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RESEARCH COMPUTING
UNIVERSITY OF MICHIGAN

Advanced Research Computing Technology Services -- ARC-TS

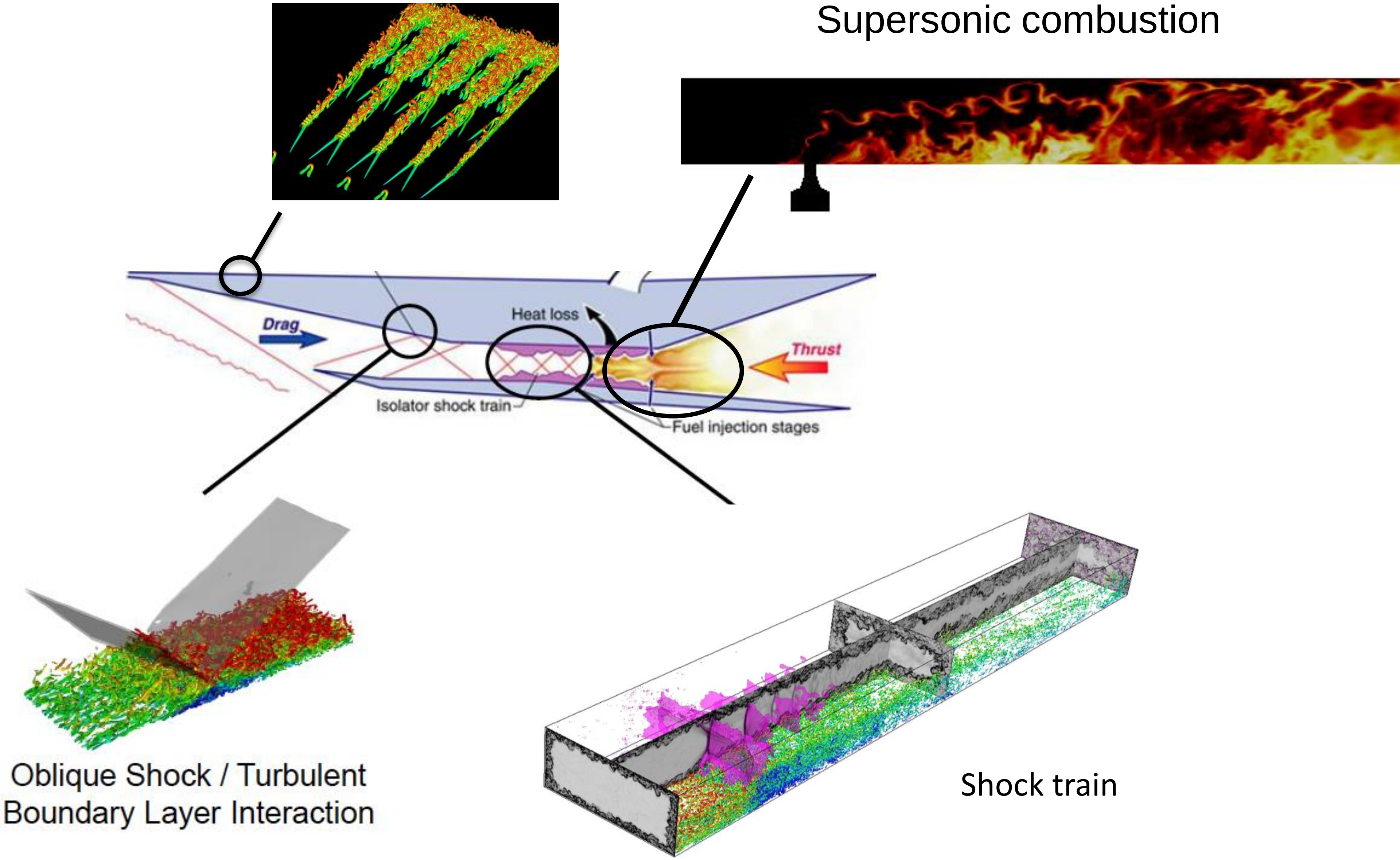
MICHIGAN INSTITUTE FOR COMPUTATIONAL DISCOVERY & ENGINEERING
UNIVERSITY OF MICHIGAN

