Multigrid Preconditioned Steepest Descent Solvers for Aviles-Giga type Energy: Application to Thin Film Epitaxy

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Outline

- Aviles-Giga Type Energy
- Thin Film Epitaxial Equations
- Convex Splitting Schemes
- Preconditioned Steepest Decent Algorithm
- Convergence Analysis
- Numerical Simulation Results

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Aviles-Giga Type Energy:

$$E(h) = \int_\Omega \left\{ \epsilon\Psi(\phi) + W(p, q) + \frac{\epsilon^2}{2}|\Delta\phi|^2 \right\} d\mathbf{x}$$

where

- $\phi : \Omega \subseteq \mathbf{R}^2 \to \mathbf{R}$ is the height of the film;
- Ψ is a height-dependent energy density;
- W is the slope energy density;
- $p = \partial_x \phi$ and $q = \partial_y \phi$ are the height function gradients;
- $\epsilon > 0$ is a constant;
- $\Delta\phi$ is a small-slope approximation of the curvature.

Outline

Thin Film Epitaxial Growth Energy:

$$E(\phi) = \int_\Omega \left\{ F(|\nabla\phi|) + \frac{\epsilon^2}{2}|\Delta\phi|^2 \right\} d\mathbf{x} \tag{0.1}$$

1. Without slope selection:

$$F_1(|\nabla\phi|) = -\frac{1}{2}\ln\left(1 + |\nabla\phi|^2\right)$$

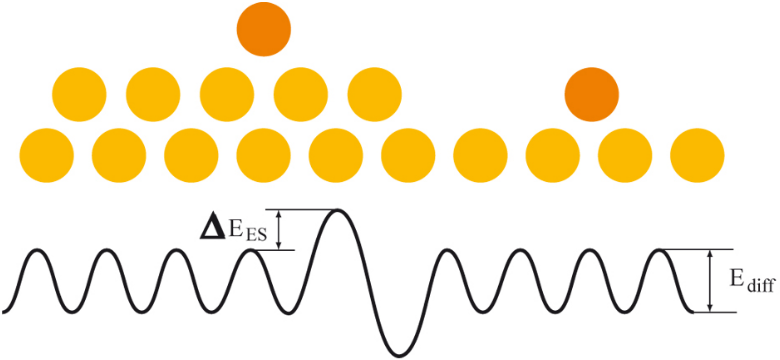
2. With slope selection:

$$F_2(|\nabla\phi|) = \frac{1}{4}(|\nabla\phi|^2 - 1)^2$$

Note:

- 1st term of (0.1) represents a continuum description of the Ehrlich-Schwoebel effect
- 2nd term of (0.1) represents the surface diffusion effect

Ehrlich-Schwoebel Effect



A schematic image of potential surface topography near a stage. ΔE_{ES} is the Ehrlich-Schwoebel barrier that the atom on the surface (a dark circle) has to bridge in addition to the E_{diff} diffuse barrier on the terrace in order to cross the edge of stage and descend to the lower terrace.

Figure from `http://eng.thesaurus.rusnano.com/wiki/article555`

Thin Film Epitaxial Equations with Slope Selection

- Energy:

$$E(h) = \int_\Omega \left\{ \frac{1}{4}(|\nabla\phi|^2 - 1)^2 + \frac{\epsilon^2}{2}|\Delta\phi|^2 \right\} d\mathbf{x}$$

- Chemical potential:

$$\mu := \frac{\delta E}{\delta\phi} = -\nabla\cdot\left(|\nabla\phi|^2\,\nabla\phi\right) + \Delta\phi + \epsilon^2\Delta^2\phi.$$

