Turbulence Simulation: Methods, Modeling, and Data to Glean Physics/Engineering Insight

Kenneth E. Jansen

Post-tenure Review
January 28th, 2019

To Compute Turbulence or to Model It, That is the Research Question

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Conceptualizing FDSI: Fluid Dynamics Software Infrastructure

A Sustainable Software Institute for the Analysis of Fluid Dynamics Data from Experiments and Computation

Support from NSF under the Software Infrastructure for Sustained Innovation: S2I2 Conceptualization -- 18 months of workshop support to engage a community in conceptualizing a software institute.
Award #1743178, Program Manager Stephan Robila

Ann and H.J. Smead Aerospace Engineering
UNIVERSITY OF COLORADO **BOULDER**

Management Team

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- Kurt K. Maute

University of Colorado Boulder

- Onkar Sahni
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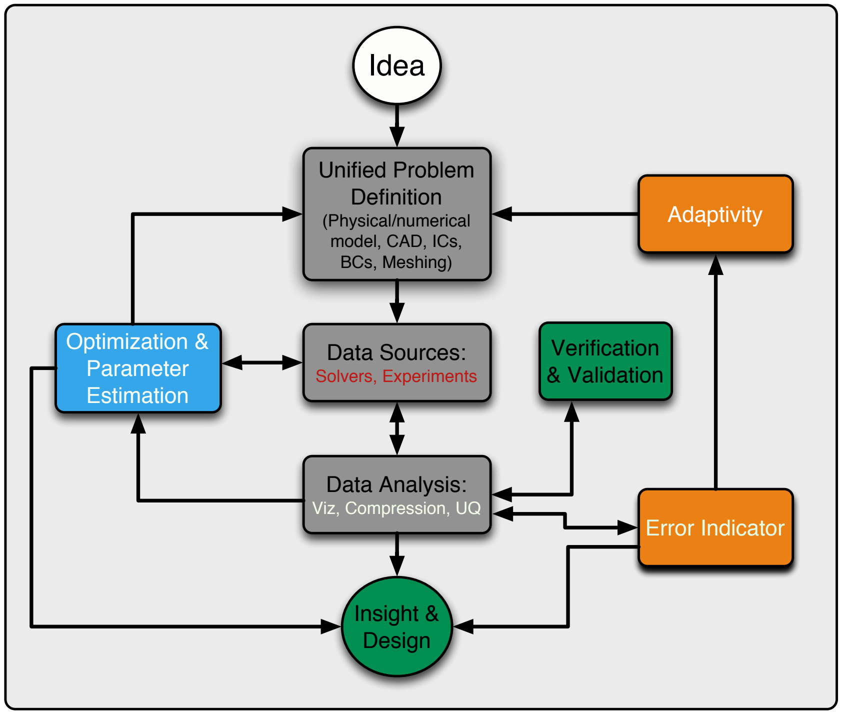
Rensselaer

Pre-Conceptualization Vision of Software Infrastructure Components



Aurora Early Science Program

The Aurora Early Science Program will prepare key applications for Aurora's scale and architecture, and will solidify libraries and infrastructure to pave the way for other production applications to run on the system.

The program has selected 15 projects, proposed by investigator-led teams from universities and national labs and covering a wide range of scientific areas and numerical methods.

In collaboration with experts from Intel and Cray, ALCF staff will train the teams on the Aurora hardware design and how to program it. This includes not only code migration and optimization, but also mapping the complex workflows of data-focused, deep learning, and crosscutting applications. The facility will publish technical reports that detail the techniques used to prepare the applications for the new system.

In addition to fostering application readiness for the future supercomputer, the Early Science Program allows researchers to pursue innovative computational science campaigns not possible on today's leadership-class supercomputers.

Aurora ESP Projects

The combination of simulation, data science, and machine learning will transform how supercomputers are used for scientific discovery and innovation.

