Bayesian Calibration of Models for Diblock Copolymers Self-Assembly with the Power Spectrum of Microscopy Image Data

Lianghao Cao, Keyi Wu, Peng Chen, J. Tinsley Oden, and Omar Ghattas

The University of Texas at Austin
Oden Institute for Computational Engineering and Sciences

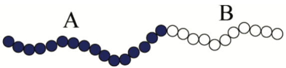
AEOLUS
Advances in Experimental Design, Optimization and Learning for Uncertain Complex Systems

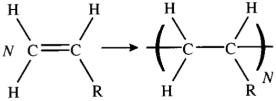
Session: Physics-Based Data-Driven Modeling and Uncertainty Quantification in Computational Materials Science and Engineering

EMI conference, 06/02/2022

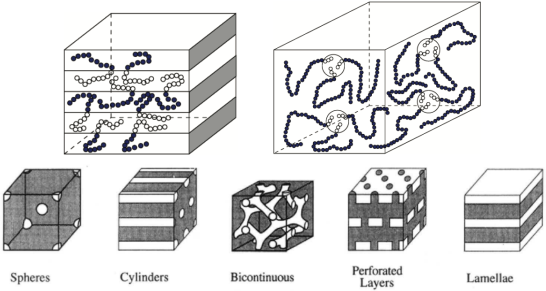
Diblock copolymer self-assembly

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

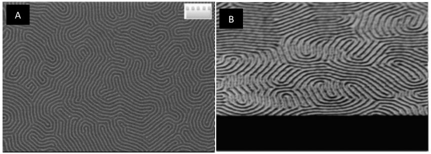




- **Self-assembly**: Below the glass-transition temperature, the two blocks spontaneously segregate and form ordered nanostructures



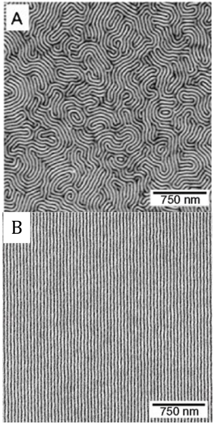
Di-BCP thin film



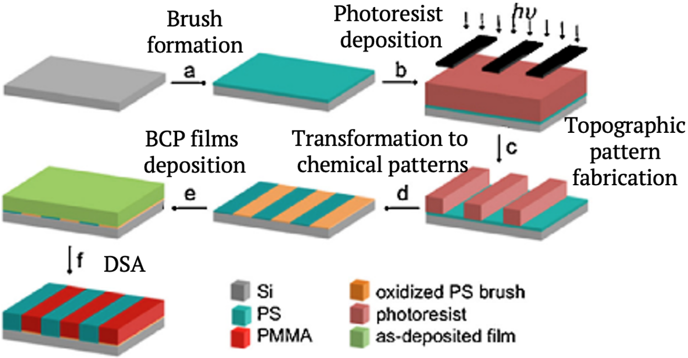
Gu et. al, *Adv. Mater.*, 2012.

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.*

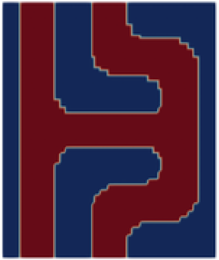
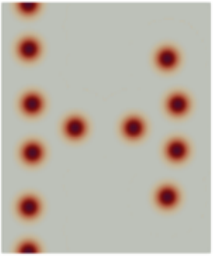
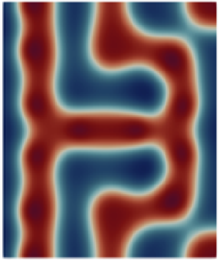


Kim et. al, *Nature*, 2003.



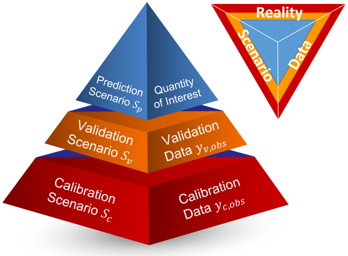
Ji et. al, *Progr. in Poly. Sci.*, 2016.

Cost effective patterning for nanolithography

Target pattern	*Guiding spots*	*Model prediction*
		

Luo et. al, in preparation.

Predictive modeling in the Bayesian framework



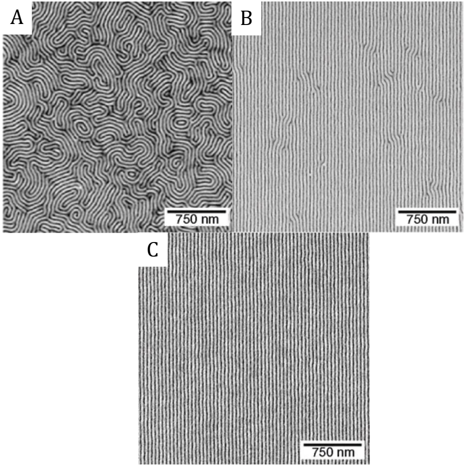
"The Prediction Triangular Pyramid"
Oden et. al, *Ency. of Comput. Mech.*, 2017.