Center for Data-Driven Computational Physics

Multiscale problems

Transitional boundary layer

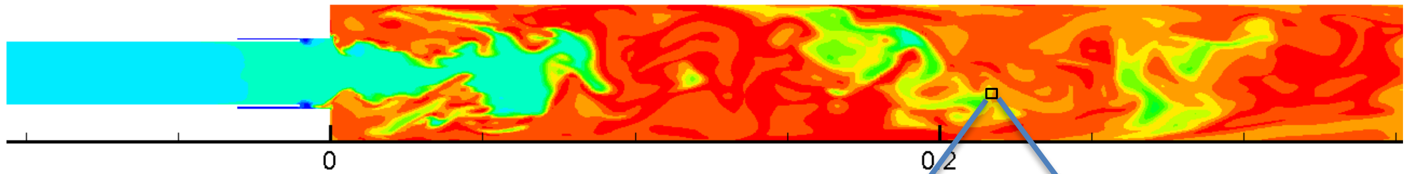
Supersonic combustion



Oblique Shock / Turbulent Boundary Layer Interaction

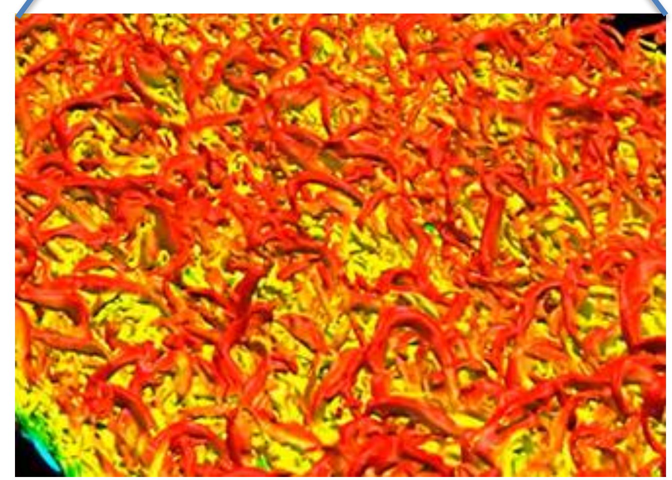
Shock train

Simulation of multiscale physics



Can compute

Macroscale model



Cannot compute everywhere

Microscale quantities

Closure problem

Macroscale model can only involve macroscale quantities

Professor Karthik Durasaimy (Aerospace Engineering)

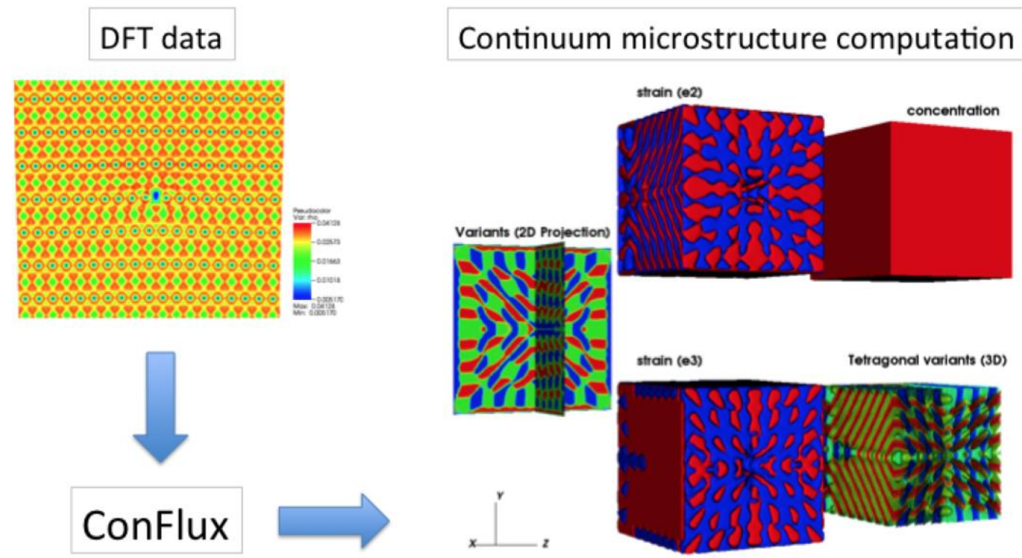
Materials Modeling

The goal is to identify, explain, predict and ultimately to design the properties and responses of these materials.

