# Computational Aerosciences Laboratory
# 2021 Highlights

2021 started with the hope of a return to normalcy, and while we didn't quite get there, CASLAB did adapt to whatever version of normal that prevailed, and produced a number of high quality publications, organized symposia and workshops and released software. We started 3 new projects and gave a total of 27 talks in international conferences & symposia. It was also a 'moving' year [1] in the sense that two PhD students and two research fellows settled into their careers, and we just started a 12 month period in which we expect 6 students to defend their PhDs. [2] Most importantly, we stayed safe and healthy and supported each other. Literally, some times!

## Publication Samples

Below are a few samples and you can find the full list here. You may click on the underlined text for your reading pleasure. Apologies in advance for the extreme length of some of these papers - we did have a lot to say!

1. *Srivastava et al., Generalizable Physics-constrained Modeling using Learning and Inference assisted by Feature Space Engineering*: This is the centerpiece of Vishal's PhD work and the latest evolution in our quest to improve the predictive accuracy of physical models by learning generalizable augmentations from sparse data. The proposed approach, referred to as LIFE focuses on a meticulously-designed feature space that is informed by the underlying physics, and a carefully constructed features-to-augmentation map.

2. *Gouasmi et al., Entropy-Stable Schemes in the Low-Mach-Number Regime: Flux-Preconditioning, Entropy Breakdowns, and Entropy Transfers*: This is from a former CASLAB'er - i.e. the last part of Ayoub's PhD work. This work focuses on an in-depth look at the behavior

[1] I might also have to mention that Michigan finally beat Ohio State and won the Big Ten Championship for the first time in the history of CASLAB.

[2] All this while the lab director was on sabbatical. Perhaps he should petition the university for one more sabbatical year.

of Entropy Stable (ES) schemes for Compressible flows in the low mach number limit. ES is desirable from a global stability perspective, but Ayoub examines the behavior from a local standpoint. Popular preconditioners are studied for their implications on ES. The budget of entropy production is analyzed and it is hypothesized that accuracy degradation is caused by discrete entropy fluctuations that are inconsistent with those of the continuous system.

3. *Xu et al., Conditionally Parameterized, Discretization-Aware Neural Networks for Mesh-Based Modeling of Physical Systems* : We generalize the idea of conditional parameterization – using trainable functions of input parameters to generate the weights of a neural network, and extend them in a flexible way to encode critical information into the network architecture. The method is implemented on different networks and applied to several scientific machine learning tasks including the discovery of unmodeled physics, super-resolution of coarse fields, and the simulation of unsteady flows with chemical reactions.

4. *Duvall, et al., Non-linear Independent Dual System (NIDS) for Discretization-independent Surrogate Modeling over Complex Geometries* : We propose non-linear independent dual system (NIDS), which is a deep learning surrogate model for discretization-independent, continuous representation of PDE solutions, and can be used for prediction over domains with complex, variable geometries and mesh topologies. NIDS leverages implicit neural representations to develop a non-linear mapping between problem parameters and spatial coordinates to state predictions by combining evaluations of a case-wise parameter network and a point-wise spatial network in a linear output layer. NOTE: This is a surrogate representation of the *solution* and is different from the DeepONet, which attempts to represent the *operator*.

5. *Duraisamy, Variational Encoders and Autoencoders: Information-theoretic Inference and Closed-form Solutions* : This work develops problem statements related to encoders and autoencoders with the goal of elucidating variational formulations and establishing clear connections to information-theoretic concepts. Specifically, four problems with varying levels of input are considered : a) The data, likelihood and prior distributions are given, b) The data and likelihood are given; c) The data and prior are given; d) the data and the dimensionality of the parameters is specified. A linear Gaussian setting is adopted within a Variational Bayesian setting, and closed form solutions are derived.

