Shane A. McQuarrie: Curriculum Vitae

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Research Interests

My research centers on the synthesis of dynamical systems and data-driven learning methods. While I have broad interests in computational mathematics and the data-enabled sciences, the main objective of my research is to develop and analyze accurate and scalable predictive computational models that continuously assimilate data and issue predictions equipped with uncertainty estimates. I have particular interest in the following topics:

- Data-driven reduced-order models with uncertainty estimates for parametric systems.
- Continuous data assimilation and active learning for dynamical systems.
- Scientific machine learning for system identification and inverse problems.
- Efficient optimization and control under PDE constraints via reduced models.

Education

PhD Computational Science, Engineering, and Mathematics   2023
Dissertation: *Data-driven Parametric Reduced-order Models: Operator Inference
    for Reactive Flow Applications*
Dissertation Committee: Karen Willcox (Chair), Rachel Ward, Omar Ghattas,
    Robert Moser, Max Gunzburger
Oden Institute for Computational Engineering and Sciences,
    The University of Texas at Austin

MS Computational Science, Engineering, and Mathematics   2020
Oden Institute for Computational Engineering and Sciences,
    The University of Texas at Austin

MS Mathematics   2018
Thesis: *Data Assimilation in the Boussinesq Approximation for Mantle Convection*
Thesis Committee: Jared Whitehead (Chair), Emily Evans, Mark Allen
Department of Mathematics, Brigham Young University

BS Mathematics (Applied and Computational Mathematics Emphasis)   2016
magna cum laude
Minors in Computer Science and Music
Department of Mathematics, Brigham Young University

Experience

Postdoctoral Fellow, John von Neumann Fellowship in Computational Science   2023
Sandia National Laboratories, Albuquerque, NM
Effective 1 September 2023.

Predictive Science Academic Alliance Program III R&D Graduate Intern   2021
Sandia National Laboratories, Albuquerque, NM (virtual)
Developed a Python/MATLAB computational framework for utilizing data-driven reduced-order models in control problems with partial differential equation constraints.

Software Systems R&D Graduate Intern   2017
Sandia National Laboratories, Albuquerque, NM
Automated data mining and supervised learning algorithm selection for text classification to reduce the cost of sharing sensitive information.

Curriculum Developer / Development Manager   2014–2018
Department of Mathematics, Brigham Young University
Led team of developers to draft and revise over 30 Python programming labs for the applied and computational mathematics curriculum; designed programmatic test driver framework to automate grading; authored student / TA instructions and managed materials distribution.

Programming Languages

Strong: Python (`numpy`, `scipy`, `matplotlib`, `sklearn`, `pandas`, `sympy`, `jupyter-notebook`, `jupyter-book`, `pytest`, etc.), bash / shell, git

Proficient: MATLAB

Familiar: Julia, C++, C, Java, SQL

Awards and Honors

2023   SIAM SEAS Student Awards, First Place, *SIAM Southeastern Atlantic Section Annual Meeting*

2023   BGCE Student Paper Prize Winner, *SIAM Conference on Computational Science and Engineering*

2021   BGCE Student Paper Prize Finalist, *SIAM Conference on Computational Science and Engineering*

2018   CSEM Graduate Student Fellowship, *Oden Institute for Computational Engineering and Sciences*

2014   Language Certificate: Spanish, Advanced Level, *ACTFL*

2010   Thomas S. Monson Scholarship, *Brigham Young University*

Teaching, Mentoring, and Service

The University of Texas at Austin

Advanced Teaching Preparation Certificate   2022
Teacher training program administered by the Center for Teaching and Learning.

CSEM Student Forum Founding Organizer   2020–2023
Oden Institute seminar series staffed by and geared toward the CSEM PhD student body.

Oden Institute Table Tennis Tournament Organizer   2022–2023
First significant post-COVID social activity, designed to foster a welcoming and collaborative culture among the CSEM PhD student body.

Directed Reading Program Graduate Mentor   2018–2020
Semester-long mentorship program organized by the Department of Mathematics.
Weekly discussions and a final project and minisymposium presentation. Mentees:

- Angela Cao, *Titanic Survival Estimation via Naïve Bayes*   Spring 2020
  K-Means in Image Clustering   Fall 2020

- Ashwin Devaraj, *An Intro to Complexity Theory: P, NP, and Reductions*   Spring 2019

- Benjamin Maccini, *Matching Networks for One Shot Learning*   Spring 2019

- Connor Brubaker, *An Introduction to Machine Learning in Practice*   Fall 2018

Brigham Young University

Laboratory Instructor
Equivalent work of instructor of record: prepared quizzes and programming assignments, taught class, held office hours, graded assignments and final projects, submitted final grades.

- Math 405: Modeling with Uncertainty and Data 2 Laboratory   Winter 2018

- Math 403: Modeling with Uncertainty and Data 1 Laboratory   Fall 2017

- Math 323: Algorithm Design and Optimization 2 Laboratory   Winter 2016

- Math 321: Algorithm Design and Optimization 1 Laboratory   Fall 2015

Graduate Teaching Assistant
Graded assignments, held office hours, taught review sessions, graded final projects.

- Math 404: Modeling with Uncertainty and Data 2   Winter 2017

- Math 402: Modeling with Uncertainty and Data 1   Fall 2016

Publications

Accepted/Published Journal Articles

13. **S. A. McQuarrie**, P. Khodabakhshi, and K. E. Willcox. Non-intrusive reduced-order models for parametric partial differential equations via data-driven operator inference. Oden Institute Report 21-17, University of Texas at Austin, 2021. arXiv preprint arXiv:2110.07653; to appear in the SIAM Journal on Scientific Computing, 2023.

