Time Stepping for Energy Gradient Flows

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UT Knoxville, March 7, 2018

Institute of Applied Mathematics

University of British Columbia

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

Overview

- Allen Cahn Dynamics [Benchmark]
- Cahn Hilliard Dynamics [Benchmarks]
- Fully Implicit Spectral Preconditioned CG Method
- Comparison to splitting methods

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

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

Time Stepping Analysis: Cheng, Li, Promislow

Allen Cahn Dynamics

$u(x,t)$, 2π-periodic in x solves

$$u_t = \epsilon^2 u_{xx} - u^3 + u$$

Allen and Cahn, Acta Metall 1979

- for discussion, consider $\epsilon = 0$
- A-C 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) time: spinodal evolution
- with $\epsilon > 0$ there is an interface of width O(ϵ) that is formed between the two phases

Allen Cahn Dynamics

Gamma Limit

$$u_t = \epsilon^2 u_{xx} - u^3 + u$$

- 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 A-C curves move with curvature motion as $\epsilon \to 0$ in an $O(\epsilon^{-2})$ time scale.

Allen Cahn Dynamics

Energy Gradient Flow

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

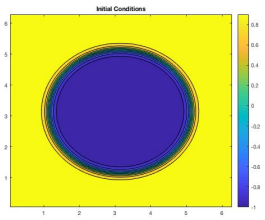
- This equation is gradient flow on the energy

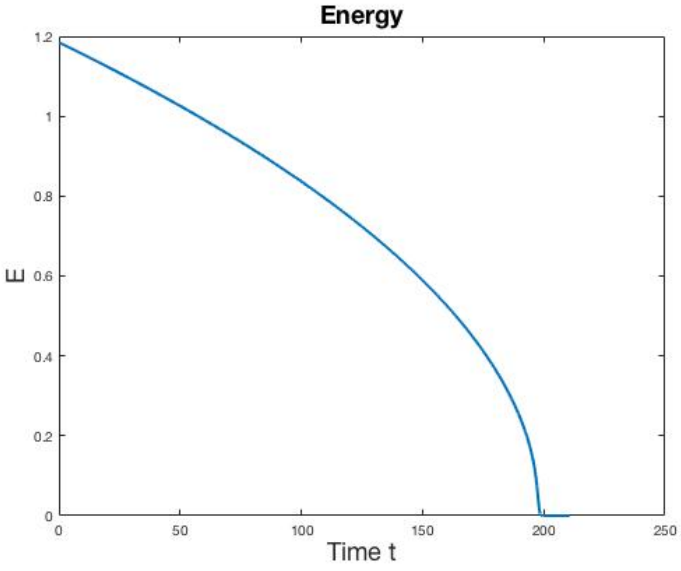
$$\mathcal{E} = \int_0^{2\pi} \left(\epsilon^2 u_x^2 + W(u)\right) dx$$

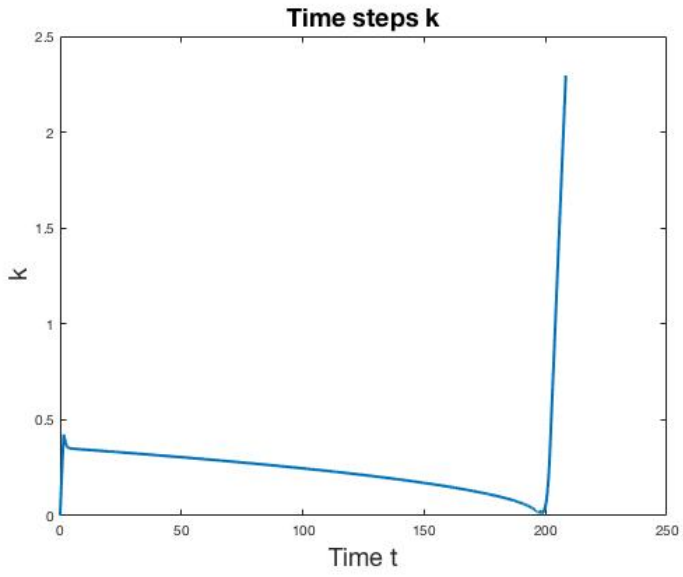
- This leads to a symmetric Jacobian matrix for the implicit time steps of the discretization
- Movie

Allen Cahn Dynamics

Details of Computational Results







The benchmark is the time the centre value changes sign.