Bayes rule

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

- $\boldsymbol{d} \in [0,1]^{M_1 \times M_2}$: image data via microscopy or X-ray scattering characterization

Aleatoric uncertainties in Di-BCP self-assembly



Kim et. al, *Nature*, 2003.

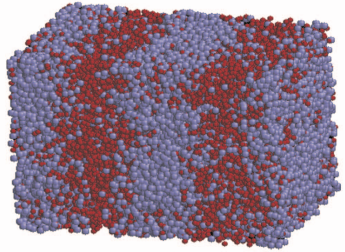
Equilibrium models of self-assembly

The forward operator $\mathcal{F}$

$$U = \mathcal{F}(\boldsymbol{x}, Z) \qquad \textbf{“Random Di-BCP structure generator”}$$

- U: random material state in a physical domain Ω
- $\boldsymbol{x}$: model parameters (material, thermal, geometrical, etc.)
- Z: auxiliary random variable

$$U \sim \nu_U \qquad \text{(canonical distribution)}$$



Pike et. al, *J. Chem. Phy.*, 2019.

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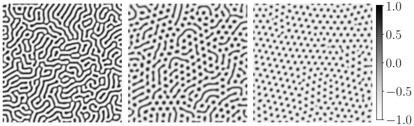
Phase field models:

- $U := U_A - U_B \in \mathcal{V}^u(\Omega; [-1, 1])$, an order parameter

$$U = \underset{u \in \mathcal{V}^u(\Omega)}{\arg\min}\ \mathcal{E}(u; \boldsymbol{x}), \text{ starting from } Z \sim \nu_{Z|\boldsymbol{x}}$$

- $\mathcal{E}$: variational free energy
- Z: random initial guess (e.g., Gauss. rand. fields)



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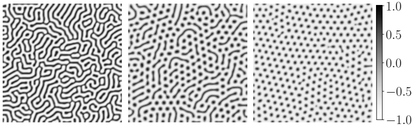
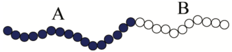


The Ohta–Kawasaki (OK) model

$$\mathcal{E}(u; \boldsymbol{x}) = \int_\Omega \Big\{ \left(1 - u(\boldsymbol{s})^2\right)^2/4) + \frac{\epsilon^2}{2}|\nabla u(\boldsymbol{s})|^2 + \frac{\sigma}{2}(u(\boldsymbol{s}) - m)(-\Delta^{-1})(u(\boldsymbol{s}) - m) \Big\}\, d\boldsymbol{s}$$



- $\boldsymbol{x} = (\epsilon, \sigma, m)$
- $\mathcal{V}^u(\Omega) := \{u \in H^1 : \int_\Omega (u(\boldsymbol{s}) - m)\, d\boldsymbol{s} = 0\}$
- “A globally convergent modified Newton method...” in SISC

Overview: Bayesian model calibration for unguided self-assembly

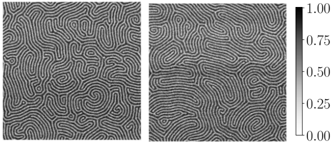
Bayes rule

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

Microscope images

$$\boldsymbol{D} \in [0,1]^{M_1 \times M_2}$$

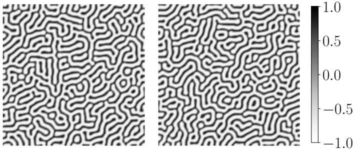
- Noisy images of random patterns



Generative forward model

$$U \stackrel{d}{=} \mathcal{F}(\boldsymbol{x}, Z) \in \mathcal{V}^u([0, L_1] \times [0, L_2])$$

- Random pattern generation



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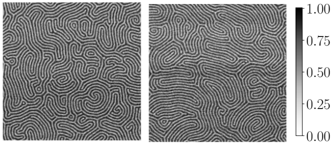

Characterization model

$$\boldsymbol{D} = \textbf{Microscopy}(U;\boldsymbol{w})$$

- $\boldsymbol{w}$: characterization model parameters

Generative forward model

$$U \stackrel{d}{=} \mathcal{F}(\boldsymbol{x}, Z) \in \mathcal{V}^u([0,L_1]\times[0,L_2])$$

