John D. Jakeman, PhD

Computational Scientist · Applied Mathematician — Scientific Machine Learning & Uncertainty Quantification

Albuquerque, NM | LinkedIn | GitHub | Scholar | quantifying-uncertainty.com

SUMMARY

Computational mathematician who builds the methods and production software that make physics-based simulations and machine-learning models reliable for high-consequence decisions. Pairs deep applied-mathematics and physics modeling with modern ML — operator learning, surrogate modeling, multifidelity methods — and software engineering. Work cited 6,000+ times (h-index 32); founding developer of the open-source PyApprox toolkit.

CORE COMPETENCIES

Methods: Scientific machine learning, operator learning (neural operators), uncertainty quantification, surrogate modeling (Gaussian processes, polynomial chaos, sparse grids, tensor decompositions), multifidelity & multilevel methods, Bayesian inference & inverse problems, optimal experimental design, sensitivity analysis.

Software & engineering: Python (NumPy, SciPy), deep-learning frameworks for operator learning, CI/CD, test automation, static typing, release engineering, AI-assisted (agentic) development.

Application domains: Fusion & plasma physics, aerospace design, earth science (ice-sheet & sea-level prediction), continuum solid mechanics, additive manufacturing, hydrology/subsurface.

EXPERIENCE

Principal Member of Technical Staff

Sandia National Laboratories, Albuquerque, NM — May 2020 – Present

- Lead research in scientific machine learning and uncertainty quantification for high-consequence engineering and national-security applications, fusing physics-based models with data to make expensive simulations and ML predictions reliable and cheaper.
- Founding developer of **PyApprox**, an open-source Python toolkit (surrogate modeling, Bayesian inference, optimal experimental design, multifidelity UQ) maintained to production standards: cross-platform CI, static typing, security scanning, automated OIDC release pipeline.
- Built multifidelity and operator-learning methods applied across fusion/plasma, aerospace, ice-sheet/sea-level, and solid mechanics; funded by DARPA, the DOE Office of Science (ASCR), and Sandia LDRD; principal investigator on multiple funded projects.

Senior Member of Technical Staff

Sandia National Laboratories, Albuquerque, NM — Oct 2014 – May 2020

- Developed foundational surrogate-modeling and sparse-approximation methods (polynomial chaos, adaptive sparse grids, compressed sensing) and data-consistent inversion, now widely used and cited in UQ research and practice.

Postdoctoral Appointee

Sandia National Laboratories — Jan 2012 – Oct 2014

Postdoctoral Researcher

Purdue University, then SAMSI (hosted by Duke University) — Feb – Dec 2011

EDUCATION

Ph.D. in Mathematics, Australian National University, Canberra, Australia — 2011

B.Sc. with First-Class Honours in Mathematics, Australian National University, Canberra, Australia — 2007

RECOGNITION & SERVICE

- 6,000+ citations; h-index 32; i10-index 52 (Google Scholar).
- Chair, DOE ASCR Basic Research Needs workshop on inverse problems; lead author of the resulting report (2025).
- Associate Editor, Journal of Machine Learning for Modeling and Computing (Begell House).
- Organizing Committee, SIAM Conference on Uncertainty Quantification (UQ26), 2026.
- Invited tutorials: IPAM Multi-Fidelity Methods for Fusion Energy (UCLA, 2026); AIAA Workshop on Multifidelity Methods for Design & UQ (2026); SIAM Conference on Uncertainty Quantification (2024).

SELECTED PUBLICATIONS

- J.D. Jakeman. PyApprox: sensitivity analysis, Bayesian inference, optimal experimental design, and multi-fidelity UQ and surrogate modeling. Environmental Modelling & Software, 2023.
- J.D. Jakeman, L.A. Barba, J.R.R.A. Martins, T. O'Leary-Roseberry. Verification and validation for trustworthy scientific machine learning. 2025.
- M. Lowery, J. Turnage, Z. Morrow, J.D. Jakeman, A. Narayan, S. Zhe, V. Shankar. Kernel neural operators (KNOs) for scalable, memory-efficient, geometrically-flexible operator learning. 2024.