- Thin Film Epitaxy Equations with Slope Selection
  - L^2 gradient flow:

$$\frac{\partial\phi}{\partial t} = -M\mu.$$

  - H^{-1} gradient flow:

$$\frac{\partial\phi}{\partial t} = \Delta(M\mu).$$

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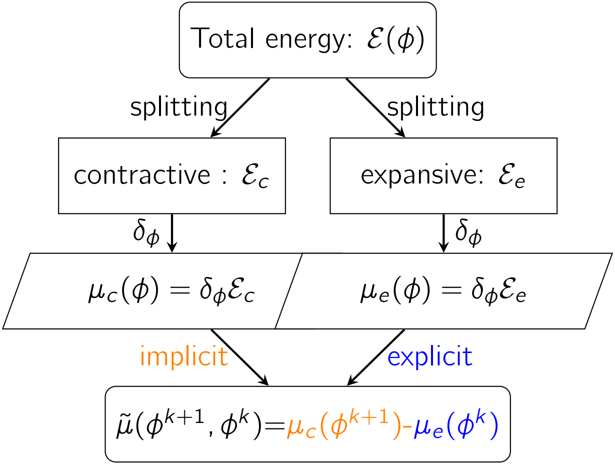
General Convex Splitting Scheme



$L^2 : \phi^{k+1} - \phi^k = -s\tilde{\mu}$ $\qquad$ $H^{-1} : \phi^{k+1} - \phi^k = s\Delta\tilde{\mu}$

Convex Splitting Scheme for TFE equation

- Free energy

$$E(\phi) = \int_\Omega \left\{ \frac{1}{4}\left(|\nabla\phi|^2 - 1\right)^2 + \frac{\epsilon^2}{2} |\Delta\phi|^2 \right\} d\mathbf{x},$$

- Convex Splitting Choice: $E(\phi) = E_c(\phi) - E_e(\phi)$

$$E_c(\phi) = \int_\Omega \frac{1}{4}|\nabla\phi|^4 + \frac{\epsilon^2}{2}|\Delta\phi|^2 d\mathbf{x}, \quad E_e(\phi) = \int_\Omega \frac{1}{2}|\nabla\phi|^2 d\mathbf{x},$$

- Convex Splitting Scheme

$$\begin{aligned}
\frac{\phi^{k+1} - \phi^k}{s} &= \nabla\cdot\left(\left|\nabla\phi^{k+1}\right|^2 \nabla\phi^{k+1}\right) - \epsilon^2\Delta^2\phi^{k+1} - \Delta\phi^k \\
\frac{\phi^{k+1} - \phi^k}{s} &= \Delta\left(-\nabla\cdot\left(\left|\nabla\phi^{k+1}\right|^2 \nabla\phi^{k+1}\right) + \epsilon^2\Delta^2\phi^{k+1} + \Delta\phi^k\right)
\end{aligned}$$

Operator Format of the Scheme for TFE equation (L^2)

- Convex Splitting Scheme (L^2)

$$\frac{\phi^{k+1} - \phi^k}{s} = \nabla \cdot \left(\left| \nabla \phi^{k+1} \right|^2 \nabla \phi^{k+1} \right) - \epsilon^2 \Delta^2 \phi^{k+1} - \Delta \phi^k$$

- Nonlinear system $\mathcal{N}(\phi) = f$, where

$$\mathcal{N}(\phi) := \phi - \phi^k - s\nabla \cdot \left(|\nabla \phi|^2 \nabla \phi \right) + s\epsilon^2 \Delta^2 \phi, \quad f = -s\Delta\phi^k$$

- Convex energy (L^2)

$$J_2(\phi) = \frac{1}{2} \left\| \phi - \phi^k \right\|_{L^2}^2 + \frac{s}{4} \left\| \nabla \phi \right\|_{L^4}^4 + \frac{s\epsilon^2}{2} \left\| \Delta \phi \right\|_{L^2}^2 - (f, \phi)$$

- Convex Splitting Scheme (H^{-1})

$$\frac{\phi^{k+1}-\phi^k}{s} \quad = \quad \Delta\left(-\nabla\cdot\left(\left|\nabla\phi^{k+1}\right|^2\nabla\phi^{k+1}\right)+\epsilon^2\Delta^2\phi^{k+1}+\Delta\phi^k\right)$$

