Computational Aerosciences Laboratory 2023 Highlights

2023 was a highly multi-dimensional year for CASLAB, and you can find a sparse and reduced order representation here. We waved farewell to four long-standing members and welcomed four new ones. Junior and Senior PhD students made major progress towards their dissertations with a long pipeline of publications. We played an important part in university and national level initiatives (some of the outcomes will be shared soon) and conducted workshops and short courses.



Snapshot of Publications & Preprints

Full list found on google scholar . We'll be uploading several preprints in the next couple of weeks.

1. CoCoGen: Physically-Consistent and Conditioned Score-based Generative Models for Forward and Inverse Problems C. Jacobsen, et al. arXiv:2312.10527: By incorporating discretized information into score-based generative models, CoCoGen generates samples closely aligned with the true data distribution. Conditioning is added so that these models generate PDE solutions by incorporating parameters, macroscopic quantities, or partial field measurements as guidance. CoCoGen is applied to several SciML tasks including surrogate modeling, probabilistic field reconstruction and inversion from sparse measurements.

- 2. Generative Artificial Intelligence Advisory Committee Report, K. Duraisamy et al. This is a publication of a different kind. To help navigate the unprecedented scale and speed of the impact of Generative AI, U-M established the Generative Artificial Intelligence Advisory (GAIA) Committee. The GAIA Committee developed an initial vision and recommendations towards the goal of ensuring that U-M is at the forefront in the responsible, ethical, legal, secure, equitable, accessible, and transparent development and use of GenAI in all aspects of our missions. The report was written in June '23. Also check out the website the committee put together.
- 3. Information Theoretic Clustering for Coarse-grained Modeling of Non-equilibrium Gas Dynamics, C. Jacobsen, et al.: We propose a machine learning framework informed by rate-distortion theory to learn optimal cluster assignments, aiming to improve the effectiveness of the coarsegraining process. The framework is end-to-end differentiable, facilitating backward pass gradient computation to flow through the ODE solve and probabilistic coarse-graining to train a classifier. We apply this technique to a 1D source quantization problem followed by the problem of isothermal relaxation of a $N_2 + N$ system with $O(10^4)$ degrees of freedom. We are making a round of revisions as per the journal review and will soon upload the preprint on arxiv.
- 4. Estimating global identifiability using conditional mutual information in a Bayesian framework, S Bhola, et al. Nature Scientific Reports: An information-theoretic approach is proposed to assess the global practical identifiability of Bayesian statistical models. The estimator has the following notable advantages: first, no controlled experiment or data is required to conduct the practical identifiability analysis; second, unlike popular variance-based global sensitivity analysis methods, different forms of uncertainties, such as model-form, parameter, or measurement can be taken into account; third, the identifiability analysis is global, and therefore independent of a realization of the parameters.
- 5. Extracting Koopman Operators for Prediction and Control of Non-linear Dynamics Using Twostage Learning and Oblique Projections, D Uchida, et al. arXiv preprint arXiv:2308.13051: Neural network-based modeling is proposed based on linear embedding with oblique projection, which is derived from a weak formulation of projection-based linear operator learning. We train the proposed model using a two-stage learning procedure, wherein the features and operators are initialized with orthogonal projection, followed by the main training process in which test functions characterizing the oblique projection are learned from data.
- 6. *Easy attention: A simple self-attention mechanism for Transformers, M Sanchis-Agudo, et al. arXiv:2308.12874.*: To improve the robustness of transformer neural networks used for temporal-dynamics prediction of chaotic systems, we propose an attention mechanism in which the scores are treated as learnable parameters. This approach produces good results when reconstructing and predicting the temporal dynamics of simple chaotic systems exhibiting more robustness and less complexity than the standard self attention architecture.
- 7. Predictive Reduced Order Modeling of Chaotic Multi-scale Problems Using Adaptively Sampled Projections, C Huang, et al. Journal of Computational Physics. : Finally in print. An adaptive projection-based formulation is presented for model-order reduction (and solver acceleration) of problems featuring chaotic and convection-dominant physics. A detailed analysis of the computational complexity is presented, and validated. *True* predictivity is demonstrated in highly complex reacting flows.

