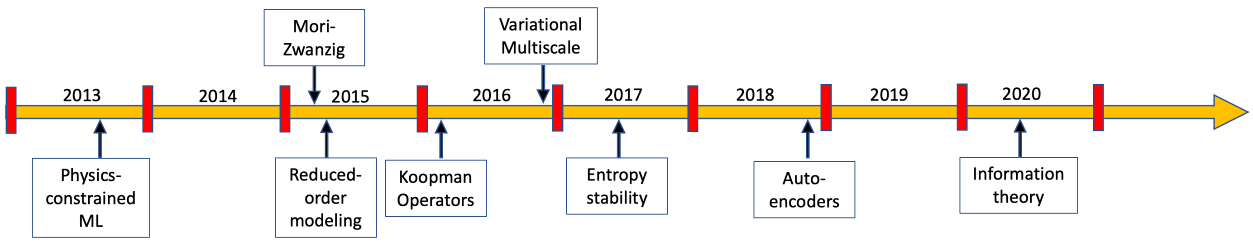
Computational Aerosciences Laboratory
2020 Highlights

2020 was a challenging, yet productive year for the group. As mentioned in the 2019 report, the journey began in 2013 with two PhD students, and here we are with 11 PhD students, a majority of whom started circa 2016-2018. In this regard, a number of students made critical progress towards their PhD degrees this year.

In terms of new research directions, we embarked on information theory. To place this in context, the figure below shows the starting points of some of the major research directions over the history of CASLAB.



Publication Samples

Below are a few samples. Full list is here. You may click on the underlined text for your reading pleasure.

1. *Model Reduction for Multi-Scale Transport Problems using Structure-Preserving Least-Squares Projections with Variable Transformation* : A reduced order modeling strategy is developed for highly non-linear problems with extreme scale disparity. Least-squares-based minimization is leveraged to guarantee symmetrization and discrete consistency with the full-order model (FOM) at the sub-iteration level. The approach allows for the selection of an arbitrary, but complete, set of solution variables while preserving the conservative form of the governing equations. Applications are presented in challenging combustion applications. Chris is also presenting a Scitech paper focused on scaling alone (and demonstrates 10000x speed up at a high level of accuracy).

2. *Sparsity-promoting algorithms for the discovery of informative Koopman invariant subspaces*: The Koopman decomposition is a non-linear generalization of eigen-decomposition, and is being increasingly utilized in the analysis of spatio-temporal dynamics. We propose a framework to extract informative Koopman invariant subspaces by removing redundant and spurious Koopman triplets. These algorithms can be viewed as sparsity promoting extensions of EDMD/KDMD. Demonstrations are performed in problems with very strong transient dynamics. Underlying physical mechanisms are analyzed, and a new type of mode - which we call as the oscillatory shift mode - is identified.

3. *Machine Learning-augmented Reynolds-averaged and Large Eddy Simulation Models of Turbulence : A Review and Perspectives* : Different approaches of applying supervised learning to represent unclosed terms, model discrepancies and sub-filter scales are discussed in the context of RANS and LES modeling. Particular emphasis is placed on the impact of

the training procedure on the consistency of ML augmentations with the underlying physical model. Techniques to promote model-consistent training, and to avoid the requirement of full fields of direct numerical simulation data are detailed. This is followed by a discussion of physics-informed and mathematical considerations on the choice of the feature space, and imposition of constraints on the ML model. The target audience for this paper is the fluid mechanics community, as well as the computational science and machine learning communities.

4. *Data-Driven discovery of Variational Multiscale Closures: A unified approach to sub-grid modeling and super-resolution*: This work proposes a Variational Multiscale Neural Network architecture that embeds physics-informed parameters and model forms in sub-scale closures for continuous and discontinuous Galerkin methods. The model is trained on on coarse and fine-scale data obtained by L_2-projection of high-fidelity data, and the super-resolved state is used to compute the flux.

