

Successes and Challenges for Machine Learning at Sandia National Laboratories



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Accelerating calculations of full-field fluid flow for fragment drag coefficient via physics-informed machine learning (ML) models

Simplified problem: Predict the flow field around rectangles flying at Mach 5

Work in progress: 3D version with real fragment geometries

Time to solution significantly reduced

- >100x faster on 2D
- >1000x faster on 3D

2D force	Avg Relative Error
Drag	1.87%
Lift	5.63%
Torque	2.29%

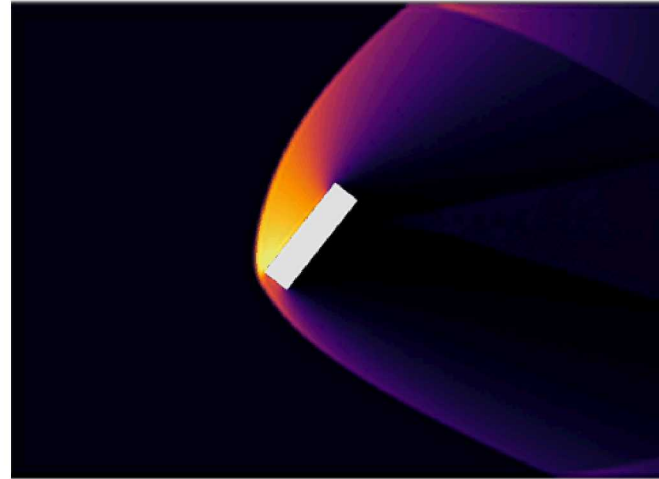
Model successfully predicted flow field and aerodynamic coefficients of simplified fragment model.

Contact:

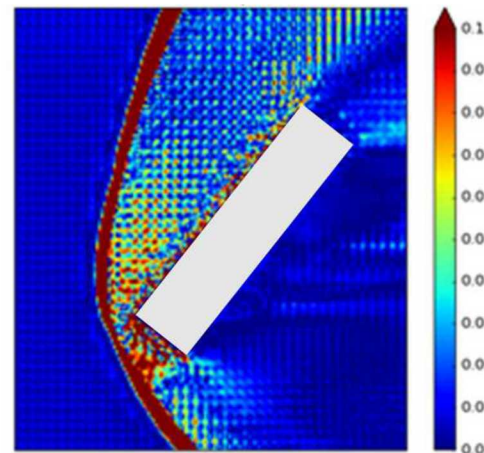
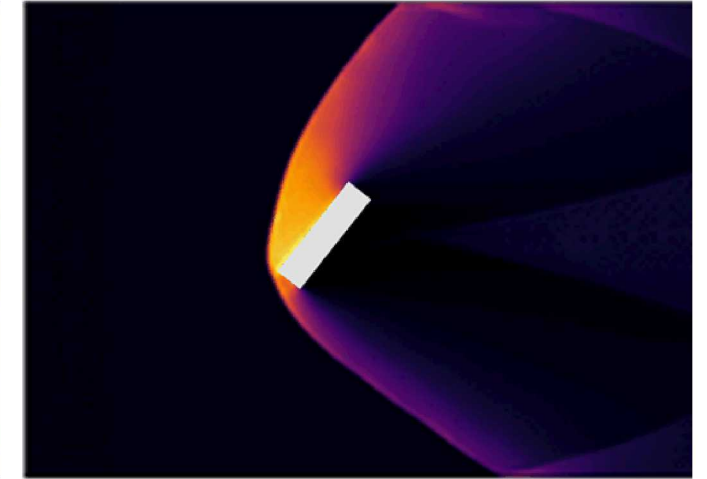
Sandia Interdisciplinary Machine Learning team (simlr@sandia.gov)

Slide courtesy Emily Donahue (eadonah@sandia.gov)

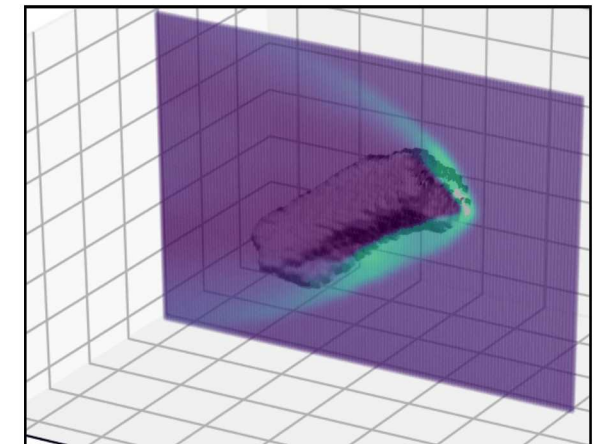
High Fidelity Simulation Pressure



ML Pressure Prediction



Relative error map of 2D ML prediction



ML predicts pressure field of complex 3D fragment

HPC Storage Systems Aren't Ready

Coming Platforms for Combined Analytics/ML and Simulation

- Burst buffers are going to be obsolete
- Workload interference is real, and will have outsized impacts

Inflection Point in I/O and ML Performance

- Inefficiencies have nowhere to hide

I/O Characterization for ML is Incomplete

- What will an ML workload look like? We can't know.
- Current ML workloads aren't comparable to simulation workloads
- N-to-1, N-to-M, ... 1-to-N?



Frustration