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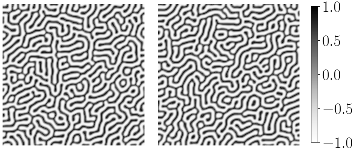
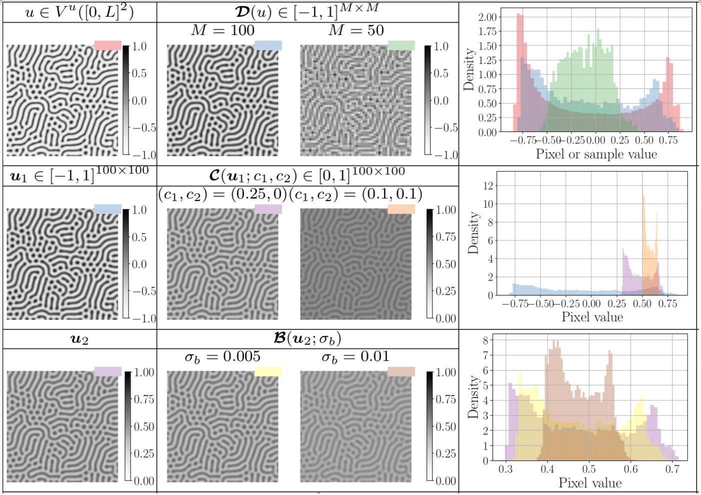


1 Define a microscopy characterization model

A model of microscopy characterization

$$\boldsymbol{D} = \boldsymbol{\mathcal{J}}(U) + \underbrace{\boldsymbol{N}(\sigma_n)}_{\text{Gaussian white noise}}, \quad \boldsymbol{\mathcal{J}} = \underbrace{\boldsymbol{\mathcal{B}}(\sigma_b)}_{\text{Gaussian blur}} \circ \underbrace{\boldsymbol{\mathcal{C}}(c_1, c_2)}_{\text{contrast and brightness}} \circ \underbrace{\boldsymbol{\mathcal{D}}}_{\text{Pixelization}}$$



Overview: Bayesian model calibration for unguided self-assembly

Bayes rule with integrated likelihood

$$\pi_{\boldsymbol{X}|\boldsymbol{d}}(\boldsymbol{x}) = \frac{\mathbb{E}_{\boldsymbol{W},Z|\boldsymbol{x}}[\mathcal{L}(\boldsymbol{x},\boldsymbol{W},Z;\boldsymbol{d})]\pi_{\boldsymbol{X}|\langle\boldsymbol{d}\rangle}(\boldsymbol{x})}{C_{\boldsymbol{d}}} \text{ a.s.}$$

Microscope images

$$\boldsymbol{D} \in [0,1]^{M_1 \times M_2}$$

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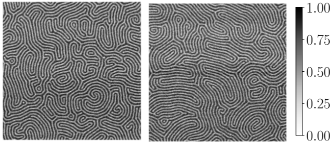


Characterization model

$$\boldsymbol{D} = \boldsymbol{\mathcal{J}}(U;\boldsymbol{w}) + \boldsymbol{N}$$

- $\boldsymbol{\mathcal{J}}(U;\boldsymbol{w})$: parameterized imaging model
- $\boldsymbol{N}$: Gaussian white noise

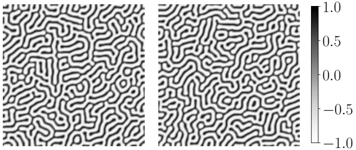
$\downarrow$

$\mathcal{L}(\boldsymbol{x},\boldsymbol{w},z;\boldsymbol{d})$by weighted l^2

Generative forward model

$$U \overset{d}{=} \mathcal{F}(\boldsymbol{x},Z) \in \mathcal{V}^u([0,L_1]\times[0,L_2])$$

- Random pattern generation



1. Define the state-to-observable map $\boldsymbol{\mathcal{J}}(U;\boldsymbol{w})$
2. Accounting for nuisance parameters by integrated likelihoods

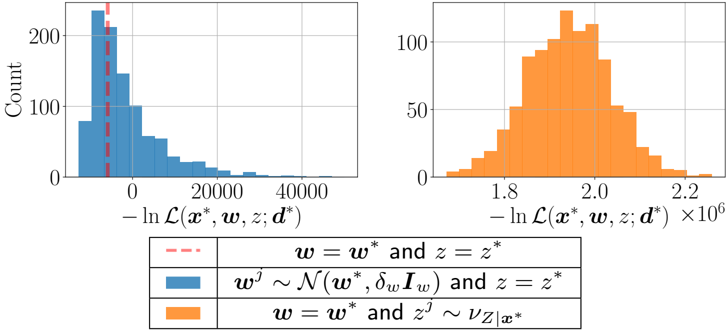
Pseudo-Marginal Metropolis–Hastings Method