Cahn-Hilliard Dynamics

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

Cahn and Hilliard, J Chem Phys 1958

- Same steady state solution as A-C

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

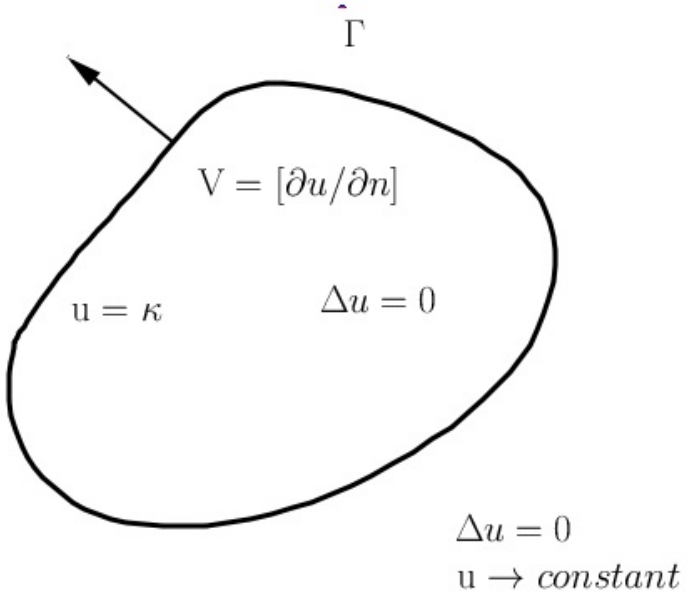
- gradient flow on the same energy $\mathcal{E}$ but in the H_{-1} norm that has inner product

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

- In higher dimensions, the gamma limit is nonlocal, Mullins-Sekerka flow, in $O(1/\epsilon)$ time scale.
- for a dilute phase, a later ripening evolution is known as Ostwald ripening
- C-H conserves the mass of the two phases