- Nonlinear system $\mathcal{N}(\phi)=f$, where

$$\mathcal{N}(\phi):=-\Delta^{-1}(\phi-\phi^k)-s\nabla\cdot\left(|\nabla\phi|^2\nabla\phi\right)+s\epsilon^2\Delta^2\phi, \quad f=-s\Delta\phi^k$$

- Convex energy (H^{-1})

$$J_{-1}(\phi) \quad = \quad \frac{1}{2}\left\|\phi-\phi^k\right\|_{H^{-1}}^2+\frac{s}{4}\|\nabla\phi\|_{L^4}^4+\frac{s\epsilon^2}{2}\|\Delta\phi\|_{L^2}^2-(f,\phi)$$

Steepest descent algorithm: minimize $J(x) : \mathbb{R}^n \to \mathbb{R}$

$$\boxed{x_{k+1} = x_k + \alpha_k d_k, \quad x_0 \in \mathbb{R}^n}$$

where

- d_k is search direction of steepest descent of J at point x_k:

$$d_k := -\nabla J(x_k) = -r_k$$

- α_k is search step $\alpha_k := \operatorname{argmin}_{\alpha \geq 0} J(x_k - \alpha \nabla J(x_k))$

Note:

- This requires one dimensional optimization over $\alpha > 0$,
- d_k is descent direction because
  $d_k^T \nabla J(x_k) = -\|\nabla J(x_k)\|^2 < 0$, whenever $\nabla J(x_k) \neq 0$.

Theorem 1 ([Braess, 2007])

Suppose A is a p.s.d. matrix with spectral condition number κ, then the gradient method to $f(x) = \frac{1}{2}x'Ax - b'x$ generates a sequence with

$$\|x_k - x^*\|_A \leq \left(\frac{\kappa-1}{\kappa+1}\right)^k \|x_0 - x^*\|_A$$

Note: Convergence behavior for large condition numbers: If the condition number κ is very large, then the convergence rate

$$\frac{\kappa-1}{\kappa+1} \approx 1 - \frac{2}{\kappa} \to 1,$$

which indicates the algorithm will be very slow.

Preconditioned Steepest Decent Algorithm

1. L^2 gradient flow [F. et al., 2015, Huang et al., 2007]
   - Nonlinear system $\mathcal{N}(\phi) = f$, where

$$\mathcal{N}(\phi) := \phi - \phi^k - s\nabla \cdot \left(|\nabla\phi|^2 \nabla\phi \right) + s\epsilon^2\Delta^2\phi$$

   - Linearized system for Search Direction $\mathcal{L}(d_k) = f - \mathcal{N}(\phi)$

$$\mathcal{L}(d^k) := d^k - s\Delta d^k + s\epsilon^2\Delta^2 d^k$$

2. H^{-1} gradient flow [F. et al., 2016]
   - Nonlinear system $\mathcal{N}(\phi) = f$, where

$$\mathcal{N}(\phi) := -\Delta^{-1}(\phi - \phi^k) - s\nabla \cdot \left(|\nabla\phi|^2 \nabla\phi \right) + s\epsilon^2\Delta^2\phi$$

   - Linearized system for Search Direction $\mathcal{L}(d_k) = f - \mathcal{N}(\phi)$

$$\mathcal{L}(d^k) := -\Delta^{-1} d^k - s\Delta d^k + s\epsilon^2\Delta^2 d^k$$

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Theorem 2

Let $\phi^{k+1,(n)}$ be the sequence generated by our algorithm. Then there exists a constant $C^* > 0$ such that