## Symposiums/Workshops:

### Symposium on Model-Consistent Data-driven Turbulence Modeling : June 22/23/24

While much of the initial work in data-driven turbulence modeling has been devoted towards different ways of representing model discrepancies using machine learning, many recent efforts have recognized the importance of enforcing model consistency. In other words, the flow solver is integrated into the training process to promote consistency between the training and prediction environments. This symposium brought together experts and participants from academia, industry and national labs. The response was very enthusiastic, with 30 speakers and more than 200 participants. More details here.

**Workshop Panel on Data-Driven Modeling for Complex Fluid Physics, Scitech 2021**

Cheng, along with Dr. Munipalli (Edwards AFB) organized a panel moving towards a workshop on data-driven modeling for Complex Fluid Physics. The goal of this workshop is to establish benchmark problems/datasets and bring together the engineering and applied math communities to a) Guide the development of improved data-driven techniques to provide fast and accurate models for many-query applications in industry, and b) Establish a pathway to accelerate the transition of fundamental research in data-driven techniques to real industry applications. More details and an upcoming panel discussion can be found here.

## Center Updates:

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

The Center was renewed for a 5th year of research. The major goal of the center is to advance the science of ROMs with the overarching goal of application in full-scale rocket engines. This year, we made progress in improving the efficiency of intrusive ROMs using scalable sampling and adaptive basis methods. Non-intrusive ROMs of various kinds have also become viable. A full list of publications can be found here.

*Prototyping Environment for Reacting Flow Order Reduction Methods (PERFORM)* : Chris Wentland spearheaded the development of PERFORM, a combination of 1D compressible reacting flow solver and modular reduced-order model (ROM) framework, designed to provide a simple, easy-to-use test bed for members of the ROM community to quickly prototype and test new methods on challenging (yet computationally-manageable) reacting flow problems. Details here.

**Center for Data-driven Computational Physics**

A full list of projects can be found here.

## New projects:

**Physics-aware Reduced order modeling for Non-equlibrium plasma flows. Sponsor: DoD**

This project, in collaboration with Prof. Marco Panesi (UIUC) seeks to develop new adaptive reduced order modeling techniques for non-equilibrium Hypersonic flows. Our contributions will be in developing coarse graining descriptions at the Master equation level and in developing supervised and unsupervised learning at multiple scales.

**Hybrid Physics-Machine Learning Models for Electrodeposition Sponsor: Ford**

This project will develop and demonstrate probabilistic machine learning techniques and optimal experimental design to identify data-driven augmentations for unknown constitutive relationships in the electric field, deposition rate and film thickness/resistance equations. The learning will be achieved by using data from parallel plate experiments of electrodeposition. The outcome will help improve model predictive capability and better analysis of the e-coating process. This is in collaboration with Prof. Xun Huan (ME).

**SAFARI – Secure Automation for Advanced Reactor Innovation. Sponsor: ARPA-E** This center-scale project develops AI-enhanced digital twins of nuclear reactors. The PI of theproject is Prof. Annalisa Manera (UM Nuclear Engineering) and the project includes partners atArgonne National Lab, Idaho National Lab, and the engineering firms Kairos Power and CurtissWright. The team will validate and demonstrate their approach using the experimental flow loop. Then, the software will be used to optimize the design of the KairosPower fluoride-salt-cooled, high-temperature reactor. CASLAB's contribution will be on surrogate and reduced order modeling for

digital twins.

## Conference/Invited Talks

1. At Scitech '21, Chris presented a paper and Cheng organized a panel discussion
2. At SIAM CSE '21, Christian, Cheng, Elnaz, Chris, David and Karthik gave invited talks
3. At Aviation '21, Bernardo presented a paper
4. At USNCCM '21, James gave a talk on NIDS.
5. At APS DFD '21, Aniruddhe, Chris, Elnaz, Cheng, Nick, James and Vishal gave talks.
6. Mohit Tekriwal presented his paper at the NASA Formal methods symposium.
7. Karthik gave invited talks at Rice University, Houston; Turing Institute, London; and at Lawrence Livermore National Labs, CA.
8. Vishal gave an invited talk at NASA Langley.
9. Karthik gave a Keynote lecture at Euromech (Machine Learning for Prediction and Control of Fluid Flows), Paris; and a 'Distinguished lecture,' at the Canadian Nuclear Society conference on Generation IV & Small reactors.

