

Imex methods for thin film equations and Cahn Hilliard equations with variable mobility

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- Spinodal decomposition is a process in which two or more materials can separate to form different compositions.
- Phase Segregation applies to liquids and solids (polymers and metals) in different fields of science.
- Theoretical and Numerical structure for such processes



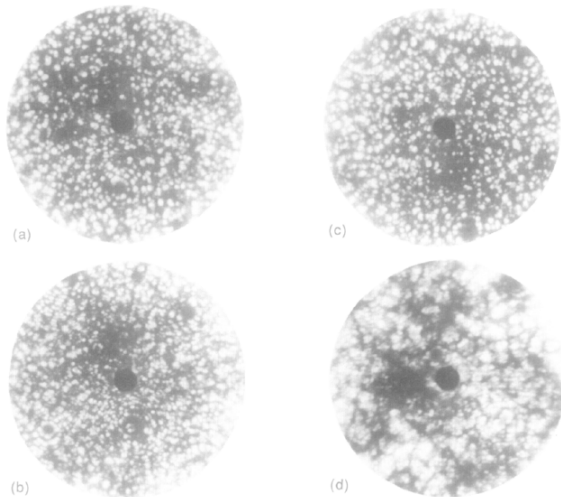
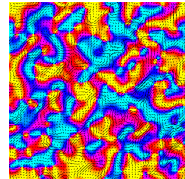
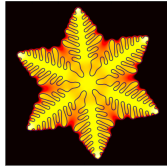
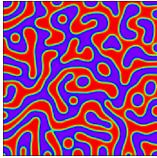


Fig. 2. Field ion micrographs from Fe-45%Cr samples aged for (a) 4, (b) 24, (c) 100 and (d) 500 h. The brightly imaging regions are Cr-enriched and the dark regions are Cr-depleted.



Part I: Models for material microstructure evolution



- Micro-structure evolution occurs during formation or processing of materials.
- Track evolution of interfaces, uniformity , pattern formation.
- Phases with different composition, crystalline structure, grain orientation, and structural defects.
- Spatial arrangement of the local structural features determine properties (mechanical, optical, electrical,...)
- Microstructure evolution : biology, hydrodynamics, chemical reactions,...
- Easy to add new physics : Instrument for material design



The solutions u evolve toward minimizers of $F(u)$ and the energy is always non-increasing. It is easy to demonstrate that any solution $u(x, t)$ in an appropriate function class will satisfy

$$\frac{d}{dt}F(u) = - \int_{\Omega} \left| \nabla \frac{\delta F}{\delta u} \right|^2 dx \leq 0.$$



Example 1: the Cahn-Hilliard equation $u_t = \Delta(-\epsilon^2 \Delta u + u^3 - u)$

The equation is the H^{-1} gradient flow of free energy

$$F(u) = \int_{\Omega} \frac{\epsilon^2}{2} |\nabla u|^2 + \frac{u^4}{4} - \frac{u^2}{2} dx.$$

Convexity splitting

$$F_+(u) = \int \frac{\epsilon^2}{2} |\nabla u|^2 + a \frac{u^2}{2} dx, \quad F_-(u) = \int \frac{u^4}{4} - [1 + a] \frac{u^2}{2} dx$$

with $F_+(u)'' > 0$ and $F_-(u)'' < 0$ for $a > 2$.

$$u_t = \Delta[\delta F(u)] = \Delta[\delta F_+(u) + \delta F_-(u)]$$

$$u_t = \underbrace{\Delta[-\epsilon^2 \Delta u + au]}_{n+1\text{-level}} + \underbrace{\Delta[u^3 - (1+a)u]}_{n\text{-level}}$$

$$\frac{u_{n+1} - u_n}{h} = (-\epsilon^2 \Delta^2 + a\Delta)u_{n+1} + \Delta[(u_n)^3 - (1+a)u_n]. \quad (\text{CS})$$

$$\frac{u_j^* - u_n}{h} = (-\epsilon^2 \Delta^2 + a\Delta)u_j^* + \Delta[(u_{j-1}^*)^3 - (1+a)u_{j-1}^*]. \quad (\text{ICS})$$



$$u_t = \nabla \cdot (M(u) \nabla \delta F(u)),$$

note: if $M(u) = 1$, we get the usual CH equation $u_t = \Delta[\delta F(u)]$

$$\mathcal{F}(u) = \int_{\Omega} \frac{\epsilon^2}{2} |\nabla u|^2 + w(u) \, dx.$$

$$u_t = \nabla \cdot (M(u) \nabla (-\epsilon^2 \Delta u + w'(u))), \quad (\text{VMCH})$$

Letting $\epsilon = 1$ gives

$$u_t = \nabla \cdot (M(u) \nabla [w'(u) - \Delta u]),$$

which can be written

$$u_t = \underbrace{\nabla \cdot (M(u) w''(u) \nabla u)}_{G(u)} - \nabla \cdot (M(u) \nabla \Delta u),$$



$$\frac{\partial u}{\partial t} = \underbrace{\Delta G(u) - \nabla \cdot (M(u) \nabla \Delta u)}_{F(u)},$$

where

$$G(u) = \int M(u) w''(u) du.$$

Introducing the splitting, the mobility coefficient function of the fourth-order operator can be written as $M(u) = M_1 + (M(u) - M_1)$ to give the form

$$\frac{\partial u}{\partial t} = \underbrace{-M_1 \Delta^2 u}_{F_{\text{im}}(u)} + \underbrace{\Delta G(u) - \nabla \cdot [(M(u) - M_1) \nabla \Delta u]}_{F_{\text{ex}}(u)}$$



The main schemes

$$\frac{U_{n+1} - U_n}{h} - F_{\text{im}}(U_{n+1}) = F_{\text{ex}}(U_n), \quad (\text{BHM})$$

$$\frac{U_{(k)} - U_n}{h} - F_{\text{im}}(U_{(k)}) = F_{\text{ex}}(U_{(k-1)}) \quad (\text{BHM-BE}_K)$$

$$\frac{U_{(k)} - U_n}{h} - \frac{1}{2}F_{\text{im}}(U_{(k)}) = \frac{1}{2}F_{\text{ex}}(U_{(k-1)}) + \frac{1}{2}F(U_n) \quad (\text{BHM-CN}_K)$$



$$U_{(0)} = U_n,$$

$$U_{(1)} = U_{(0)} + h \left(F_{\text{ex}}(U_{(0)}) + F_{\text{im}}(U_{(1)}) \right),$$

$$U_{(2)} = \frac{3}{2}U_{(0)} - \frac{1}{2}U_{(1)} + h \left(\frac{1}{2}F_{\text{ex}}(U_{(1)}) + \frac{1}{2}F_{\text{im}}(U_{(2)}) \right),$$

$$U_{(3)} = U_{(2)} + h \left(F_{\text{ex}}(U_{(2)}) + F_{\text{im}}(U_{(3)}) \right),$$

$$U_{n+1} = U_{(3)}$$

(Huailing Song, 2015)



$$U_{(0)} = U_n,$$

$$U_{(1)} = U_{(0)} + h \left(\gamma F_{\text{ex}}(U_{(0)}) + \gamma F_{\text{im}}(U_{(1)}), \right),$$

$$U_{(2)} = U_{(0)} + h \left(\delta F_{\text{ex}}(U_{(0)}) + (1 - \delta) F_{\text{ex}}(U_{(1)}) \right. \\ \left. + (1 - \gamma) F_{\text{im}}(U_{(1)}) + \gamma F_{\text{im}}(U_{(2)}) \right),$$

$$U_{n+1} = U_{(2)},$$

where $\gamma = (2 - \sqrt{2})/2$ and $\delta = 1 - 1/(2\gamma)$.
(Hector D. Cenicer0s 2013)



Approximate by Fourier series

$$u \approx \sum_{k_x=1}^N \sum_{k_y=1}^N \hat{u}(k, t) \exp [2\pi i(\omega_{k_x}x + \omega_{k_y}y)] ,$$

where $\hat{u}$ is computed via FFT.

Discrete Fourier transform is linear map $\hat{u} = \mathcal{F}u$, and Laplacian is discretized

$$\Delta u \approx \mathcal{F}^{-1} \Lambda \mathcal{F} u, \quad \Lambda \hat{u} = -(\omega_{k_x}^2 + \omega_{k_y}^2) \hat{u}$$

Operator inverses are easy by spectral mapping, e.g.

$$(I + h\Delta)^{-1} u \approx \mathcal{F}^{-1} (1 + h\Lambda)^{-1} \mathcal{F} u.$$



