Finite element approximations of moving interface in electro-static field

Edward Tucker

Applied Mathematics & Mathematical Physics Section
Department of Mathematics
Imperial College London

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1 Introduction

2 The Cahn-Hilliard equation with electric field

3 Finite element approximations
- Decoupled F.E.A. with energy bounded below
- Decoupled F.E.A. with energy decrease
- Coupled F.E.A. with energy decrease, stability, and existence results
- Decoupled F.E.A. with stability terms

4 Numerical results

5 Future work: coupling with kinetics

6 Conclusions

Motivating industrial problem

- Interface movement problems arise in many physical phenomena and industrial processes.
- Often modelled using a phase-field approach to cope with changes in topology.

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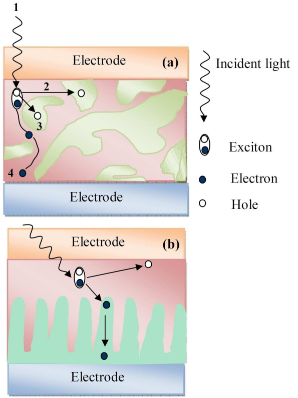
- Bi-layer organic solar cells make use of such an arrangement of dielectric polymer layers, with an electrostatic field across their interface.
- Organic cells are cheap to produce in large quantities, but have low efficiency ($\sim 1\%$).

Efficient organic solar panel morpholgy

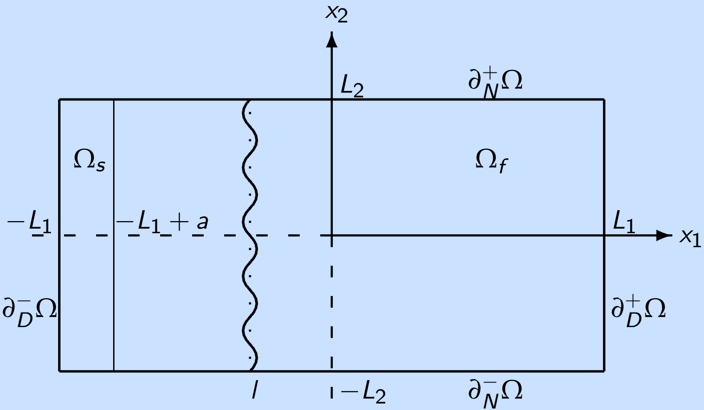
- Efficiency can be significantly improved by a particular "finger-like" film morphology.
- It is difficult to produce and control this morphology in practice.

1. Incident light creates exciton
2. Hole diffusing towards electrode
3. Hole trapped in an isolated island of organic molecule
4. Electron moving towards electrode



(a): Highly folded Hetero-junction
(b): Hetero-junction with controlled growth

Domain diagram in 2D



Phase field model

Find functions $u : \Omega_T \to [-1, 1]$, and $w, \phi : \Omega_T \to \mathbb{R}$ such that

$$\gamma \frac{\partial u}{\partial t} - \underline{\nabla} \cdot (b(\underline{x}, u) \underline{\nabla}\, w) = 0 \qquad \text{in } \Omega_T,$$

$$w = -\gamma \Delta u + \gamma^{-1} \Psi'(u) - \tfrac{1}{2} \alpha c'(\underline{x}, u) |\underline{\nabla}\, \phi|^2 \qquad \text{on } \{|u| < 1\},$$

$$u(\underline{x}, 0) = u^0(\underline{x}) \in [-1, 1] \qquad \forall \underline{x} \in \Omega,$$

$$\underline{\nabla} \cdot (c(\underline{x}, u) \underline{\nabla}\, \phi) = 0 \qquad \text{in } \Omega_T,$$

$$b(\underline{x}, u) \underline{\nabla}\, w \cdot \underline{\nu}_{\partial\Omega} = \underline{\nabla}\, u \cdot \underline{\nu}_{\partial\Omega} = 0 \qquad \text{on } \partial\Omega_T,$$

$$c(\underline{x}, u) \underline{\nabla}\, \phi \cdot \underline{\nu}_{\partial\Omega} = 0 \quad \text{on } \partial_N \Omega_T, \qquad \phi = g^{\pm} \quad \text{on } \partial_D^{\pm} \Omega_T.$$