Cahn Hilliard Dynamics

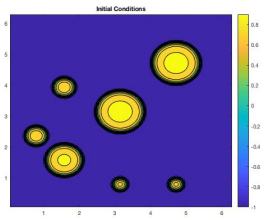
Mullins-Sekerka Flow

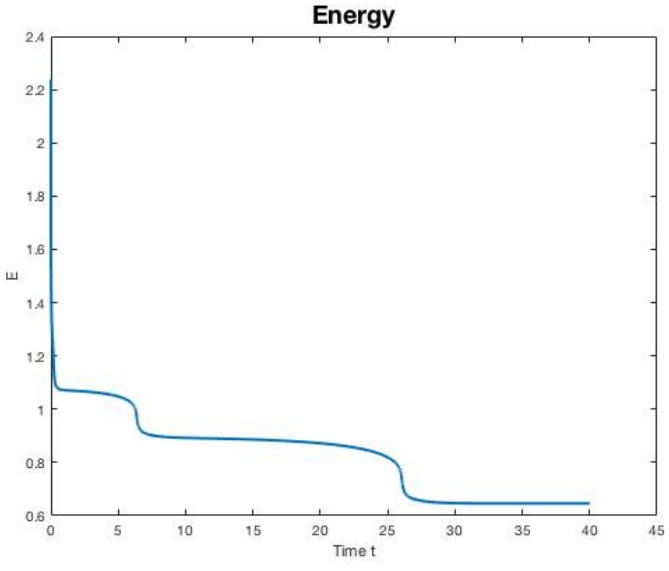


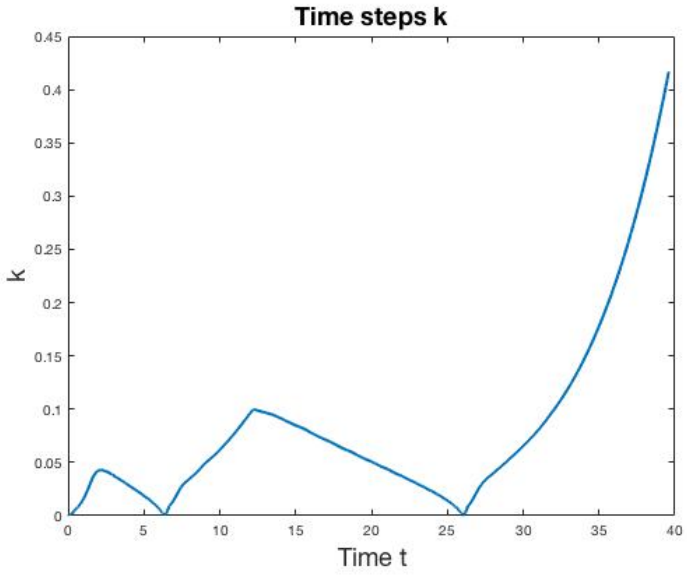
- Mullins and Sekerka 1963
- Sharp interface limit of Cahn Hilliard equations, Pego 1989 and Alikakos, Bates, and Chen 1994

Cahn-Hilliard Dynamics

2D Benchmark Problem #1





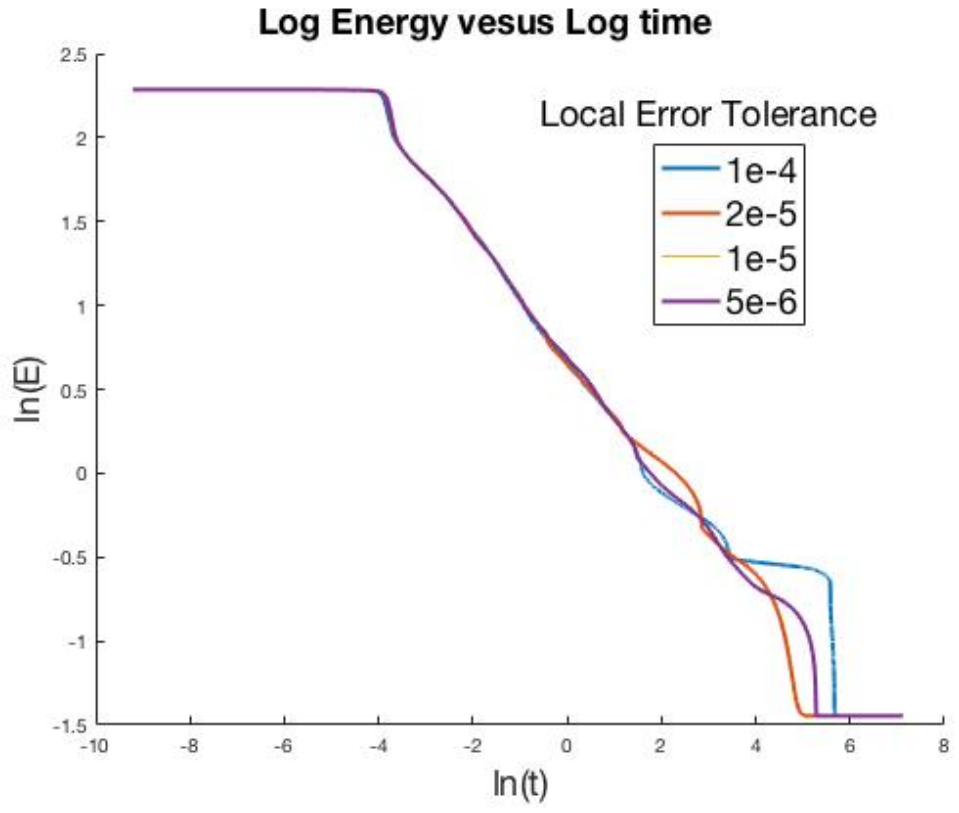


Benchmark is the times the values at $(\pi/2, \pi/2)$ and $(3\pi/2, 3\pi/2)$ change sign.