Simulation Co-PIs CO:
Jed Brown CS
John Evans
John Farnsworth
Philippe Spalart

Simulation

Extending Moore's Law Computing with Quantum Monte Carlo
PI: Anouar Benali, Argonne National Laboratory
DOMAIN: Materials Science

High-Fidelity Simulation of Fusion Reactor Boundary Plasmas
PI: C.S. Chang, Princeton Plasma Physics Laboratory
DOMAIN: Physics

NWChemEx: Tackling Chemical, Materials, and Biochemical Challenges in the Exascale Era
PI: Thomas Dunning, Pacific Northwest National Laboratory
DOMAIN: Chemistry

Extreme-Scale Cosmological Hydrodynamics
PI: Katrin Heitmann, Argonne National Laboratory
DOMAIN: Physics

Extreme-Scale Unstructured Adaptive CFD
PI: Kenneth Jansen, University of Colorado at Boulder
DOMAIN: Engineering

Data

Exascale Computational Catalysis
PI: David Bross, Argonne National Laboratory
DOMAIN: Chemistry

Dark Sky Mining
PI: Salman Habib, Argonne National Laboratory
DOMAIN: Physics

Data Analytics and Machine Learning for Exascale Computational Fluid Dynamics
PI: Ken Jansen, University of Colorado Boulder
DOMAIN: Engineering

Simulating and Learning in the ATLAS Detector at the Exascale
PI: James Proudfoot, Argonne National Laboratory
DOMAIN: Physics

Extreme-Scale In-Situ Visualization and Analysis of Fluid-Structure-Interaction Simulations
PI: Amanda Randles, Duke University and Oak Ridge National Laboratory
DOMAIN: Biological Sciences

Learning

Machine Learning for Lattice Quantum Chromodynamics
PI: William Detmold, Massachusetts Institute of Technology
DOMAIN: Physics

Enabling Connectomics at Exascale to Facilitate Discoveries in Neuroscience
PI: Nicola Ferrier, Argonne National Laboratory
DOMAIN: Biological Sciences

Many-Body Perturbation Theory Meets Machine Learning to Discover Singlet Fission Materials
PI: Noa Marom, Carnegie Mellon University
DOMAIN: Materials Science

Virtual Drug Response Prediction
PI: Rick Stevens, Argonne National Laboratory
DOMAIN: Biological Science

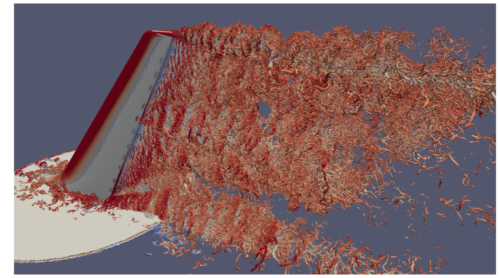
Accelerated Deep Learning Discovery in Fusion Energy Science
PI: William Tang, Princeton Plasma Physics Laboratory
DOMAIN: Physics

Data Co-PIs CO:
Stephen Becker APPM
Jed Brown CS
Alireza Doostan
John Evans
John Farnsworth
Philippe Spalart

https://aurora.alcf.anl.gov

Argonne NATIONAL LABORATORY

in situ Visualization Unlocks Unsteady Dynamics at Extreme Scale on Xeon PHI KNL 5B elements on 128Ki cores



Scientific Achievement

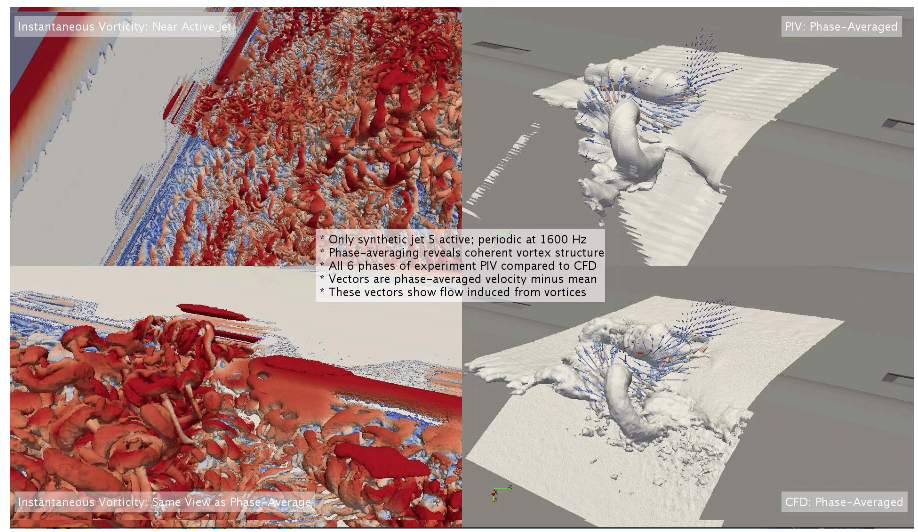
Unsteady synthetic jet flow control simulations create data streams so large that dynamics are only practical to access with *in situ* visualization.