Parameters

- $\gamma \in \mathbb{R}_{>0}$ is the interfacial parameter.
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- Diffusion coefficient $c(\underline{x}, u)$ is non-degenerate and linear,

$$c(\underline{x}, \chi) := \begin{cases} c_0 + \frac{1}{2} c_1 (1 + \chi) & -L_1 + a \leq x_1 \leq L_1, \\ c_2 & -L_1 \leq x_1 \leq -L_1 + a. \end{cases}$$

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- Obstacle potential given by

$$\Psi(s) := \begin{cases} \frac{1}{2}(1 - s^2) & \text{if } s \in [-1, 1], \\ \infty & \text{if } s \notin [-1, 1]. \end{cases}$$

Parameters and Free energy

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$$J(v,\eta) = \int_{\Omega} \{ \tfrac{1}{2}\gamma |\underline{\nabla}\, v|^2 + \gamma^{-1}\Psi(v) - \tfrac{1}{2}\alpha c(\underline{x}, v) |\underline{\nabla}\, \eta|^2 \} \mathrm{d}x.$$

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- The continuous solution satisfies the following energy bound:

$$\tfrac{\partial}{\partial t}[J(u,\phi)] + \tfrac{1}{\gamma}(b(\underline{x},u)\underline{\nabla}\, w, \underline{\nabla}\, w) \leq 0.$$

Finite element spaces and discrete energy

Let $\{\mathcal{T}^h\}_{h>0}$ be a family of partitionings of Ω into disjoint open regular non-obtuse simplices σ. We introduce the finite element spaces:

$$S^h := \{\chi \in C(\overline{\Omega}) : \chi|_\sigma \text{ is linear } \forall \sigma \in \mathcal{T}^h\} \subset H^1(\Omega);$$

$$S^h_0 = \{\chi \in S^h \ : \quad \chi = 0 \text{ on } \partial_D \Omega\};$$

$$S^h_g = \{\chi \in S^h \ : \quad \chi = g^\pm \text{ on } \partial^\pm_D \Omega\};$$

$$K^h := \{\chi \in S^h : |\chi| \leq 1 \text{ in } \Omega\} \subset K := \{\eta \in H^1(\Omega) : |\eta| \leq 1 \text{ a.e. in } \Omega\}.$$

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Discrete energy for all F.E.A.s given by

$$\mathfrak{I}(U^n, \Phi^n) = \tfrac{1}{2}\{\gamma|U^n|_1^2 - \gamma^{-1}|U^n|_h^2\} - \tfrac{1}{2}\alpha \int_\Omega c(\underline{x}, U^n)|\underline{\nabla}\,\Phi^n|^2 \mathrm{d}x.$$

Decoupled F.E.A. with energy bounded below

Scheme A

Given $U^0 \in K^h$**, for** $n \geq 1$ **find** $\{U^n, W^n, \Phi^n\} \in K^h \times S^h \times S^h_g$ **such that**

$$\left(c(\underline{x}, U^{n-1})\underline{\nabla}\,\Phi^n, \underline{\nabla}\,\chi\right) = 0 \qquad \forall \chi \in S^h_0,$$

$$\gamma\left(\frac{U^n - U^{n-1}}{\tau_n}, \chi\right)^h + \left(b(\underline{x}, U^{n-1})\underline{\nabla}\,W^n, \underline{\nabla}\,\chi\right) = 0 \qquad \forall \chi \in S^h,$$

$$\gamma\left(\underline{\nabla}\,U^n, \underline{\nabla}\,(\chi - U^n)\right) \geq \left(W^n + \gamma^{-1}U^{n-1}, \chi - U^n\right)^h + \tfrac{1}{2}\alpha\left(c'(\underline{x}, U^{n-1})|\underline{\nabla}\,\Phi^n|^2, \chi - U^n\right) \qquad \forall \chi \in K^h,$$