Hierarchical models have been developed at several scales

These methods have thus far provided insight and qualitative connections to parameters and phenomena from lower scales, but have not been predictive

Quantum Monte Carlo <-> Density Functional Theory <-> Continuum physics



Profs. Vikram Gavini and Krishna Garikipati (Mech Engineering and Materials Science)

Subject-specific blood flow modeling

Biggest challenges
- lack of physiologic data to inform the boundary conditions
- lack of data on mechanical properties of the vascular model

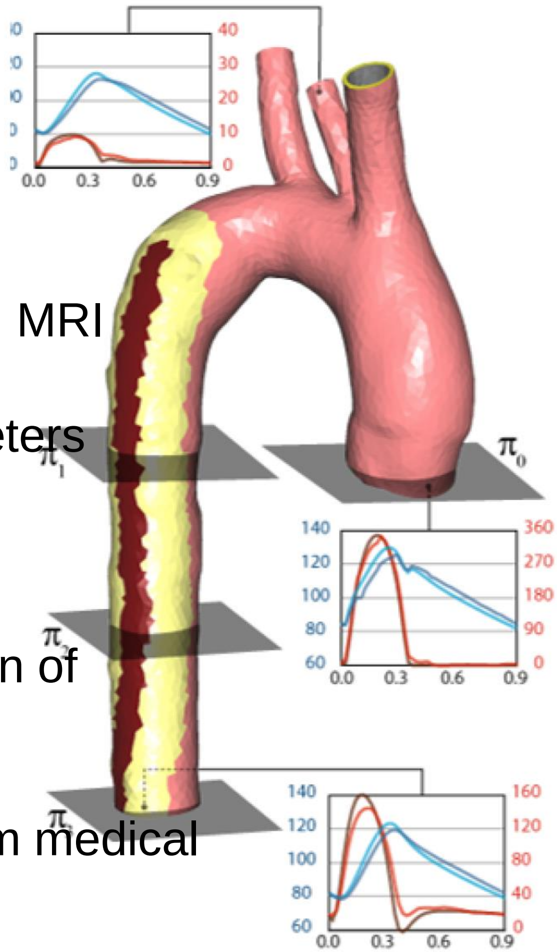
Obtain data from tomography and MRI

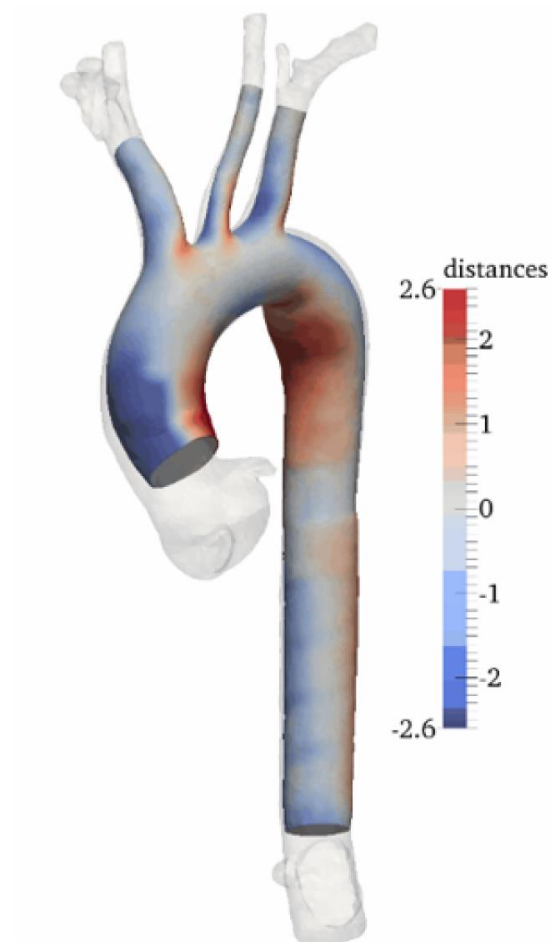
Solve inverse problem for parameters

Massive data size

On-the-fly Lagrangian computation of Motion

Evaluation of arterial stiffness from medical Images !





