

Malik Hassanaly

Computational Science, Scientific Machine Learning & Uncertainty Quantification
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🔗 [Google Scholar](https://scholar.google.com/citations?user=malik-hassanally)

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ℹ️ [ResearchGate](https://www.researchgate.net/profile/malik-hassanally)

RESEARCH PROFILE

I develop physics-based simulators and their outer-loop applications: simulation-based inference, uncertainty quantification and propagation, rare-event probability estimation, and machine-learning surrogates. **I work across a broad set of domains** — Li-ion batteries, atmospheric flows, power-system security, bioreactors, photovoltaic manufacturing, and reacting flows — and release the resulting methods as maintained open-source software.

EDUCATION

- **PhD University of Michigan, USA** August 2019
Aerospace Engineering — Dissertation: “*Extreme Events in Turbulent Combustion*”
- **MSE University of Texas at Austin, USA** January 2015
Aerospace Engineering — Master Thesis: “*Large-eddy simulations of boundary layer flashback*”
- **MSE École Centrale de Lille, France** January 2015
General Engineering — Thesis project: “*Design and testing of a new tidal turbine*”

SKILLS

- **Uncertainty Quantification:** Bayesian inference, simulation-based inference, inverse problems, model calibration, uncertainty propagation, sensitivity analysis, rare-event probability estimation, multi-fidelity methods, design of experiments
- **Machine learning:** Generative models (GANs, diffusion models), physics-informed neural networks, Bayesian neural networks, normalizing flows, reinforcement learning, anomaly detection, reduced-order modeling
- **Programming:** Python, C++, Fortran, Bash, Git
- **ML libraries:** PyTorch, TensorFlow
- **Physics modeling tools:** OpenFOAM, AMReX, ParaView
- **Languages:** English (Fluent), French (Native), Spanish (Intermediate)

EXPERIENCE

- **National Laboratory of the Rockies (NLR), USA** September 2022 – Current
Staff Researcher — AI & Physics modeling
 - Adversarial Machine Learning for automated red-teaming of power-system controllers (Project lead, \$550k)
 - Sample-efficient uncertainty propagation and rare/extreme event generation
 - Physics-informed ML and uncertainty-aware inverse parameter identification for Li-ion batteries
 - Bioreactor design optimization, Bayesian calibration, and cost-aware experimental design
 - Reduced chemical kinetics for heterogeneous (CPU/GPU) exascale hardware
 - Mentored 4 graduate interns and 2 postdoctoral researchers
- **National Laboratory of the Rockies (NLR), USA** September 2019 – September 2022
Post-doctoral researcher — AI & Physics modeling
 - Uncertainty quantification of super-resolved atmospheric flow fields; measuring and enforcing generative-model diversity
 - Physics-based solver development for heterogeneous HPC (CPU/GPU)
 - Intelligent data-reduction for data-based physics surrogates
 - Inverse modeling of surface chemistry kinetics and deposition reactor optimization
- **University of Michigan, USA** January 2015 – August 2019
Graduate Research Assistant
 - Chaotic dynamics of turbulent combustion
 - Information extraction from large simulation and experimental datasets; predictive model from combustor observations
 - Developed a minimally-dissipative low-Mach solver for variable-density reacting flows
- **University of Texas at Austin, USA** August 2013 – December 2014
Graduate Research Assistant
 - Boundary-layer flame flashback modeling in channel and swirl combustors
 - Maintained and developed structured and unstructured large-eddy simulation codes
- **Maïa Eolis (now Engie Green), France** November 2012 – May 2013
Physics Modeling Intern
 - Computational fluid dynamics modeling of wind turbine blades
- **RTE (French Electrical Grid), France** May 2012 – November 2012
Software Development Intern
 - Developed a generic gateway from a UML model to a C++ library used in a large-scale power grid code.

