Malik Hassanaly

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EDUCATION

PhD University of Michigan, USA

Aerospace Engineering - Dissertation: "Extreme Events in Turbulent Combustion"

MSE University of Texas at Austin, USA

Aerospace Engineering - Master Thesis: "Large-eddy simulations of boundary layer flashback"

MSE Ecole Centrale de Lille, France

GPA: 3.89

General Engineering - Thesis project: "Design and testing of a new tidal turbine"

January 2015

SKILLS

• **Programming**: Python, C₊₊, Fortran, Bash, Git

• ML Libraries: TensorFlow, PyTorch

• Physics modeling tools: OpenFOAM, Paraview

• Languages: English (Fluent), French (Native), Spanish (Intermediate)

EXPERIENCE

National Renewable Energy Laboratory (NREL), USA

September 2019 - Current

Researcher - Computational Science and Machine Learning

o Data augmentation for atmospheric modeling and probability estimation: Developed a method that estimates the amount of diversity that must be observed when super-resolving atmospheric data. The a priori diversity is used to evaluate and regularize Generative Adversarial Networks (GANs).

Adversarial sampling of unknown and high-dimensional conditional distributions, M. Hassanaly et al. *Journal of Computational Physics*, 2022 •

Scaled up the conditional moment estimation method to large spatiotemporal atmospheric datasets.

🖒 Coarse-graining uncertainty in atmospheric spatio-temporal super-resolution 🔾

The method is also useful when multiple realizations need to be generated. I demonstrated that it reduces the variance of rare-event probability estimators when using importance splitting.

🖒 GANISP: a GAN-assisted Importance Splitting Probability Estimator, M. Hassanaly et al. AAAI-ADAM, 2022, 🗘

o Downsampling of large and high-dimensional datasets: Developed a method to downsample large datasets while incurring minimal information loss. The method first estimates the probability density of a high-dimensional and large dataset with a normalizing flow and uses it to decide how aggressive downsampling needs to occur. An iterative treatment helps mitigate errors in low-probability regions. The method achieves uniform-in-phase space sampling even in high dimensions and outperforms SOTA for combustion modeling.

Uniform-in-phase-space data selection with iterative normalizing flows, M. Hassanaly et al. Data-Centric Engineering, 2023, ••

- Physics-informed surrogate model of Li-ion batteries: Accelerate Bayesian calibration of Li-ion battery parameters to help diagnose the cause of battery degradation and formulate degradation models for parameters. The surrogate model is constructed with a physics-informed neural network that uses sparse available data. The method accelerates inverse problem solving by at least two orders of magnitude.
- Physics-Informed Neural Network Modeling of Li-Ion Batteries, M. Hassanaly et al. 242nd ECS Meeting, 2022
- Analytically reduced chemistry for heterogeneous high-performance computing (HPC): Generation of chemical Jacobian for analytically reduced chemistry. The Jacobian is symbolically encoded allowing to automate memory-efficient pre-computations to balance memory and register pressure on CPU/GPU architectures. The method has been successfully deployed on exascale machines \mathbf{Q}
- Uncertainty propagation of data-driven models: Estimate reducible and non-reducible uncertainties with Bayesian neural networks. Developed a method for including extrapolative uncertainty in regression models.
- Optimization of deposition reactors: Developed a chemistry surrogate model for accelerating numerical simulations of III-V deposition reactors used for solar cell manufacturing. The chemistry model was calibrated with a Bayesian approach. The model was used to optimize the reactor geometry and the reactant injection scheme.

🖒 Surface chemistry models for GaAs epitaxial growth and hydride cracking using reacting flow simulations, M. Hassanaly et al. Journal of Applied Physics, 2021

