

A Globally Convergent Modified Newton Method for Direct Minimization of the Ohta–Kawasaki Energy¹: Application to Diblock Copolymer Self-Assembly

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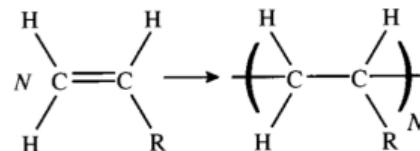
Session: Phase Field Study of Microstructures and Behaviours of Advanced Materials

USNC/TAM, 06/24/2022

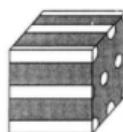
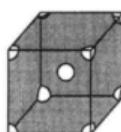
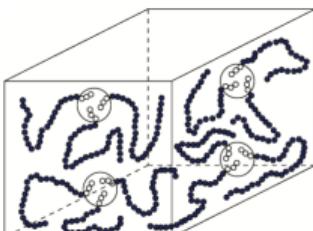
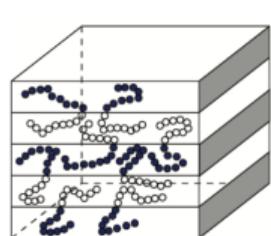
¹Cao, L., Ghattas, O., & Oden, J. T. (2022). A globally convergent modified Newton method for the direct minimization of the Ohta–Kawasaki energy with application to the directed self-assembly of diblock copolymers. *SIAM Journal on Scientific Computing*, 44(1), B51–B79. doi:10.1137/20M1378119.

Diblock copolymer self-assembly

- **Diblock copolymers (Di-BCPs):** Linear polymers consist of two blocks of thermodynamically incompatible monomers.



- **Self-assembly:** Below the glass-transition temperature, the two blocks spontaneously segregate and form ordered nanostructures



Spheres

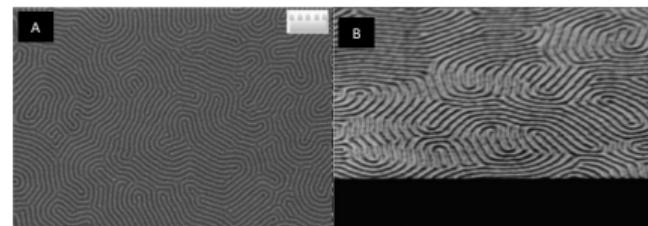
Cylinders

Bicontinuous

Perforated Layers

Lamellae

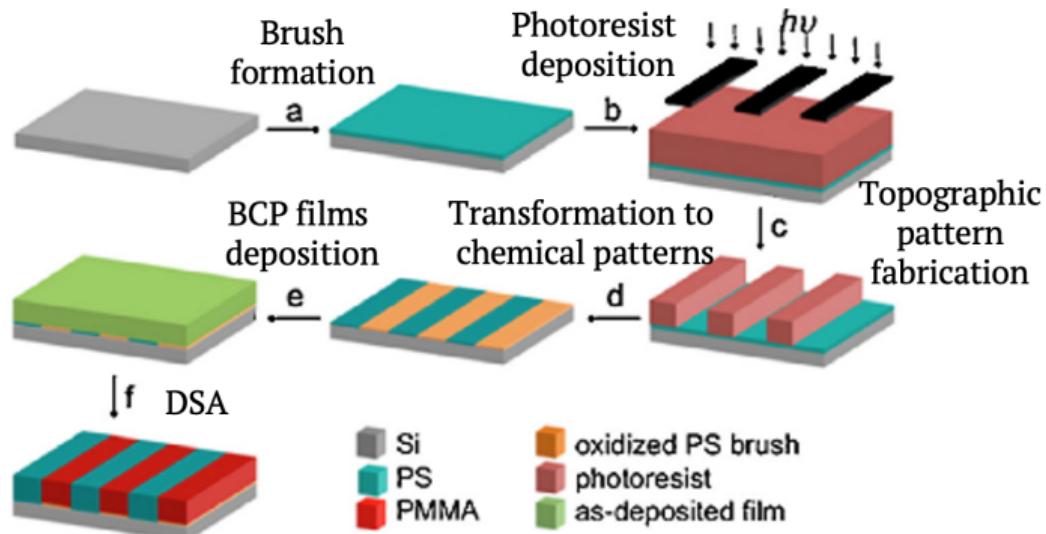
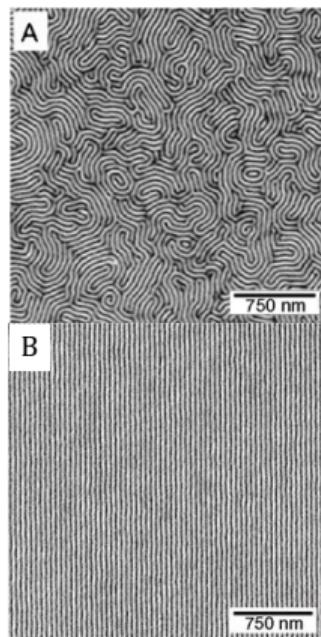
Di-BCP thin film



Gu et. al, *Adv. Mater.*, 2012.