## Awards

Behdad was recognized as a Gupta Values Scholar: This award is in recognition of 'integrity, commitment to human dignity, and dedication to excellence among graduate students at UM,' (2 awards/year of $7500 each for the entire university). Here is an article on Behdad's research.

## New members

1. Niloy Gupta (PhD student): Niloy is a double major in Aerospace Engineering & Applied mathematics from the University of Maryland.
2. Daisuke Uchida (PhD student): Daisuke has a Bachelors in Aerospace (Osaka) & Masters in Precision Engineering (U. Tokyo).
3. Mehdi Khalloufi (Post doctoral scholar ): Mehdi has a PhD in Computational Mechanics and Material Science, from Mines ParisTech & was formerly a post doctoral scholar at Duke.
4. Mohammad Amin Khodkar (Visiting Post doctoral scholar ): Amin has a PhD from UCSB and spent 4 months working with us on vortex instabilities.

## On the move

1. Cheng Huang (Assistant Research Scientist): Cheng joined the Dept. of Aerospace Engineering at the University of Kansas as an Assistant Professor in Fall 2021.
2. Behdad Davoudi (PhD student): Behdad defended his PhD in April and founded Watts Motors, Inc. (based in Raleigh, NC).

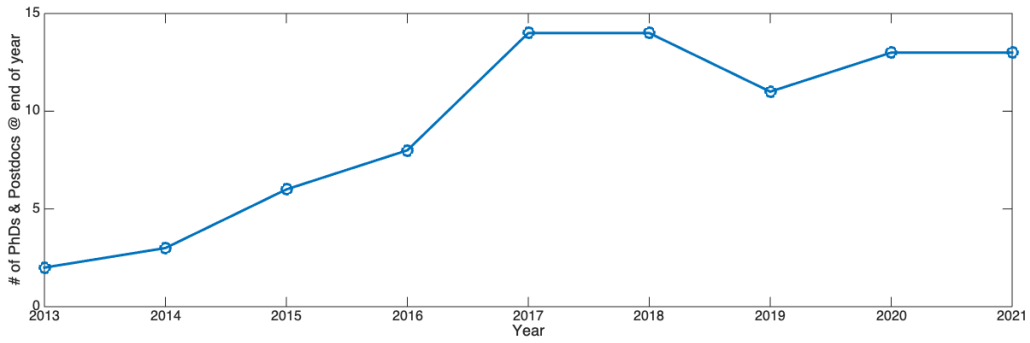
3. Jiayang Xu (PhD student): David defended his PhD in December and will start as a research scientist in Meta Reality Labs, Seattle, WA.

4. Rajarshi Biswas (Post doctoral fellow): Raj joined Cargill as a data scientist and is based in the Minneapolis-St. Paul area.

5. Ashish Nair (Masters student): Ashish joined the department of Mechanical Engineering at Notre Dame as a PhD student.

## CASLAB team of 2021

*Research Scientists:* Cheng Huang
*Post Doctoral Fellows:* Elnaz Rezaian, Rajarshi Biswas, Mehdi Khalloufi, Behdad Davoudi, Mohammad Amin Khodkar (Visiting).
*PhD Students:* Nicholas Arnold-Medabalimi, Jiayang Xu, Behdad Davoudi, Vishal Srivastava, Christopher Wentland, Aniruddhe Pradhan, James Duvall, Christian Jacobsen, Bernardo Pacini, Jasmin Lim, Niloy Gupta, Daisuke Uchida, Sahil Bhola.
*Affiliated PhD Students:* Mohit Tekriwal (Aero), Christiana Mavroyiakoumou (Applied Math), Brandon Lefleur (Nuclear).
*Lead:* Karthik Duraisamy.




Prior newsletters:
Newsletter from 2020
Newsletter from 2019
Newsletter from 2018
Newsletter from 2017

Visit us at `https://caslab.engin.umich.edu/`.