Prof. Alberto Figueroa (Biomedical Engineering & Surgery)

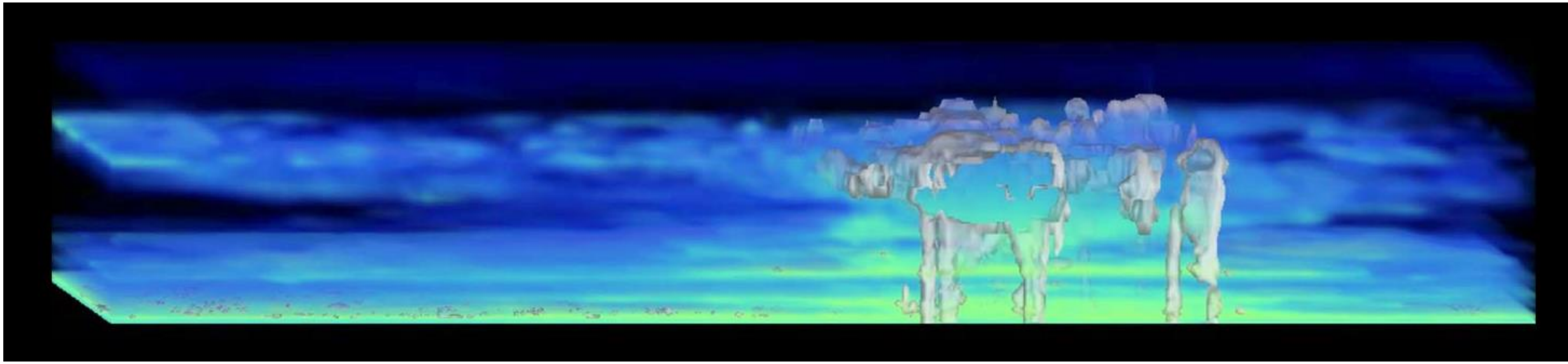
Climate system interactions

The Earth's climate system is composed of multiple interacting components that span spatial scales of 13 orders of magnitude and temporal scales that range from microseconds to centuries.

key responses and feed backs in the system are not well characterized

Understanding how clouds interact with the
larger scale circulation, thermodynamic state, and radiative balance is one of the most challenging problems

We use statistical inversion and machine learning to explore the interaction between changes in the Earths climate system and the radiative fluxes, circulation, and precipitation generated by large scale organized cloud systems.



Profs. Derek Posselt and Allison Steiner (Atmospheric Oceanic & Space Sciences)

Common problem:

Highly complex systems (many variables and often unknown relationship)

Multi-Scale (time and space)

Require extreme hi-resolution for accuracy in the details

Proposed approach to the problem

Merge Machine Learning with traditional HPC

Large scale data-driven simulations to enable accurate construction of models

“Infer” the modeling link between micro and macro scales

Procedure

Assembly — Collection of relevant / necessary data

Data

Inverse modeling — Extreme-scale optimization

Information

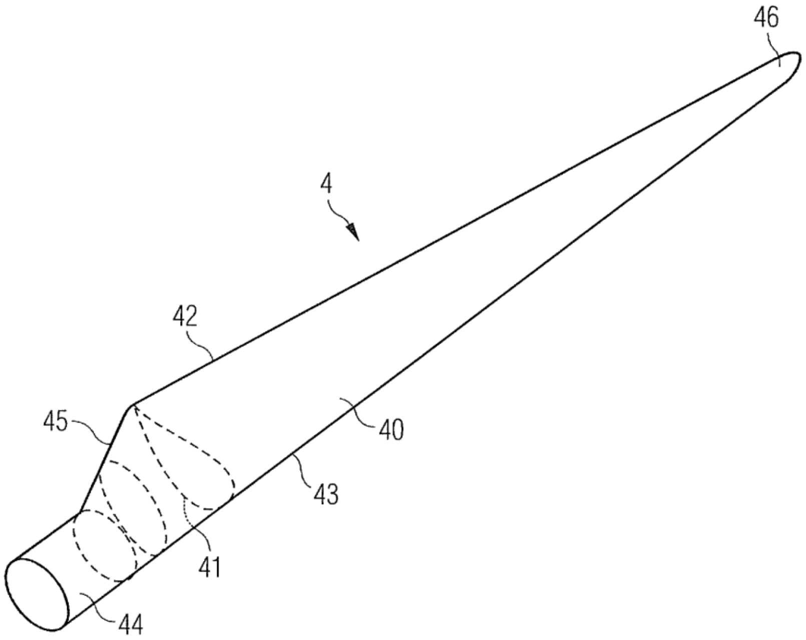
Machine Learning — Noisy, Complex, Extreme-scale data, feature set selection