Directed self-assembly of Di-BCP thin films

- **Directed self-assembly (DSA):** Guiding Di-BCP self-assembly to form long-range ordered structures with desired nanoscale features.
- **Chemoepitaxy DSA:** Di-BCP thin film self-assembly on *chemically patterned surfaces*.

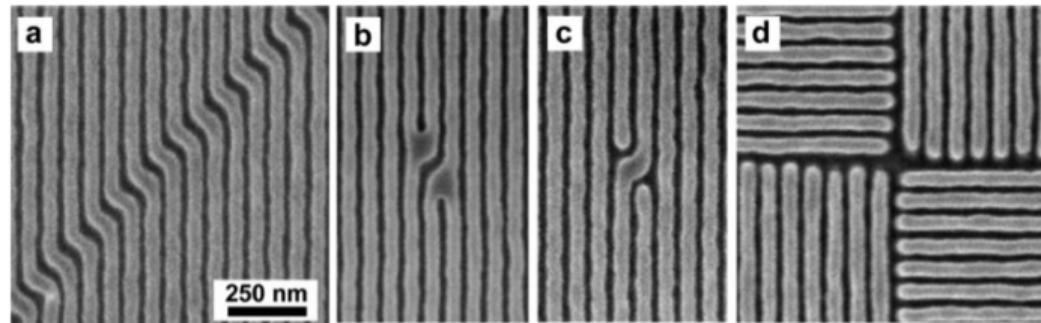


Ji et. al, *Progr. in Poly. Sci.*, 2016.

Kim et. al, *Nature*, 2003.

Key application: Patterning for nanofabrication

Example: Integrated circuits geometry by Di-BCP



Stoykovich et.al, *ACS Nano*, 2007.

Phase field models for diblock copolymer self-assembly

Density functional theory

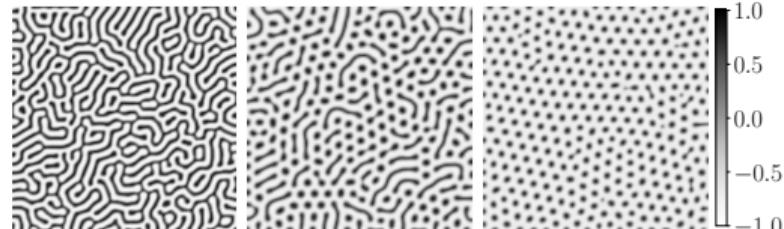
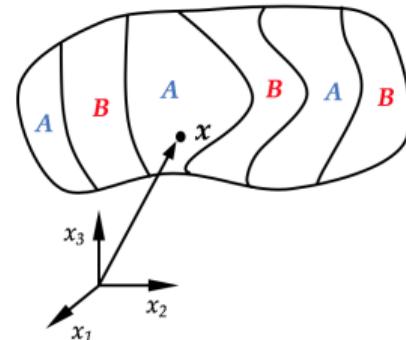
$$u^* = \arg \min_{u \in \mathring{H}_m^k} F_{\text{PF}}(u)$$

$$\mathring{H}_m^k := \{u \in H^k : \int (u - m) d\mathbf{x} = 0\}$$

Model	Free energy
OK	$F_{\text{OK}}(u) = \int_{\Omega} \left(\frac{1}{4}(1-u^2)^2 + \frac{\epsilon^2}{2} \nabla u ^2 + \frac{\sigma}{2}(u-m)(-\Delta)^{-1}(u-m) \right) d\mathbf{x}$
SH	$F_{\text{SH}}(u) = \int_{\Omega} \left(\frac{1}{4}u^4 - \frac{\epsilon}{2}u^2 + \frac{1}{2}((1+\Delta)u)^2 \right) d\mathbf{x}$
gOK	$F_{\text{gOK}}(u) = \int_{\Omega} \left(\frac{1}{4}(1-u^2) + \frac{c_1}{2}\sqrt{1-u^2} + \frac{c_2}{2}(1+u)\ln((1+u)/2) + \frac{c_3}{2}(1-u)\ln((1-u)/2) + \frac{c_4 \nabla u ^2}{(1-u^2)} + \frac{c_5}{2}v(-\Delta)^{-1}v \right) d\mathbf{x},$ $v = \sqrt{(1-m)(u+1)} - \sqrt{(m+1)(1-u)}$

Uneyma and Doi, *Macromolecules*, 2005.