Significance and Impact

***in situ* visualization allows dynamic comparison of instantaneous vortical structures with phase averaged quantities from experiment (PIV) and simulation. Animations of images help engineers understand how jets improve flow and scale that improvement to flight/turbine conditions.**

Details

- **Catalyst compiled into PHASTA, provides isosurfaces at every time step at 3% overhead to simulation- far less than writing full data.**
- **Communication of parameter changes back to simulation (computational steering) in progress.**



Comparison to experimental results.

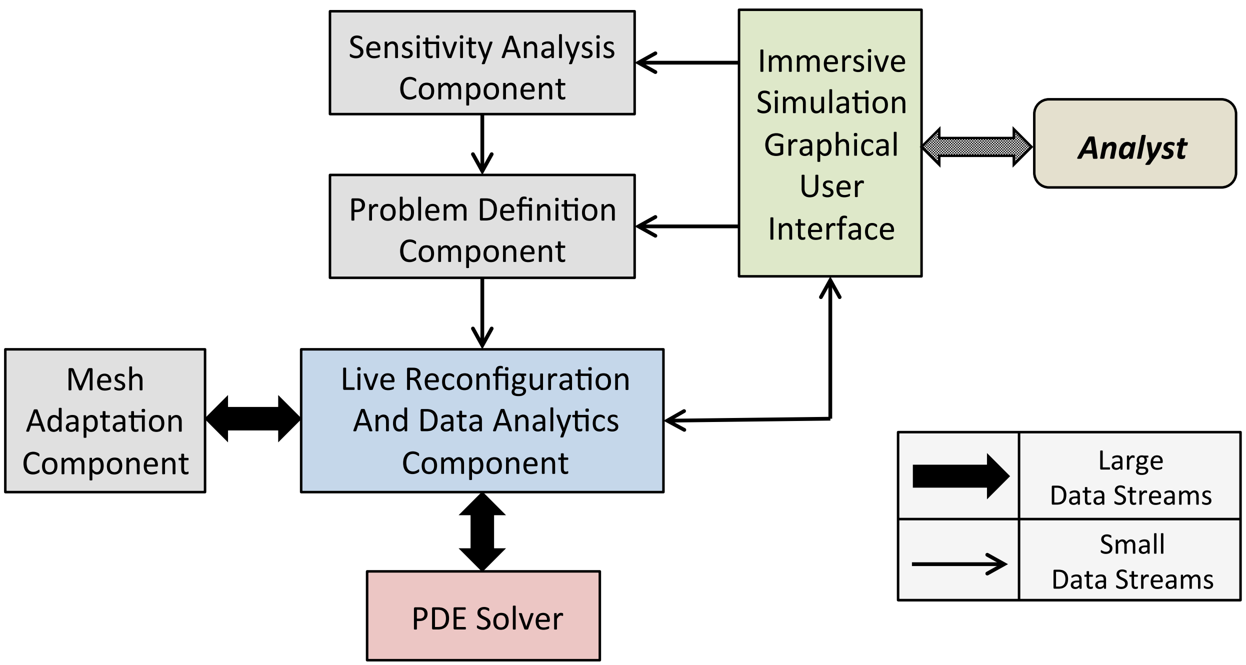
Ann and H.J. Smead Aerospace Engineering
UNIVERSITY OF COLORADO BOULDER