Unbiased integrated likelihood estimator

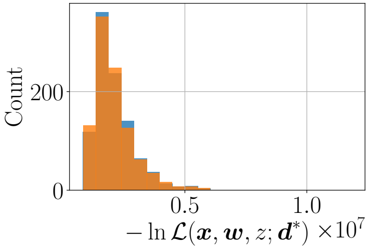
$$\widehat{\mathcal{L}}(\boldsymbol{x}, \widehat{\boldsymbol{W}}, \widehat{\boldsymbol{Z}}; \boldsymbol{d}) = \sum_{j=1}^{n_{\boldsymbol{w}}} \sum_{k=1}^{n_z} \frac{1}{n_{\boldsymbol{w}} n_z} \mathcal{L}(\boldsymbol{x}, \widehat{\boldsymbol{W}}_j, \widehat{\boldsymbol{Z}}_k; \boldsymbol{\mathcal{P}}_r(\boldsymbol{d}))\,, \quad \widehat{\boldsymbol{W}} \sim \otimes_{j=1}^{n_{\boldsymbol{w}}} \nu_{\boldsymbol{W}}\,, \quad \widehat{\boldsymbol{Z}} \sim \otimes_{k=1}^{n_z} \nu_Z$$

- Mixing time and sample efficiency depends on variance of the estimator

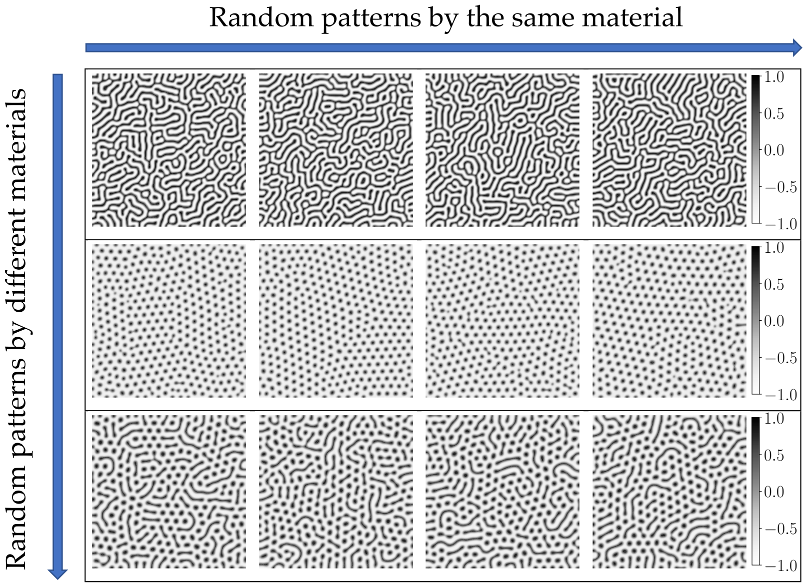
Ineffective sampling-based estimation: Hypersensitivity to Z



Ineffective parameter inference: Insensitivity to X



(blue)	$\boldsymbol{x} = \boldsymbol{x}^*, \boldsymbol{w}^j \sim \mathcal{N}(\boldsymbol{w}^*, \delta_w \boldsymbol{I}_w)$ and $z^j \sim \nu_{Z\vert\boldsymbol{x}^*}$
(orange)	$\boldsymbol{x}^j \sim \mathcal{N}(\boldsymbol{x}^*, \delta_x \boldsymbol{I}_x)$, $\boldsymbol{w}^j \sim \mathcal{N}(\boldsymbol{w}^*, \delta_w \boldsymbol{I}_w)$ and $z^j \sim \nu_{Z\vert\boldsymbol{x}^j}$


Random patterns by the same material
Random patterns by different materials
1.0
0.5
0.0
−0.5
−1.0

Overview: Bayesian model calibration for unguided self-assembly

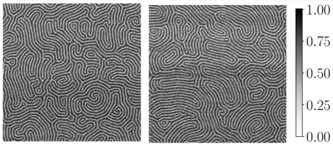
Bayes rule with integrated likelihood

$$\pi_{\boldsymbol{X}|\boldsymbol{d}}(\boldsymbol{x}) = \frac{\mathbb{E}_{Z|\boldsymbol{x}}\left[\mathcal{L}(\boldsymbol{x}, \boldsymbol{W}, Z; \overline{\boldsymbol{\mathcal{P}}_r}(\boldsymbol{d}))\right] \pi_{\boldsymbol{X}|\langle \boldsymbol{d}\rangle}(\boldsymbol{x})}{C_{\boldsymbol{d}}} \text{ a.s.}$$

Microscope images

$$\boldsymbol{D} \in [0,1]^{M_1 \times M_2}$$

- Noisy images of random patterns



Characterization model

$$\boldsymbol{D} = \boldsymbol{\mathcal{J}}(U; \boldsymbol{w}) + \boldsymbol{N}$$

- $\boldsymbol{\mathcal{J}}(U; \boldsymbol{w})$: parameterized imaging model
- $\boldsymbol{N}$: Gaussian i.i.d. noise.

