Thomas O'Leary-Roseberry

CONTACT INFORMATION

The University of Texas at Austin
Oden Institute for Computational Engineering and Sciences
201 E. 24th Street, Stop C0200
Austin, TX, 78712-0027

https://tomoleary.github.io

✉ tom.olearyroseberry@utexas.edu

EDUCATION

The University of Texas at Austin — Austin, TX
PhD in Computational Science, Engineering, and Mathematics — **August 2020**
MSc in Computational Science, Engineering, and Mathematics — **December 2017**

University of Wisconsin – Madison — Madison, WI.
BA in Mathematics — **May 2015**
BSE in Engineering Mechanics — **May 2015**

POSITIONS

The University of Texas at Austin — Austin, TX
Research Associate — **September 2021 – present**
Postdoctoral Research Fellow — **September 2020 – August 2021**
Graduate Research Assistant — **August 2016 – August 2020**

PUBLICATIONS AND MANUSCRIPTS

Preprints

1. T. O'Leary-Roseberry and R. Bollapragada, Fast Finite-Sum Optimization via Cyclically-Sampled Hessian Averaging Methods, (see technical report arXiv:2408.07268), (2024) in review at *Mathematical Programming*.
2. J. Kirchhoff, D. Luo, T. O'Leary-Roseberry and O. Ghattas, Inference of Heterogeneous Material Properties via Infinite-Dimensional Integrated DIC arXiv preprint arXiv:2408.10217 (2024) [`math.NA`] (to be submitted)
3. L. Cao, T. O'Leary-Roseberry and O. Ghattas, Derivative-informed neural operator acceleration of geometric MCMC for infinite-dimensional Bayesian inverse problems, arXiv preprint arXiv:2403.08220, (2024) [`math.NA`] (in review at *Journal of Machine Learning Research*)
4. D. Luo, T. O'Leary-Roseberry, P. Chen and O. Ghattas, Efficient PDE-constrained optimization under high-dimensional uncertainty using derivative-informed neural operators, arXiv preprint arXiv:2305.20053, (2023) [`math.OC`] (first round of revisions at *SIAM Journal on Scientific Computing*)

Journal Papers

5. B. Keith, T. O'Leary-Roseberry, B. Sanderse, R. Scheichl, B. van Bloemen Waanders, Scientific Machine Learning: A Symbiosis. To appear in American Institute for Mathematical Sciences *Foundations of Data Science*, (2025).
6. D. Luo, P. Chen, T. O'Leary-Roseberry, U. Villa and O. Ghattas. SOUPy: Stochastic PDE-constrained optimization under high-dimensional uncertainty in Python. *Journal of Open Source Software* (2024).
7. T. O'Leary-Roseberry, P. Chen, U. Villa, and O. Ghattas, Derivative-Informed Neural Operator: An Efficient Framework for High-Dimensional Parametric Derivative Learning. *Journal of Computational Physics* (2024).
8. L. Cao, T. O'Leary-Roseberry, P. Jha, J. T. Oden, and O. Ghattas, Residual-based error correction for neural operator accelerated infinite-dimensional Bayesian inverse problems. *Journal of Computational Physics* (2023).
9. K. Wu, T. O'Leary-Roseberry, P. Chen, and O. Ghattas, Large-scale Bayesian optimal experimental design with derivative-informed projected neural network. *Journal of Scientific Computing* (2023).

10. T. O'Leary-Roseberry, X. Du, A. Chaudhuri, J. R. Martins, K. Willcox, and O. Ghattas, Learning high-dimensional parametric maps via reduced basis adaptive residual networks, *Computer Methods in Applied Mechanics and Engineering*, 402 (2022), p. 115730.
11. T. O'Leary-Roseberry, U. Villa, P. Chen, and O. Ghattas, Derivative-Informed Projected Neural Networks for High-Dimensional Parametric Maps Governed by PDEs, *Computer Methods in Applied Mechanics and Engineering*, 388 (2022), p. 114199.

Conference Papers

12. V. Sella, A. Chaudhuri, T. O'Leary-Roseberry, X. Du, M. Guo, J. R. R. A. Martins, O. Ghattas & K.E. Willcox. Improving neural network efficiency with multifidelity and dimension reduction techniques. In *AIAA SciTech 2025 Forum*.
13. X. Du, J. R. R. A. Martins, T. O'Leary-Roseberry, A. Chaudhuri and O. Ghattas, & K.E. Willcox. Learning Optimal Aerodynamic Designs through Multi-Fidelity Reduced-Dimensional Neural Networks. In *AIAA SciTech 2023 Forum* (p. 0334).
14. P. Chen, K. Wu, J. Chen, T. O'Leary-Roseberry, and O. Ghattas, Projected Stein Variational Newton: A Fast and Scalable Bayesian Inference Method in High Dimensions. *Advances in Neural Information Processing Systems* 32 (2019).

