Computational Aerosciences Laboratory
2019 Highlights

2019 was a great year for the group from many perspectives. Frankly, it is a bit difficult to believe that this group was established in 2013 with two fresh graduate students. For the first time, more than half the students are closer to the end of their PhD journeys than the beginning, and it shows! We managed to touch many aspects of predictive modeling at depth (also a note that we arent a "data-driven modeling group" :) . In short, some of our research became more fundamental and some of our research became more applied than in the past! We also saw the use of some of our ideas in the industry and at national labs.

Publication Samples

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

1. **Physics-informed Operator modeling:** *Physics-Informed Probabilistic Learning of Linear Embeddings of Non-linear Dynamics With Guaranteed Stability*: Shaowu's novel autoencoder architecture for the continuous Koopman decomposition that learns the residual of the dynamic mode decomposition (akin to res-nets). Physical and structural constraints are enforced in the network architecture, and uncertainty bounds are derived.

2. **Physically-constrained numerical modeling:** *A minimum entropy principle in the compressible multicomponent Euler equations* and *Formulation of Entropy-Stable schemes for the multicomponent compressible Euler equations*: Ayoub brings entropy stable methods to multi-component flows at great depth.

3. **Physical modeling:** *A Hybrid Blade Element Momentum Model for Flight Simulation of Rotary Wing Unmanned Aerial Vehicles*: Behdad's very neat idea for aerodynamic modeling of rotor performance that consistently combines Blade Element and Momentum theories with a linear inflow model, and can be executed in near-real time. Also, he conducted detailed physical experiments for validation. That's a first for CASLAB.

4. **Reduced-order modeling:** *The Adjoint Petrov-Galerkin Method for Non-Linear Model Reduction*: Eric and Chris developed a projection-based ROM using the Mori-Zwanzig formalism to derive a reduced-order representation of the coarse-scales. Theoretical analysis examining a priori error bounds and computational cost is presented along with numerical results.

5. **Data-driven modeling theory:** *On the Structure of Time-delay Embedding in Linear Models of Non-linear Dynamical Systems*: Shaowu presents analytical results on the minimal number of time delays required for perfect recovery of attractor dynamics using linear time delay embedding. This paper also explicitly shows that the underlying dynamics can be accurately recovered using only a partial period of trajectory data.

6. **Data-driven modeling applications:** *Multi-level Convolutional Autoencoder Networks for Parametric Prediction of Spatio-temporal Dynamics*: Jiayang presents our very first modeling paper from the dark-side (i.e. no physics constraints). Spatial and temporal autoencoders

are used to build compact non-linear latent spaces, and predictive results appear quite compelling.

7. **Turbulence modeling:** *Turbulence modeling in the age of data*: A review paper on recent developments in the use of data for turbulence modeling. Turned out to be the most cited Annual Review of Fluid Mechanics paper in 2019.

Center Updates:

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

The Center which was initiated in April 2017 had a very productive year. We were renewed for the second phase of the effort. 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. We demonstrated this framework for a 5-injector model combustor. We took major strides in improving the robustness of intrusive ROMs for reacting flows. Perhaps most importantly, we learnt many lessons regarding training dynamics, chaotic behavior, scaling, coupled/uncoupled formulations, limiting, hybridization, etc. We also initiated a new angle of research on hybrid & non-intrusive ROM approaches using multi-level convolutional autoencoder networks. A list of publications can be found here.

Center for Data-driven Computational Physics

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

The 4 year/ $3.5M NSF project that enabled Conflux concluded in November. This project established a hardware and software ecosystem at UM to support data-enabled modeling of complex physical problems, by enabling High Performance Computing (HPC) clusters to communicate seamlessly and at interactive speeds with data-intensive operations. Conflux is a unique resource that was designed with the view that computational physics and large-scale predictive modeling are natural allies whose tight integration would benefit the scientific endeavor greatly. On the software side, a new memory disaggregation protocol has been developed to pool together unused memory across the cluster to improve application-level performance and overall cluster memory utilization. A fast job switching and memory sharing routine has also been developed to achieve fine-grained GPU sharing among multiple distributed deep learning applications.

Conflux has been used in several applications of data-driven computational physics. Examples include materials modeling and discovery, turbulence modeling, hydrogen storage, cardiovascular modeling, repair and surgery planning. This research has resulted in several high impact journal publications, publicly available data respositories and software repositories. Conflux is now a well-established computing resource at the University of Michigan. It has been continuously utilized at high operational rates over the past 3 years by around 100 users from different parts of the campus as well as from other universities. A number of students have been exposed to the interface between HPC and machine learning. Further, workshops and courses have been conducted using Conflux.

Talks

1. At the *AIAA Scitech* conference in San Diego, Cheng, Jon, Adam and Ankit presented their papers.

2. At the *SIAM CSE* conference in Spokane, Yaser, Cheng, Jiayang, Shaowu, Ayoub, Aniruddhe and Karthik had invited presentations. We also organized a special session on Entropy Stable methods with Scott Murman (NASA).