$\downarrow$

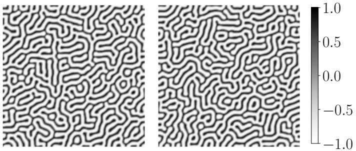
Learn parameters from
length scale and phase information

$\longleftrightarrow$

Generative forward model

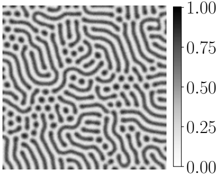
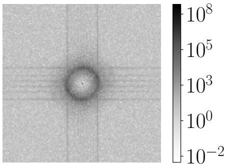
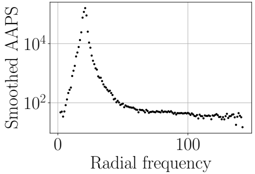
$$U \overset{d}{=} \mathcal{F}(\boldsymbol{x}, Z) \in \mathcal{V}^u([0, L_1] \times [0, L_2])$$

- Random pattern generation



1. Define the state-to-observable map $\boldsymbol{\mathcal{J}}(U; \boldsymbol{w})$
2. Account for nuisance parameters by integrated likelihoods
3. Extract the *azimuthally-averaged power spectrum* (AAPS) $\overline{\boldsymbol{\mathcal{P}}_r}(\boldsymbol{d})$ for inference
4. Extract *the mean pixel value* $\langle \boldsymbol{d}\rangle$ for the prior

Azimuthally-averaged power spectrum (AAPS) of image data

$\boldsymbol{d}^* \in [0,1]^{200\times 200}$	$\boldsymbol{\mathcal{P}}(\boldsymbol{d}^*)$	$\overline{\boldsymbol{\mathcal{P}}_r}(\boldsymbol{d}^*)$
		

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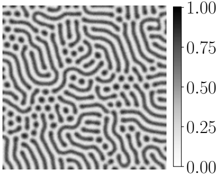	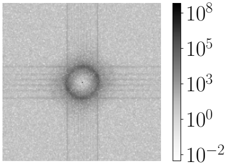	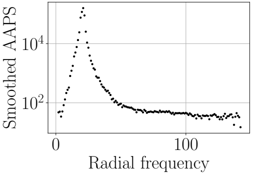

1. Discrete Fourier transform, zero-centering, and compute entrywise complex modulus

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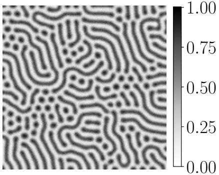
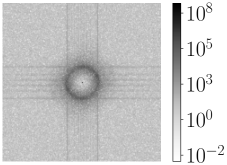
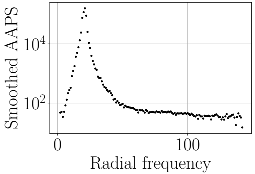
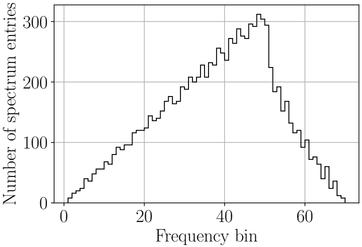
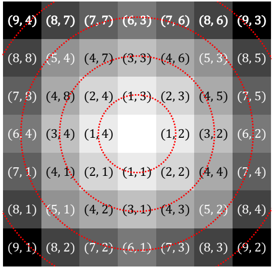
		

1. Discrete Fourier transform, zero-centering, and compute entrywise complex modulus
2. Averaging $(\overline{\boldsymbol{N}_\theta})_j$ PS entries in the j-th unit bin of radial frequencies





Radial coordinate (r_j, θ_{jk}) indexing of a 7×7 image

The probability distribution of AAPS

$$\boldsymbol{D} = \boldsymbol{\mathcal{J}}(u) + \boldsymbol{N}\,, \quad \boldsymbol{D}_{jk} \sim \mathcal{N}\left(\left(\boldsymbol{\mathcal{J}}\,(u) \right)_{jk}, \sigma_n^2 \right)$$

$$\overline{\boldsymbol{\mathcal{P}}_r}(\boldsymbol{D}) \sim \quad ?$$

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- Discrete Fourier transform $\boldsymbol{\mathcal{T}}_s(\boldsymbol{D})$

$$\left(\boldsymbol{\mathcal{T}}_s(\boldsymbol{D})\right)_{jk} \sim \mathcal{CN}\left(\left(\left(\boldsymbol{\mathcal{T}}_s \circ \boldsymbol{\mathcal{J}}\right)(u)\right)_{jk}, M_1 M_2 \sigma_n^2\right)$$

