Leveraging Argonne Computing Facilities and Expertise for Industry Challenges

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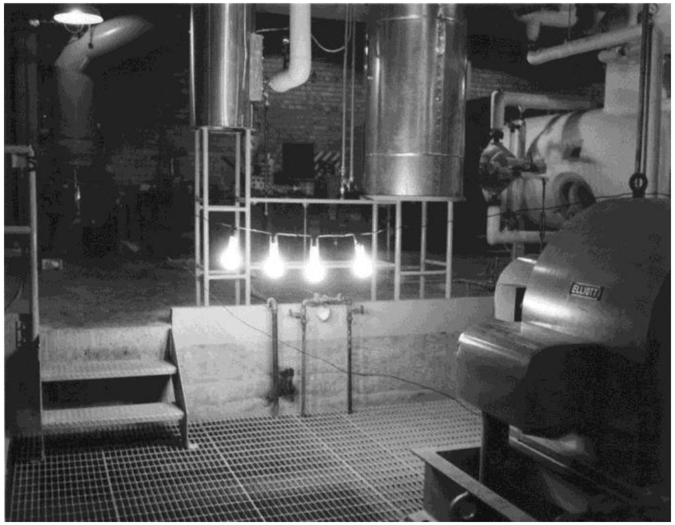
VERIFI Workshop

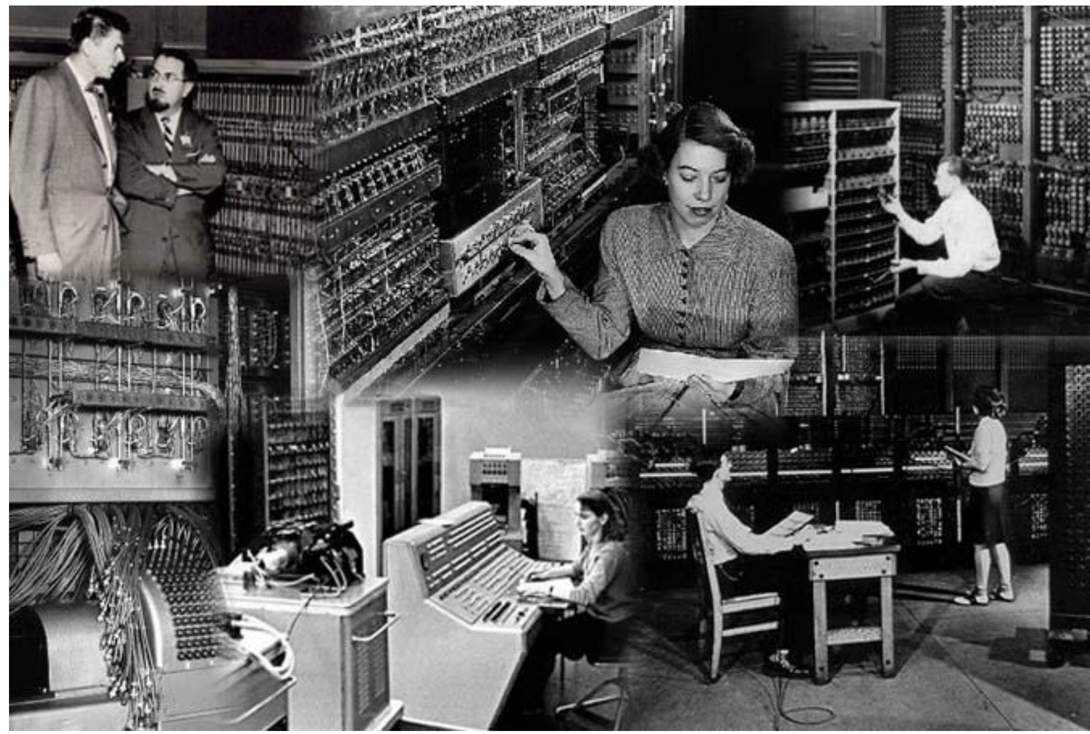
November 12, 2014

Argonne’s History

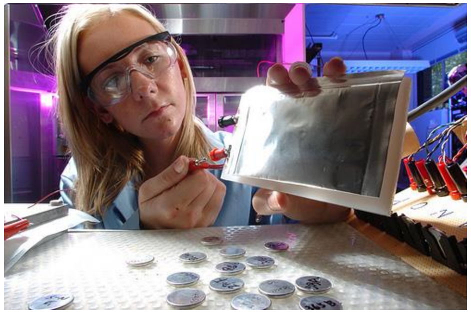


The world’s first usable amount of electricity from nuclear energy was produced by Experimental Breeder Reactor 1 in Southeastern Idaho and used to light these four light bulbs on December 21, 1951.

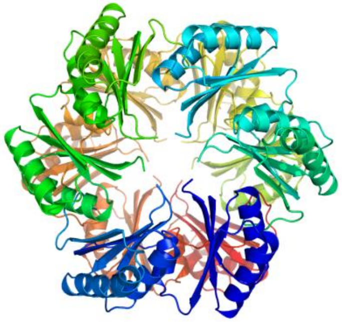
AVIDAC, Argonne’s first digital computer, began operation in January 1953. It was built by the Physics Division for $250,000. Pictured is pioneer Argonne computer scientist Jean F. Hall.



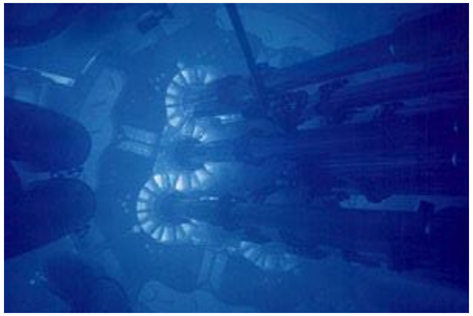
Argonne: Science-based Solutions to Global Challenges



Energy production, conversion, storage and use



Environmental Sustainability

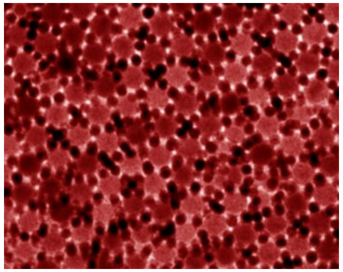


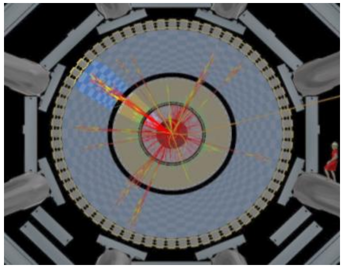
National Security

Use-inspired science and engineering…

… Discovery and transformational science and engineering

Major User Facilities

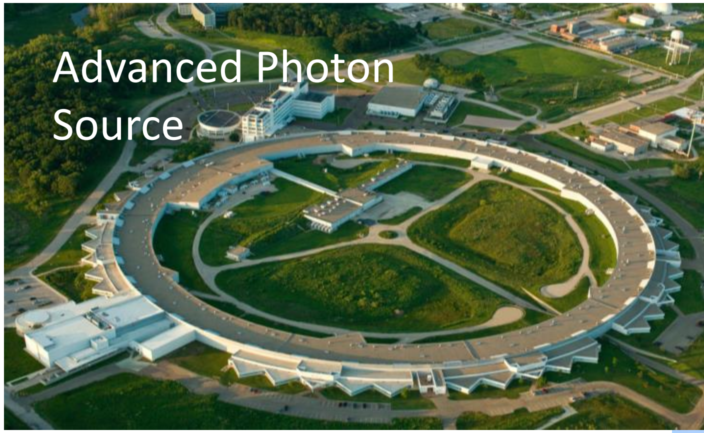


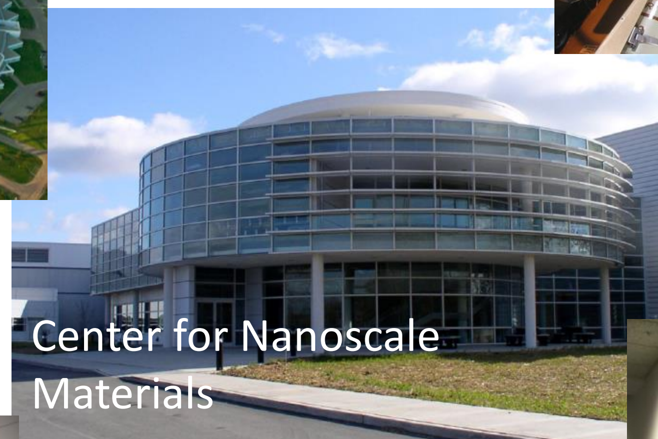


S&T Programs

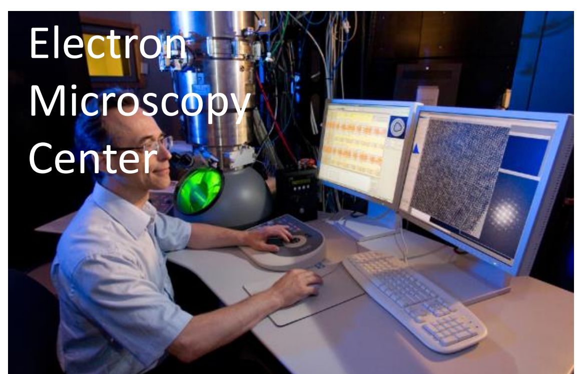
Argonne User Facilities


Argonne Tandem-Linac Accelerator System


Advanced Photon Source


Center for Nanoscale Materials


Argonne Leadership Computing Facility


Electron Microscopy Center


Transportation Research and Analysis Computing Center

DOE User Facilities

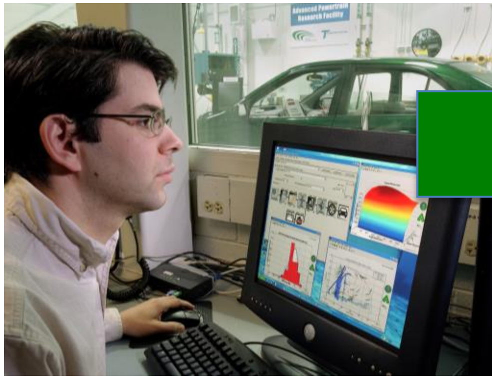
- Open to all
  - No restriction on organization, funding source, nationality, or research area
- No charge for open science
  - Cost recovery for proprietary work
- Access through peer-reviewed proposal process
  - Rapid Access/Discretionary access available
- Expert support
  - Dedicated staff help to users utilize unique resources
  - Collaborative work with domain experts

How Industry Works with Argonne

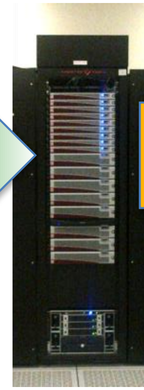
- A primary objective of the U.S. Department of Energy (DOE) laboratories is to promote the economic interests of the United States
  - By facilitating development, transfer, and use of federally owned or originated technology to industry for public benefit and to leverage DOE resources through partnering with industry.
- Argonne Technology Development and Commercialization
  - Exchanging Information or Materials
  - Use of Argonne-developed IP
  - Cost-Shared Research Collaboration (CRADA)
  - Reimbursable Research and Development (sponsored research)
  - Short-Term Technical Assistance Program
  - Using Argonne's Scientific and Technical Facilities
  - Small Business Innovative Research and Small Business Technology Transfer
  - Regional Economic Development Programs

http://www.anl.gov/techtransfer/

Innovation Often Requires New Scales



Desktop



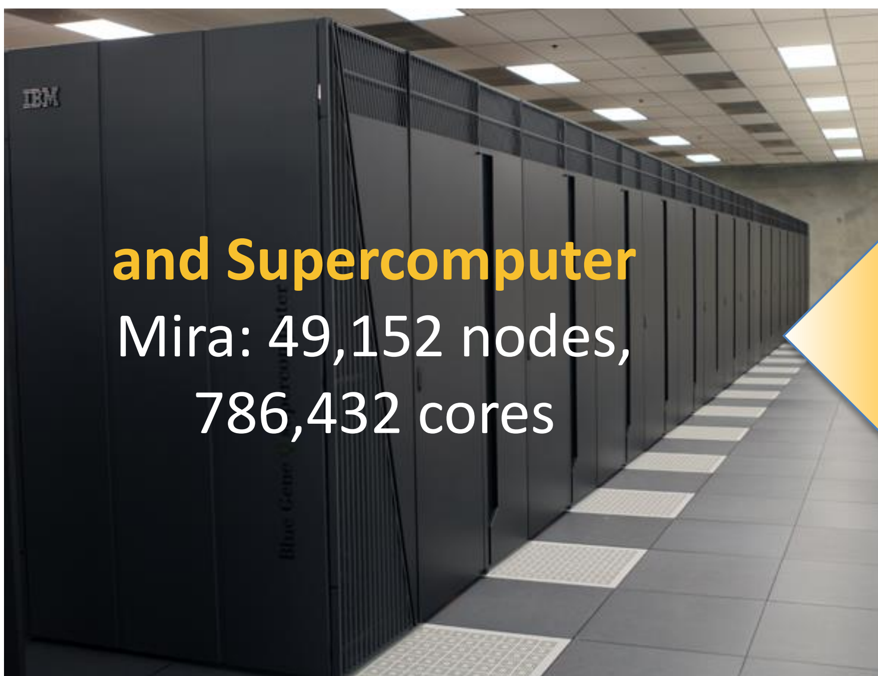
Work Group

Medium Cluster

Fusion: 344 nodes, 2,824 cores

Large Cluster

Blues: 308 nodes, 4,928 cores



and Supercomputer

Mira: 49,152 nodes, 786,432 cores

Computer Architecture this Decade: Challenges and Opportunities

- CPU/GPU core speed improves slowly
- Many more cores per processor package
- In-package memory boosts performance
- Another tier (or two) added to memory hierarchy
- CPU performance gains continue to outpace network/interconnect
- Time step/checkpoint output speed boosted by NVRAM
- Bulk synchronous algorithms hinder apps
- Petaflops in a rack

Argonne is already at work

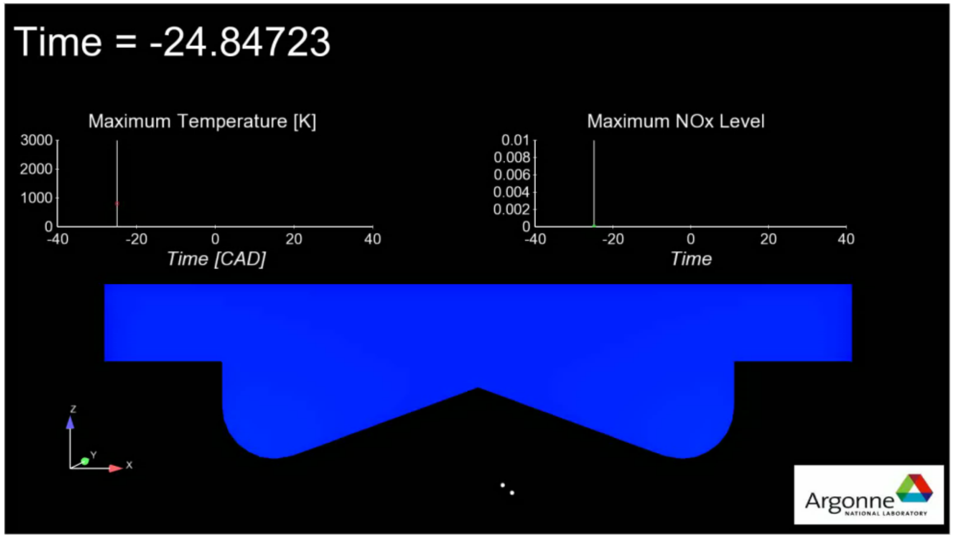
- Co-designing computers
- Evaluating alternatives
- Developing new algorithms, libraries, tools – for engineering and science

The Laboratory Computing Resource Center

Delivering end-to-end computing since 2003

Dedicated to science and engineering (technical) computing solutions

- **Project Planning**: identify approaches, applications, and resource require-ments to solve your specific problem; SOW development; info security
- **Project Startup:** code installation, test, support – many codes are available
- **User Training:** transfer data, set up workflow, schedule and run jobs, retrieve results, debug problems
- **Advanced Tutorials:** moving to more scalable apps, using advanced features



- **Project Execution:** optimizing throughput and run time for your problem
- **Deep Expertise:** facilitate lab-wide access to collaborators and contract researchers

LCRC Industrial Partnerships with dedicated Fusion Cluster

High performance Intel cluster

- 342 compute nodes, 2824 cores, 27 teraflops
- Fast network fabric
- Many tools & applications

Open or Proprietary R&D

- No charge for open R&D
- Reasonable fee for proprietary use

Try approaches that cannot be done in house

- Solve a critical problem with Argonne's help
- Prototype accurate models or deep analyses
- Evaluate accuracy vs. design margin

User Facility Agreement

- One agreement for all Argonne facilities

Argonne Leadership Computing Facility

Mira – 10PF IBM Blue Gene/Q Supercomputer

- 48 Racks
- 1,024 Nodes per Rack
- 1.6 GHz 16-core processors
- 16 GB RAM per Node
- 384 I/O Nodes
- Two-Ton Water Cooled Racks

Overall

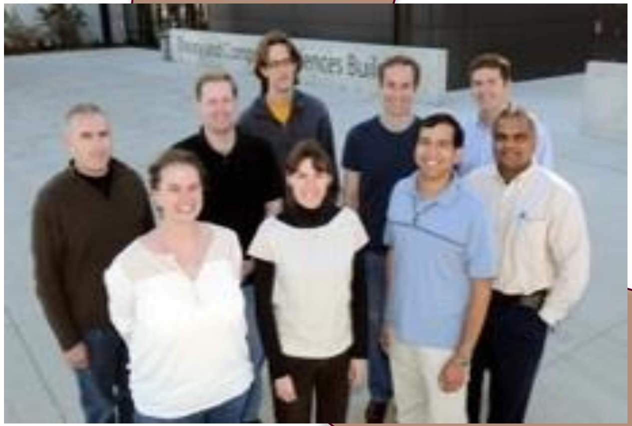
- 786,000 Cores
- 768 Terabytes of Memory
- Peak of 10 petaFLOPS
- 240 GB/s Network
- 35 PB of Storage
- #5 on June 2013 Top500 List

Allocations @ ALCF

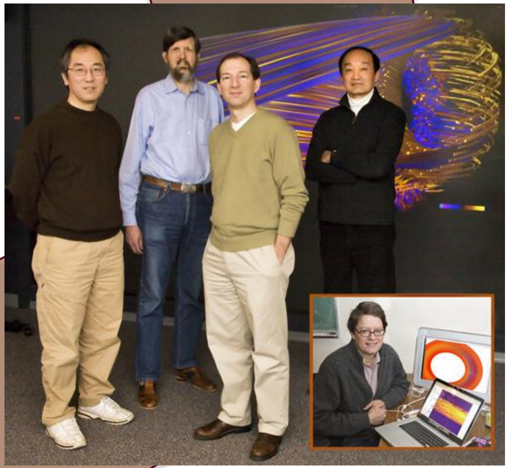
	60% INCITE	30% ALCC	10% ALCF Discretionary
Mission	High-risk, high-payoff science that requires LCF-scale resources*	High-risk, high-payoff science aligned with DOE mission	Strategic ANL and ASCR use
Call	1x/year – (Closes June)	1x/year – (Closes February)	Rolling
Duration	1-3 years, yearly renewal	1 year	3m,6m,1 year
Typical Size	30 - 40 projects 10M - 100M core-hours/yr.	5 - 10 projects 1M – 75M core-hours/yr.	100s of projects 10K – 1M core-hours
Review Process	Scientific Peer-Review Computational Readiness	Scientific Peer-Review Computational Readiness	Strategic impact and feasibility
Managed By	INCITE management committee (ALCF & OLCF)	DOE Office of Science	LCF management
Availability	Open to all scientific researchers and organizations ***Capability >20% of cores***		

Argonne Collaborative Strategy

Computer Scientists



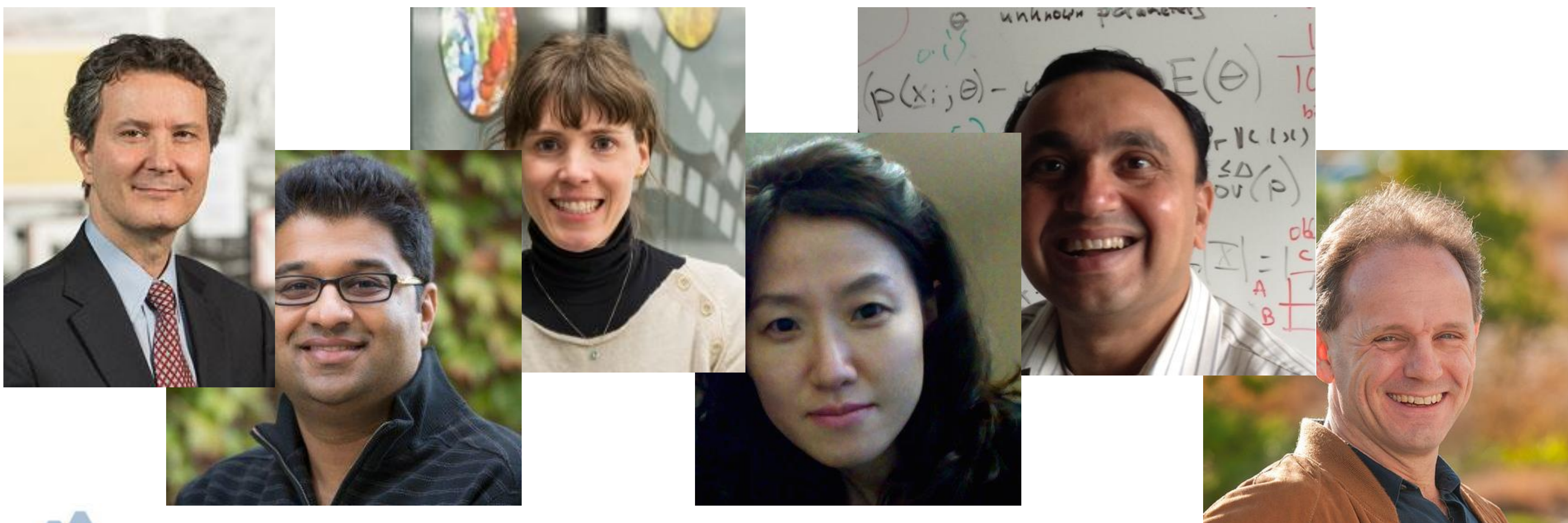
Computational Scientists



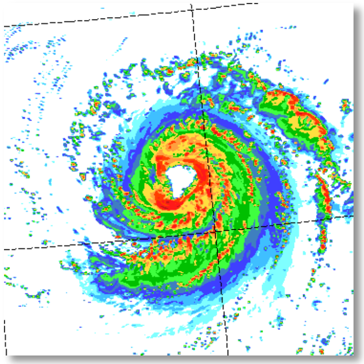
Domain Scientists

Argonne Has Deep CFD Expertise

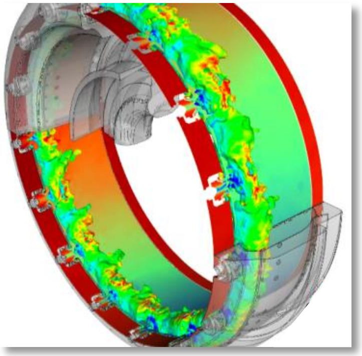
- Software Development, Porting, Optimization, Uncertainty Quantification, Verification
- Spread Across Many Divisions – ES, ALCF, MCS, CELS, NE, …
- Integration with Chemistry, FEA, Visualization
- Future: New Architectures, Increased Scale, New Algorithms



Argonne Projects Span Many Domains

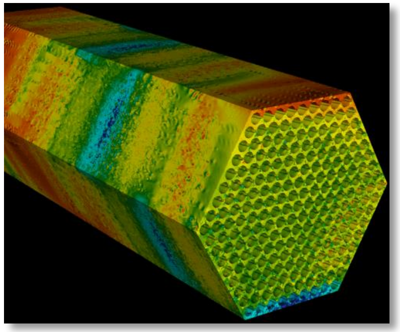


Climate
Predicting hurricane tracks to mitigate risks, hindcasting with climate model data to gauge impact of global change.

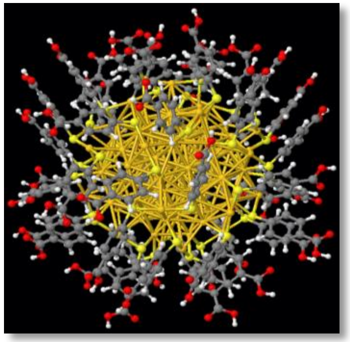


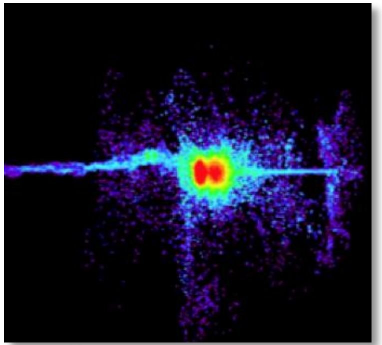
Gas Turbines
Modeling two-phase flow and combustion for the design of more efficient aircraft engines.

Nuclear Energy
High-fidelity fluid flow and heat transfer simulation of next-generation reactor designs, aiming to reduce the need for costly experimental facilities.

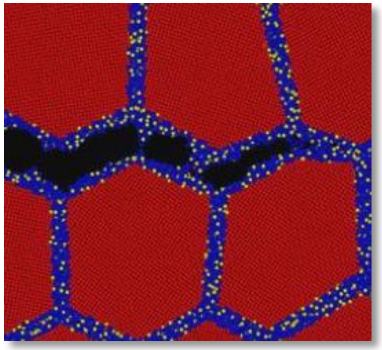


Nano Catalysts
Mapping out properties of gold nanoparticles to design catalysts for fuel cells and methane conversion.





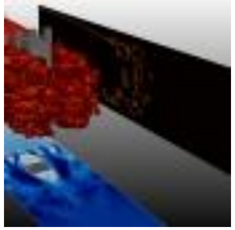
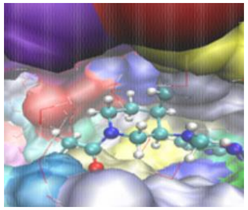
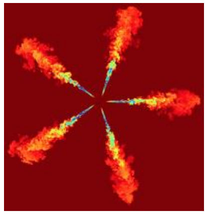
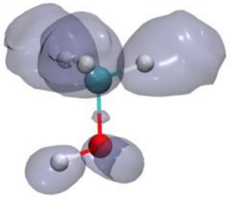
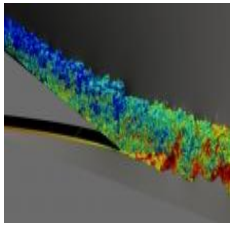
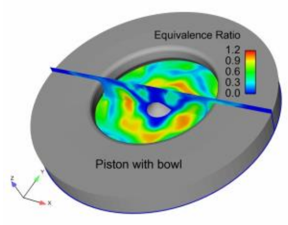
Fusion Energy
Understanding the detailed physics of Fast Ignition inertial confinement fusion.



Materials Science
Molecular simulation of fracture dynamics in structural materials in next-generation nuclear reactors.

Innovation through Industrial Partnerships

Oil Platform Safety	Drug Design	Engine Design	Catalysis	Wind Turbines	CFD Software
Predict flame spread in confined spaces in an effort to avoid catastrophic explosions on offshore oil platforms	Identify leading drug candidates for broad-impact, anti-parasitic therapeutics targeting several orphan diseases including malaria	Develop more powerful combustion engine simulation capabilities to allow shorter development times and reduce need for multi-cylinder test programs	Improve the production of synthetic gas products by simulating the catalytic properties of cluster-based materials	Enable the design of quieter, more efficient wind turbines by accurate simulations of the complex behavior of air flows around wind turbine blades	Improve scaling of combustion simulations to allow unprecedented number of simultaneous jobs, providing a valuable design tool for engine manufacturers

Simulation of Massively Separated Flow

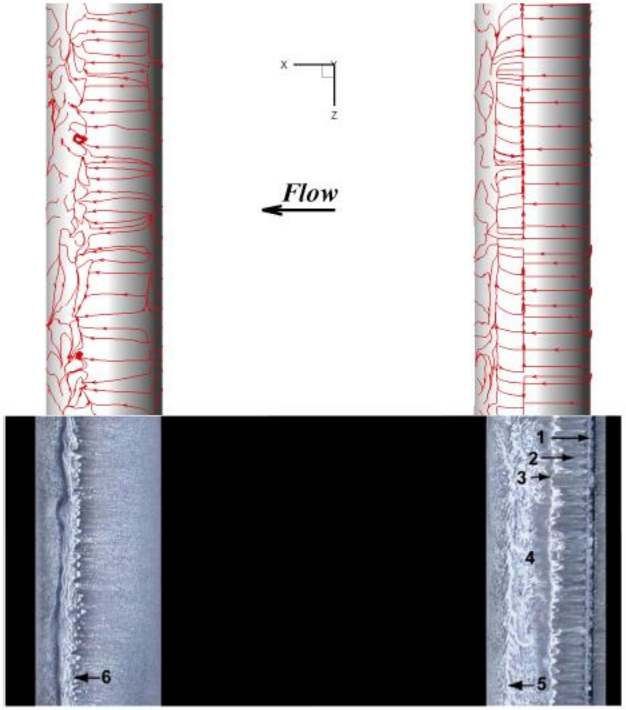
- Discretionary, PI Philippe Spalart (Boeing)
  - Innovative blending of RANS and LES techniques for massively separated flows
    - *Largest Detached Eddy Simulation (DES) of tandem cylinder configuration (to mimic turbulent flows past a non-proprietary landing gear-like configuration)*
    - Excellent comparison with experiments conducted at NASA Langley
  - NTS: RANS+LES on Overlapping Cartesian Grids
    - 3D Navier-Stokes
    - Improved wall model

IMPACT

- Improved Detached Eddy Simulation
  - RANS + LES (with wall model)
  - Improved noise prediction

ALCF Contribution

- Production runs on 32,768 cores
- Hybrid MPI+OpenMP



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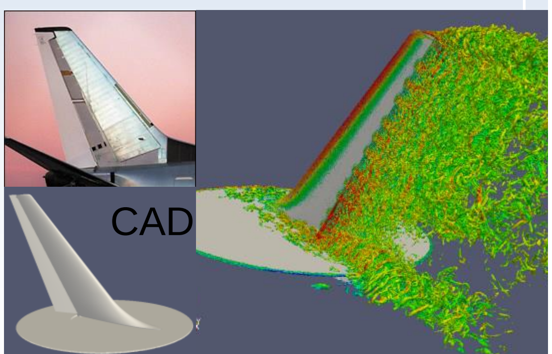
Predicting Aerodynamic Active Flow Control
Kenneth Jansen, U. Colorado

Science and Accomplishments

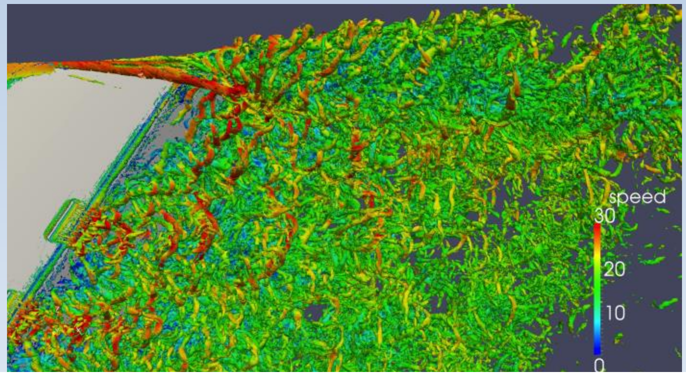
- Synthetic jet flow control can dramatically alter aerodynamic flow with very small power input.
- Turbulent flow simulated over a real tail-rudder assembly that matches experiment.
- Unsteady, separated flow with active flow control is not accurately simulated with time-averaged models.
- Adaptive, unstructured grid flow solver resolves large range of spatial and temporal scales.

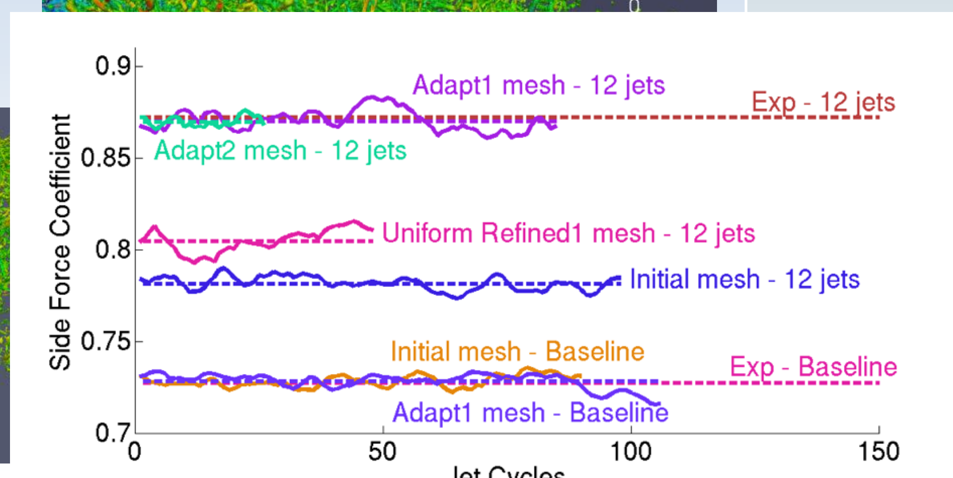


Recent Presentations: Rasquin, *Title, ANL* Postdoc Symposium…

Key Impact

- Experiments show flow control can produce 20% improvement/increase in side force





- *Initial mesh for flow control difficult; misses the expected improvement*
- *Uniform refinement: Cost (# of elements) rises unacceptably fast, accuracy improvement too slow.*
- *Local mesh adaptivity efficiently captures required physical scales for accurate prediction.*

ALCF Contributions

- ESP Postdoc Michel Rasquin essential to this work
- MIRA simulation hardware, software and support
- TUKEY visualization hardware, software, and support
- Co-Visualization work with Mike Papka, Mark Herald and Venkat Vishwanath
- Dedicated resources for full scale studies with Ray Loy

Faster Design of Better Jet Engines

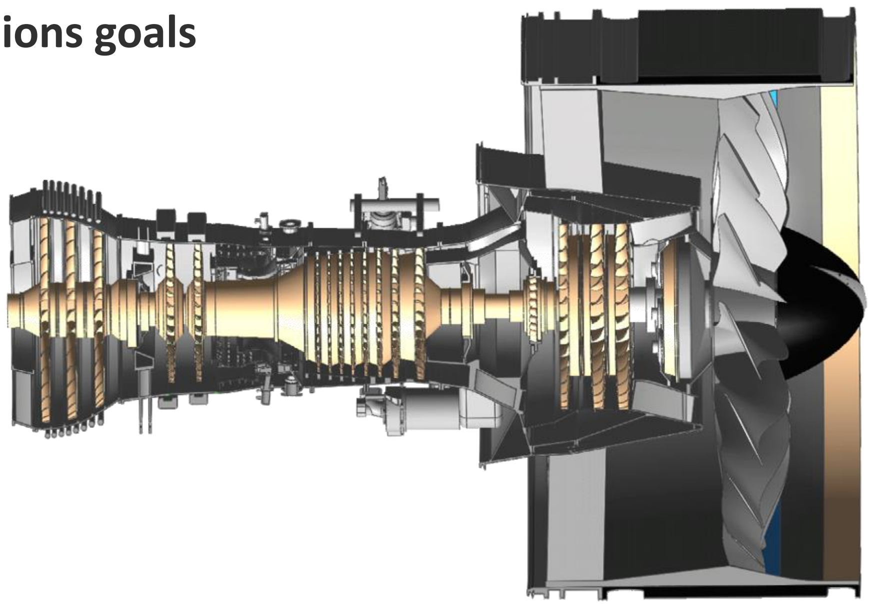
Peter Bradley
Pratt & Whitney

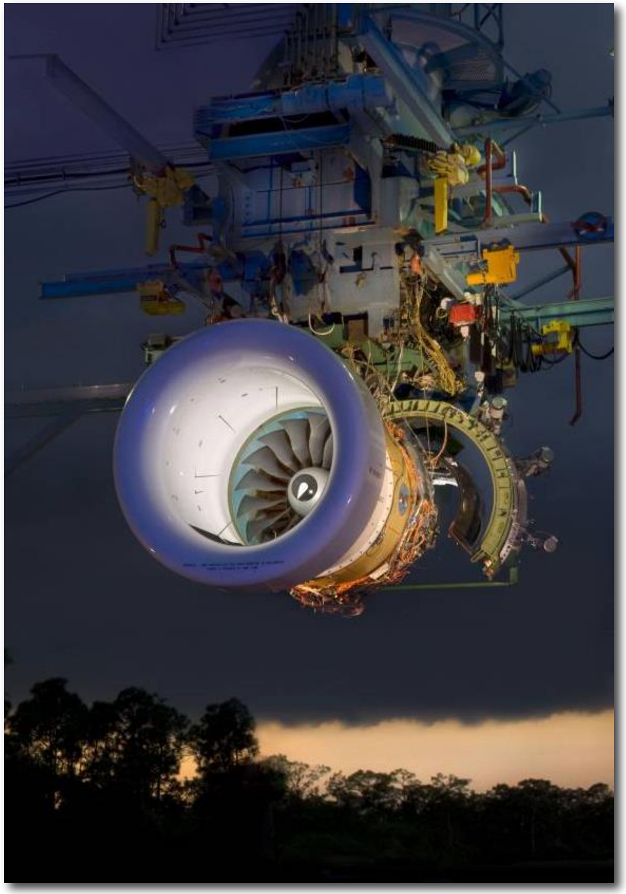
Science

- Save cost and time by designing engines through simulation rather than building models
- Technologies from simulations now being applied to next generation high-efficiency low-emission engines
- A key enabler for the depth of understanding needed to needed to meet emissions goals

Challenges

- I/O algorithm redesign speeds up simulations by 3x





Multiscale Blood Flow Simulations

George E. Karniadakis, Brown University

Science and Approach

- Couple hydro solver NεκTαr with Dissipative Particle Dynamics, DPD-LAMMPS
- Performed first multiscale simulation of blood flow in the brain of a patient with an aneurysm

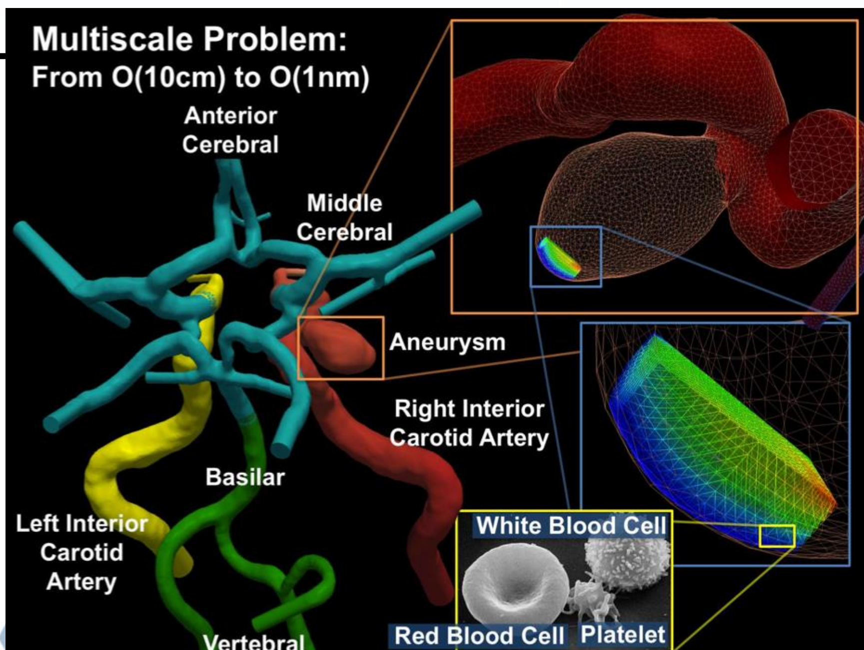
Key Impact

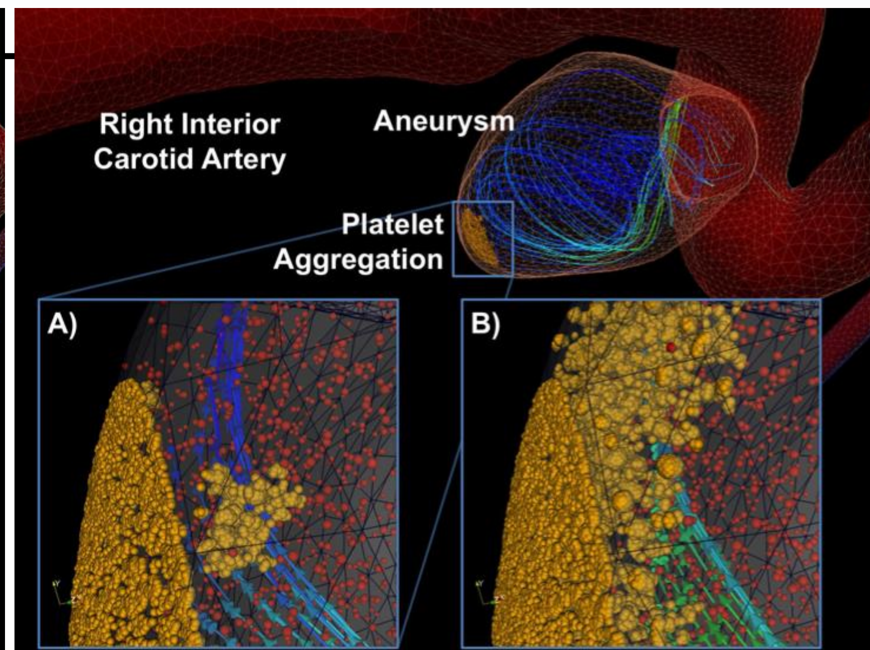
- Improve the diagnosis and treatment of diseases with brain blood flow complications such as cerebral malaria, sickle cell anemia and cerebral aneurysms

Gordon Bell Finalist, SC11

ALCF Contributions

- New multi-part visualization of blood flow simulation combining continuum hydro and immersed material (SC10 and ASAC 2010 Fall Report)
- Collaborated with the team to perform simulations on 131,072 cores

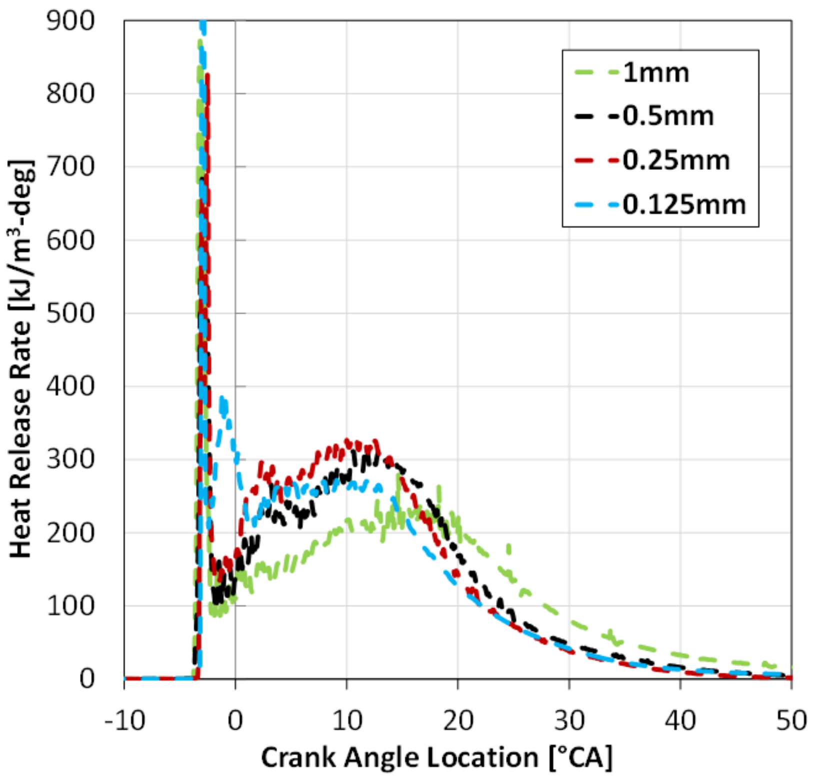




High Fidelity Engine Modeling with Caterpillar and Convergent Science

Doug Longman (ESD), Sibendu Som (ESD), Shashi Aithal (LCRC), Marcus Weber (CAT), Tushar Shethaji (CAT), Peter Senecal (CSI), Keith Richards (CSI), Marta Garcia Martinez (ALCF), Ray Bair (CELS)

- **Challenge**
  - Quantify relationships between CFD precision and model accuracy (T, P, emissions, etc.)
  - Realistic moving piston models
- **Benefit**
  - More efficient ICE; alternative fuels
  - Relevant to both Argonne and CAT
- **Argonne Engagement**
  - LCRC: Identify scaling bottlenecks, recommend approaches
  - LCRC+ESD+CAT: analyze results
  - ALCF+CSI: Discretionary Project to port CONVERGE to Blue Gene



Advanced Energy Storage Systems

Combined effort of 5 Argonne divisions (MSD, CSE, CNM, ALCF, MCS)

Lithium-air Batteries

- Potential for much larger energy densities than current batteries, e.g., 400 mile electric vehicles (CSE)

High Performance Computing

- DFT calculations predict electronic structure properties of Li_2O_2 nanoparticles that may explain electronic conductivity
- Predictions confirmed by experiment

Future

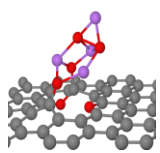
- Multi-scale modeling to improve efficiency and cyclability of electrochemical processes in Li-air batteries (combined MSD, CNM, ALCF, MCS effort)

GPAW

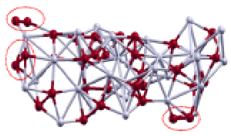
- Highly parallelized electronic structure code (GPAW)
- DFT calculations on Li_2O_2 nanoparticles with over 1000 atoms (MSD, CNM)

New Insight into Li-O_2 Chemistries

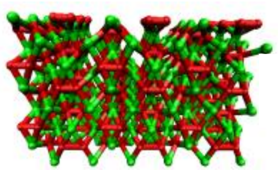
- Surface superoxide species provides clues to discharge/charge mechanisms



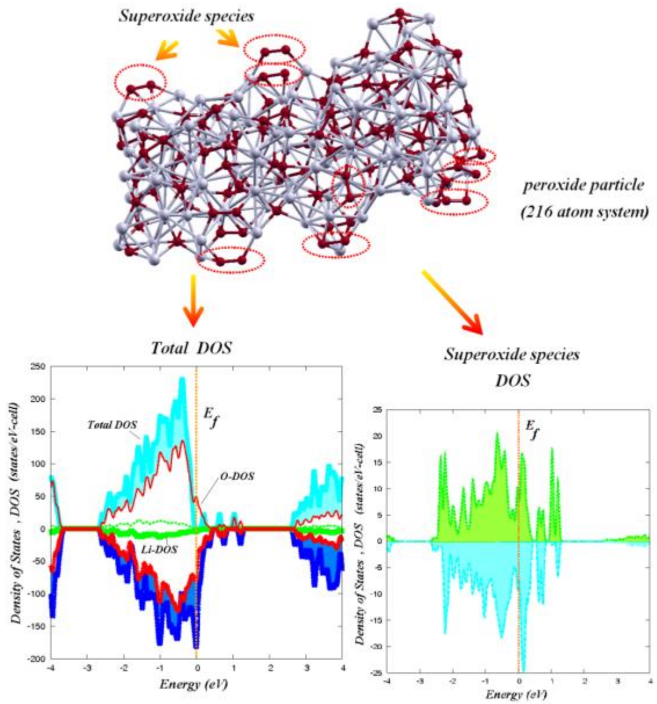
Li_2O_2 nucleation



Li_2O_2 nanoparticle



Li_2O_2 bulk surface



Minimizing the Acoustic Signature of Jet Engines and Wind Turbines

Umesh Paliath, G.E. Global Research, Niskayuna, USA

Science and Approach

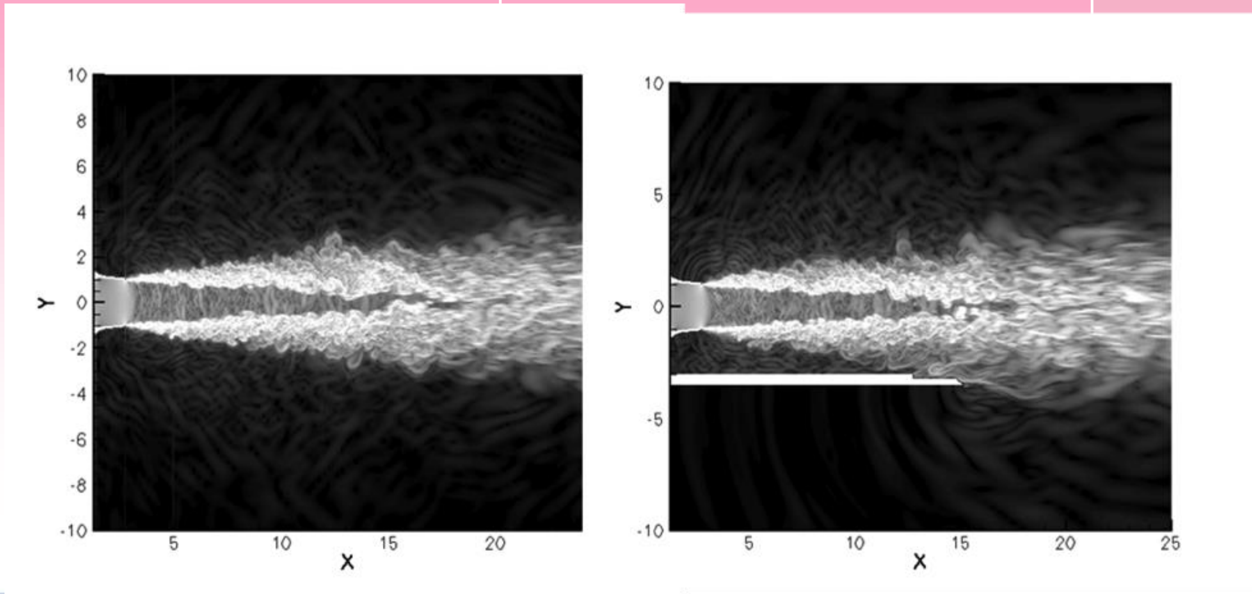
- Carry out large-eddy simulations on jet nozzles to understand noise generation
- Completed a proof-of-concept problem that proved the LES approach captures the acoustics

Key Impact

- Design improved, lighter engines with more fuel savings and fewer CO_2 emissions
- Reduce ear damage for these working near engines
- Decrease noise impact and improve design of wind turbines

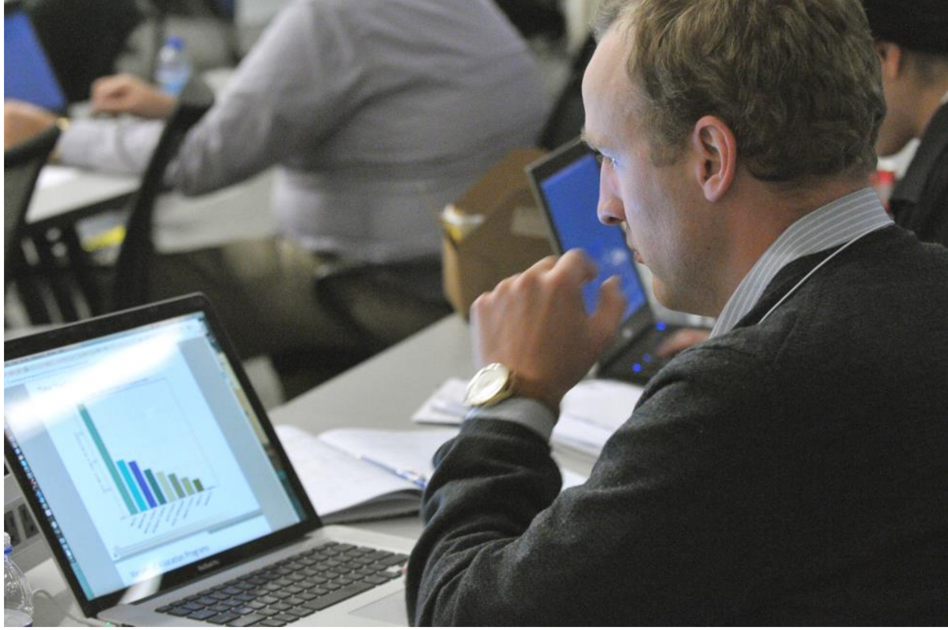
ALCF Contributions

- The ALCF ported and performed performance optimizations of the code CharLES.
- The team is tightly engaged getting this and a preferred software package ready for Mira.



Density gradient contours for simulation of conic nozzle with and without the presence of flat plane. The density gradient is a qualitative picture of noise.

Benefits of working with Argonne



- **Evaluating pathways to innovation and greater ROI**
- **Improving time to market, and product performance**
  - Design for higher performance, efficiency, reliability
  - Explore new materials and approaches
  - Reduce cost, design margins
  - Quantify uncertainty, validate models
- **Tackling problems that cannot be done in house**
- **Extending computational skills**
- **Building the business case for use of HPC**

Questions and Discussion