12. M. Guo, **S. A. McQuarrie**, and K. Willcox. Bayesian operator inference for data-driven reduced-order modeling. *Computer Methods in Applied Mechanics and Engineering*, 402:115336, 2022. `doi:10.1016/j.cma.2022.115336`.

11. B. Pachev, J. P. Whitehead, and **S. A. McQuarrie**. Concurrent multiparameter learning demonstrated on the Kuramoto–Sivashinsky equation. *SIAM Journal on Scientific Computing*, 44(5):A2974–A2990, 2022. `doi:10.1137/21M1426109`.

10. **S. A. McQuarrie**, C. Huang, and K. E. Willcox. Data-driven reduced-order models via regularised operator inference for a single-injector combustion process. *Journal of the Royal Society of New Zealand*, 51(2):194–211, 2021. `doi:10.1080/03036758.2020.1863237`.

9. A. Farhat, N. E. Glatt-Holtz, V. R. Martinez, **S. A. McQuarrie**, and J. P. Whitehead. Data assimilation in large-Prandtl Rayleigh-Bénard convection from thermal measurements. *SIAM Journal on Applied Dynamical Systems*, 19(1):510–540, 2020. `doi:10.1137/19M1248327`.

8. P. Bartholomew, **S. A. McQuarrie**, J. S. Purcell, and K. Weser. Volume and geometry of homogeneously adequate knots. *Journal of Knot Theory and Its Ramifications*, 24(08):1550044, 29, 2015. `doi:10.1142/S0218216515500443`.

Conference Proceedings

7. P. Jain, **S. A. McQuarrie**, and B. Kramer. Performance comparison of data-driven reduced models for a single-injector combustion process. In *AIAA Propulsion and Energy 2021 Forum*, Virtual event, 2021. AIAA Paper 2021-3633. `doi:10.2514/6.2021-3633`.

6. **S. A. McQuarrie**, J. Hart, B. van Bloemen Waanders, and K. Willcox. Data-driven model reduction for physics-constrained optimization. In *CSRI Summer Proceedings 2021*, pages 101–111, 2021.

Software and Projects

5. Python package `opinf`: Operator inference for data-driven, non-intrusive model reduction of dynamical systems.
https://willcox-research-group.github.io/rom-operator-inference-Python3

4. Reduced-order modeling via operator inference for 2D combustion.
github.com/Willcox-Research-Group/ROM-OpInf-Combustion-2D

3. Labs for the *Foundation of Applied Mathematics* curriculum.
   github.com/Foundations-of-Applied-Mathematics/Labs

Other Publications

2. **S. A. McQuarrie**. Data assimilation in the Boussinesq approximation for mantle convection. Master's thesis, Brigham Young University, 2018.

1. **S. A. McQuarrie**, A. X. Garcia, and J. E. Spomer. Information extraction and logical inference for derivative classifier assistance. Technical report, Sandia National Lab (SNL-NM), Albuquerque, NM (United States), 2017.

Presentations

Conference Presentations

15. *Non-intrusive parametric reduced-order modeling via operator inference.* SIAM SEAS Sectional, Blacksburg, VA, 25 March 2025.

14. *Operator inference for affine-parametric systems of partial differential equations.* SIAM Conference on Computational Science and Engineering, Amsterdam, The Netherlands, 28 February 2023.

13. *Bayesian operator inference for data-driven reduced-order modeling.* SIAM TX/LA Sectional, Houston, TX, 5 November 2022.

12. *Bayesian operator inference for data-driven reduced-order modeling.* American Mathematical Society Western Sectional, Salt Lake City, UT, 22 October 2022.

11. *Non-Intrusive parametric reduced-order modeling via operator inference.* SIAM Conference on the Mathematics of Data Science, San Diego, CA, 28 September 2022.

10. *Non-intrusive parametric reduced-order modeling via operator inference.* U.S. National Congress on Theoretical and Applied Mechanics, Austin, TX, 22 June 2022.

9. *Non-intrusive parametric reduced-order modeling via operator inference.* SIAM Conference on Uncertainty Quantification, Atlanta, GA, 14 April 2022.

8. *Non-intrusive parametric reduced-order modeling via operator inference.* U.S. National Congress on Computational Mechanics, Virtual, 28 July 2021.

7. *Data-driven reduced-order models via regularized operator inference for a single-injector combustion process.* SIAM Conference on Control and Its Applications, Virtual, 21 July 2021.

6. *Data-driven reduced-order models via regularized operator inference.* SIAM Conference on Computational Science and Engineering, Virtual, 1 March 2021.

SEMINARS AND INVITED TALKS

5. *An introduction to non-intrusive model reduction via operator inference.* CSEM Student Forum, Oden Institute for Computational Engineering and Sciences, Austin, TX, 2 October 2020.

4. *Data assimilation in the Boussinesq approximation for mantle convection.* Applied and Computational Mathematics Research Seminar, Tulane University, New Orleans, LA, 23 April 2017.

POSTERS

3. *Bayesian operator inference for data-driven reduced-order models.* Chesapeake Large Scale Analytics Conference, Annapolis, MD, 26 October 2022.

2. *RaISE: A framework to characterize surrogate models in scientific machine learning.* SIAM Conference on the Mathematics of Data Science, San Diego, CA, 28 September 2022.

1. *Data-driven reduced-order models via regularized operator inference for a single-injector combustion process.* Model Order Reduction Summer School (MORSS), École polytechnique fédérale de Lausanne (EPFL), Virtual, 8 September 2020.