$$u := u_A - u_B \in [-1, 1]$$



Outer-loop: Bayesian model calibration, validation, and selection

Model	Free energy
OK	$F_{OK}(u) = \int_{\Omega} \left(\frac{1}{4}(1-u^2)^2 + \frac{\epsilon^2}{2} \nabla u ^2 + \frac{\sigma}{2} (u-m)(-\Delta)^{-1}(u-m) \right) d\mathbf{x}$
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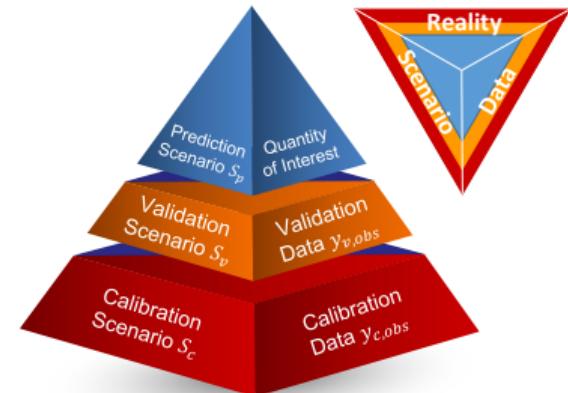
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Bayes rule

$$\pi_{X|d}(x) = \frac{\mathcal{L}(x; d)\pi_X(x)}{C_d} \text{ a.s.}$$

- X : uncertain model parameters

Cao, Baptista, et. al, *arXiv pre-print*, 2022



"The Prediction Triangular Pyramid"

Oden et. al, *Ency. of Comput. Mech.*, 2017.

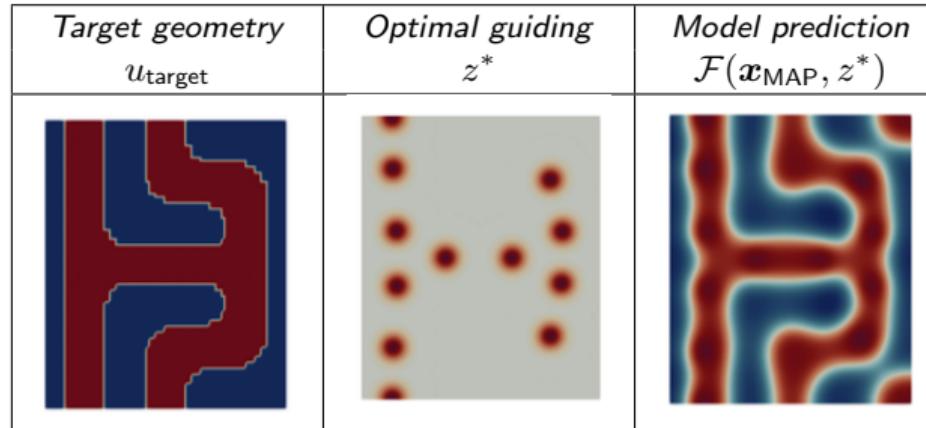
- d : image data via microscopy or X-ray scattering
- $\mathcal{L}(x; d)$: likelihood function, **requires (repeatedly) solving model at x**
- $C_d = \mathbb{E}_X [\mathcal{L}(X; d)]$: *evidence* used in model selection

Outer-loop: Optimal design of chemoepitaxy under uncertainty

Empirical risk minimization

$$z^* = \arg \min_{z \in \mathcal{V}^z} \mathbb{E}_{\mathbf{X}, \delta Z} [\|u_{\text{target}} - \mathcal{F}(\mathbf{X}, z + \delta Z)\|_{L^2}] + \mathcal{P}(z)$$

- δZ : uncertainty in chemical pattern placement
- $\mathcal{P}(z)$: penalty inducing sparse pattern
- \mathcal{F} : the model solution operator



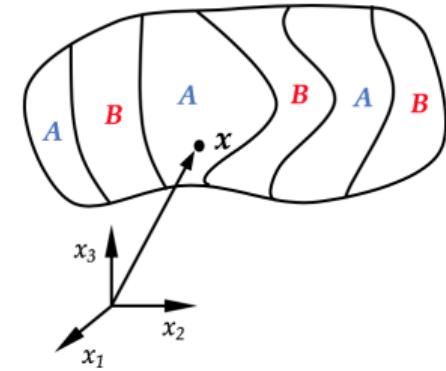
Luo, Cao, et. al, arXiv pre-print, 2022.

The Ohta–Kawasaki (OK) energy (Ohta & Kawasaki, 1986)

$$F_{\text{OK}}(u) = \frac{1}{2} \int_{\Omega} \left\{ 2\kappa W(u) + \epsilon^2 |\nabla u|^2 + \sigma(u - m)(-\Delta_N)^{-1}(u - m) \right\} d\mathbf{x}$$

