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

January 2015

#### SKILLS

- **Programming**: Python, C<sub>++</sub>, 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
  - 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 **Q**

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

Coarse-graining uncertainty in atmospheric spatio-temporal super-resolution •

We used the method to show that diffusion models are able to natively generate a sufficient amount of diversity

- Generating Initial Conditions for Ensemble Data Assimilation of Large-Eddy Simulations with Latent Diffusion Models, A. Rybchuk, M. Hassanaly et al. *Physics of Fluids*, 2023
- 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, 🗘
- 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.
  - C 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 •
- 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 ♥

• Synergistic activities: Developed a variety of funding proposals for solving inverse problems, data reduction, parameter estimation and extreme event prediction. Mentored two summer interns.

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.
  - Used experimental observations in swirl-combustors to formulate a predictive model for flame lift-off and access state variables non-measurable.
  - 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.
- 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.
  - À 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

- Visualizations of a methane/diesel RCCI engine using PeleC and PeleLMeX: N. T. Wimer, [...], M. Hassanaly et al., Physical Review Fluids, 2023
- Bi-fidelity Modeling of Uncertain and Partially Unknown Systems using DeepONets: S. De, M. Reynolds, M. Hassanaly et al. *Computational Mechanics*, 2023
- An Approximate Inertial Manifold (AIM) Based Closure for Turbulent Flows: M. Akram, M. Hassanaly et al. AIP Advances, 2022
- 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
- Probabilistic Modeling of Forced Ignition of Alternative Jet Fuels: Y. Tang, M. Hassanaly et al. Proceedings of the Combustion Institute, 2021
- Data-driven Classification and Modeling of Combustion Regimes in Detonation Waves: S. Barwey, S. Prakash, M. Hassanaly et al. Flow Turbulence and Combustion, 2020
- A priori analysis of reduced description of dynamical systems using approximate inertial manifolds: M. Akram, M. Hassanaly et al. *Journal of Computational Physics*, 2020
- Data-based analysis of multimodal partial cavity shedding dynamics: S. Barwey, H. Ganesh, M. Hassanaly et al. Experiments in Fluids, 2020
- 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
- Using Machine Learning to Construct Velocity Fields from OH-PLIF Images: S. Barwey, M. Hassanaly et al. Combustion Science and Technology, 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

# Honors and Awards

- $\bullet$  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"