	2580 (3.04)	8273	39,942
1e-6	8072 (3.13)	8304	87,563
1e-7	25446 (3.15)	8314	227,799

ES – exponentially (in ϵ) less accurate than FI:

σ	time steps	ripening time	total CG
1e-4	70,517	13147	1,039,676
1e-5	202,549 (2.87)	9582	2,368,051
1e-6	618,431(3.06)	8695	5,205,739

Summary

1. Analytic, Asymptotic, and Numerical results that show FI is energy stable with time steps chosen appropriately to the dynamics.
2. Evidence that FI is more efficient than widely used ES methods for AC and CH problems.