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- Sum of $2(\overline{\boldsymbol{N}_\theta})_j$ normal RV squared $\implies$ noncentral chi square RV $\chi_k^2(\lambda)$

$$\frac{2(\overline{\boldsymbol{N}_\theta})_j}{M_1 M_2 \sigma_n^2} \left(\overline{\boldsymbol{\mathcal{P}}_r}\,(\boldsymbol{d}) \right)_j \sim \chi^2_{2(\overline{\boldsymbol{N}_\theta})_j} \left(\frac{2(\overline{\boldsymbol{N}_\theta})_j}{M_1 M_2 \sigma_n^2} \left(\left(\overline{\boldsymbol{\mathcal{P}}_r} \circ \boldsymbol{\mathcal{J}} \right)(u) \right)_j \right)$$

The probability distribution of AAPS

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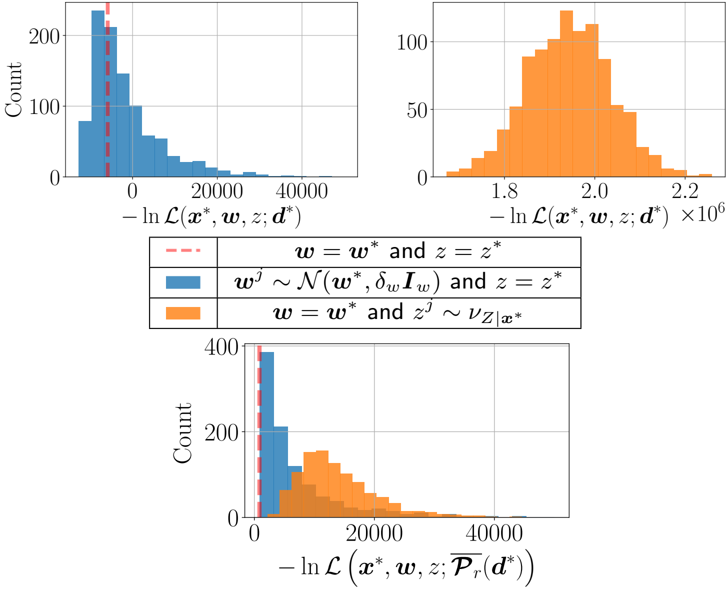
- Sum of $2(\overline{\boldsymbol{N}_\theta})_j$ normal RV squared $\implies$ noncentral chi square RV $\chi_k^2(\lambda)$

$$\frac{2(\overline{\boldsymbol{N}_\theta})_j}{M_1 M_2 \sigma_n^2}\left(\overline{\boldsymbol{\mathcal{P}}_r}\,(\boldsymbol{d})\right)_j \sim \chi^2_{2(\overline{\boldsymbol{N}_\theta})_j}\left(\frac{2(\overline{\boldsymbol{N}_\theta})_j}{M_1 M_2 \sigma_n^2}\left(\left(\overline{\boldsymbol{\mathcal{P}}_r} \circ \boldsymbol{\mathcal{J}}\right)(u)\right)_j\right)$$

- Normal approximation: $k, \lambda \to \infty$ in $\chi_k^2(\lambda)$

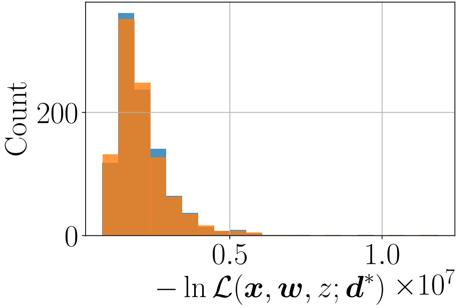
$$\left(\overline{\boldsymbol{\mathcal{P}}_r}\,(\boldsymbol{d})\right)_j \dot{\sim}\, \mathcal{N}\left(M_1 M_2 \sigma_n^2 + \left(\left(\overline{\boldsymbol{\mathcal{P}}_r} \circ \boldsymbol{\mathcal{J}}\right)(u)\right)_j, \frac{M_1 M_2 \sigma_n^2}{2(\overline{\boldsymbol{N}_\theta})_j}\left(2 M_1 M_2 \sigma_n^2 + \left(\left(\overline{\boldsymbol{\mathcal{P}}_r} \circ \boldsymbol{\mathcal{J}}\right)(u)\right)_j\right)\right)$$

