Industrial HPC Partnerships Program

Presented by

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NICS

OLCF
Oak Ridge Leadership Computing Facility

Oak Ridge National Laboratory
Managed by UT-Battelle for the U.S. Department of Energy

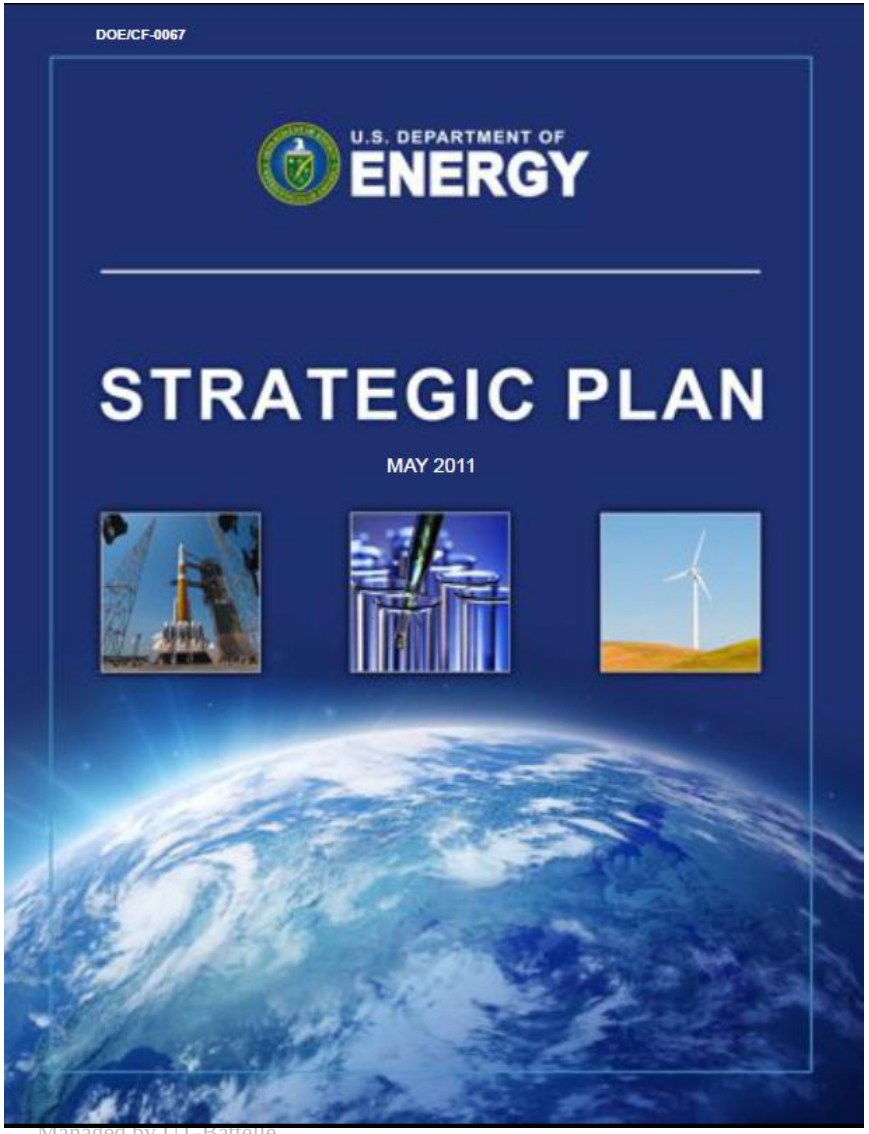
U.S. Department of Energy | Office of Science

NSF

Topics

- Kick off of new series of Lab-Industry Workshops
- Update on ORNL Industry HPC Industry Partnerships Program

Advancing DOE's Strategic Plan



Goal 1: Catalyze the timely, material, and efficient transformation of the nation's energy system and secure U.S. leadership in clean energy technologies.