3. Karthik gave a plenary lecture at the *ECCOMAS Computational Science and AI* Conference in Jyvaskyla, Finland.

4. At the *AIAA Aviation* conference in Dallas, Jon and Behdad presented their papers.

5. Karthik gave an invited talk at the *ENUMATH* conference in Egmond-an-Zee, Netherlands and ONERA, Paris.

6. At the *American Physical Society Fluids Meeting* in Seattle, Vishal, Danny, Nick, Shaowu, Jiayang and James gave talks. We also organized an extremely popular focus session (with Pedro Milani, Stanford) on data-driven modeling with 45 talks and an average audience of 250! Karthik gave an invited mini-symposium talk with 350+ attendees.

7. Karthik gave invited talks at Penn State, RPI, MIT (Data centric Engineering) and Univ of Washington (PIML).

8. Karthik was an invited speaker at a Digital twins for semi-conductors forum in San Jose.

New projects:

Data-driven fuel cell modeling for real time engine control. Sponsor: Toyota Motors, Inc. The goal of this research is to develop a data-driven real-time fuel cell modeling approach that is optimized for real-time operation aimed at direct market engine control unit implementation. We are using Field Inversion and Machine Learning (FIML) to improve the accuracy of fuel cell models. Once hardware is available, focused sets of real-world data will be used to refine the model. This is in collaboration with Dr. Jason Seigel, a Research Scientist in the ME department at UMich.

Artificial Intelligence guided multi-scale multi-physics framework for discovering complex emergent materials phenomena. Sponsor: DARPA This project targets the challenges in material physics associated with systematic attempts to abstract complexity from a hierarchy of scales into predictive model forms, and to delineate mechanisms of coupled materials physics. FIML is being applied to improve models based on density functional theory. Our part is on segmentation and learning algorithms to help convert microstructure images into useful data for inference. This is a larger project with Profs. Huan, Garikipati, Gorodetsky, Marquis and Gavini at UMich.

Visitors to/from CASLAB

1. Felix Kohler (PhD student at TU Darmstadt, Germany) visited us to collaborate on data-driven turbulence modeling.

2. Aniruddhe spent the summer at NASA Ames research center, working with Scott Murman's group on Discontinouous Galerkin methods.

3. Vishal spent time at NASA Langley giving tutorials and hands-on help on the implementation of data-driven turbulence modeling algorithms. Vishal did the same at CMSOFT Inc., Palo Alto.

4. Shaowu spent a week at Univ of Washington with Nathan Kutz and Steve Brunton.

5. Bernardo spent the summer at Airbus Silicon Valley, helping them with aeroacoustic modeling of their UAM vehicle.

New members

1. Bernardo Pacini (PhD student): Bernardo has a Bachelors in Mechanical & Aerospace Engineering from Princeton. His work is on distributed propulsion systems.

2. Christian Jacobsen (PhD student): Christian has a Bachelors in Mechanical Engineering from UC San Diego. He is currently exploring Variational Inference.

3. James Duvall (PhD Candidate) : James has a Bachelors in Mechanical Engineering from Colorado State. James research is on learning algorithms for unstructured data.

4. Rajarshi Biswas (Post-doctoral Fellow) : Rajarshi has a PhD in Aerospace Engineering from Iowa State. Rajarshis research is on turbulence modeling.

5. Ashish Nair (Masters student): Ashish is working on reduced order modeling on non-linear manifolds.

6. Rohan Vemula (Masters student): Rohan worked on data-driven modeling applied to automobile aerodynamics.

On the move

1. Ayoub Gouasmi (PhD student): Ayoub defended his PhD - a tour-de-force on entropy stability and will join NASA Ames Research Center.

2. Danny Foti (Post-doctoral Fellow): Danny is now an assistant professor close to his family at Univ of Memphis.

3. Yaser Afshar (Post-doctoral Fellow): Yaser is a research scientist at OPENKIM foundation in Minnesota, continuing his work on learning molecular potentials.

4. Rohan Vemula (Masters Student): Rohan graduated and joined ANSYS as a CFD developer.

5. Jonathan Holland (Co-advised PhD Student, Maryland): Jon defended his thesis and continued his job at Applied Physics Laboratories.

CASLAB team in 2019

Light font: Departing members; *Italics*: New members
Research Scientist: Cheng Huang
Post Doctoral Fellows: Daniel Foti, Yaser Afshar, *Rajarshi Biswas*.
PhD Students: Ayoub Gouasmi, Nicholas Arnold-Medabalimi, Jiayang Xu, Behdad Davoudi, Shaowu Pan, Vishal Srivastava, Christopher Wentland, Aniruddhe Pradhan, *James Duvall, Christian Jacobsen, Bernardo Pacini.*
Co-advised PhD Students: Mohit Tekriwal, Jonathan Holland (Maryland).
Masters Students: Rohan Vemula, *Ashish Nair*, Adam Comer.
Lead: Karthik Duraisamy.

Prior newsletters:
Newsletter from 2018
Newsletter from 2017

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