Energy properties for scheme A

The following energy properties hold for all $n \geq 1$:

$$\mathfrak{I}(U^{n-1}, \Phi^n) = \mathfrak{I}(U^{n-1}, \Phi^{n-1}) + \tfrac{1}{2}\alpha \int_\Omega c(\underline{x}, U^{n-1}) |\underline{\nabla}(\Phi^n - \Phi^{n-1})|^2 \mathrm{d}x.$$

$$\mathfrak{I}(U^n, \Phi^n) + \tfrac{\gamma}{2}|U^n - U^{n-1}|_1^2 + \tfrac{1}{2}\gamma^{-1}|U^n - U^{n-1}|_h^2 + \tfrac{\tau_n}{\gamma}(b(\underline{x}, U^{n-1})\underline{\nabla} W^n, \underline{\nabla} W^n) \leq \mathfrak{I}(U^{n-1}, \Phi^n).$$

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so we have a bound on the energy increase at each time-level,

$$\begin{aligned}\mathfrak{I}(U^n, \Phi^n) &+ \tfrac{1}{2}\left[\gamma|\underline{\nabla}(U^n - U^{n-1})|_{0,\Omega}^2 + \gamma^{-1}|U^n - U^{n-1}|_h^2\right] \\ &+ \tfrac{\tau_n}{\gamma}\left(b(\underline{x}, U^{n-1})\underline{\nabla} W^n, \underline{\nabla} W^n\right) \\ &\leq \mathfrak{I}(U^{n-1}, \Phi^{n-1}) + \tfrac{1}{2}\alpha \int_\Omega c(\underline{x}, U^{n-1}) |\underline{\nabla}(\Phi^n - \Phi^{n-1})|^2 \mathrm{d}x.\end{aligned}$$

Properties and limitations of scheme A

- The following discrete maximum principle holds.

$$g^- \leq \Phi^n \leq g^+ \qquad \text{in } \Omega, \ \forall n \in \mathbb{N}.$$

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- However, no stability result can be shown.

Decoupled F.E.A. with energy decrease

Scheme B

Given $\{U^0, \Phi^0\} \in K^h \times S^h_g$**, for** $n \geq 1$ **find** $\{U^n, W^n, \Phi^n\} \in K^h \times S^h \times S^h_g$ **such that**

$$\left(c(\underline{x}, U^{n-1})\underline{\nabla}\left(\tfrac{1}{2}(\Phi^n + \Phi^{n-1})\right), \underline{\nabla}\chi\right) = 0 \qquad \forall \chi \in S^h_0,$$

$$\gamma\left(\frac{U^n - U^{n-1}}{\tau_n}, \chi\right)^h + \left(b(\underline{x}, U^{n-1})\underline{\nabla}(W^n), \underline{\nabla}\chi\right) = 0 \qquad \forall \chi \in S^h,$$

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$\Phi^0 \in S^h_g$ is required, $\left(c(\underline{x}, U^0)\underline{\nabla}\,\Phi^0, \underline{\nabla}\,\chi\right) = 0 \qquad \forall \chi \in S^h_0$.

Energy decrease for scheme B

Due to the form of the discrete electric field we have the following energy properties, for all $n \geq 1$:

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Combining the above we have discrete energy decrease at each timestep,

$$\mathfrak{I}(U^n, \Phi^n) \leq \mathfrak{I}(U^{n-1}, \Phi^n) = \mathfrak{I}(U^{n-1}, \Phi^{n-1}).$$

Electric field properties

- Discrete maximum principle for electric field

$$g^- \leq \frac{1}{2}(\Phi^n + \Phi^{n-1}) \leq g^+ \qquad \text{in } \overline{\Omega} \quad \forall n \geq 1.$$

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- The discrete electric field also satisfies

$$\int_\Omega c(\underline{x}, U^{n-1}) |\underline{\nabla}\, (\tfrac{1}{2}(\Phi^n + \Phi^{n-1}))|^2 \leq \int_\Omega c(\underline{x}, U^{n-1}) \quad \forall n \geq 1.$$

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- Crucially, there is no way to bound the term $-\frac{1}{2}\alpha \int_\Omega c(\underline{x}, U^n)|\underline{\nabla}\,\Phi^n|^2 dx$ from below in the discrete energy. Therefore we have unbounded energy decrease so there is no possibility of proving a steady state exists.

Coupled F.E.A. with energy decrease, stability, and existence results

Scheme C

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$$\gamma\left(\frac{U^n - U^{n-1}}{\tau_n}, \chi\right)^h + \left(b(\underline{x}, U^{n-1})\underline{\nabla}\,W^n, \underline{\nabla}\,\chi\right) = 0 \qquad \forall \chi \in S^h,$$

$$\gamma\left(\underline{\nabla}\,U^n, \underline{\nabla}\,(\chi - U^n)\right) \geq \left(W^n + \gamma^{-1}U^{n-1}, \chi - U^n\right)^h + \tfrac{1}{2}\alpha\left(c'(\underline{x}, U^{n-1})|\underline{\nabla}\,\Phi^n|^2, \chi - U^n\right) \qquad \forall \chi \in K^h,$$

Energy decrease for scheme C

Due to the form of the discrete electric field we have the following energy properties, for all $n \geq 1$:

$$\mathfrak{I}(U^{n-1}, \Phi^n) = \mathfrak{I}(U^{n-1}, \Phi^{n-1}) - \tfrac{\alpha}{2}\left(c(\underline{x}, U^{n-1}), |\underline{\nabla}\,(\Phi^n - \Phi^{n-1})|^2\right),$$

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- Stability for the scheme C follows from the energy decrease.
- Convergence for this system is still to be done, but should be attainable!
- Discrete maximum principle for electric field holds.
- The following holds

$$\int_\Omega c(\underline{x}, U^n)|\underline{\nabla}\,\Phi^n|^2 \leq \int_\Omega c(\underline{x}, U^n) \leq c_{\max}|\Omega| =: C,$$

and so the discrete energy is bounded below.

Practical considerations limitations of scheme C

- The highly non-linear scheme at each time level is solved using a fixed-point approach.
- Existence of solutions $\{U^n, \Phi^n\}$ is proved using a Brouwer-fixed point argument.

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Limitations:

- Solving scheme C requires much larger CPU times, especially in 3D.

Decoupled F.E.A. with stability terms

Scheme D

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$$\gamma \left(\frac{U^n - U^{n-1}}{\tau_n}, \chi \right)^h + \left(b(\underline{x}, U^{n-1}) \underline{\nabla}\, W^n, \underline{\nabla}\, \chi \right) = 0 \qquad \forall \chi \in S^h,$$

$$\begin{aligned}(\rho + \gamma) \left(\underline{\nabla}\, U^n, \underline{\nabla}\, (\chi - U^n) \right) \geq & \left(W^n + \gamma^{-1} U^{n-1}, \chi - U^n \right)^h \\ & + \tfrac{1}{2}\alpha \left(c'(\underline{x}, U^{n-1}) |\underline{\nabla}\, \Phi^n|^2, \chi - U^n \right) \\ & + \rho \left(\underline{\nabla}\, U^{n-1}, \underline{\nabla}\, (\chi - U^n) \right) \qquad \forall \chi \in K^h,\end{aligned}$$