$$\mathring{H}_m^1 := \{u \in H^1 : \int (u - m) d\mathbf{x} = 0\}$$

$$u = \textcolor{blue}{u_A} - \textcolor{red}{u_B} \in [-1, 1]$$



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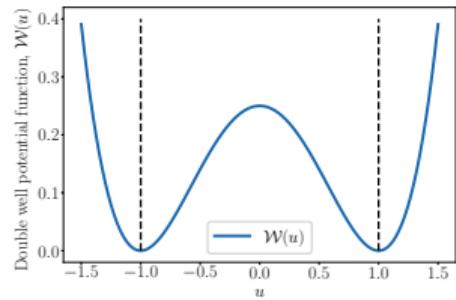
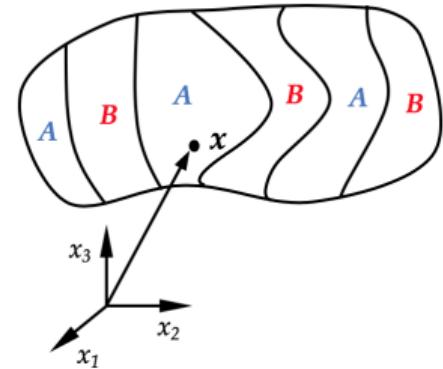
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- **Effect:** Enforcing phase separation at ± 1

$$W(u) = (1 - u^2)^2$$

Interpretation: Repulsion between distinct monomers

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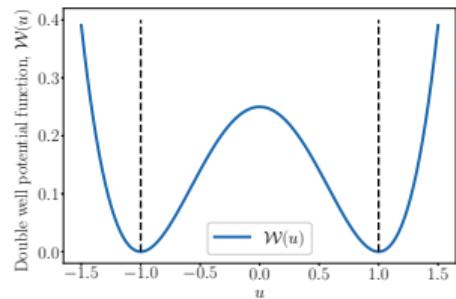
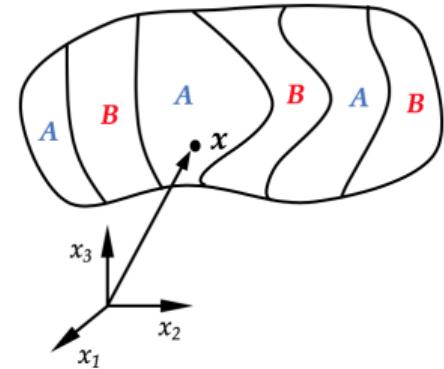
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- **Effect:** Prefer smooth interface

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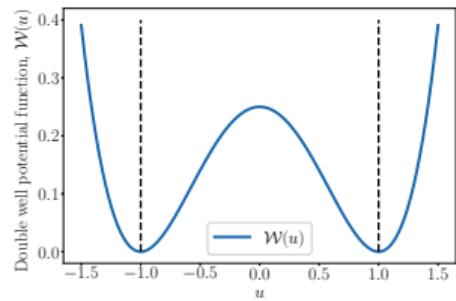
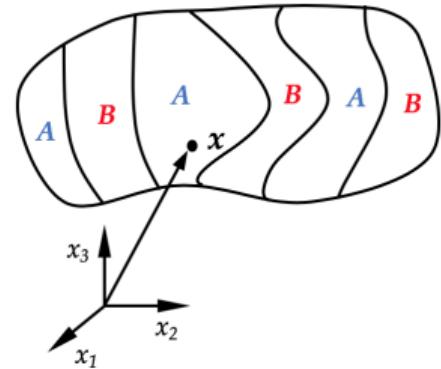
Interpretation: Characterize short range interaction of polymer chains.

- **Effect:** Prefer small phase domains

$$w = (-\Delta_N)^{-1}(u - m) \iff \begin{cases} -\Delta w = u - m & \text{in } \Omega \\ \nabla w \cdot \nu = 0 & \text{on } \partial\Omega \end{cases}$$

Interpretation: Characterize long range interaction of polymer chains

$$u = \textcolor{blue}{u_A} - \textcolor{red}{u_B} \in [-1, 1]$$



Solving phase field models via \mathring{H}^{-1} gradient flow

List of terminology

\mathring{H}^1	$\left\{ u \in H^1 : \int_{\Omega} u \, d\mathbf{x} = 0 \right\}$
\mathring{H}^{-1}	$\{f \in (H^1)^* : \langle f, \text{constant} \rangle = 0\}$

\mathring{H}^{-1} gradient flow (strong form)

$$\begin{aligned}\partial_t u(t) &= -\Delta DF_{\text{PF}}(u(t)) && \text{in } \Omega, \quad t \in \mathbb{R}_+ \\ \nabla u(t) \cdot \nu &= \nabla(\Delta u(t)) \cdot \nu = 0 && \text{on } \partial\Omega, \quad t \in \mathbb{R}_+ \\ u(0) &= m + \text{ random field } && \text{in } \Omega\end{aligned}$$

- $-\Delta_N : \mathring{H}^1 \rightarrow \mathring{H}^{-1}$ (weak form of Poisson problem)
- Evolves until $\partial_t u(T) \approx 0 \implies DF_{\text{PF}}(u(T)) \approx 0$

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What's good

- “Mass” conservation

$$\int_{\Omega} u(t) \, d\mathbf{x} = \int_{\Omega} u(0) \, d\mathbf{x} \quad \forall t \in \mathbb{R}_+$$

- Energy stability (i.e. globally convergent)

$$F(u(t_1)) \geq F(u(t_2)), \quad 0 \leq t_1 < t_2$$

What's bad:

- Stiffness: requires small time steps \implies slow progress towards steady states
- Linearly convergent
- Mesh dependence: slower convergence rate for denser mesh

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FOK: Non-local Cahn–Hilliard (mixed strong form)

$$\begin{aligned}\partial_t u(t) &= \Delta \mu(t) - \sigma(u(t) - m) && \text{in } \Omega, \quad t \in \mathbb{R}_+ \\ \mu(t) &= \kappa W'(u(t)) - \epsilon^2 \Delta u(t) && \text{in } \Omega, \quad t \in \mathbb{R}_+\end{aligned}$$

Direct minimization with Newton's method

List of terminology

R	\mathring{H}^1	(\cdot, \cdot)	$\langle \cdot, \cdot \rangle$
L^2 Riesz map	$\left\{ u \in H^1 : \int_{\Omega} u \, d\mathbf{x} = 0 \right\}$	L^2 -inner product	duality paring

Gradient and Hessian

$$\begin{aligned}\langle DF_{OK}(u), \tilde{u}_0 \rangle &:= (\kappa W'(u), \tilde{u}_0) + (\epsilon^2 \nabla u, \nabla \tilde{u}_0) + (\sigma(-\Delta_N)^{-1} R(u - m), \tilde{u}_0) \quad \forall \tilde{u}_0 \in \mathring{H}^1 \\ \langle D^2 F_{OK}(u) \hat{u}_0, \tilde{u}_0 \rangle &:= (\kappa W''(u) \hat{u}_0, \tilde{u}_0) + (\epsilon^2 \nabla \hat{u}_0, \nabla \tilde{u}_0) + (\sigma(-\Delta_N)^{-1} R(\hat{u}_0), \tilde{u}_0) \quad \forall \hat{u}_0, \tilde{u}_0 \in \mathring{H}^1\end{aligned}$$

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What's bad

- Hard to directly implement in \mathring{H}^1
- Not globally convergent (no energy stability)

- 1 δu_n may not point to descent direction
- 2 If it does, need to determine t_n

Newton's method

$$u_{n+1} = u_n + t_n \delta u_n \quad \forall n \in \mathbb{N} \cup \{0\}$$

Find $\delta u_n \in \mathring{H}^1$ such that:

$$\langle D^2 F_{OK}(u_n) \delta u_n, \tilde{u}_0 \rangle = -\langle DF_{OK}(u_n), \tilde{u}_0 \rangle \quad \forall \tilde{u}_0 \in \mathring{H}^1$$

What's good

- “Mass” conservative
- If converges, converges quadratically ($t = 1$)
- If converges, rate is mesh independent

\mathring{H}^{-1} Newton step problem (solve in H^1)

\mathring{H}^1 Newton step problem

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Inspiration: \mathring{H}^{-1} gradient flow $\partial_t u = DF(u) \rightarrow \partial_t u = \Delta DF(u_n) \in \mathring{H}^{-1}$

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\mathring{H}^{-1} Newton step problem

Find $(\delta u_n, \hat{\mu}_n) \in H^1 \times H^1$ such that:

$$(\nabla \hat{\mu}_n, \nabla \tilde{u}) + (\sigma \delta u_n, \tilde{u}) = -(\nabla \mu_n, \nabla \tilde{u}) - (\sigma(u_n - m), \tilde{u}) \quad \forall \tilde{u} \in H^1$$

$$(\hat{\mu}_n, \tilde{\mu}) - (\kappa W''(u_n) \delta u_n, \tilde{\mu}) - (\epsilon^2 \nabla(\delta u_n), \nabla \tilde{\mu}) = 0 \quad \forall \tilde{\mu} \in H^1$$

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We proved...

If $u_n \in \mathring{H}_m^1$:

- Solutions to the \mathring{H}^{-1} problem solve the \mathring{H}^1 problem
(Independent to form of W'')

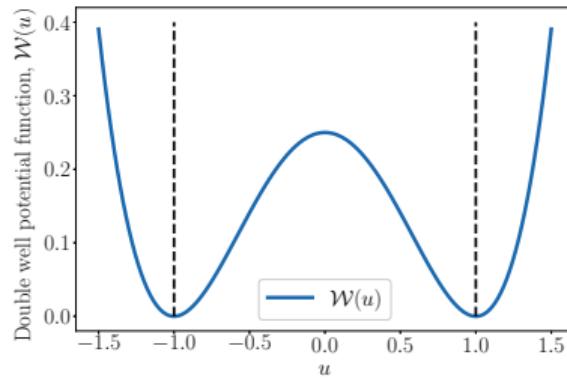
If $u_n \notin \mathring{H}_m^1$:

- $u_n + \delta u_n \in \mathring{H}_m^1$ (a correction step!)