$$e_n \le (C^*)^n e_0, \quad \textit{with} \quad C^* = 1 - \frac{1}{2C_3C_4}.$$

Corollary 3

Let $\phi^{k+1,(n)}$ be the sequence generated by our algorithm. Then

$$\frac{1}{2}\|\phi^{k+1,(n)} - \phi\|_{\Box,h}^2 + \frac{\epsilon^2 s}{2}\|\Delta_h(\phi^{k+1,(n)} - \phi)\|_2^2 \le s(C^*)^n R_k,$$

where

$$R_k = \frac{1}{4}\left(\left\|\nabla_h\phi^k\right\|_4^4 - \|\nabla_h\phi\|_4^4\right) + \frac{\epsilon^2}{2}\left(\left\|\Delta_h\phi^k\right\|_2^2 - \|\Delta_h\phi\|_2^2\right) - (\Delta_h\phi^k, \phi^k - \phi).$$

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In this test, $\Omega = [0, 3.2]^2$, $\epsilon = 0.1$, $dt = 0.1h^2$ and $T = 3.2 \times 10^{-2}$ [F. et al., 2016]

$$\phi_0(x, y) = 0.1\Big(\sin(3\pi x/3.2)\sin(2\pi y/3.2) + \sin(5\pi x/3.2)\sin(5\pi y/3.2)\Big).$$

		PSD-L^2		PSD-H^{-1}	
h_c	h_f	$\left\Vert\delta_\phi\right\Vert_2$	Rate	$\left\Vert\delta_\phi\right\Vert_2$	Rate
$\frac{3.2}{16}$	$\frac{3.2}{32}$	6.191×10^{-3}	-	5.0305×10^{-3}	-
$\frac{3.2}{32}$	$\frac{3.2}{64}$	1.121×10^{-3}	2.47	1.0290×10^{-3}	2.29
$\frac{3.2}{64}$	$\frac{3.2}{128}$	2.449×10^{-4}	2.19	2.4184×10^{-4}	2.09
$\frac{3.2}{128}$	$\frac{3.2}{256}$	5.842×10^{-5}	2.07	5.9421×10^{-5}	2.02
$\frac{3.2}{256}$	$\frac{3.2}{512}$	1.441×10^{-5}	2.02	1.4789×10^{-5}	2.01

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Animation of the evolution with PSD solver for L^2 gradient flow up to $t = 10^4$.

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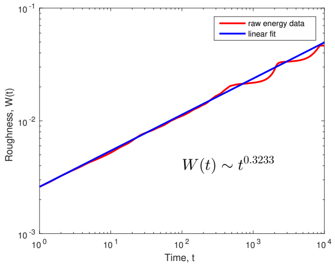
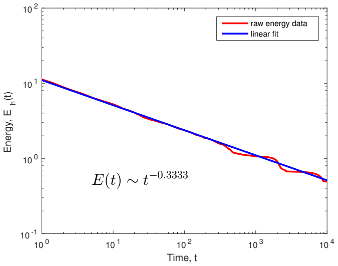
Animation of the evolution with PSD solver for H^{-1} gradient flow up to $t = 10^4$.

Numerical Results: One third power law verification L^2



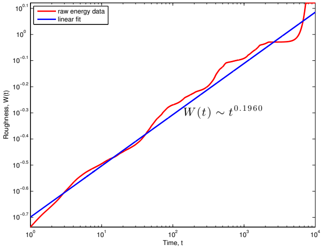
(a) Roughness evolution



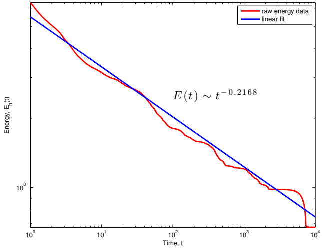
(b) Energy evolution

Loglog plot of Roughness and energy evolution for L^2 simulation

Numerical Results: One third power law verification H^{-1}



(a) Roughness evolution



(b) Energy evolution

Loglog plot of Roughness and energy evolution for H^{-1} simulation

Main reference

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Preliminary Results for Squared Phase Field Crystal Equation

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Thank you!

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