IXPUG MIDDLE EAST MEETING

HIGH PERFORMANCE COMPUTING IN INDUSTRY, AGENCIES AND SMALL BUSINESS

DAVID E MARTIN
President, IXPUG

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KAUST

WORKSHOP QUESTIONS

- Experiences
  - What are some examples of collaborations with industry?
  - What were the outcomes?
  - What can we learn?

- Models for industry collaboration
  - How do you structure a collaboration?
  - What roles are needed in a successful collaboration?

- Organization
  - How are you organized to facilitate industry collaborations?
  - What other resources do you leverage?
  - What more would you like to do?

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WORKSHOP AGENDA

- Group 1 – Examples of Industry Collaborations
  - David Keyes, KAUST
  - Richard Gerber, NERSC/Berkeley Lab
  - Thierry Tonellot, Aramco

- Group 2 – How to Work with Industry
  - Belal Fayad, KAUST
  - Rob Farber, TechEnablement
  - David Martin, Argonne National Laboratory

- Group 3 – National Industry Collaboration Efforts
  - Taisuke Boku, University of Tsukuba
  - Jaysoo Lee, KAUST (and reporting on KISTI)
  - David Martin, Argonne National Laboratory

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HPC FOR INDUSTRY IS A DOE PRIORITY

- Public Law 108-423 - Department of Energy High-End Computing Revitalization Act of 2004
  - "…ensure that the high-end computing activities of the Department of Energy are **coordinated with relevant activities in industry**…"
  - Office of Science shall provide "… Leadership Systems, on a competitive, merit-reviewed basis, **access to researchers in United States industry**, institutions of higher education, national laboratories, and other Federal agencies."

- DOE Secretary Moniz - November 2014
  - "High-performance computing is an essential component of the science and technology portfolio required to **maintain U.S. competitiveness** and ensure our economic and national security," Secretary Moniz said."

- President Obama Executive Order - Creating a National Strategic Computing Initiative, July 2015
  - "The United States **must foster public-private collaboration**, relying on the respective strengths of government, industry, and academia to maximize the benefits of HPC."

DOE INDUSTRY COLLABORATION MODELS

- Strategic Partnership Project (SPP) agreement, formerly referred to as Work for Others (WFO)
  - Partner pays full cost recovery
  - Retain to inventions, protect generated data as proprietary
- Cooperative Research and Development Agreement (CRADA)
  - Collaborative research and development agreements for the mutual benefit of both parties.
  - The lab and partner share costs and inventions

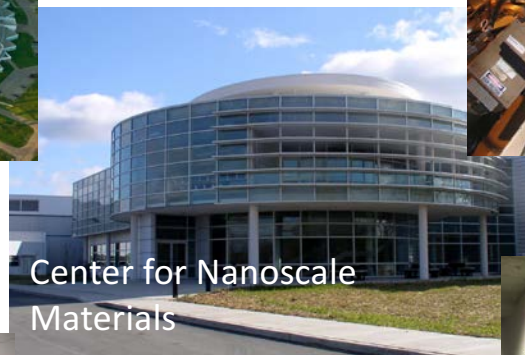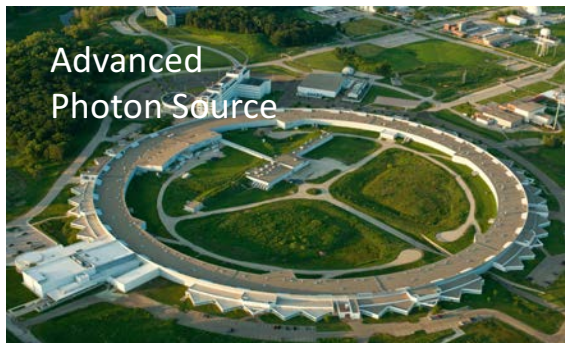# DOE INDUSTRY COLLABORATION MODELS (2)

- Non-Proprietary User Agreement (NPUA)
  - Researchers who engage in non-proprietary research are able to access unique scientific User Facilities without paying a user fee.
  - Users commit to publishing research results in the open literature
  - Access granted on a competitive and peer-reviewed basis

- Proprietary User Agreement (PUA)
  - Research is kept confidential and proprietary
  - Partner pays full cost recovery
  - Access is granted by facility out of discretionary time

USER FACILITIES (DOE DEFINITION)

A user facility is a federally sponsored research facility available for external use to advance scientific or technical knowledge under the following conditions:

- The facility is **open to all** interested potential users without regard to nationality or institutional affiliation.

