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)
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 feedbacks 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 Earth's climate system and the radiative fluxes, circulation, and precipitation generated by large scale organized cloud systems.
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

“Inf"er” the modeling link between micro and macro scales
Procedure

Data
  ↓
Assembly

Information
  ↓
Inverse modeling

Modeling
  ↓
Machine Learning

Knowledge
  ↓
Embedding
Predictive capability

Collection of relevant / necessary data
Extreme-scale optimization
Noisy, Complex, Extreme-scale data, feature set selection
UQ and Computational Efficiency
Example: Wind turbine predictions

Get data from some blade shapes
Predict for other blade shapes

![Graph showing Cp vs X/C with legend: Experiment, Base SA, Inverse SA, Neural Net SA.](image1)

(a) Base SA  
(b) Inverse SA  
(c) NN-augmented SA (prediction)
What does it take?

Physics & Modeling

Data & Computational Science

High Performance Computing
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!