We will facilitate the transfer of our computer simulation capability to industry *with the goal of accelerating energy technology innovation by improving designs, compressing the design cycle and easing the transitions to scale, thereby enhancing US economic competitiveness.*

Industry-Laboratory Workshops

U.S. DEPARTMENT OF ENERGY

- Outgrowth of meeting between Secretary Chu and CTOs
- Increase industry awareness of relevant research capabilities within the DOE national laboratory system,
- Deepen the national laboratories' understanding of the technical challenges facing industry, and
- Identify and improve paths forward for collaboration.
- 4 topics in first wave: materials for energy applications, modeling and simulation, cybersecurity, sensors
  - Materials Jan 30 – Feb 1 Berkeley, CA
  - Mod-Sim: March 7-8 Austin, TX

Modeling and Simulation Workshop

- Applications and challenges that are driving industrial use of modeling and simulation for increased competitiveness,
- Unique computational tools and expertise within DOE's national laboratories that are or can be made available to industry, and
- Opportunities for collaboration that can leverage national laboratory and industrial capabilities in order to strengthen the nation's innovation capacity and drive economic growth.

Modeling and Simulation Workshop

- 180 attendees; approximately 45% industry
- All 17 labs represented, and at the executive level
- Keynote by Secretary Chu
- 9 Panels; Poster session
- Tours AMD laboratories

- https://www.ornl.gov/modeling_simulation
- http://www.lbl.gov/mfea/

Industrial HPC Partnership Program

Important Program Updates (since my presentation at the April 2011 HPC User Forum)

Problems to Bring to Our User Facilities:
High Risk – High Return

Competitive Opportunity
(Break out of the Pack!)

Strategic

High Risk

Breakthrough Innovation

High Return

Moderate Risk and Innovation

Routine Low Risk

New DOE Industry Partnership Program User Agreement for OLCF

Projects whose output is a blend of proprietary and non - proprietary data receive no-cost access if they can make public meaningful science

Key Points

- **Protects proprietary output (like the proprietary user agreement)**
- **Collaboration not permitted (like the proprietary user agreement)**
- **Must make public meaningful science (like the non-proprietary user agreement)**
- **No-cost access (like the non-proprietary user agreement)**

New DOE Industry Partnership Program User Agreement for OLCF ctd

Why this new user agreement?

- DOE recognizes that, unlike university and lab projects, many industry projects are not starkly non-proprietary or proprietary.

Benefit to Industry

- This gives companies flexibility to operate at OLCF in a way that more closely resembles their business environment

Which Programs Does it Apply To?

- ASCR Leadership Computing Challenge (30%)
- Director's Discretionary Awards (10%)
- (INCITE continues as a non-proprietary program)

New INCITE Guidelines

- 2012 call for proposals outlines new policy on ensembles
- Opens the door for broader range of industrial problems to be considered
- Recognizes that these are the leadership problems within industry, in keeping with the focus on leadership computing required by Congress/OMB

How industry can access NICS
(NSF-funded National Institute for Computational Sciences)

XSEDE

Extreme Science and Engineering Discovery Environment

XSEDE

- Assumption that work is non proprietary
- Apply quarterly via NSF TeraGrid
- "the principal investigator (PI) must be a researcher or educator at a U.S.-based institution, including federal research labs or commercial organizations, though additional information may be needed …"

Note: no-cost access, project output is considered non proprietary and available to public

Turbo Compressor Innovation

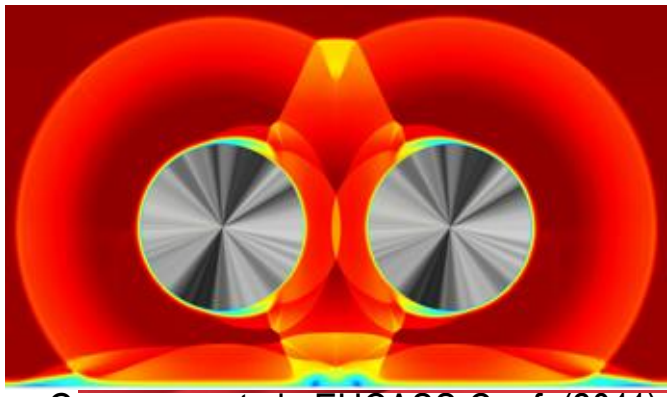
Scaling CFD code to machining titanium for a new turbo compressor in a few months