Energy properties for scheme D

We have the following energy properties, for all $n \geq 1$:

$$\mathfrak{I}(U^{n-1}, \Phi^n) = \mathfrak{I}(U^{n-1}, \Phi^{n-1}) + \tfrac{1}{2}\alpha \left(c(\underline{x}, U^{n-1}), |\underline{\nabla}\,(\Phi^n - \Phi^{n-1})|^2 \right),$$

$$\begin{aligned} \mathfrak{I}(U^n, \Phi^n) + (\rho + \tfrac{\gamma}{2})|\underline{\nabla}\,(U^n - U^{n-1})|^2_{0,\Omega} + \tfrac{1}{2}\gamma^{-1}|U^n - U^{n-1}|^2_h \\ + \tfrac{\tau_n}{\gamma}(b(\underline{x}, U^{n-1})\underline{\nabla}\,W^n, \underline{\nabla}\,W^n) \leq \mathfrak{I}(U^{n-1}, \Phi^n), \end{aligned}$$

Energy properties for scheme D

We have the following energy properties, for all $n \geq 1$:

$$\mathfrak{I}(U^{n-1}, \Phi^n) = \mathfrak{I}(U^{n-1}, \Phi^{n-1}) + \tfrac{1}{2}\alpha \left(c(\underline{x}, U^{n-1}), |\underline{\nabla}\,(\Phi^n - \Phi^{n-1})|^2 \right),$$

$$\begin{aligned} \mathfrak{I}(U^n, \Phi^n) + (\rho + \tfrac{\gamma}{2})|\underline{\nabla}\,(U^n - U^{n-1})|^2_{0,\Omega} + \tfrac{1}{2}\gamma^{-1}|U^n - U^{n-1}|^2_h \\ + \tfrac{\tau_n}{\gamma}(b(\underline{x}, U^{n-1})\underline{\nabla}\,W^n, \underline{\nabla}\,W^n) \leq \mathfrak{I}(U^{n-1}, \Phi^n), \end{aligned}$$

$$\begin{aligned} \Longrightarrow \mathfrak{I}(U^n, \Phi^n) &+ \tfrac{1}{2}\left[(2\rho + \gamma)|\underline{\nabla}\,(U^n - U^{n-1})|^2_{0,\Omega} + \gamma^{-1}|U^n - U^{n-1}|^2_h\right] \\ &+ \tfrac{\tau_n}{\gamma}\left(b(\underline{x}, U^{n-1})\underline{\nabla}\,W^n, \underline{\nabla}\,W^n\right) \\ &\leq \mathfrak{I}(U^{n-1}, \Phi^{n-1}) + \tfrac{1}{2}\alpha \int_\Omega c(\underline{x}, U^{n-1})|\underline{\nabla}\,(\Phi^n - \Phi^{n-1})|^2 \mathrm{d}x. \end{aligned}$$

Stability conditions of Scheme D

Attempt to obtain stability for the system leads to

$$\mathfrak{I}(U^n, \Phi^n) + \frac{1}{2}\sum_{k=1}^{n}\left[(2\rho+\gamma)|\underline{\nabla}(U^k - U^{k-1})|_{0,\Omega}^2 + \gamma^{-1}|U^k - U^{k-1}|_h^2\right]$$

$$\leq \mathfrak{I}(U^0, \Phi^1) + \frac{\alpha(c'_{\max})^2}{2c_{\min}} \max_{k=1\to n-1} \|\underline{\nabla}\,\Phi^k\|_{0,p,\Omega}^2 \sum_{k=1}^{n-1} \|U^k - U^{k-1}\|_{0,q}^2.$$

for $p > 2$, and $q = \frac{2p}{p-2}$. Applying the Sobolev embedding theorem for $d = 2$, we can get the following bound

$$\|U^k - U^{k-1}\|_{0,q}^2 \leq C\|U^k - U^{k-1}\|_1^2 \qquad \text{for } q < \infty$$
$$\leq C^*|U^k - U^{k-1}|_1^2.$$

Crucially, we can bound $\|\underline{\nabla}\,\Phi^k\|_{0,p,\Omega}^2 \leq C, \qquad \text{for } p \in [2, 2+\delta].$

Further properties and limitations of Scheme D

- As with scheme A, we have a bound on the energy increase.
- Discrete maximum principle for electric field Φ^n holds.
- Discrete energy bounded below.