Adaptive Gauss–Newton convexification (energy descent direction)

Issue: δu_n may not be a energy descent direction, due to **non-convex double well**

$$\underbrace{\langle DF_{OK}(u_n), \delta u_n \rangle < 0}_{\text{local energy descent}} \iff \underbrace{\langle D^2 F_{OK}(u_n) \delta u_n, \delta u_n \rangle > 0}_{\text{Hessian-weighted product}},$$



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Strategy: adaptively convexify double well by backtracking search

- 1 Introduce a weight parameter $\gamma \in [0, 1]$

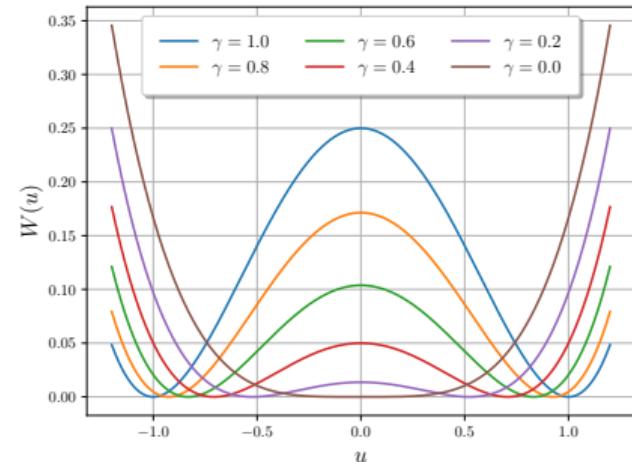
$$W''(u) = 2u^2 + (u^2 - 1) \rightarrow W''_\gamma(u) = 2u^2 + \underbrace{\gamma(u^2 - 1)}_{\leq 0}$$

- 2 Solve \mathring{H}^{-1} Newton step with $\gamma_0 = 1$

- 3 Check if the step is in descent direction

- 4 If not, re-solve the modified problem with $\gamma_{n+1} \in [0, \gamma_n]$

- 5 Repeat 3–4 until a descent direction is found.



Adaptive Gauss–Newton convexification (energy descent direction)

Issue: δu_n may not be a energy descent direction, due to non-convex double well

$$\underbrace{\langle DF_{\text{OK}}(u_n), \delta u_n \rangle < 0}_{\text{local energy descent}} \iff \underbrace{\langle D^2 F_{\text{OK}}(u_n) \delta u_n, \delta u_n \rangle > 0}_{\text{Hessian-weighted product}},$$

Strategy: adaptively convexify double well by backtracking search

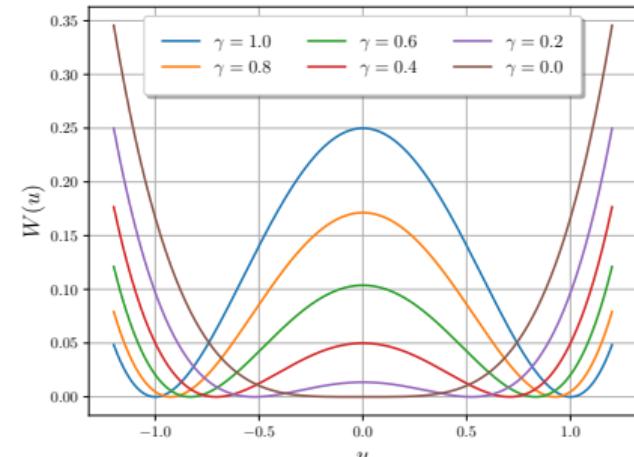
- 1 Introduce a weight parameter $\gamma \in [0, 1]$

$$W''(u) = 2u^2 + (u^2 - 1) \rightarrow W''_\gamma(u) = 2u^2 + \underbrace{\gamma(u^2 - 1)}_{\leq 0}$$

- 2 Solve \mathring{H}^{-1} Newton step with $\gamma_0 = 1$
- 3 Check if the step is in descent direction
- 4 If not, re-solve the modified problem with $\gamma_{n+1} \in [0, \gamma_n)$
- 5 Repeat 3–4 until a descent direction is found.

We proved...

There exists a constant $\gamma_c(\kappa, \epsilon, \Omega) > 0$ such that $\gamma \in [0, \gamma_c)$ gives us a descent direction



Inexact line search on the OK energy (finding step size)

Newton iteration

$$u_{n+1} = u_n + t_n \delta u_n \quad \forall n \in \mathbb{N} \cup \{0\}$$

Goal: find a step size t_n that returns *sufficient energy descent*

Armijo inexact line search

$$F_{OK}(u_n + \alpha \delta u_n) \leq F_{OK}(u_n) + c\alpha \langle DF_{OK}(u_n), \delta u_n \rangle, \quad c = 10^{-4}$$