5. *Sub-grid scale characterization and asymptotic behavior of multi-dimensional upwind schemes for the vorticity transport equations*: We establish the properties of a multi-dimensional upwind scheme for the vorticity transport equations in the under-resolved regime. The asymptotic behavior of key turbulence statistics of velocity gradients, vorticity, and invariants is studied in detail. The enstrophy budget highlights the remarkable ability of the truncation terms to mimic the true sub-grid scale dissipation and diffusion. The modified equation also reveals diffusive terms that are similar to several commonly employed sub-grid scale models including tensor-gradient and hyper-viscosity models.

Center Updates:

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

The Center which was initiated in April 2017 had another fruitful year. This is a collaboration with Profs. Willcox (UT Austin), Anderson (Purdue) and Peherstorfer (NYU).

The major goal of the center is to develop mathematically formal reduced order models of full-scale rocket engines that Airforce engineers can use in detailed design studies. Note that we will not have access to the full order simulations of the entire engine. Thus we established a multi-component ROM framework, where traditional geometry-specific training is replaced by the response generated by perturbing the characteristics at the boundary of the truncated component domains. The sub-component ROMs are then integrated as part of a multi-fidelity full system ROM. This year, we made major progress in ROM stability and accuracy, adaptive basis, and showed that non-intrusive (data-driven) reduced order models can be competitive with intrusive ROMs. A list of publications can be found here.

Center for Data-driven Computational Physics

The center for data-driven computational physics had another good year in terms of publications and impact. A full list of projects can be found here.

New projects:

MULTI-source LEarning-Accelerated Design of high-Efficiency multi-stage compRessor (MULTI-LEADER). Sponsor: ARPA-E

The goal of this project is to accelerate and augment the multi-disciplinary detailed design of a more energy-efficient multi-stage compressors, via machine learning, with considerations of aerodynamics, structures and additive manufacturability. This proposal addresses the following key design challenges: (1) concurrent optimization of multiple stages under many non-linear constraints; (2) multitude of evaluation of high-fidelity and expensive solvers and their gradients during optimization convergence in high-dimensional design; (3) multi-disciplinary design to maximize aerodynamic performance while guaranteeing structural integrity and additive manufacturability; (4) utilization of multiple fidelity of solvers with disparate parameterization and modeling assumptions. This is in collaboration with UTRC, Univ of Maryland and Univ of Pennsylvania.

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 the project is Prof. Annalisa Manera (UM Nuclear Engineering) and the project includes partners at Argonne National Lab, Idaho National Lab, and the engineering firms Kairos Power and Curtiss Wright. The team will validate and demonstrate their approach using the experimental flow loop. The loop runs molten salt as the coolant, emulating cooling loops inside an advanced reactor type called a molten salt reactor. Then, the software will be used to optimize the design of the Kairos Power fluoride-salt-cooled, high-temperature reactor.

Machine Learning for Cooling Pack Design Optimization for Electrified Vehicles. Sponsor: Ford

Machine learning methods will be applied to develop ROMs for front air inlet / cooling pack designs for electrified vehicles. The output will be a set of ODE's which can be easily incorporated into a system level model for design.

New members

1. Elnaz Rezaian (Post doctoral scholar): Elnaz finished her PhD in Kansas State University and worked on stabilization approaches in linear and non-linear reduced order models.

2. Jasmin Lim (PhD student): Jasmin finished her Bachelor's degree in computational engineering from UT Austin.

3. Sahil Bhola (Masters student): Sahil is working on adaptive ROMs.

On the move

1. Shaowu Pan (PhD student): Shaowu defended his PhD in December. Shaowu was prolific during his PhD and did leading edge work on operator theory and many other topics. He will join the University of Washington as a Post doctoral fellow.

CASLAB team in 2020

Research Scientists: Cheng Huang
Post Doctoral Fellows: Elnaz Rezaian, Rajarshi Biswas.
PhD Students: Nicholas Arnold-Medabalimi, Jiayang Xu, Behdad Davoudi, Shaowu Pan, Vishal Srivastava, Christopher Wentland, Aniruddhe Pradhan, James Duvall, Christian Jacobsen, Bernardo Pacini, Jasmin Lim.
Masters Students: Sahil Bhola, Ashish Nair.
Lead: Karthik Duraisamy.

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

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