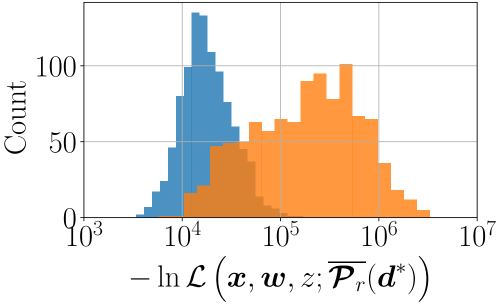
AAPS: Likelihood insensitivity to Z



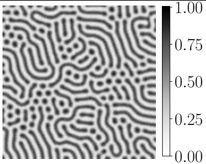
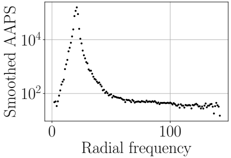
AAPS: Likelihood sensitivity to X

	$\boldsymbol{x} = \boldsymbol{x}^*, \boldsymbol{w}^j \sim \mathcal{N}(\boldsymbol{w}^*, \delta_w \boldsymbol{I}_w)$ and $z^j \sim \nu_{Z\vert\boldsymbol{x}^*}$
	$\boldsymbol{x}^j \sim \mathcal{N}(\boldsymbol{x}^*, \delta_x \boldsymbol{I}_x)$, $\boldsymbol{w}^j \sim \mathcal{N}(\boldsymbol{w}^*, \delta_w \boldsymbol{I}_w)$ and $z^j \sim \nu_{Z\vert\boldsymbol{x}^j}$





Accounting for the lost information: Marginal priors

$\boldsymbol{d}^* \in [0,1]^{200\times 200}$	$\overline{\boldsymbol{\mathcal{P}}_r}(\boldsymbol{d}^*)$
	

$$\overline{\boldsymbol{\mathcal{P}}_r}(\boldsymbol{d}) \equiv \overline{\boldsymbol{\mathcal{P}}_r}(\boldsymbol{d} + \text{constant})$$

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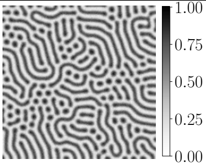	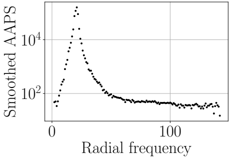

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$$\langle \boldsymbol{D} \rangle = \langle \boldsymbol{\mathcal{J}}(u) \rangle + \langle \boldsymbol{N} \rangle \sim \mathcal{N}\left(\langle \boldsymbol{\mathcal{J}}(u) \rangle, \frac{\sigma_n^2}{M_1 M_2}\right)$$

Mean pixel value of image data

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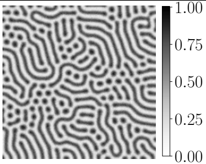	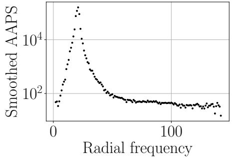

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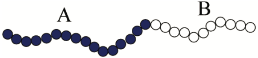
Mean pixel value of image data

$$\langle \boldsymbol{D} \rangle \sim \mathcal{N}\left(\underbrace{\mathcal{C}\left(\int_\Omega u(\boldsymbol{s})\, d\boldsymbol{s}; c_1, c_2 \right)}_{\text{contrast and brightness}}, \frac{\sigma_n^2}{M_1 M_2} \right)$$

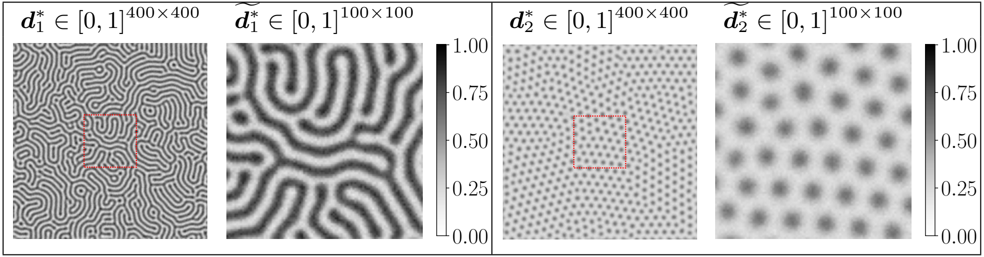
Commutative property

Imcompressibility of Di-BCP films

$$\mathcal{V}^u(\Omega) := \left\{ u \in H^1 : \int_\Omega (u(\boldsymbol{s}) - m)\, d\boldsymbol{s} \right\} \qquad \text{(The OK model)}$$