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- In practice, the stability bound μ is unknown, so analysis of the discrete energy behaviour is required.
- The artificial stabilisation parameter may have an unwanted effect upon the morphology of solutions!

Practical implementation of schemes A-D

We present results for scheme D (decoupled, with stability terms).

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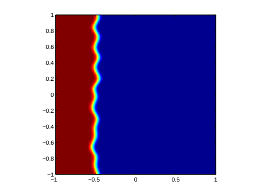
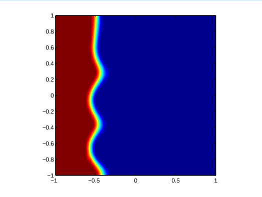
- Linear system for Φ^n is easily solved using conjugate gradient or multigrid solvers.
- $\{U^n, W^n\}$ solved using Gauss-Seidel iterative solver.
- h-adaptivity used to track the interface.
- Elements (σ) are marked according to $\max_{\underline{x}\in\sigma}|U^n(\underline{x})| - 1$.
- Computations done with adaptive finite element code Alberta-3.0-rc6.

Morphology evolution in 2D

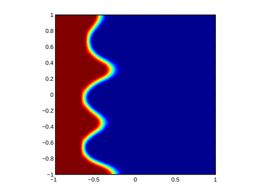
Scheme D with $\rho = 0.1$, $\alpha = 80$, $\gamma = 1/8\pi$, and $\tau = 5 * 10^{-7}$.



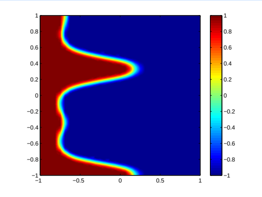
$t = 0$



$t = 2 * 10^{-4}$



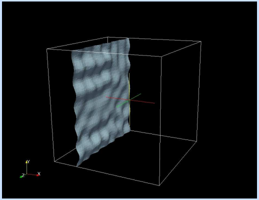
$t = 4 * 10^{-4}$



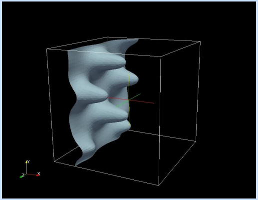
$t = 10^{-3}$

Morphology evolution in 3D

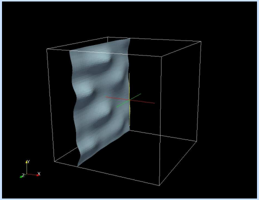
Scheme D with $\rho = 1.0$, $\alpha = 100$, $\gamma = 1/8\pi$, and $\tau = 10^{-5}$. movie



$t = 0$



$t = 5 * 10^{-4}$



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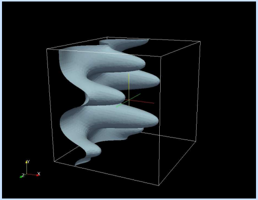

$t = 10^{-3}$

Coupling with kinetics

Find functions $u : \Omega_T \to \mathcal{K}$, $w, \phi : \Omega_T \to \mathbb{R}$, and $\underline{v} : \Omega_T \to \mathbb{R}^d$, $p : \Omega_T \to \mathbb{R}$ such that

$$\gamma \frac{\partial u}{\partial t} + \beta \underline{v} \cdot \underline{\nabla}\, u - \underline{\nabla} \cdot (b(\underline{x}, u) \underline{\nabla}\, w) = 0 \qquad \text{in } \Omega_T,$$