Modeling Knowledge

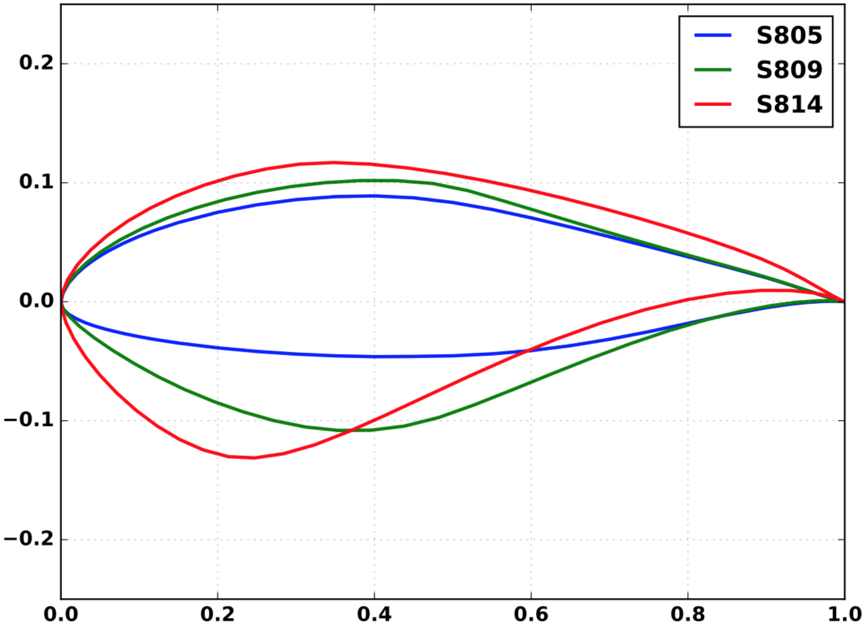
Embedding UQ and Computational Efficiency