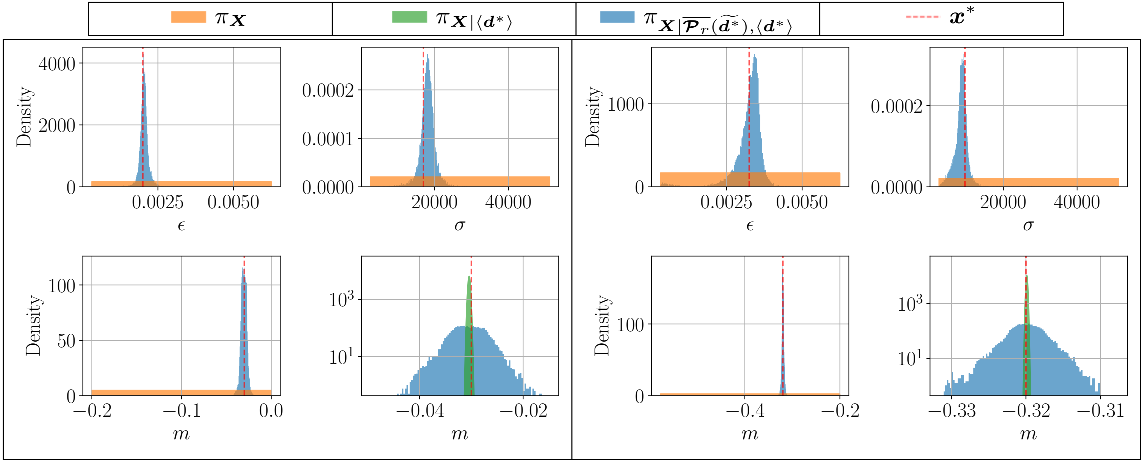


Numerical experiments: Set up



- $\boldsymbol{W} \sim \delta_{\boldsymbol{w}_i^*}$: known characterization model parameters
- $n_z = 5$ for integrated likelihood estimator

Numerical experiments: Marginal posteriors



Ongoing work: Surrogate modeling (with Keyi W. and Peng C.)

Challenge: solving the forward problem *hundreds of thousands times* for parameter inference

Surroagte parameter-to-observable (PtO) maps

$\overline{\boldsymbol{\mathcal{O}}_r}(\boldsymbol{x}, \boldsymbol{w}, Z) := \overline{\boldsymbol{\mathcal{P}}_r} \circ \boldsymbol{\mathcal{J}}(\boldsymbol{w}) \circ \mathcal{F}(\boldsymbol{x}, Z)$ (AAPS of simulated noise-free images)

$\overline{\boldsymbol{\mathcal{O}}_r}(\boldsymbol{x}, \boldsymbol{w}, Z) \dot{\sim} \text{Lognormal}\left(\boldsymbol{\mathcal{S}}_m(\boldsymbol{x}, \boldsymbol{w}), \boldsymbol{\mathcal{S}}_\sigma^2(\boldsymbol{x}, \boldsymbol{w}) \boldsymbol{I}_{\lceil \boldsymbol{r}_{N_r} \rceil}\right)$ (Independent log-normal spectrum response to Z)

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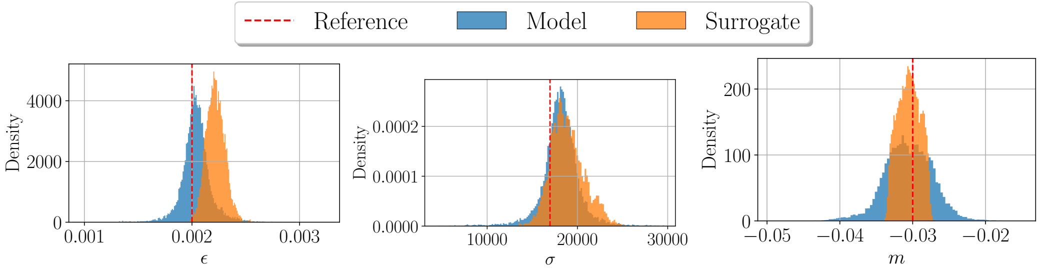
Preliminary results

- Use two (mean and std) four-layers neural networks (3 dim to 50 dim):



Conclusion

We discussed...

- Bayesian model calibration for diblock copoymer thin film self-assembly with microscopy image data

We introduced...

- a generic model for microscopy characterization
- integrated likelihoods that account for aleatoric uncertainties
- the AAPS of noisy image data and its probability distribution

We showed that...

- the AAPS of image data is suitable for model calibration in the presence of aleatoric uncertainties
- mean pixel values of image data can be used to build informative marginal priors

Ongoing works

- Building surrogates of PtO map to accelerate model calibration
- Bayesian model calibration for DSA
- Bayesian model validation and selection

Contact

Lianghao Cao (lianghao@oden.utexas.edu)