# Computational Aerosciences Laboratory 2024 Highlights

2024 was another highly productive year for CASLAB. This also feels like a year of generational shift as the lab got a whole lot younger. Over the past 18 months, we waved goodbye to 6 CASLABers and welcomed 6 new ones. What an amazing feeling to see students grow into mature researchers and to work with new minds every year. Given several high-profile initiatives, 2024 might sound like it was dominated by AI, but CASLAB did have a very balanced portfolio. Here are some highlights:



Figure 1: Sahil's photo of the total eclipse of April 2024

#### **Book**

Data-driven Analysis and Modeling of Turbulent Flows, Edited by K. Duraisamy, including contributions from Kunihiko Taira & Steven Brunton, Tim Colonius & Aaron Towne, Ati Sharma & Beverley McKeon, Mengze Wang & Tamer Zaki, Peter Schmid, Paul Durbin, Richard Dwight & Heng Xiao, Vishal Srivastava, Paola Cinnella. This is in final production and should be out very soon.

This book emerges from a recognition that the field of turbulence is experiencing a renaissance driven by three key developments: the explosive growth in computational capabilities generating massive datasets, the maturation of machine learning and data science techniques, and the continued need for improved turbulence models in engineering applications. Our goal is to provide a comprehensive introduction to modern data-driven approaches for analyzing, modeling, and controlling turbulent flows while maintaining strong connections to the underlying physics.

The material is organized into three complementary parts, each addressing fundamental challenges in turbulence research. Part A, *Quest to Find Structure*, focuses on extracting coherent patterns from turbulent flows. Part B, *Estimation and Control*, addresses the critical challenge of reconstructing and manipulating turbulent flows from limited observations. Part C, *Modeling and Prediction*, delves into the heart of turbulence modeling, examining both traditional Reynolds-averaged approaches and modern data-driven alternatives.

# **Journal Publications & Preprints**

# **Information Theory**

- Information theoretic clustering for coarse-grained modeling of non-equilibrium gas dynamics, C Jacobsen, I Zanardi, S Bhola, K Duraisamy, M Panesi, *Journal of Computational Physics*
- Variational Bayesian optimal experimental design with normalizing flows, J Dong, C Jacobsen, M Khalloufi, M Akram, W Liu, K Duraisamy, X Huan, Computer Methods in Applied Mechanics and Engineering

## **Numerical Verification & Stochastics**

- Finite Sample Analysis and Bounds of Generalization Error of Gradient Descent in In-Context Linear Regression, K Duraisamy, *arXiv*:2405.02462.
- Variance-informed Rounding Uncertainty Analysis for Floating-point Statistical Models, S Bhola, K Duraisamy, *arXiv:2404.12556*
- Deterministic and Probabilistic Rounding Error Analysis for Mixed-Precision Arithmetic on Modern Computing Units, S Bhola, K Duraisamy, *arXiv:2411.18747*.

# **Machine Learning**

- Zhuang, Y., Cheng, S. and Duraisamy, K. "Spatially-aware diffusion models with cross-attention for global field reconstruction with sparse observations," *Computer Methods in Applied Mechanics and Engineering*.
- Jacobsen, C., Zhuang, Y., and Duraisamy, K., "CoCoGen: Physically-consistent and conditioned score-based generative models for forward and inverse problems," *SIAM Journal on Scientific Computing*.
- Duvall, J., Pan. S., and Duraisamy, K., "Discretization-independent surrogate modeling of physical fields around variable geometries using coordinate-based networks," *Data Centric Engineering*.
- A hybrid surrogate modeling framework for the Digital Twin of a Fluoride-salt-cooled High-temperature Reactor, Lim, J., Li, J., O'Grady, D., Downar, T., and Duraisamy, K., *Nuclear Engineering Design*.
- Design-Variable Hypernetworks for Flowfield Emulation and Shape Optimization of Compressor Airfoils, J Duvall, M Joly, K Duraisamy, S Sarkar, *AIAA Journal*.

## **Turbulence Modeling**

Data-Driven Turbulent Prandtl Number Modeling for Hypersonic Shock—Boundary-Layer Interactions, E Parish, DS Ching, C Jordan, G Nicholson, NE Miller, S Beresh, N Gupta, K Duraisamy, AIAA Journal.

- Recent developments and research needs in turbulence modeling of hypersonic flows, P Raje, E Parish, JP Hickey, P Cinnella, K Duraisamy, *arXiv:2412.13985*.
- Stochastic Wavevector Model for Rapidly-Distorted Compressible Turbulence, N Zambrano, K Duraisamy, arXiv:2409.12791.
- A new dynamic slip approach for wall-modeled Large Eddy Simulations in a Consistent Discontinuous Galerkin Framework, P Raje, K Duraisamy, *arXiv*:2405.15899.