SOFTWARE

Full list: github.com/malihass

- **PINNSTRIPES** — lead author, 60+ stars: Physics-informed neural network surrogates of Li-ion battery models for parameter identification
- **BioReactorDesign (BiRD)** — lead author, 40+ stars: OpenFOAM toolbox for bioreactor simulation, Bayesian calibration and design optimization
- **Phase-space-sampling**, **diversity_SR**, **GANISP**, **mluq-prop**, **BatFIT** — lead author: Normalizing-flow data downselection; GAN diversity measurement and enforcement; GAN-assisted rare-event probability estimation; ML uncertainty propagation; neural posterior estimation for battery inference
- **PelePhysics** — contributor, 80+ stars: Chemistry and transport for the Pele exascale reacting-flow suite; authored the symbolic QSS Jacobian generator
- **sup3r** — contributor, 130+ stars: Generative adversarial super-resolution for synthetic high-resolution wind and solar data
- **BATMODS-lite** — contributor: SPM and P2D battery models

PUBLICATIONS

- **Generative Machine Learning:**
 1. **Super resolution with generative adversarial nets:** Adversarial sampling of unknown and high-dimensional conditional distributions, M. Hassanaly et al. *Journal of Computational Physics*, 2022  
 2. **Inpainting with diffusion models:** Ensemble flow reconstruction in the atmospheric boundary layer from spatially limited measurements through latent diffusion models, A. Rybchuk, M. Hassanaly et al. *Physics of Fluids*, 2023 
 3. **Extreme event generation:** GANISP: a GAN-assisted Importance Splitting Probability Estimator, M. Hassanaly et al. *AAAI-ADAM*, 2022 
 4. **Data reduction:** Uniform-in-phase-space data selection with iterative normalizing flows, M. Hassanaly et al. *Data-Centric Engineering*, 2023 
- **Predictive surrogate modeling:**
 5. **Physics-informed neural networks:** PINN surrogate of Li-ion battery models for parameter inference, Part I: Implementation and multi-fidelity hierarchies for the single-particle model, M. Hassanaly et al. *Journal of Energy Storage*, 2024 
 6. **Bayesian neural networks:** A Priori Uncertainty Quantification of Reacting Turbulence Closure Models using Bayesian Neural Networks, G. Pash, M. Hassanaly et al. *Engineering Applications of Artificial Intelligence*, 2025 
 7. **Bayesian neural network visualization:** BNNVis: Towards Visual Analytics for Bayesian Neural Networks, G. Appleby, M. Hassanaly et al. *IEEE Visualization and Visual Analytics (VIS)*, 2025
 8. **Mixture of experts:** Data-driven Classification and Modeling of Combustion Regimes in Detonation Waves, S. Barwey, S. Prakash, M. Hassanaly et al. *Flow Turbulence and Combustion*, 2020
 9. **Multifidelity neural operators:** Bi-fidelity Modeling of Uncertain and Partially Unknown Systems using DeepONets, S. De, M. Reynolds, M. Hassanaly et al. *Computational Mechanics*, 2023
- **Bayesian inverse modeling:**
 10. **Neural posterior estimation:** Neural posterior estimation for scalable and accurate inverse parameter inference in Li-ion batteries, M. Hassanaly et al. *Journal of Energy Storage*, 2026 
 11. **Physics-informed neural networks:** PINN surrogate of Li-ion battery models for parameter inference, Part II: Regularization and application of the pseudo-2D model, M. Hassanaly et al. *Journal of Energy Storage*, 2024 
 12. **Population balance modeling:** Bayesian calibration of bubble size dynamics applied to CO₂ gas fermenters, M. Hassanaly et al. *Chemical Engineering Research and Design*, 2025 
 13. **Reaction kinetics:** Surface chemistry models for GaAs epitaxial growth and hydride cracking using reacting flow simulations, M. Hassanaly et al. *Journal of Applied Physics*, 2021
- **Adversarial ML:**
 14. **Multi-agent reinforcement learning:** Adversarial Multi-Agent Reinforcement Learning for Proactive False Data Injection Detection, K. Chen, T. Nguyen, M. Hassanaly, *Under Review*, 2025
 15. **Discrete reinforcement learning:** Discovering the Most Severe K-Point Failure Based on Reinforcement Learning, K. Chen, A. Sahu, T. Nguyen, M. Hassanaly, *IEEE Green Tech*, 2026
 16. **Reinforcement learning + continual learning:** Continual Adversarial Reinforcement Learning (CARL) of False Data Injection detection: forgetting and explainability, P. Aslami, K. Chen, T. Hansen, M. Hassanaly, *IEEE Power Tech*, 2025
 17. **Reinforcement learning:** Discovery of False Data Injection Attacks on Power Grid Frequency Controllers with Reinforcement Learning, R. Prasad, M. Hassanaly et al. *IEEE PES GM*, 2024
- **Anomaly detection:**
 18. **Reinforcement learning + variational autoencoder:** Swift Hydra: Self-Reinforcing Generative Framework for Anomaly Detection with Multiple Mamba Models, N. H. K. Do, T. Nguyen, M. Hassanaly et al. *ICLR*, 2025
 19. **LSTM:** Detection of False Data Injection (FDI) attacks on power dynamical systems with a state prediction method, A. Sahu, [...], M. Hassanaly *IEEE Access*, 2024