L_1 errors vs timestep h

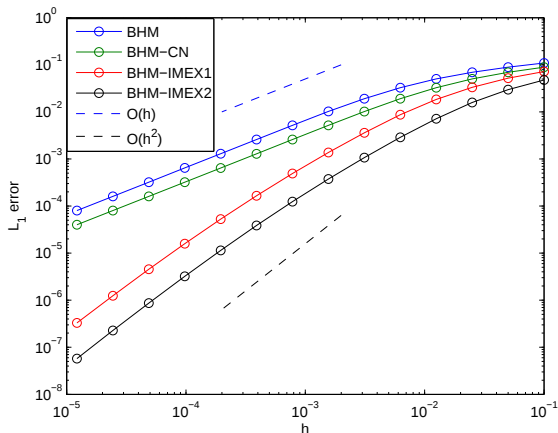
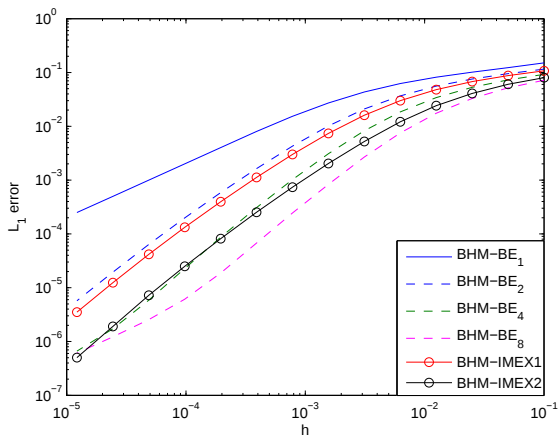


Figure: L^1 -norm errors versus h of the four time-stepping schemes for the test problem using TF equation on the computational domain $[0, 12\pi]^2$ with 256×256 elements, $\epsilon = 0.1$, $t_f = 1.0$ and $M_1 = 0.32275$.





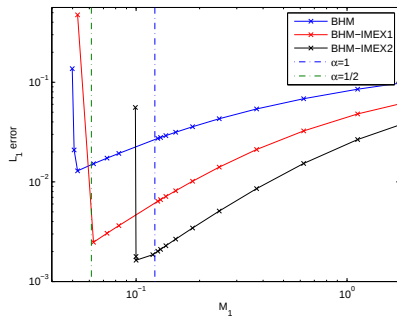
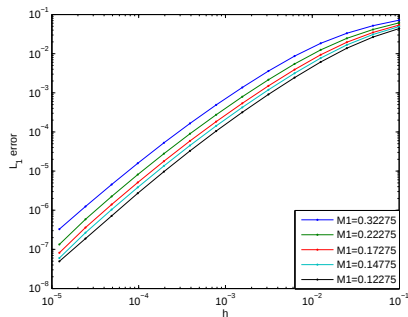


Figure: (left) BHM-IMEX1 method and various values for M_1 . (right) The error for the time-stepping methods at fixed $h = 0.125$ over a range of values of M_1 .



Closer look at BHM-BE_k

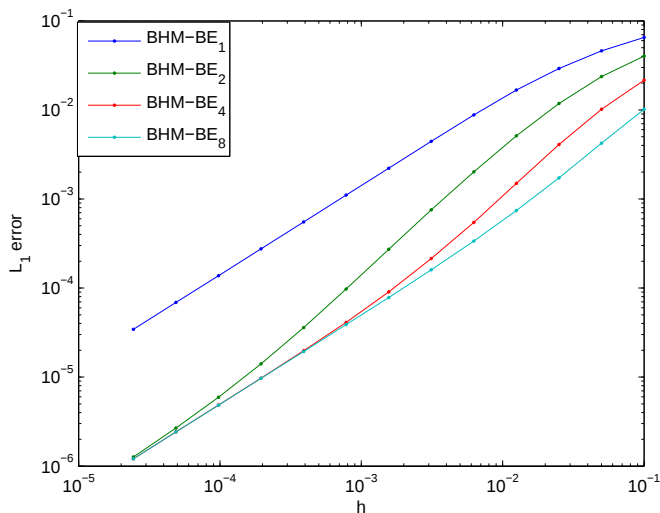


Figure: BHM-BE_k using $M_1 = 0.07$.



$$u_e = 0.3 + 0.1 \sin(x) \sin(y) e^{0.5t}$$

$$\frac{\partial u_e}{\partial t} = F(u_e) + \tilde{f}(x, y, t),$$

where $F(u)$ is the right hand side of the original PDE and $\tilde{f}(x, y, t) = u_{et} - F(u_e)$ is the forcing term.