University of Michigan, USA

January 2015 - August 2019

Graduate Research Assistant

- Chaotic dynamics of turbulent combustion: Characterized the dynamics of turbulent flames using Lyapunov exponent (LE). I identified that extinction and reignition in turbulent flames mainly participated in the amplification of perturbations. In absence of combustion, perturbation amplification is mostly localized near strong vortices. I provided the first estimate of the attractor dimension of turbulent flames.
 - 🖒 Ensemble-LES Analysis of Perturbation Response of Turbulent Partially-Premixed Flames, M. Hassanaly et al. Proceedings of the Combustion Institute, 2019
 - I adapted the LE computation algorithm to variable density low-Mach CFD solvers and rigorously assessed the convergence properties of the algorithm.
 - Numerical convergence of the Lyapunov spectrum computed using low Mach number solvers, M. Hassanaly et al. *Journal of Computational Physics*, 2019
- Information extraction from large datasets: Identify turbulent features that influence ignition of jet fuels using data from numerical simulations.
 - 🖒 Data-driven Analysis of Relight variability of Jet Fuels induced by Turbulence, M. Hassanaly et al. Combustion and Flame, 2021.
- Efficient numerical solvers for variable density flows: Developed a numerical solver that reduces the amount of numerical dissipation and mass conservation inaccuracies in variable density low-Mach solvers. The solver has been used by 4 corporations and 15 universities.
 - A minimally-dissipative low-Mach number solver for complex reacting flows in OpenFOAM, M. Hassanaly, Computer and Fluids, 2018.

Maïa Eolis (now Engie Green), France

November 2012 - May 2013

Physics Modeling Intern

 Computational fluid dynamics modeling of wind turbine blades. I quantified the mechanical stress induced by a novel blade spoiler.

RTE (French Electrical Grid), France

May 2012 - November 2012

Software Development Intern

• Developed of a generic gateway from a UML model to a C++ library used in a large-scale power grid code.

OTHER JOURNAL PUBLICATIONS

Data-driven modeling

- Bi-fidelity Modeling of Uncertain and Partially Unknown Systems using DeepONets: S. De, M. Reynolds, M. Hassanaly et al. Computational Mechanics, 2023
- Data-driven Classification and Modeling of Combustion Regimes in Detonation Waves: S. Barwey, S. Prakash, M. Hassanaly et al. Flow Turbulence and Combustion, 2020
- Data-based analysis of multimodal partial cavity shedding dynamics: S. Barwey, H. Ganesh, M. Hassanaly et al. Experiments in Fluids, 2020

Information Extraction

- Using Machine Learning to Construct Velocity Fields from OH-PLIF Images: S. Barwey, M. Hassanaly et al. Combustion Science and Technology, 2019
- Experimental Data Based Reduced Order Model for Analysis and Prediction of Flame Transition in Gas Turbine Combustors: S. Barwey, M. Hassanaly, Q. An, V. Raman, A. Steinberg Combustion Theory and Modelling, 2019.

Reacting flows modeling

- Surface chemistry models for GaAs epitaxial growth and hydride cracking using reacting flow simulations: M. Hassanaly et al. *Journal of Applied Physics*, 2021
- Probabilistic Modeling of Forced Ignition of Alternative Jet Fuels: Y. Tang, M. Hassanaly et al. Proceedings of the Combustion Institute, 2021
- Emerging Trends in Numerical Simulations of Combustion Systems: V. Raman, M. Hassanaly, Proceedings of the Combustion Institute, 2019
- A Comprehensive Modeling Procedure for Estimating Statistical Properties of Forced Ignition: Y. Tang, M. Hassanaly et al. Combustion and Flame, 2019
- 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
- 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

Turbulence modeling

- A priori analysis of reduced description of dynamical systems using approximate inertial manifolds: M. Akram, M. Hassanaly et al. *Journal of Computational Physics*, 2020
- An Approximate Inertial Manifold (AIM) Based Closure for Turbulent Flows: M. Akram, M. Hassanaly et al. AIP Advances, 2022

Chaotic dynamics

- Classification and Computation of Extreme Events in Turbulent Combustion: M. Hassanaly et al. Progress in Energy and Combustion Science, 2021
- A self-similarity principle for the computation of rare event probability: M. Hassanaly et al. Journal of Physics A: Mathematical and Theoretical, 2019
- Lyapunov spectrum of forced homogeneous isotropic turbulent flows: M. Hassanaly et al. Physics Review Fluids, 2019

Honors and Awards

- 2019: Richard and Eleanor Towner Prize for Distinguished Academic Achievement
- 2022: Milton Van Dyke Video Award, "Simulation of an RCCI Engine Using the Pele Suite of Exascale Codes"