RAMGEN POWER SYSTEMS™

Science Objectives and Impact

- Ramgen Power Systems is developing shock wave compression turbo machinery to meet DOE goals for reducing Carbon Capture and Sequestration costs
- Complementary goal: design a gas turbine with dramatically lower costs and higher efficiency

Image on right:
3.7 billion grid cell simulation of two-body shock-wave, boundary layer interaction, showing high-resolution shock capture



Grosvenor et al., EUCASS Conf. (2011)

Application Performance

- **50x improvement in code scalability** with more efficient memory utilization
- Accelerated I/O by 10x with optimizations and ADIOS
- Intelligent use of **ensembles to explore parameter space using over 120,000 cores**

Science Results

- Advanced Ramgen's aerodynamic design process
- Observed designs with valuable new characteristics, from ensembles not possible without Jaguar
- Created a new workflow paradigm that accelerates design of compressors
- **Accelerated computational design cycle for turbo machinery from months to 8 hours!**

OLCF contributions:
Mike Matheson guided Ramgen and Numeca to improve scalability, I/O performance, memory utilization and workflow design to fully exploit Jaguar. Larger XK6 memory helped.

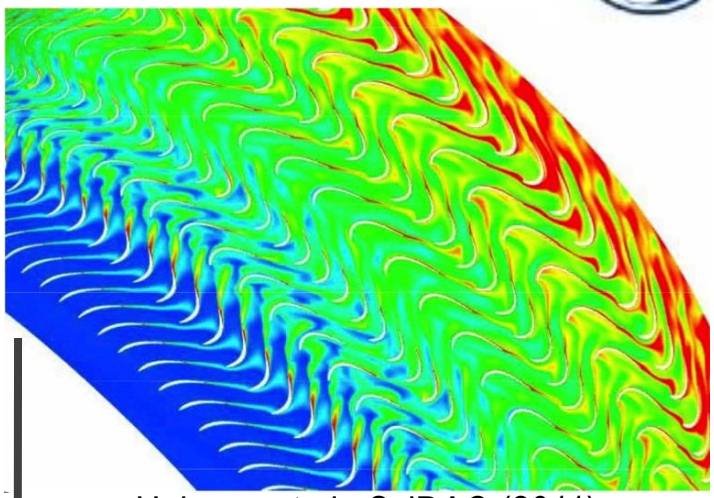
Turbo Machinery Efficiency

Removing Steady-Flow Assumptions Helps Improve Efficiency and Reduce Noise

Science Objectives and Impact

- Design efficient turbo machinery generating less noise
  - 1% reduction in fuel consumption can save $20B
- What is the "steady-flow" assumption hiding?

Image on right:
Computational Fluid Dynamics results depicting entropy for unsteady flow through turbine with fan blades removed.



Holmes, et al., SciDAC (2011)

Application Performance

- Scaled GE's TACOMA CFD code from ~1K cores to 8K cores
- TACOMA has good weak scaling

OLCF contributions:

- Guide them in porting TACOMA.

Science Results

- GE ran their largest ever CFD simulation on Jaguar
- Unsteady flow and efficiency losses localize at end walls
- **On the basis of the success of these calculations, GE Global Research has purchased a Cray XE6**

"Jaguar has allowed us to see phenomena we have never seen before." -- Graham Holmes, GE Global Research

2011-2012 Industry Users

Companies ranged from small to large:

- **Small Business**
  - Ramgen
  - SmartTruck Systems
- **Larger Firms**
  - Boeing
  - Corning
  - GE
  - Ford
  - Global Foundries
  - Procter & Gamble
  - United Technologies
  - Pratt & Whitney

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