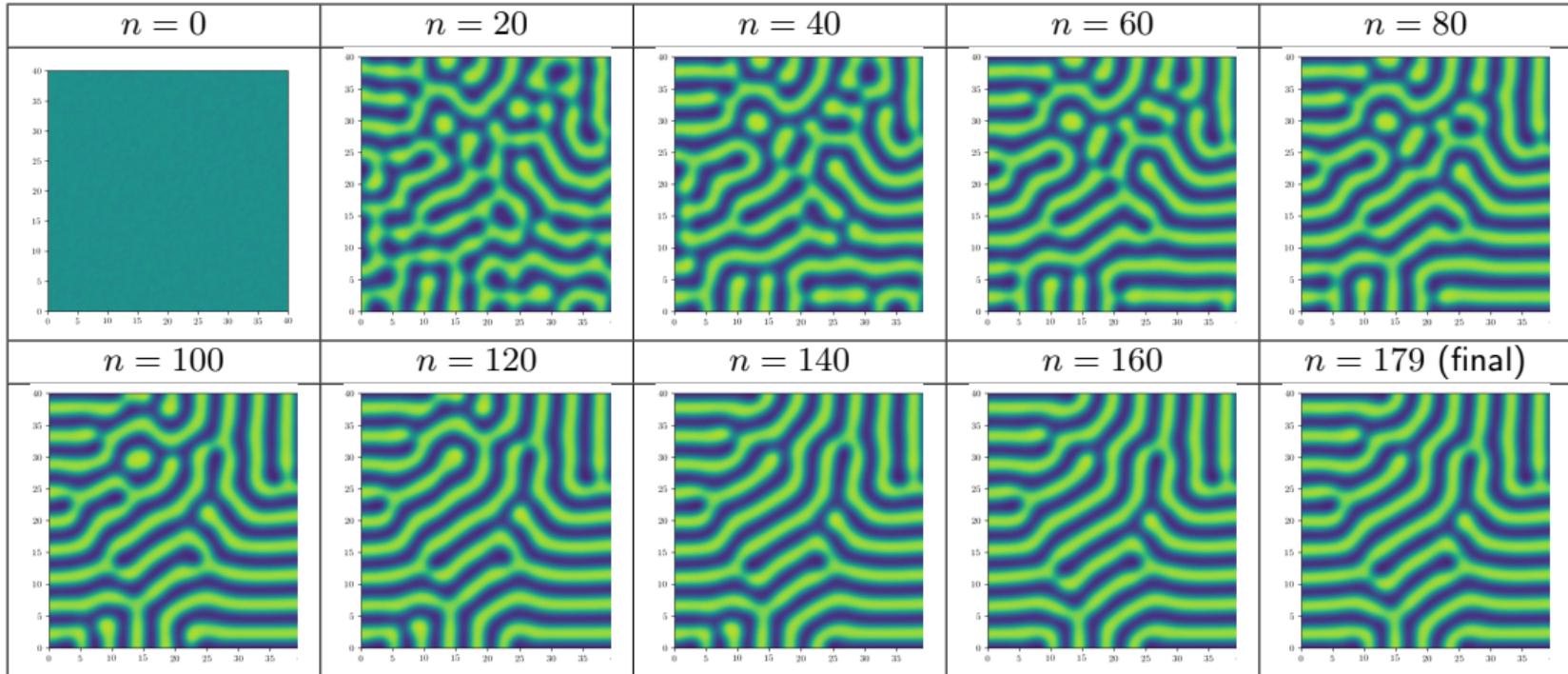
- 1 Solve $\delta w_n = (-\Delta_N)^{-1} \delta u_n$ and $w = (-\Delta_N)^{-1} u_n$ (one time at $n = 0$)
- 2 Try $\alpha = 1$
- 3 Check condition above
- 4 If not satisfied, try $\alpha = \alpha/2$
- 5 Repeat 3–4 until the condition satisfied