Cahn-Hilliard Dynamics

2D Benchmark Problem #2

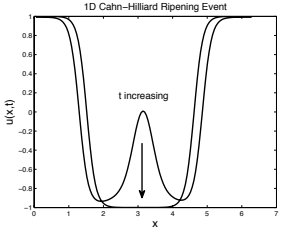
Modified from: Jokisaari et. al., Computational Materials Science **126** (2016)

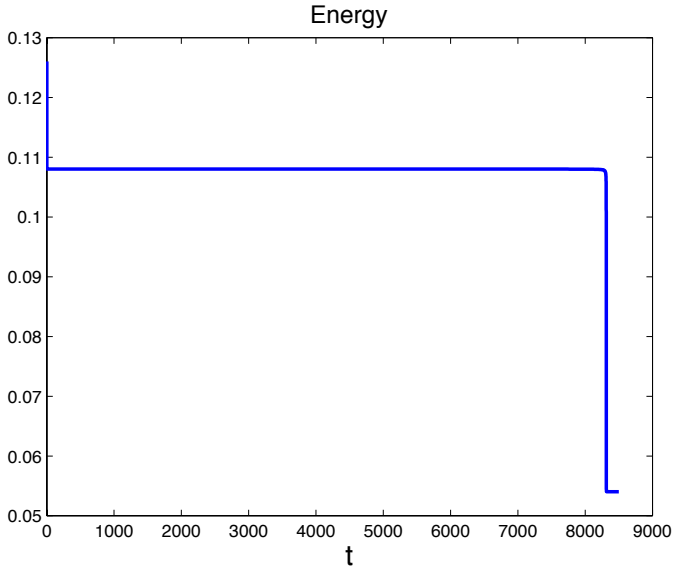


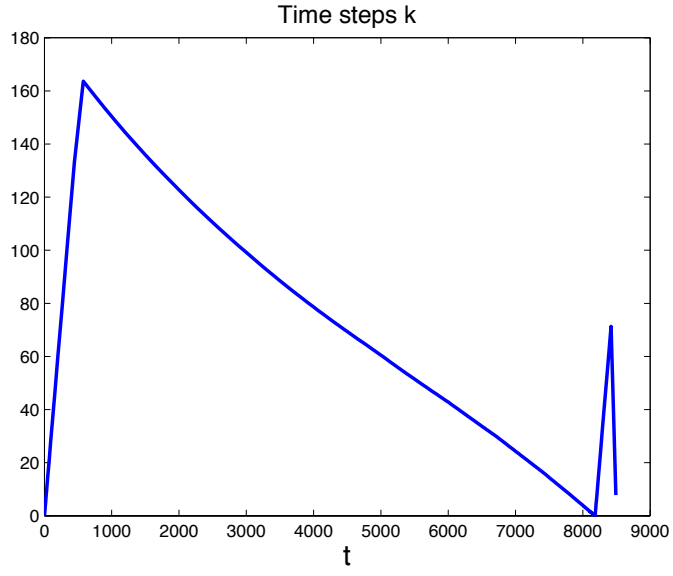
Benchmark is the L_1 error in $\ln E(\ln t)$.

Cahn-Hilliard Dynamics

1D Benchmark Problem







Benchmark is the times 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).

Numerical Approximation

Spectral approximation in space

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

Dual form of the approximation:

$$\begin{aligned} u(jh, t) &\approx U_j(t), \quad j = 1, \ldots N \\ u(x, t) &\approx \sum_{\alpha=-N/2+1}^{N/2} \hat{U}_\alpha(t) e^{i\alpha x} \end{aligned}$$

- N is the number of spatial grid points
- $h = 2\pi/N$ is the grid spacing
- $\hat{\mathbf{U}}$ is the DFT of $\mathbf{U}$, $\hat{\mathbf{U}} = \mathcal{F}\mathbf{U}$

Approximation of RHS above (Λ_α is diag$(-\alpha^2)$):

$$-\mathcal{F}^{-1}\Lambda_\alpha\mathcal{F}(\epsilon^2\mathcal{F}^{-1}\Lambda_\alpha\mathcal{F}\mathbf{U} - \mathbf{U}^{<3>} + \mathbf{U})$$