- **Image processing:**
 - 20. **Data augmentation:** Using Machine Learning to Construct Velocity Fields from OH-PLIF Images, S. Barwey, M. Hassanaly et al. *Combustion Science and Technology*, 2019
 - 21. **Cluster-reduced order modeling:** Experimental Data Based Reduced Order Model for Analysis and Prediction of Flame Transition in Gas Turbine Combustors, S. Barwey, M. Hassanaly et al. *Combustion Theory and Modelling*, 2019
 - 22. **Discriminant analysis:** Data-driven Analysis of Relight Variability of Jet Fuels induced by Turbulence, M. Hassanaly et al. *Combustion and Flame*, 2021
 - 23. **Cluster-reduced order modeling:** Data-based analysis of multimodal partial cavity shedding dynamics, S. Barwey, H. Ganesh, M. Hassanaly et al. *Experiments in Fluids*, 2020
- **Numerical methods for high-performance computing:**
 - 24. **Chemistry integration:** SUNDIALS Time Integrators for Exascale Applications with Many Independent ODE Systems, C. Balos, [...], M. Hassanaly et al. *International Journal of High Performance Computing Applications*, 2024
 - 25. **Symbolic computations:** Symbolic construction of the chemical Jacobian of quasi-steady state (QSS) chemistries for Exascale computing platforms, M. Hassanaly et al. *Combustion and Flame*, 2024 
 - 26. **Exascale computing methods:** The Pele Simulation Suite for Reacting Flows at Exascale, M. Henry de Frahan, [...], M. Hassanaly et al. *SIAM Conference on Parallel Processing for Scientific Computing*, 2024 
 - 27. **Exascale computing demo:** Visualizations of a methane/diesel RCCI engine using PeleC and PeleLMEx, N. T. Wimer, [...], M. Hassanaly et al., *Physical Review Fluids*, 2023
 - 28. **Secondary conservation:** A minimally-dissipative low-Mach number solver for complex reacting flows in OpenFOAM, M. Hassanaly, *Computers & Fluids*, 2018 — *in use by 4 corporations and 15 universities*
- **Topical reviews:**
 - 29. **Extreme and rare events:** Emerging Trends in Numerical Simulations of Combustion Systems, V. Raman, M. Hassanaly, *Proceedings of the Combustion Institute*, 2019
 - 30. **Combustion modeling:** Classification and Computation of Extreme Events in Turbulent Combustion, M. Hassanaly et al. *Progress in Energy and Combustion Science*, 2021
- **Design optimization:**
 - 31. **Surrogate-based optimization:** Optimal sparging and mixing for enhanced mass transfer in U-loop bioreactors, M. Hassanaly et al. *Under Review*, 2026 
 - 32. **Sensitivity analysis:** Low embodied energy and carbon, high lifetime silicon boules via a combined chemical vapor deposition/float zone process, D. L. Young, [...], M. Hassanaly et al. *Solar Energy Materials and Solar Cells*, 2026
- **Turbulence modeling:**
 - 33. **Ignition:** Probabilistic Modeling of Forced Ignition of Alternative Jet Fuels, Y. Tang, M. Hassanaly et al. *Proceedings of the Combustion Institute*, 2021
 - 34. **Ignition:** Simulation of gas turbine ignition using large eddy simulation approach, Y. Tang, M. Hassanaly et al., *ASME Turbo Expo*, 2020
 - 35. **Ignition:** A Comprehensive Modeling Procedure for Estimating Statistical Properties of Forced Ignition, Y. Tang, M. Hassanaly et al. *Combustion and Flame*, 2019
 - 36. **Soot:** Large Eddy Simulation of Pressure and Dilution Jet Effects on Soot Formation in a Model Aircraft Swirl Combustor, S. T. Chong, M. Hassanaly et al. *Combustion and Flame*, 2018
 - 37. **Soot:** Large-Eddy Simulation of Soot Formation in a Model Gas Turbine Combustor, H. Koo, M. Hassanaly et al. *Journal of Engineering for Gas Turbines and Power*, 2017
 - 38. **Flashback:** Large eddy simulation of flame stabilization in a multi-jet burner using a non-adiabatic flamelet approach, Y. Tang, M. Hassanaly et al., *54th AIAA Aerospace Sciences Meeting*, 2016
 - 39. **Boundary layer flashback:** Large Eddy Simulation of Flame Flashback in Swirling Premixed CH₄/H₂-Air Flames, C. F. Lietz, M. Hassanaly et al., *53rd AIAA Aerospace Sciences Meeting*, 2015
 - 40. **Stratified combustion:** Influence of Fuel Stratification on Turbulent Flame Propagation, M. Hassanaly et al., *53rd AIAA Aerospace Sciences Meeting*, 2015
 - 41. **Boundary layer flashback:** LES of Premixed Flame Flashback in a Turbulent Channel, C. F. Lietz, M. Hassanaly et al., *52nd AIAA Aerospace Sciences Meeting*, 2014
 - 42. **Inertial manifolds:** An Approximate Inertial Manifold (AIM) Based Closure for Turbulent Flows, M. Akram, M. Hassanaly et al. *AIP Advances*, 2022
 - 43. **Inertial manifolds:** A priori analysis of reduced description of dynamical systems using approximate inertial manifolds, M. Akram, M. Hassanaly et al. *Journal of Computational Physics*, 2020
- **Chaotic dynamics and rare event modeling:**

