Computational Aerosciences Laboratory
2025 Highlights

Phew! What a breathless year. We said 2024 was a generational shift as the lab got a whole lot younger, but in 2025, depth *and* breadth of outcomes kept getting better, and impact kept accelerating. Here are some highlights.

Figure 1: CASLAB (minus those at internships) 4th of July bbq. Also doubled as a sendoff for Jasmin.

Publications [1]

Fluid Dynamics

- *Gauss Principle in Incompressible Flow: Unified Variational Perspective on Pressure and Projection,* K Duraisamy, arXiv:2510.22925

- *Two-point Turbulence Closures in Physical Space,* N Zambrano, K Duraisamy, arXiv:2511.00669.

- *Stochastic wavevector model for rapidly distorted compressible turbulence,* N Zambrano, K Duraisamy, Journal of Fluid Mechanics.

- *Recent developments and research needs in turbulence modeling of hypersonic flows,* P Raje, E Parish, JP Hickey, P Cinnella, K Duraisamy, Physics of Fluids.

- *A new dynamic slip approach for wall-modelled large eddy simulations in a consistent discontinuous Galerkin framework*, P Raje, K Duraisamy, Journal of Fluid Mechanics 1017.

Machine Learning & AI

- *Active Inference AI Systems for Scientific Discovery,* K Duraisamy, arXiv:2506.21329.

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[1] Some of these were listed in last year's report as preprints, but they're now improved and published

- *Flow-matching Operators for Residual-Augmented Probabilistic Learning of Partial Differential Equations*, S Bhola, K Duraisamy, arXiv:2512.12749.

- *Foundation Models for Discovery and Exploration in Chemical Space,* A Wadell, A Bhutani, V Azumah, AR Ellis-Mohr, C Kelly, H Zhao, ... arXiv:2510.18900.

- *LaDCast: A Latent Diffusion Model for Medium-Range Ensemble Weather Forecasting,* Y Zhuang, K Duraisamy, arXiv:2506.09193.

- *Easy attention: A simple attention mechanism for temporal predictions with transformers,* M Sanchis-Agudo, Y Wang, R Arnau, L Guastoni, J Lim, K Duraisamy, R. Vinuesa, APL Computational Physics.

- *Spatially-aware diffusion models with cross-attention for global field reconstruction with sparse observations,* Y Zhuang, S Cheng, K Duraisamy, Computer Methods in Applied Mechanics and Engineering.

- *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 Methods & Applications

- *Asymptotic-preserving semi-implicit finite volume scheme for Extended Magnetohydrodynamics,* YH Toh, J Dolence, K Duraisamy, arXiv:2511.15937.

- *Investigating the benefit of aerodynamic shape optimization for a wing with distributed propulsion,* B Pacini, M Prajapati, K Duraisamy, JRRA Martins, P He Meccanica 60.

Non-linear dynamics & control

- *A digital twin framework for Generation-IV reactors with reinforcement learning-enabled health-aware supervisory control,* JY Lim, D Pylorof, HE Garcia, K Duraisamy, Progress in Nuclear Energy.

- *Extracting Koopman Operators for Prediction and Control of Nonlinear Dynamics Using Two-Stage Learning and Oblique Projections,* D Uchida, K Duraisamy SIAM Journal on Applied Dynamical Systems.

- *Coarse-Graining Turbulence Using the Mori–Zwanzig Formalism* E Parish, K Duraisamy, Book Chapter, Cambridge University Press.

Data-driven 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.

- *Enhancing dynamical system modeling through interpretable machine-learning augmentations: a case study in cathodic electrophoretic deposition,* C Jacobsen, J Dong, M Khalloufi, X Huan, K Duraisamy, M Akram, W Liu, Data-Centric Engineering.

- *Computational and physical considerations for the development of machine learning augmented turbulence models,* N Gupta, K Duraisamy, International Journal of Heat and Fluid Flow.

- The book *Data-driven Analysis and Modeling of Turbulent Flows* is now in print. It includes 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.*

New Projects started in 2025

- Extreme scale bridging in magnetic plasmas (Los Alamos): We will be working on advancing computational science to handle the transition from kinetic to continuum physics (both regimes happening in the same problem at the same time!).

Figure 2: Dr. Jonah Miller talking about a typical challenge: the incredible range of physics and spatio-temporal scales in an X pinch

- Prediction, Reasoning and Intelligence for Multi-physics explorations (PSAAP center): Read more about it here

- Formal Verification in Scientific Computing (NSF): Our objective is to develop a *scalable, end-to-end* verification pipeline for scientific computing.

