Lianghao Cao

Ph.D. candidate

Oden Institute for Computational Engineering & Sciences

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Education

2017–2022 (exp.) Ph.D. in Comput. Sci. Eng. & Math. The University of Texas at Austin

Supervisor: Dr. J. Tinsley Oden Co-supervisor: Dr. Omar Ghattas

2013–2017 B.S. in Engineering Mechanics University of Illinois at Urbana-Champaign

Minor in Comput. Sci. & Eng.

Research Interests

Topics:

Uncertainty quantification, predictive modeling, PDE-constrained optimization, phase-field modeling.

Recent work:

- 1. Uncertainty quantification for model-based predictions of material self-assembly.
- 2. Fast minimization solvers for phase-field models for material self-assembly.
- 3. Neural network surrogates and error estimation for infinite-dimensional inverse problems.

Publications

Peer-reviewed

- Lianghao Cao, Omar Ghattas, and J. Tinsley Oden. "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". In: SIAM Journal on Scientific Computing 44.1 (2022), B51– B79. DOI: 10.1137/20M1378119.
- 2. Prashant K. Jha, **Lianghao Cao**, and J. Tinsley Oden. "Bayesian-based predictions of COVID-19 evolution in Texas using multispecies mixture-theoretic continuum models". In: *Computational Mechanics* 66.5 (2020), pp. 1055–1068. ISSN: 14320924. DOI: 10.1007/s00466-020-01889-z.

In pre-print (submitted for peer-review)

- Ricardo Baptista*, Lianghao Cao*, Joshua Chen*, Omar Ghattas, Fengyi Li*, Youssef M. Marzouk, and J. Tinsley Oden. Bayesian model calibration for block copolymer self-assembly: Likelihood-free inference and expected information gain computation via measure transport. *Equal contribution. 2022. DOI: 10.48550/ARXIV.2206.11343.
- 2. Dingcheng Luo, **Lianghao Cao**, Peng Chen, Omar Ghattas, and J. Tinsley Oden. *Optimal design of chemoepitaxial guideposts for the directed self-assembly of block copolymer systems*. 2022.

In preparation for submission (share upon request)

- 1. Lianghao Cao, Daniil Bochkov, Omar Ghattas, Robert D. Moser, and J. Tinsley Oden. "Polymer self-consistent field theory calculations: Analysis and a real-space semi-implicit Seidel scheme".
- Lianghao Cao, Keyi Wu, Peng Chen, J. Tinsley Oden, and Omar Ghattas. "Fast Bayesian model calibration for diblock copolymer self-assembly using the power spectrum of microscopy image data".
 Full results presented at EMI Conference 2022.
- 3. Pratyush Kumar Singh, **Lianghao Cao**, Jingye Tan, and Danial Faghihi. "A Nonlocal Theory of Heat Transfer and Micro-Phase Separation of Nanostructured Copolymers".

Presentations

- 1. <u>Conference talk</u>: "Bayesian Calibration of Models for the Self-Assembly of Diblock Copolymers: Likelihood-Free Inference and Expected Information Gain Computation via Measure Transport", 16th U.S. National Congress on Computational Mechanics, virtual, 07/26/2021.
- 2. <u>Conference talk</u>: "Bayesian Calibration of Models for Diblock Copolymers Self-Assembly with Power Spectrum of Microscopy Image Data", *The Engineering Mechanics Institute Conference 2022*, Baltimore, MD, USA, 06/02/2022.
- 3. <u>Conference talk</u>: "A Globally Convergent Modified Newton Method for the Direct Minimization of the Ohta–Kawasaki Energy", 19th U.S. National Congress on Theoretical and Applied Mechanics, Austin, TX, USA, 06/24/2022.

Professional Activities

Teaching/Mentoring

Aug. 2018–Dec. 2018	Teaching assistant	M 408 K: Calculus I	UT Austin
Aug. 2016–Dec. 2016	Course assistant	ME 370: Mechanical Design I	UIUC
Mar. 2015–Jun. 2017	NetMath mentor	MATH 415: Applied Linear Algebra	UIUC

Peer review

Computer Methods in Applied Mechanics and Engineering (12 reviews)

Membership

American Institute for Chemical Engineers (AIChE)

Society for Industrial and Applied Mathematics (SIAM)

U.S. Association for Computational Mechanics (USACM)

Awards and Honors

2021	USNCCM16 Conference Award	U.S. Association for Computational Mechanics
2017	O'Donnell Fellowship (1 year)	Institute for Comput. Eng. & Sci., UT Austin
2017	James Scholar Honors	The College of Engineering, UIUC
2016	NetMath Award for Best Student Retention	NetMath Program, UIUC

Open-Sourced Softwares

- 1. **BayesForSEIRD** (Python): Bayesian calibration and validation of PDE-based SEIRD epidemic models. (with P. K. Jha)
- 2. *OKNewton* (Python): A fast and robust direct minimization solver of the Ohta–Kawasaki model for the microphase separation of diblock copolymers.
- 3. **DRAM** (Python): A delayed-rejection adaptive Metropolis algorithm compatible with hIPPYlib for PDE-based finite-dimensional Bayesian inverse problem.

References

1. Dr. J. Tinsley Oden

Professor, Department of Aerospace Engineering & Engineering Mechanics, Department of Computer Science, Department of Mathematics, Oden Institute for Computational Engineering & Sciences, The University of Texas at Austin.

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2. Dr. Omar Ghattas

Professor, Walker Department of Mechanical Engineering, Oden Institute for Computational Engineering & Sciences, The University of Texas at Austin.

Email: omar@oden.utexas.edu

3. Dr. Youssef M. Marzouk

Professor, Department of Aeronautics & Astronautics, Massachusetts Institute of Technology.

Email: ymarz@mit.edu

4. Dr. Danial Faghihi

Assistant professor, Department of Mechanical and Aerospace Engineering, University at Buffalo.

Email: danialfa@buffalo.edu