Predictive capability

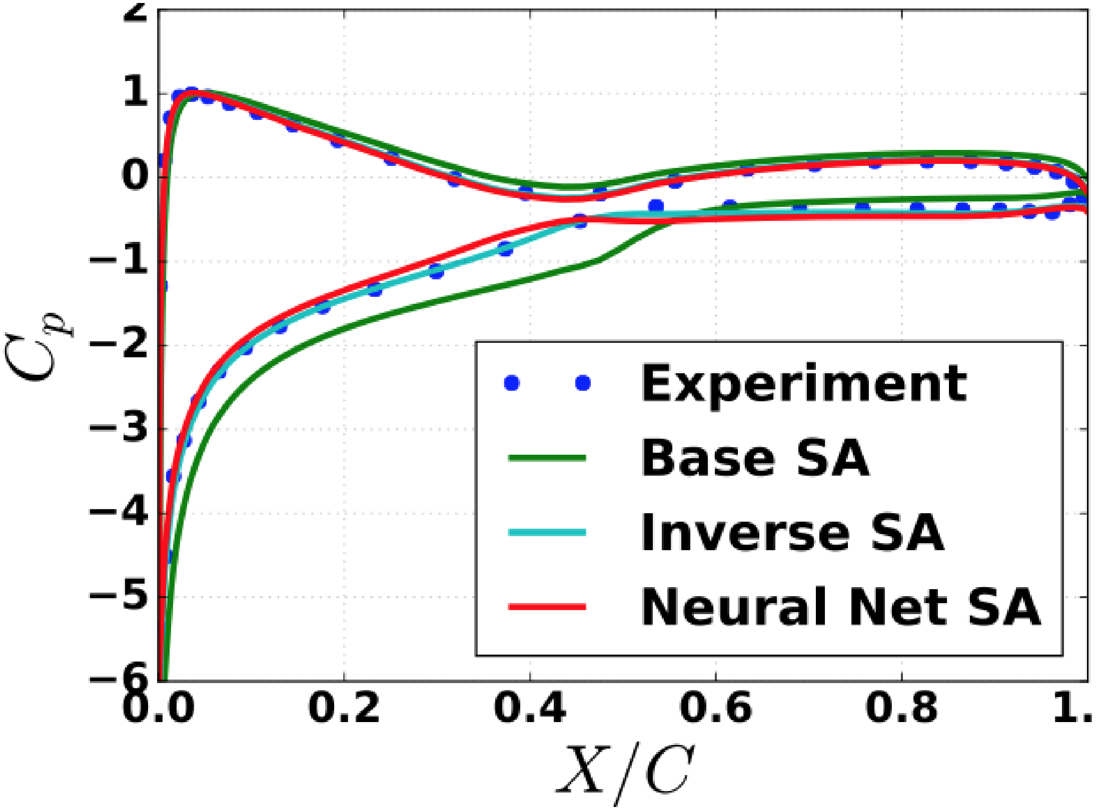
Example: Wind turbine predictions



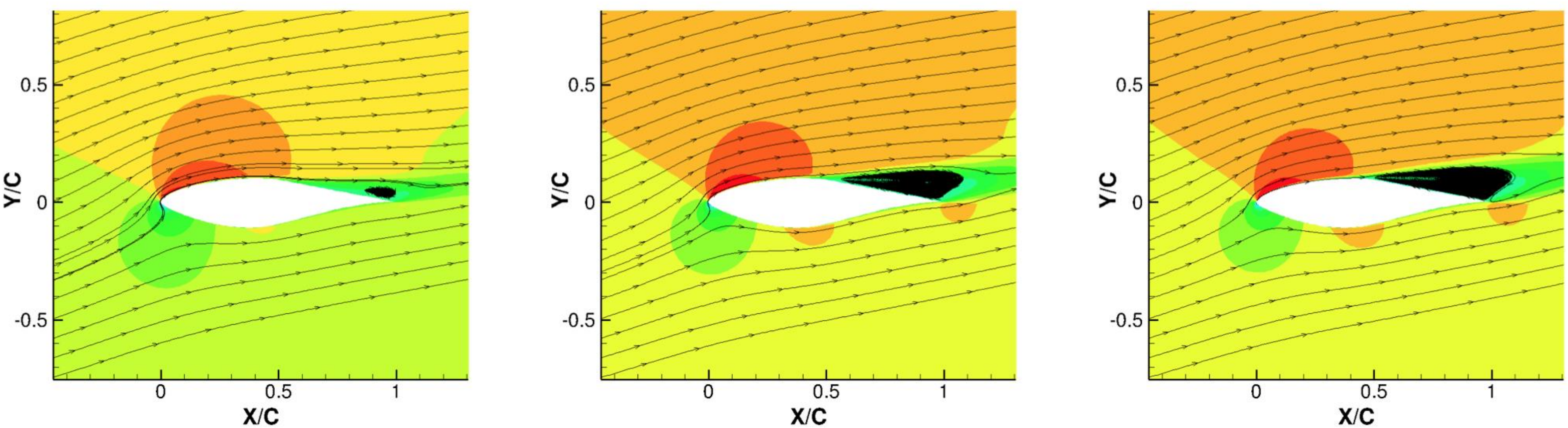
Get data from some blade shapes
Predict for other blade shapes



prediction !