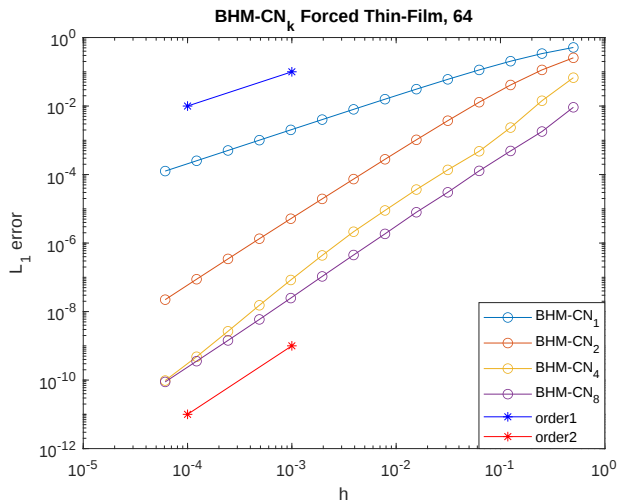


Figure: L_1 errors vs h using the forced Thin-film Equation for BHM-CN_k using $M_1 = 1$.



Simulations for larger t values

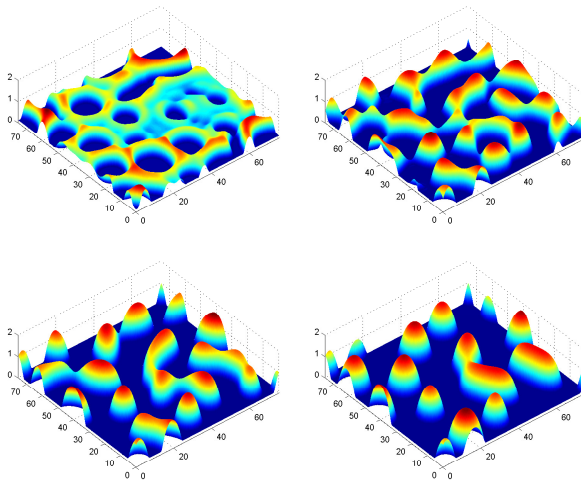


Figure: Nonlinear evolution for the solution to the thin film equation using the BHM-IMEX 2 method with $M_1 = 1$, $h = 0.1$ and $t_f = 1250$.



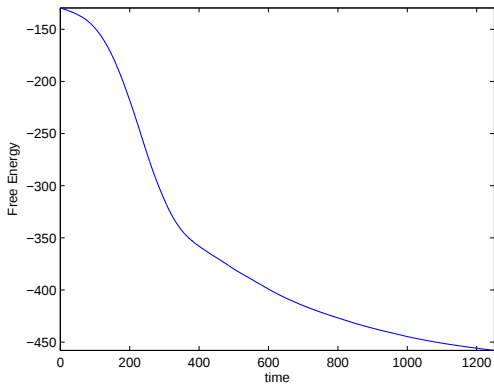
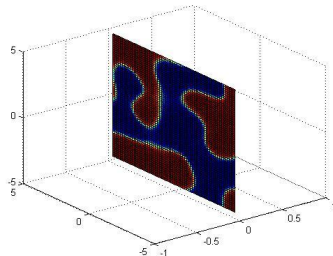
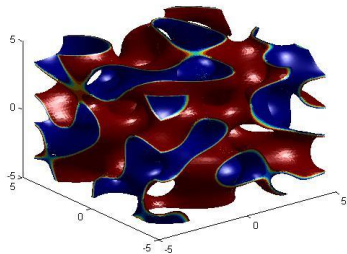
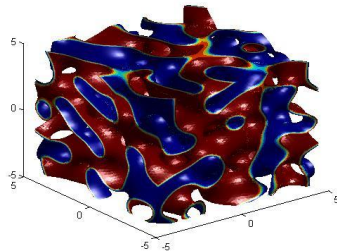
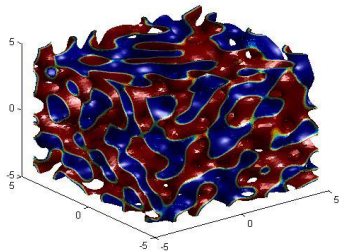


Figure: Energy evolution versus time t for the Thin film equation using BHM-IMEX 2 method with $M_1 = 5$, $h = 0.1$ and $t_f = 1250$.



Cahn-Hilliard : 3D Numerical Simulation



Future Work

- Cahn-Hilliard with variable mobility in 3D
- Thin-film Equation (TFE)
- Coarsening dynamics

References

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