- Diffusion Models for Automotive Aerodynamics (General Motors): Exploring new diffusion model architectures for exploration of aerodynamic design spaces.

Los Alamos Collaboration

U-M and Los Alamos National Laboratory have established a very deep research collaboration. Karthik is the research partnership lead for this activity. We now have 25+ researchers involved in this activity, and around 10 LANL staff are co-located with us. Expect this number to increase significantly. CASLAB students and postdocs are involved in Foundation Models, Numerical Methods and Physics Modeling.

Conference/Workshops

In-person: AIAA Scitech (Orlando), USACM (Chicago), SIAM CSE (Fort Worth), DOE CoDA(Santa Fe, Plenary), IUTAM (Okinawa), ISC-HPC (Hamburg), NATO ML & AI in Military Vehicle Design (DC, Keynote), SciFM25 (Ann Arbor), AIAA Aviation (Las Vegas), TPC25 (San Jose, Plenary), Allerton Conference (Champaign-Urbana), AI Work (Ann Arbor), Supercomputing 25, APS DFD (Houston, Plenary).
Online: AIAA Journal Keynote, DOE Basic Energy Sciences.

Colloquia

Robert W Courter Lecture (LSU), Special Seminar (Univ of Maryland).

Panels

- Creativity / Novelty / Emergence at SciFM25, Ann Arbor.

- National Ecosystem on AI for Science, Energy & Security at SciFM25, Ann Arbor.

- Vision 2030: Integrating Artificial Intelligence/Machine Learning and CFD, AIAA Aviation, Las Vegas.

- Industry/Government/Academia Ecosystem for AI, Trillion Parameter Consortium 2025, San Jose.

- Future of Science and Society in the Age of Artificial Superintelligence, Trillion Parameter Consortium 2025, San Jose.

- Accelerating Basic Research into Applied Innovation, MSU Research Foundation Data Science & AI Summit, East Lansing.

- Science behind the 2024 Nobel Prizes & role of AI, MICDE Nobel Prize Event, Ann Arbor.

- AI-enhanced Reasoning and Agentic Systems in Fluid Dynamics Research, APS DFD, Houston. Probably the first ever panel at DFD!

- Bay Area Campaign Council with Samir Kaul, Los Altos.

SciFM25: Scientific Discovery in the Age of AI

The second Conference on Foundation Models and AI Agents for Science (SciFM25), organized by MICDE, brought together more than 500 scientists and engineers from U-M and beyond at the end of May. Attendees were headlined by Thomas Mason (Director, Los Alamos National Lab), Paul Kearns (Director, Argonne National Lab), Bill Dally (SVP & Chief Scientist NVIDIA) and traded ideas on the foundations of generative AI, methods that can be applied now, avenues for improvement, ways to

integrate AI with other computational tools, and the future of AI in scientific discovery. Read more here.

This conference series has become the premier venue for in-depth discussions around the theory and applications of generative AI to scientific problems, and will be held in Chicago in 2025 (May 27–29).

A detailed summary can be found here and can be cited as: V. Kocevski & K. Duraisamy, *Summary of the 2nd conference on Foundation Models and AI Agents for Science,* MICDE Perspective Report, 2025.

The MICDE center for foundation models and AI agents for science scifm.ai is kicking into high gear and looking to actively contribute to DOE's Genesis mission and beyond.

Team Updates

1. Jasmin Lim completed her PhD

2. James Duvall and Pratik Raje completed their Post-doctoral fellowships

3. Ling Xiao is a new incoming student from General Motors, where he is a key part of the new Cadillac F1 team.

4. Internships: Noah Zambrano (Los Alamos), Moon Hazarika (Los Alamos), Sahil Bhola (Argonne), Daisuke Uchida (Mitsubishi Electric).

5. Karthik Duraisamy recognized with an endowed chair (Arthur B. Modine Professor of Engineering) and Fellowship of the American Physical society.

CASLAB team of 2025

Post Doctoral Fellows: James Duvall, Pratikkumar Raje.
PhD Students: Jasmin Lim, Niloy Gupta, Daisuke Uchida, Sahil Bhola, Noah Zambrano, Tony Zhuang, Amirpasha Hedayat, Moon Hazarika, Yi Han Toh, Curtis Maxon, Ling Xiao.
Lead: Karthik Duraisamy.

Prior CASLAB Newsletters

Newsletter from 2024
Newsletter from 2023
Newsletter from 2022
Newsletter from 2021
Newsletter from 2020
Newsletter from 2019
Newsletter from 2018
Newsletter from 2017

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