Numerical Approximation

Implicit time stepping

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

Fully discrete approximation

$$u(jh, t_m) \approx U_j^m, \; j = 1, \ldots N \text{ and } j = 0, \ldots M$$

with time steps $k_m = t_m - t_{m-1}$

- explicit FE predictor (here $\Delta_h = \mathcal{F}^{-1}\Lambda_\alpha \mathcal{F}$):

$$\mathbf{U}^* = \mathbf{U}^{m-1} - k_m \Delta_h \left[\epsilon^2 \Delta_h \mathbf{U}^{m-1} - W'(\mathbf{U}^{m-1})\right]$$

- implicit BE step

$$\mathbf{G}(\mathbf{U}^m) := \mathbf{U}^m + k_m \Delta_h \left[\epsilon^2 \Delta_h \mathbf{U}^m - W'(\mathbf{U}^m)\right] - \mathbf{U}^{m-1} = \mathbf{0}$$

Numerical Approximation

Adaptive time stepping

- Prescribe a tolerance δ for the error for *each* time step
- For the BE step the error is approximately $\sigma = \|u_{tt}\| k_m^2/2$
- $\sigma \approx \|\mathbf{U}^m - \mathbf{U}^*\|/2$
- Reject the step and repeat with time step $k_m/2$ if
  - if $\sigma > \delta$ *or*
  - Newton iterations fail to converge *or*
  - $\mathcal{E}$ increases
- Otherwise accept the step and take

$$k_{m+1} = 0.8 k_m \sqrt{\frac{\delta}{\sigma}}$$

Numerical Approximation

PCG solution of the implicit system

$$\mathbf{G}(\mathbf{U}^m) := \mathbf{U}^m + k_m \Delta_h \left[\epsilon^2 \Delta_h \mathbf{U}^m - W'(\mathbf{U}^m)\right] - \mathbf{U}^{m-1} = \mathbf{0}$$

- Newton's method with symmetric (in H^{-1}) Jacobian matrix

$$\mathcal{J} = I + k_m \Delta_h (\epsilon^2 \Delta_h - \Lambda_2)$$

where Λ_2 is the diagonal matrix with entries

$$W''(U_j^{(r)}) = 3[U_j^{(r)}]^2 - 1.$$

- Symmetric preconditioner (Scott Maclachlan and Zhengfu Xu)

$$\mathcal{Q} = I + k_m \Delta_h (\epsilon^2 \Delta_h - 2k_m I)$$

- $\mathcal{J}$ and $\mathcal{Q}^{-1}$ are dense but can multiply by these matrices efficiently

Numerical Approximation

Basic numerical tests

1D Cahn-Hilliard model, $\epsilon = 0.18$, fixed time step computations to time $t = 0.2$.

$E_k = \|U_k - U_{k/2}\|$, results for $N = 128$:

k	E_k
2e-4	1.32e-5
1e-4	6.6e-6
5e-5	3.3e-6

$E_k = \|U_N - U_{2N}\|$, results for $k = 1e-4$:

N	E_N	E_N for $\epsilon = 0.09$
32	2.0e-3	0.139
64	9.3e-7	4.4e-3
128	9.0e-13	1.3e-6

First order convergence in time, spectral in $N = O(1/\epsilon)$.

Consider only temporal accuracy for the remainder of the talk.