44. **Lyapunov spectrum calculation:** Numerical convergence of the Lyapunov spectrum computed using low Mach number solvers, M. Hassanaly et al. *Journal of Computational Physics*, 2019
45. **Rare event probability:** A self-similarity principle for the computation of rare event probability, M. Hassanaly et al. *Journal of Physics A: Mathematical and Theoretical*, 2019
46. **Lyapunov spectrum of non-reacting flows:** Lyapunov spectrum of forced homogeneous isotropic turbulent flows, M. Hassanaly et al. *Physical Review Fluids*, 2019
47. **Lyapunov spectrum of reacting flows:** Ensemble-LES Analysis of Perturbation Response of Turbulent Partially-Premixed Flames, M. Hassanaly et al. *Proceedings of the Combustion Institute*, 2019

ACADEMIC SERVICE

- **Reviewer:**
 - Project proposals (DOE ASCR, Lab-directed R&D projects, NLR's HPC allocations)
 - Peer reviewer for journals in AI/ML, numerical methods, inverse methods, uncertainty quantification, combustion modeling and Li-ion battery modeling
- **Mentorship:**
 - 4 graduate interns, 2 post-doctoral researchers
- **Professional societies:**
 - SIAM, American Physical Society, AIChE, AIAA, The Combustion Institute

HONORS AND AWARDS

- 2026: R&D 100 Winner (Pele exascale simulation suite)
- 2024: NLR President's Award
- 2024: NLR Outstanding Mentor Award
- 2022: Milton Van Dyke Video Award — "Simulation of an RCCI Engine Using the Pele Suite of Exascale Codes"
- 2019: Richard and Eleanor Towner Prize for Distinguished Academic Achievement