- 8. Design-Variable Hypernetworks for Flowfield Emulation and Shape Optimization of Compressor Airfoils, J Duvall, et al. AIAA Journal. : Design-variable hypernetworks, which are capable of learning from hetereogeneous snapshots of data (e.g.from different mesh topologies) provide continuous field predictions. These are used as emulators to predict parametric subsonic and transonic compressor flows in an industrial design use case. Some of the results (eg. Fig 18) certainly surprised us.
- 9. Towards Mixed-Fidelity Aero-Structural-Acoustic Optimization for Urban Air Mobility Vehicle Design, B Pacini et al. AIAA AVIATION. : This work details an aero-structural-acoustic optimization toolchain that utilizes multiple model fidelities, including hybrid blade element momentum theory, CFD, FEM and an aeroacoustic analogy. With this toolchain, this work presents gradient-based aero-structural-acoustic optimization, minimizing required flight power while ensuring structural integrity and respecting acoustic considerations. The toolchain is applied to the NASA tiltwing concept vehicle to optimize the wing and propeller designs, yielding a 17.8% reduction in required power for cruise flight while considering aerodynamic, structural, andacoustic constraints.
- 10. A unified understanding of scale-resolving simulations and near-wall modelling of turbulent flows using optimal finite-element projections, A Pradhan, et al. Journal of Fluid Mechanics : Taking a turbulent channel flow as an example, optimal finite element projections are used to assess the wall-resolved limit, the hybrid RANS–LES limit and the WMLES limit, via projections at different resolutions suitable for these approaches. We further characterise the slip velocity in WMLES in terms of the near-wall under-resolution and develop a universal scaling relationship which is verified in a posteriori tests. Guidance for the development of improved slip-wall models is provided, including a target for the dynamic procedure. A follow on paper is coming on using this for dynamic slip modeling in predictive LES.

Center of Excellence on Multi-fidelity Modeling of Rocket Combustor Dynamics

The center made it to six years! and is awaiting confirmation of a further two year extension. Meanwhile, we are pushing forth on adaptive ROMs and non-intrusive ROMs. We organized 2.5 day short course for Air Force (and DoD) researchers in Dayton in August. All of the slides (sans video) can be found here. A full list of publications can be found on the center website.

Conference/Invited Talks/Workshops

- 1. Conference presentations: AIAA Scitech (Washington, DC), AAAI (Washington, DC), SIAM CSE (Amsterdam), AIAA Aviation (San Diego), APS DFD (Washington, DC).
- 2. <u>Tutorial workshop on Mathematical and Statistical Foundations of Digital Twins</u>, Isaac Newton Institute, Cambridge University.
- 3. National Academies Workshop on Digital Twins. The slide on the next page shows at a high level our idea of what Digital Twins can be.
- 4. Workshop on Data-driven Analysis, Modeling and Control for Fluid Mechanics, Isaac Newton Institute, Cambridge University.
- 5. Short course on Model Order reduction for Complex Multi-scale problems at AFRL Dayton.

Туре	Outcome	Example	Decision/Cognitive ability
Level 0	Assist the 'designer'	High fidelity simulations	None
Level 1	Assist the 'user'	Numerical weather prediction	None
Level 2	Assist the `operator'	Predictive maintenance	Decision-support
Level 3	Empower the `manager'	Adaptively evolve parametrization	(high-value) Decision-making with confidence
Level 4	Assist the `organization'	Digitizing the entire product life cycle, adaptively evolve form	Designing, Planning and decision-making w/ confidence
Level 5	Empower the 'organization'	Causal reasoning, Collaboration, adaptively evolve behavior	Communicate, Plan, Consume knowledge
Level 6	Define the `organization'	Autonomously evolve digital form and behavior; generate knowledge	Define decisions, Create knowledge

Classes of digital twins based on decision/cognitive ability

* Not to be interpreted as levels of difficulty. e.g. level 0 may be harder than level 2 in some applications

- 6. Rigorous Reproducible Scientific Reasoning at University of Colorado, Boulder.
- 7. Colloquium talks at Johns Hopkins University (Baltimore) and Imperial College (London).
- 8. Also, Karthik gave at least 8 talks on the implications of Generative AI on various aspects of academia.

Career Transitions

- 1. Elnaz Rezaian began her career as a Research Scientist at KLA Tencor
- 2. Nicholas Arnold Medabalimi began his career as Computational Physicist at Lawrence Livermore National Laboratories
- 3. Chris Wentland began his career as Post doctoral fellow at Sandia National Laboratories
- 4. Mohit Tekriwal began his career as Post doctoral fellow at Lawrence Livermore National Laboratories

New members

- 1. Moon Bakaya Hazarika (PhD student): Moon got her Masters's degree in Aerospace Engineering at U-M.
- 2. Pratik Kumar Raje (Post doc fellow): Pratik got his PhD in Aerospace Engineering from IIT, Bombay.
- 3. Tony Zhuang (PhD student): Tony got his Bachelors in Chemical Engineering at Imperial College.

4. Amirpasha Hedayat (PhD student): Amir got his Masters in Mechanical Engineering from University of British Columbia.

CASLAB team of 2023

Post Doctoral Fellows: Elnaz Rezaian, Pratikkumar Raje.

PhD Students: Nicholas Arnold-Medabalimi, Christopher Wentland, James Duvall, Christian Jacobsen, Bernardo Pacini, Jasmin Lim, Niloy Gupta, Daisuke Uchida, Sahil Bhola, Noah Zambrano, Tony Zhuang, Amirpasha Hedayat.

Masters Students: Achu Shankar, Moon Bakaya Hazarika, Sai Charan Malladi, Malhar Prajapati. Affiliated PhD Students: Mohit Tekriwal (Aero), Brandon Lefleur (Nuclear). Lead: Karthik Duraisamy.

Prior CASLAB Newsletters

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. Here are the latest editions of the MICDE magazine

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