Numerical Approximation

Tests of adaptive time stepping

1D Cahn-Hilliard, $\epsilon = 0.18$, $N = 128$ to time $t = 8500$

δ	time steps	ripening time	total CG
1e-4	848	8180	19,105
1e-5	2580 (3.04)	8273	39,942 (2.09)
1e-6	8072 (3.13)	8304	87,563 (2.19)
1e-7	25446 (3.15)	8314	227,799 (2.60)

- Confirmation of adaptive time stepping strategy ($\sqrt{10} \approx 3.16$)
- Solver improves as $k \to 0$ [asymptotic condition number $O(k/\epsilon)$]
- Ripening times can be approximated accurately
- solver iterations are independent of N

Numerical Approximation

Extensions allowed by the Framework

- Easily adapted to different models:
  - Vector models
  - Additional terms and well shapes
  - Different PDE order
- Higher Order Implicit Time Stepping
- GPU implementation

Comparison to splitting methods

Eyer's method in Allen-Cahn Framework

our implicit BE step

$$\mathbf{G}(\mathbf{U}^m) := \mathbf{U}^m - k_m \left[\epsilon^2 \Delta_h \mathbf{U}^m - \mathbf{U}^{m,<3>} + \mathbf{U}^m\right] - \mathbf{U}^{m-1} = \mathbf{0}$$

Convex-concave splitting method Eyer, 1998

$$\mathbf{G}_E(\mathbf{U}^m) := \mathbf{U}^m - k_m \left[\epsilon^2 \Delta_h \mathbf{U}^m - \mathbf{U}^{m,<3>}\right] - (1 + k_m)\mathbf{U}^{m-1} = \mathbf{0}$$

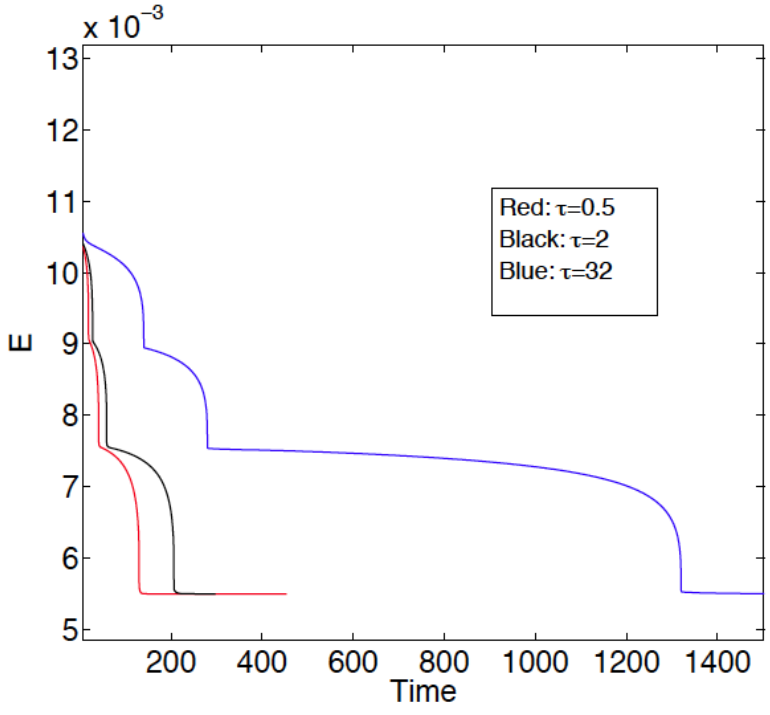
The splitting technique has some desirable properties

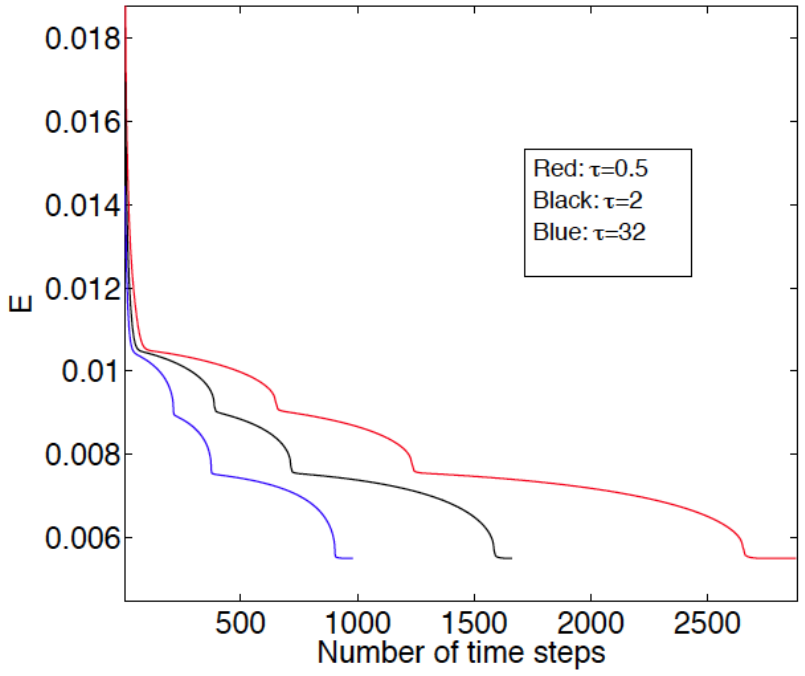
- Unique solution for any k that decreases energy $\mathcal{E}$
- Condition number of PCG iterations independent of ϵ and k (MSU fixed point method)