$$w = -\gamma \Delta u + \gamma^{-1} \Psi'(u) - \tfrac{1}{2} \alpha c'(\underline{x}, u) |\underline{\nabla}\, \phi|^2 \qquad \text{on } \{|u| < 1\},$$

$$u(\underline{x}, 0) = u^0(\underline{x}) \in \mathcal{K} \qquad \forall \underline{x} \in \Omega,$$

$$\underline{\nabla} \cdot (c(\underline{x}, u) \underline{\nabla}\, \phi) = 0 \qquad \text{in } \Omega_T,$$

$$\begin{cases} -\Delta \underline{v} + \underline{\nabla}\, p = \beta w \underline{\nabla}\, u \\ \underline{\nabla} \cdot \underline{v} = 0 \end{cases} \qquad \text{in } \Omega_T,$$

$$b(\underline{x}, u) \underline{\nabla}\, w \cdot \underline{\nu}_{\partial\Omega} = \underline{\nabla}\, u \cdot \underline{\nu}_{\partial\Omega} = 0 \qquad \text{on } \partial\Omega_T,$$

$$c(\underline{x}, u) \underline{\nabla}\, \phi \cdot \underline{\nu}_{\partial\Omega} = 0 \quad \text{on } \partial_N \Omega_T, \qquad \phi = g^{\pm} \quad \text{on } \partial_D^{\pm} \Omega_T,$$

$$(\underline{\underline{\nabla}}\, \underline{v})\, \underline{\nu}_{\partial\Omega} - p\, \underline{\nu}_{\partial\Omega} = \underline{0} \quad \text{on } \partial_N \Omega_T, \qquad \underline{v} = 0 \quad \text{on } \Omega_s \cup \partial_D \Omega_T.$$

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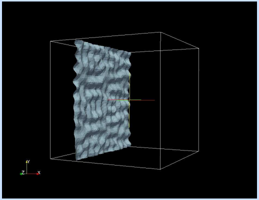
  ... but Algebraic Multigrid preconditioner might be quicker.

Morphology evolution in 3D

Parameters $\beta = 2 * 10^{-3}, \rho = 0.1, \ \alpha = 100, \ \gamma = 1/8\pi$, and $\tau = 2 * 10^{-6}$.



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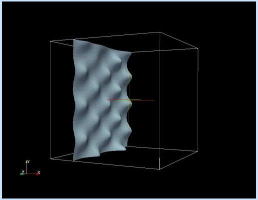

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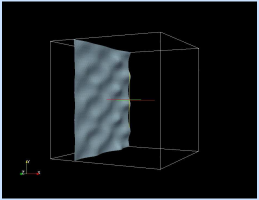
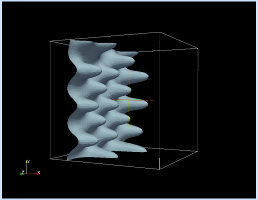
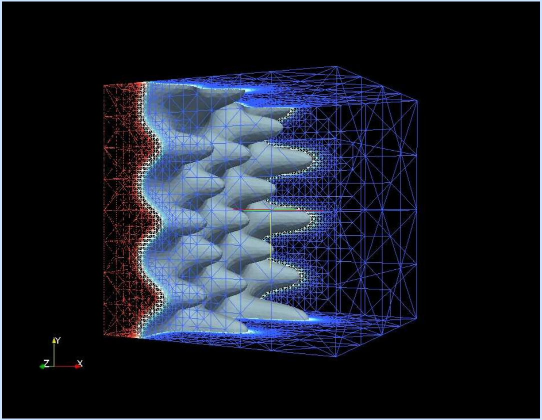


$t = 5 * 10^{-5}$



$t = 2.7 * 10^{-4}$

Morphology evolution in 3D



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Conclusions

Have introduced four finite element approximations for model of interface in an electro-static field, displaying varying properties:

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Future work includes coupling with kinetics, and completing convergence proofs.