LLNL Subcontract **B626938 of**
Prime DE-AC52-07NA27344 from DOE: PI Lori Diachen

SI2-SSE: Software Elements to Enable Immersive Simulation

Kenneth Jansen, John A. Evans, Alireza Doostan, Kurt Maute,

Students: Corey Nelson and Felix Newberry



Award #1740330,
Program Manager
Stephan Robila

CDS&E: A Data-centric Approach to Turbulence Simulation

Kenneth Jansen, John A. Evans, Alireza Doostan and Philippe Spalart

Students: Riccardo Balin, Eric Peters, and Ryan Skinner[1]

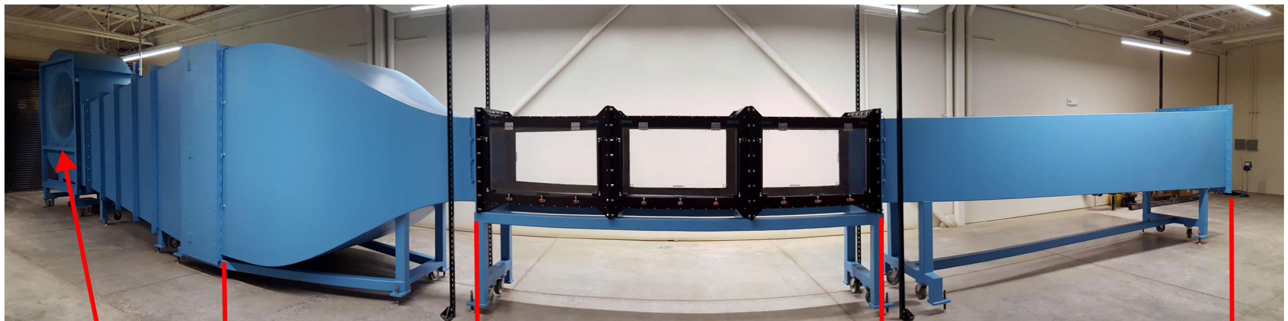
- Leverage Multi-Fidelity Modeling (MFM) to increase the efficiency of design space exploration
- Enhance low fidelity modeling (LFM) with the use of machine learning (ML) to better inform turbulence modeling closures such as RANS
- Couple MFM with ML to more accurately uncover trends present in the design space
- Contribute to the understanding and direct numerical simulation (DNS) data base of separating turbulent boundary layers with very high-fidelity simulations

Award #1710670,
Program Manager
Dr. Ron Joslin

(1) Ryan Skinner supported under a NDSEG fellowship in related work

A Coordinated Experimental and Computational Study of Global and Convective Gusts on Swept Wings

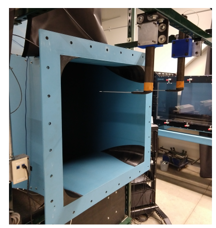
John Farnsworth (PI) and Kenneth Jansen (Co-PI)

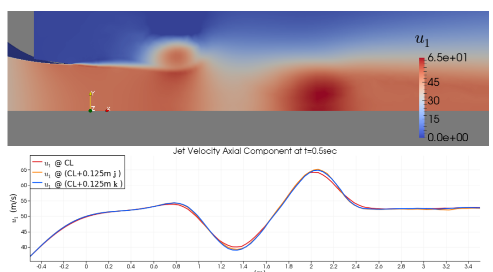


Fan Inlet Contraction Test-Section Diffuser

Closed Tunnel
+
Louvers
= Global Gust

- Test section
= Free Jet with Convective Gusts





Award #FA9550-18-1-0311
Program Manager: Dr. Doug Smith
transitioned to Dr. Gregg Abate

Effects of wall curvature on hypersonic turbulent spatially-developing boundary layers

Guillermo Araya[1] and Kenneth Jansen[2]

[1]Department of Mechanical Engineering, University of Puerto Rico at Mayaguez (UPRM), PR 00681

[2]Department of Aerospace Engineering Sciences, University of Colorado at Boulder (UCB), CO 80309