Technical Reports, Theses and Miscellaneous

15. T. O'Leary-Roseberry and R. Bollapragada, Fast Unconstrained Optimization via Hessian Averaging and Adaptive Gradient Sampling Methods, arXiv preprint arXiv:2408.07268, (2024) [`math.OC`] (comprises two different works)
16. U. Villa and T. O'Leary-Roseberry, A note on the relationship between PDE-based precision operators and Matérn covariances, arXiv preprint arXiv:2407.00471 [`math.NA`] (2024)
17. T. O'Leary-Roseberry, Efficient and dimension independent methods for neural network surrogate construction and training, PhD dissertation, *The University of Texas at Austin* (2020).
18. A. Ames, D. Belongia, K. Callan, J. O'Donnell and T. O'Leary-Roseberry, Epimetheus EGA: Design and Analysis of Novel Electric General Aviation Plane, 2015

Funding

Principal Investigator and Co-Principal Investigator

1. O. Ghattas (PI), T. Becker (Co-PI) and T. O'Leary-Roseberry (Co-PI), NSF-CAIG: A Bayesian Inference Framework for Learning Earthquake Cycle Deformation Processes Across Scales via Novel Neural Operators (RISE 2425922), 09/24-08/27 **$832,277**
2. O. Ghattas (PI) and T. O'Leary-Roseberry (Co-PI), The Best of Both Worlds: Deep Neural Operators as Preconditioners for Physics-Based Forward and Inverse Problems, National Science Foundation, Office of Advanced Cyberinfrastructure (OAC), award 2313033, 09/23–08/26, **$600,000**.
3. V.R. Bollapragada (PI), O. Ghattas (Co-PI) and T. O'Leary-Roseberry (Co-PI), Co-Design of Neural Operators and Stochastic Optimization Algorithms for Learning Surrogates for PDE-Constrained Optimization Under Uncertainty, National Science Foundation, Division of Mathematical Sciences (DMS), award 2324643, 09/23–08/26, **$499,792**.

Co-Investigator

4. (Co-I) M2dt: Multifaceted Mathematics for Predictive Digital Twins, Department of Energy, Office of Advanced Scientific Computing Research, Mathematical Multifaceted Integrated Capability Centers (MMICCs) program, award number DE-SC0023171, 9/1/22–8/31/27. $5,997,000 for UT. ($13.5M collaboration with Argonne, Brookhaven, MIT, and Sandia)

Technologies & Patents

1. J. Kirchhoff, D. Luo, T. O'Leary-Roseberry and O. Ghattas, Infinite-dimensional integrated digital image correlation (IDIC), (patent pending).

Professional Involvement

Editorial Service

Special Issue Chief Editor

"Scientific Machine Learning", AIMS Foundations of Data Science (FODS) Journal. 2024

Paper referee

- SIAM Journal on Scientific Computing (SISC)
- Computer Methods in Applied Mechanics and Engineering (CMAME)
- Computational Intelligence
- AIAA Journal
- AIAA Journal of Aircraft
- Mathematical and Scientific Machine Learning (MSML)
- International Conference on Machine Learning (ICML)
- International Journal for Numerical Methods in Engineering (IJNME)
- AIMS Foundations of Data Science (FoDS)
- Finite Elements in Analysis and Design (FEAD)
- Transactions on Machine Learning Research (TMLR)

Conference and Workshop Organization

Lead-organizer: National University of Singapore IMS Workshop on SciML for UQ 2027

Co-organizer: Banff International Research Station Workshop on Scientific Machine Learning 2023

Co-creator: The Texas Applied Mathematics and Engineering Symposium 2017

Student Positions

Host for Oden Institute Babuška Forum. September 2018 - January 2020

Treasurer for UT Austin chapter of SIAM. September 2016-August 2019

Advising Mentorship & Dissertation Service

Supervisor and co-supervisor

1. Boyuan (John) Yao, CSEM PhD student (co-supervising with advisor Omar Ghattas). Topics in derivative-informed neural operators for optimal control of PDEs.
2. Xindi Gong, CSEM PhD student (co-supervising with advisor Omar Ghattas). Topics in derivative-informed neural operators for PDE-constrained optimization under uncertainty.

Research Mentor

3. Josephine Westermann, Heidelberg mathematics PhD student (advisor Jakob Zech). Topics in high-dimensional approximation with neural operators and sparse polynomials.
4. Ziheng (Marshall) Zhang, CSEM PhD student (advisor Omar Ghattas). Topics in derivative-informed neural operators for massive scale Bayesian inverse problems.
5. Joseph Kirchhoff, UT Austin ME PhD student (advisor Omar Ghattas). Infinite-dimensional integrated digial image correlation.
   - Inference of Heterogeneous Material Properties via Infinite-Dimensional Integrated DIC
6. Blake Christierson, CSEM PhD student (advisor Omar Ghattas). Topics in derivative-informed neural operators for Bayesian inverse problems.
7. Bassel Saleh, CSEM PhD student (advisor Omar Ghattas). Topics in machine learning for graviational wave astronomy.
8. Dingcheng Luo, CSEM PhD student (advisor Omar Ghattas). Derivative-informed neural operators for PDE-constrained optimization under uncertainty.
   - SOUPy: Stochastic PDE-constrained optimization under high-dimensional uncertainty in Python, JOSS 2024
   - Efficient PDE-Constrained optimization under high-dimensional uncertainty using derivative-informed neural operators (in review, SISC)
9. Lianghao Cao, CSEM PhD (2022, advisors J. Tinsley Oden and Omar Ghattas). Neural operator accelerated solution of Bayesian inverse problems.
   - Residual-based error correction for neural operator accelerated infinite-dimensional Bayesian inverse problems, JCP 2024
   - Derivative-informed neural operator acceleration of geometric MCMC for infinite-dimensional Bayesian inverse problems (in review, JMLR)

Reader and Dissertation Committee Service

1. Thesis reader. Gradient-based dimension reduction for Bayesian inverse problems and simulation-based inference, Michael Brennan, PhD dissertation in Computational Science and Engineering, Massachusetts Institute of Technology (2023). Advisor: Youssef Marzouk.
2. External examiner. Neural Operator-Based Optimal Control. Ivar Lønning, Masters dissertation in Computer Science, University of Oslo (2024). Advisors: Thomas Surowiec and Morten Hjorth-Jensen.

Directed Reading Program, UT Austin mathematics department

Nari Jeong: Universal approximation theory for neural networks — Fall 2017
Antonio Farah: The Babuška-Lax-Milgram theorem — Fall 2018

Selected Presentations and Invited Talks

- The Ohio State University Math Department Seminar. — Columbus, OH, USA, 2024
- Oden Institute Babuška Forum. — Austin, TX, USA, 2024
- World Congress on Computational Mechanics. — Vancouver, CA, 2024
- SciComp Seminar, Heidelberg University Mathematics Department. — Heidelberg, DE, 2024
- SIAM Conference on Uncertainty Quantification. — Trieste, IT, 2024
- International Congress on Industrial and Applied Mathematics. — Tokyo, JP, 2023
- Massachusetts Institute of Technology ACDL Seminar. — Cambridge, MA, USA, 2023
- Weierstrass Institute for Applied Analysis and Stochastics Seminar. — Berlin, DE, 2023
- SIAM Conference on Computational Science & Engineering. — Amsterdam, NL, 2023
- SIAM Conference on Mathematics of Data Science 2022. — San Diego, CA, USA, 2022
- International Conference on Continuous Optimization. — Bethlehem, PA, USA, 2022
- New York University Courant Seminar. — New York, NY, USA, 2022
- SIAM Conference on Uncertainty Quantification. — Atlanta, GA, USA, 2022
- Mechanistic ML & Digital Twins for Computational Science. — San Diego, CA, USA, 2021
- SIAM Annual Conference. — Virtual, 2021
- SIAM Conference on Optimization. — Virtual, 2021
- EUROPT Workshop on Advances in Continuous Optimization. — Virtual, 2021
- Oden Institute Babuška Forum — Austin, TX, USA, 2021
- SIAM Conference on Computational Science & Engineering, — Virtual, 2021
- California Institute of Technology CliMA Seminar. — Virtual, 2021
- Argonne National Laboratory LANS Seminar. — Virual, 2020
- SIAM Mathematics of Data Science, (cancelled, COVID-19), — Cincinnati, OH, USA, 2020
- TU Munich Numerical Mathematics Chair Seminar, (cancelled, COVID-19), — Munich, DE, 2020
- SIAM Conference on Uncertainty Quantification, (cancelled, COVID-19), — Munich, DE, 2020
- SIAM Conference on Computational Science & Engineering. — Atlanta, GA, USA, 2017

Selected Workshops and training

Argonne Training Program on Extreme-Scale Computing, — Summer 2017
NSF REU in Mathematics, University of Wisconsin–Madison, — Summer 2014

Fellowships

CSEM Fellowship, The University of Texas at Austin, Austin, TX — August 2015 – July 2019

Selected Scientific Software

Creator

1. `hessianaveraging`: Hessian-averaged Newton methods for stochastic optimization in jax.
2. `dino`: Derivative-informed neural operator training in TensorFlow.
3. `hippyflow`: Dimension reduced surrogate construction for parametric PDE maps in Python.
4. `hessianlearn`: Hessian-based stochastic optimization in TensorFlow and keras.

Co-creator

5. `soupy` Stochastic PDE-constrained Optimization under high-dimensional Uncertainty in Python.

Contributor

6. `hIPPYlib`: An Extensible Software Framework for Large-Scale Inverse Problems.