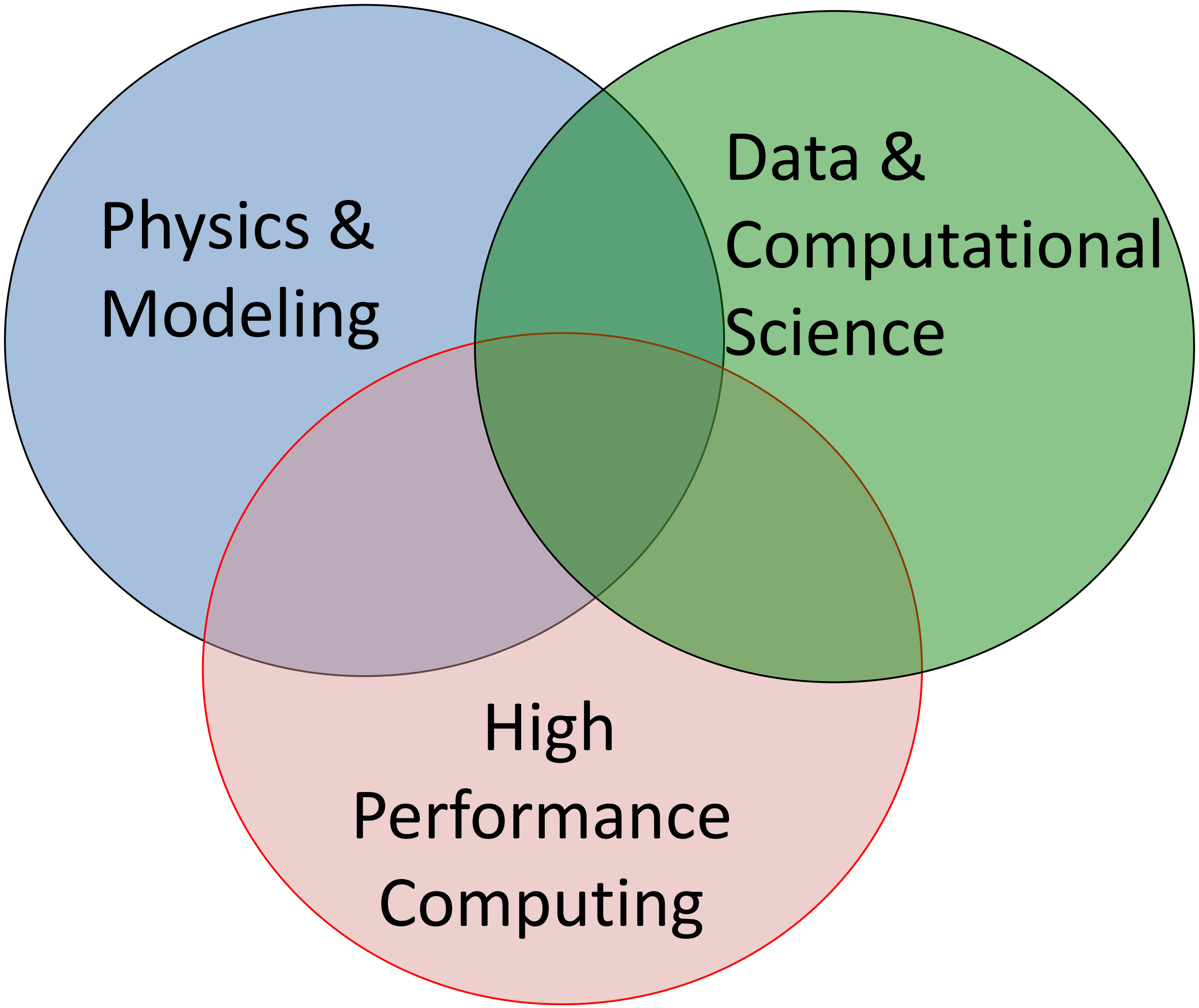


Singh, A., Medida, S. & Duraisamy, K., Data-augmented Predictive Modeling of Turbulent Separated Flows over Airfoils Submitted, AIAA Journal, 2016 (arXiv)



(a) Base SA (b) Inverse SA (c) NN-augmented SA (prediction)

What does it take ?



NSF funded PoC
What do we need ?

- ❑ Significant Computational Capability
  - CPU
  - GPU
- ❑ Extremely Fast Communication
  - Node ⟷ Node
  - CPU ⟷ GPU
  - GPU ⟷ GPU
- ❑ Flexible Storage
  - Large
  - Fast
  - Efficient Shared Filesystem
  - Can Handle HPC and Data Intensive Workloads

- ✓ Fast Multi-process/thread systems
- ✓ HPC & Big Data scheduling
- ✓ NVIDIA GPU (P100)

- ✓ ~100 Gb/s for High Speed Network
- ✓ NVIDIA NVLink

- ✓ ~1.5 PB growing to >3 PB over time
- ✓ HDFS Support

What we got from IBM

- 47 x POWER8 S822LC Systems
- 15 x POWER8 S822LC with 4 x NVIDIA P100 & NVLink
- 100 Gb/s EDR Infiniband non-blocking fat-tree
- CAPI
- Elastic Storage Server
- Spectrum Scale
- Platform LSF

What we learned so far

- Power8 is ~ 2-3 x faster for most of our code
  - Intel Centric
  - Special options for PPC (MASS, ESSL)
- SMT8 is a real thing, but ...
- Just now trying the P100s and NVLink –> **fast**!