# Non-linear Dynamics & Control theory

- On the lifting and reconstruction of nonlinear systems with multiple invariant sets, S Pan, K Duraisamy, *Nonlinear Dynamics*.
- Model Predictive Control of Nonlinear Dynamics Using Online Adaptive Koopman Operators D Uchida, K Duraisamy, *arXiv:2412.02972*.
- Extracting Koopman Operators for Prediction and Control of Non-linear Dynamics Using Twostage Learning and Oblique Projections, D Uchida, K Duraisamy, SIAM Journal on Applied Dynamical Systems.

## **Honors and Distinctions**

- Sahil Bhola and Yi Han Toh won MICDE fellowships. MICDE roughly awards 20 / year across the entire university and CASLAB has only had two fellows prior to this year.
- Karthik's MICDE directorship is now endowed by Samir and Puja Kaul.

#### **Los Alamos Collaboration**

U-M and Los Alamos National Laboratory have established a very deep collaboration in Computational Science, AI and HPC. Some information can be found in scattered news articles, but more will be forthcoming in the next few months. On the ground, Karthik is the PI of a \$15M research contract, and CASLAB students and postdocs are involved in Scientific Foundation Models, Multi-fidelity Modeling and Solver acceleration, with topics spanning multi-physics applications including inertial confinement fusion, stellar astrophysics and weather prediction. Watch this space next year.

## **Conference/Workshops**

AIAA Scitech (Orlando), WCCM (Vancouver), Model Reduction & Surrogate Modeling (San Diego), Scale-Bridging (Los Alamos), SciML (Brown U.), ML for Fluids (Madison), TSFP (Montreal), APS DFD (Salt Lake City), AI4Science (Harvard).

## **Colloquia**

Fluids (Stanford), Fluids (Penn State), AI Forum (Los Alamos), TPC (Argonne National Labs), Special (ETH, Zurich).

#### **Panels**

- 1. AI for Science, Energy and Security Panel at the NVIDIA AI Summit (Washington DC); Special Remarks by DOE Secretary Granholm.
- 2. Panel on Geothermal energy & Bloomberg Interview at the World Economic Forum (Davos) .
- 3. Panel on People and Technology at the SLB Digital Forum (Monaco).

# **Conferences & Workshops (Organized by MICDE)**

1. Conference on Scientific Foundation Models.

This conference focused on scientific foundation models (SciFM) that aim to have a similar transformative impact on science as Generative AI has had on natural language. This event was the first of its kind, dedicated exclusively to this exciting and nascent field.

A special issue of the MICDE magazine covered the proceedings.

Videos can be found at the bottom of the conference page

SciFM25 is going to be an order of magnitude bigger. Mark the dates: May 28-30.

- 2. Summer School on Scientific Foundation Models. Based on the feedback from SciFM24, meeting and further discussions with National Lab and academic partners, we organized the SciFM Summer School 2024. We wish for this to be a recurring event hosted at different locations across the country. The first instance was run in parallel at the University of Michigan (UM) and at Argonne National Laboratory (ANL). The summer school involved:
  - a) Developing technical plans for specific instances of SciFMs; b) A hackathon to jumpstart the construction of SciFMs; c) Furthering a vision for a national SciFM ecosystem.

Videos of talks here

### **Career Transitions**

- 1. Christian Jacobsen defended his doctoral dissertation titled 'Enhancing Physical Modeling with Interpretable Physics-Aware Machine Learning' and started as a research engineer at NVIDIA.
- 2. Bernardo Pacini (co-advised with Joaquim Martins) defended his dissertation titled 'Aerodynamic, Aeroacoustic, and Aerostructural Design Optimization for Propeller-Driven Aircraft,' and started as a Aerodynamics Engineer at Joby Aviation.
- 3. James Duvall defended his doctoral dissertation titled 'Development and Application of Hypernetworks for Discretization-Independent Surrogate Modeling of Physical Fields,' and continued as a post doctoral fellow in CASLAB.

## **New members**

- 1. Yi Han Toh (PhD student) got his BEng in Aerospace at Nanyang (Singapore) and Masters in Aero at Georgia Tech and comes in with a strong publication record.
- 2. Curtis Maxon (PhD student) got his Bachelors and Masters in Mechanical and Aerospace Engineering from the Univ of Missouri and has significant research experience at Los Alamos and work experience at Honeywell.

## CASLAB team of 2024

Post Doctoral Fellows: James Duvall, Pratikkumar Raje.

*PhD Students:* James Duvall, Christian Jacobsen, Bernardo Pacini, Jasmin Lim, Niloy Gupta, Daisuke Uchida, Sahil Bhola, Noah Zambrano, Tony Zhuang, Amirpasha Hedayat, Moon Hazarika, Yi Han Toh, Curtis Maxon.

Lead: Karthik Duraisamy.

## **Prior CASLAB Newsletters**

Newsletter from 2023

Newsletter from 2022

Newsletter from 2021

Newsletter from 2020

Newsletter from 2019

Newsletter from 2018

Newsletter from 2017

Thank you for reading our newsletter. Visit us at https://caslab.engin.umich.edu/.

P.S. If you are interested in knowing more about Computational science, AI & HPC at the U. of Michigan, please check out the MICDE website and the latest editions of the MICDE magazine