Operation counts: Gradient flow versus Newton

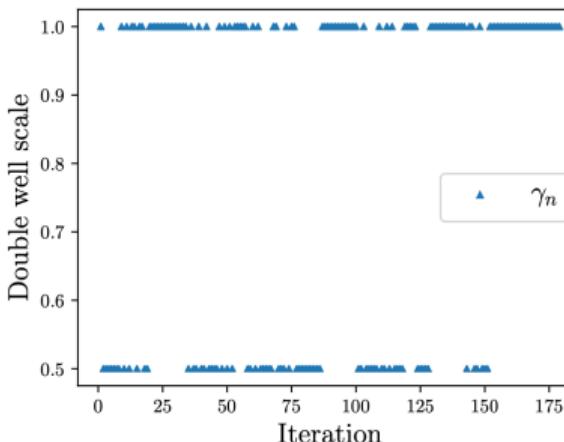
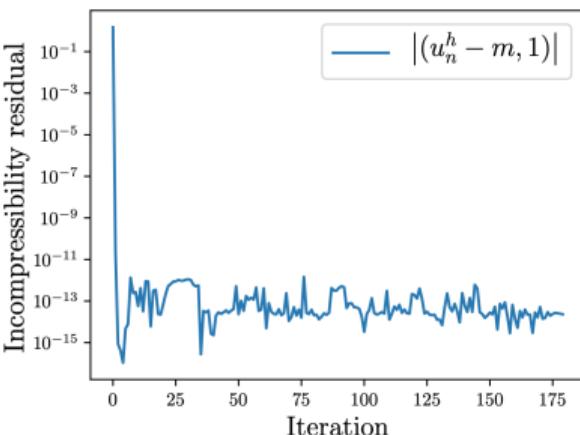
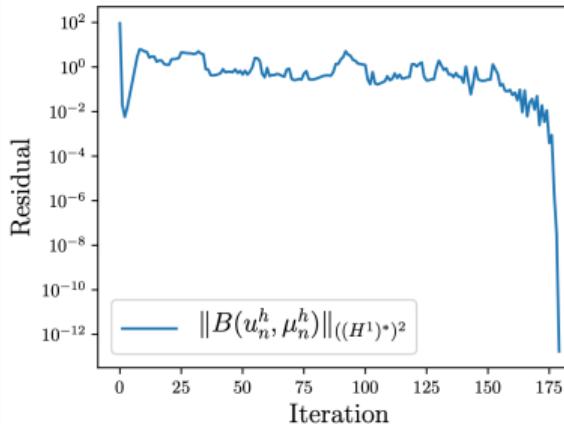
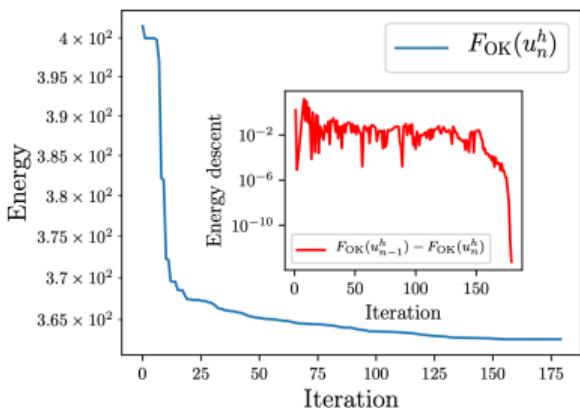
Main idea: the dominant cost in terms of degrees of freedoms N are similar

	Linear system solves per time step or iteration	Operation counts
Gradient flow approach	Solving a nonlinear algebraic system with $2N \times 2N$ Jacobian via an iterative method	$\mathcal{O}(N^{3/2}) \times \text{number of iterative solves}$
Proposed Newton scheme	Solving $2N \times 2N$ Newton step problems with backtracking on the double well	$\mathcal{O}(N^{3/2}) \times \text{number of double well backtracking steps}$
	Solving a $(N + 1) \times (N + 1)$ linear system for δw_n	$\mathcal{O}(N \log N)$ with pre-factorization
	Solving an $N \times N$ linear system for μ_n	$\mathcal{O}(N \log N)$ with pre-factorization

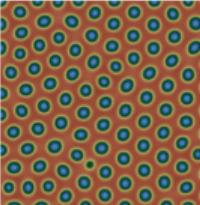
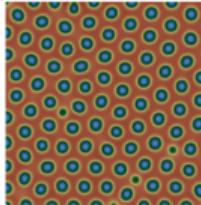
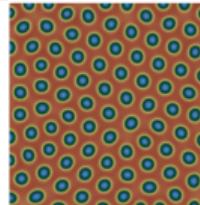
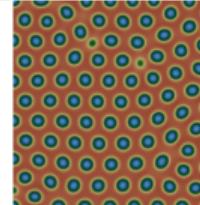
Numerical examples: Evolution



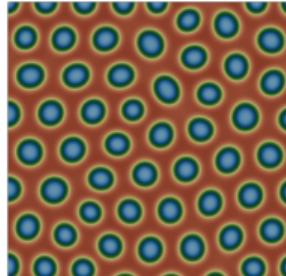
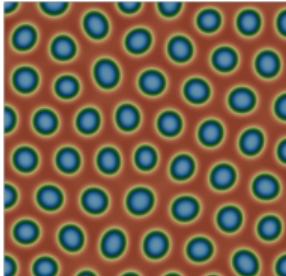
Numerical results: Evolution, cont.



Numerical results: Mesh independent convergence

Discretization (cells)	200×200	400×400	600×600	800×800
Number of iterations	118	103	102	111
Model solutions				

Numerical results: Comparison with gradient flow

	Gradient flow approach	Proposed Newton scheme
$(m, \kappa, \epsilon, \sigma) = (0, 1, 0.01, 500)$		
Number of time steps or iterations	6.54×10^5	160
$(m, \kappa, \epsilon, \sigma) = (0.3, 1, 0.01, 500)$		
Number of time steps or iterations	1.36×10^5	141

Conclusion

We are interested in...

- using phase field models in inverse and design problems for Di-BCP self-assembly

The challenges to address...

- develop fast and robust model solvers
- conventional \mathring{H}^{-1} gradient flow is robust but slow

Our proposed method...

- a modified \mathring{H}^{-1} Newton method
- retains the robustness of gradient flow via adaptive convexification and inexact line search
- exhibits quadratic and mesh-independent convergence
- shows typically three orders of magnitude speed up

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Link to the published and pre-print paper
with open-sourced code:

