Leveraging Argonne Computing Facilities and Expertise for Industry Challenges

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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

Advanced Photon Source

Center for Nanoscale Materials

Argonne Leadership Computing Facility

Electron Microscopy Center

Argonne Tandem-Linac Accelerator System

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

and Supercomputer
Mira: 49,152 nodes, 786,432 cores

Large Cluster
Blues: 308 nodes, 4,928 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 requirements 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
<table>
<thead>
<tr>
<th><strong>Allocations @ ALCF</strong></th>
<th><strong>INCITE</strong></th>
<th><strong>ALCC</strong></th>
<th><strong>ALCF Discretionary</strong></th>
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</thead>
<tbody>
<tr>
<td><strong>Mission</strong></td>
<td>High-risk, high-payoff science that requires LCF-scale resources*</td>
<td>High-risk, high-payoff science aligned with DOE mission</td>
<td>Strategic ANL and ASCR use</td>
</tr>
<tr>
<td><strong>Call</strong></td>
<td>1x/year – (Closes June)</td>
<td>1x/year – (Closes February)</td>
<td>Rolling</td>
</tr>
<tr>
<td><strong>Duration</strong></td>
<td>1-3 years, yearly renewal</td>
<td>1 year</td>
<td>3m,6m,1 year</td>
</tr>
<tr>
<td><strong>Typical Size</strong></td>
<td>30 - 40 projects</td>
<td>10M - 100M core-hours/yr.</td>
<td>5 - 10 projects</td>
</tr>
<tr>
<td><strong>Review Process</strong></td>
<td>Scientific Peer-Review</td>
<td>Computational Readiness</td>
<td>Scientific Peer-Review</td>
</tr>
<tr>
<td><strong>Managed By</strong></td>
<td>INCITE management committee (ALCF &amp; OLCF)</td>
<td>DOE Office of Science</td>
<td>LCF management</td>
</tr>
<tr>
<td><strong>Availability</strong></td>
<td>Open to all scientific researchers and organizations</td>
<td><strong>Capability &gt;20% of cores</strong></td>
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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

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

**Key Impact**

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

**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

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

- 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.

![Graph showing mesh adaptivity](image-url)

![CAD model](image-url)
Faster Design of Better Jet Engines

**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 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

## 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

### Multiscale Problem: From O(10cm) to O(1nm)

- Anterior Cerebral
- Middle Cerebral
- Left Interior Carotid Artery
- Basilar
- Vertebral
- Aneurysm
- White Blood Cell
- Red Blood Cell
- Platelet
- Right Interior Carotid Artery
- Aneurysm
- Platelet Aggregation
- B)

### Gordon Bell Finalist, SC11
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$_2$O$_2$ 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$_2$O$_2$ nanoparticles with over 1000 atoms (MSD, CNM)

New Insight into Li-O$_2$ Chemistries
- Surface superoxide species provides clues to discharge/charge mechanisms
Minimizing the Acoustic Signature of Jet Engines and Wind Turbines
Umesh Paliath, G.E. Global Research, Niskayuna, USA

Science and Approach | Key Impact | ALCF Contributions
--- | --- | ---
- Carry out large-eddy simulations on jet nozzles to understand noise generation | - Design improved, lighter engines with more fuel savings and fewer CO₂ emissions | - The ALCF ported and performed performance optimizations of the code CharLES.
- Completed a proof-of-concept problem that proved the LES approach captures the acoustics | - Reduce ear damage for these working near engines | - The team is tightly engaged getting this and a preferred software package ready for Mira.
- Decrease noise impact and improve design of wind turbines | - Decrease noise impact and improve design of wind turbines | 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