Award #FA9550-17-1-0051

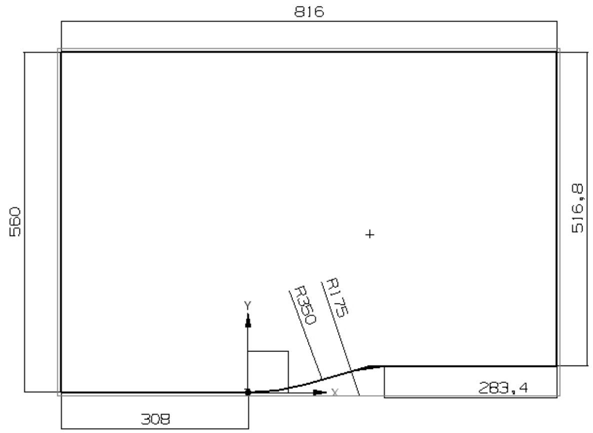
Program Manager: Dr. Ivett Leyva

Project Background

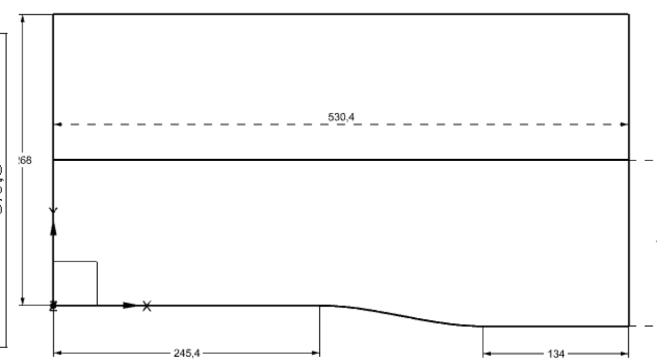
Spatially-developing turbulent boundary layers (SDTBL) are ubiquitous.

Computational challenges

- ✓ Time-dependent inflow turbulence information.
- ✓ Flow compressibility.
- ✓ Wall-curvature driven pressure gradient.



Concave wall, $M_\infty = 2.86$, Donovan et al. (JFM, 259, 1994)



Convex wall, $M_\infty = 4.9$, Tichenor et al. (JFM, 722, 2013)

Summary: Investigate concave/convex wall curvature on supersonic/hypersonic SDTBL (Mach numbers up to 5) in a suite of high spatial/temporal resolution Direct Numerical Simulation (DNS) as well as Wall Resolved Large Eddy Simulation (LES) at experimental Reynolds numbers.

Research Objectives: The extensive information supplied by DNS will be used to evaluate the downstream influence of concave (adverse pressure gradient) and convex (favorable pressure gradient) wall curvatures on:
(i) Low/high order statistics of flow parameters, particularly on the thermal transport.
(ii) Coherent structures.
Additionally, the DNS database will be employed on the improvement of sub-grid scale (SGS) turbulence models for the LES approach.

Improving the Accuracy and Efficiency of Scale-Resolving Simulations for Favorable and Adverse Pressure Gradient Flows

Kenneth E. Jansen, John Evans,
University of Colorado, Boulder

Philippe R. Spalart
The Boeing Company

Students: Riccardo Balin, Corey Nelson and John Patterson

Grant Number: 80NSSC18M0147
Program Manager:
Dr. Christopher Rumsey

Overview of PHASTA CFD Solver

- Massively parallel MPI Navier-Stokes flow solver
- Models compressible or incompressible, turbulent, unsteady flows
- Finite element discretization in space => Complex geometries
- Accuracy h^{k+1}; k=polynomial order, e.g., k=1 linear, 2nd order accurate
- Minimally dissipative stabilization key to scale-resolving turbulence
- Fully implicit in time => Δt governed by the physics
- Mesh adaptivity => - Grid matches physical scale
  - Anisotropic (boundary and shear layers)
- Variety of scale resolving (DNS, LES), turbulence models (RANS), and hybrids (DES, DDES, IDDES).
- Parallel scaling to 768K cores and 3.1M MPI instances
- Applied to a number of flows that demonstrate the progress but additional need for improved scale-resolving simulations