But suffers from poor accuracy!

Comparison to splitting methods

Anecdotal: splitting methods are inaccurate – 2D CH





Christlieb et. al., Commun. Math. Sci. **11** (2013)

Comparison to splitting methods

Anecdotal: splitting methods are inaccurate – FCH

Doelman, Hayrapetyan, Promnislow, Wetton, SIMATH **48** (2014)

Splitting methods cannot capture this pearling bifurcation.

Comparison to splitting methods

Benchmark: Splitting methods are inaccurate

Our implicit BE step applied to 1D C-H model (reprise)

δ	time steps	ripening time	total CG
1e-4	848	8180	19,105
1e-5	2580 (3.04)	8273	39,942 (2.09)
1e-6	8072 (3.13)	8304	87,563 (2.19)
1e-7	25446 (3.15)	8314	227,799 (2.60)

Eyer's splitting method (similar poor performance from other IMEX methods)

δ	time steps	ripening time	total CG
1e-4	70,517	13147	1,039,676
1e-5	202,549 (2.87)	9582	2,368,051 (2.27)
1e-6	618,431(3.06)	8695	5,205,739 (2.19)

Comparison to splitting methods

Benchmark: Splitting methods are inaccurate II

Our implicit BE step applied to 2D AC Benchmark Problem (shrinking circle) $\epsilon = 0.05$

δ	time steps	ripening time	total CG
1e-4	2,461	797.1	17,731
1e-5	7,714	797.3	35,010
1e-6	24,339	797.4	71,988

Eyer's splitting method

δ	time steps	ripening time	total CG
1e-4	13,108	853	64,130
1e-5	40,491	815	151,031
1e-6	127,084	803	379,429

Eyre performs increasingly worse compared to fully implicit as $\epsilon \to 0$.

Comparison to splitting methods

Large errors from splitting: simple explanation

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

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

with $\gamma \ll 1$ and $\gamma = \alpha - \beta$ with α, β size $O(1)$. 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 $\gamma \ll 1$, the IMEX scheme is much less accurate that the fully implicit scheme, although they are the same order.

Comparison to splitting methods

Large errors from splitting: asymptotic analysis for AC case

Asymptotic ripening solution

$$u \approx \tanh\left(\frac{z - x(s, \epsilon^2 t)}{\epsilon\sqrt{2}}\right)$$

so $u_t = O(\epsilon)$ and $u_{tt} = O(\epsilon^2)$.

Backward Euler:

$$\mathbf{U}^m = k_m\left[\epsilon^2 \Delta_h \mathbf{U}^m - \mathbf{U}^{m,<3>} + \mathbf{U}^m\right] - \mathbf{U}^{m-1}$$

standard local error $k^2 u_{tt} = k^2 O(\epsilon^2)$.

Convex-concave splitting method Eyer, 1998

$$\mathbf{U}^m = \text{same as above} - k_m(\mathbf{U}^m - \mathbf{U}^{m-1})$$

local error from the last term $k^2 u_t = k^2 O(\epsilon)$.

Summary

1. General framework for solving energy gradient problems from materials science
2. Applied to several benchmark problems
3. More efficient than widely used splitting methods