- Allocation of facility resources is **determined by merit review** of the proposed work.

- **User fees are not charged** for non-proprietary work if the user intends to publish the research results in the open literature. Full cost recovery is required for proprietary work.

- The facility **provides resources** sufficient for users to conduct work safely and efficiently.

- The facility supports a **formal user organization** to represent the users and facilitate sharing of information, forming collaborations, and organizing research efforts among users.

- The facility capability **does not compete with an available private sector** capability.

ARGONNE USER FACILITIES

Advanced Photon Source

Argonne Tandem-Linac Accelerator System

Center for Nanoscale Materials

Argonne Leadership Computing Facility

Electron Microscopy Center

Transportation Research and Analysis Computing Center

ALCF ALLOCATION PROGRAMS

	INCITE **60%**		ALCC **30%**		ALCF Discretionary **10%**	
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	

ALCF – A NATIONAL USER FACILITY FOR COMPUTING AND COMPUTATIONAL SCIENCES

- 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 Discretionary access available

- Expert support
  - Dedicated staff help to users utilize unique resources
  - Collaborative work with domain experts

DRIVING INNOVATION FOR U.S. INDUSTRY

ALCF industrial partnerships help strengthen the nation's innovation infrastructure
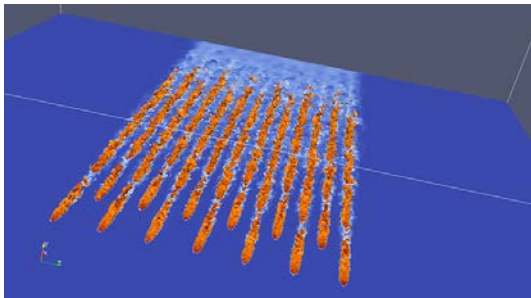
- GE Global Research is using ALCF resources to study the physics of an engine's combustor liner flows. Their findings will help guide the design of improved aircraft engines.
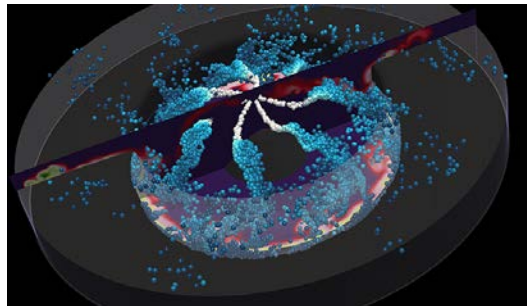
- Convergent Science is developing HPC engine modeling capabilities to provide U.S. automotive manufacturers with a tool to accelerate the development of more energy-efficient engines.
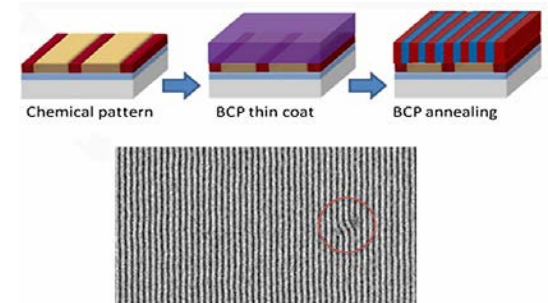
- Brewer Science is partnering with the ALCF to use simulations to gain insights into the development of new materials that will benefit the semiconductor industry.

ALCF INDUSTRY PARTNERSHIP PROGRAM

WORKING TOGETHER

ALCF Provides
- Leadership Computing
- Computational Science Expertise
- Optimization and Visualization
- Collaboration with Domain Scientists Across Argonne

Industry Achieves
- Accelerated Innovation
- Reduced Design Time
- Improved Products
- Engineering Breakthroughs

Our Partners

GE | BOEING | DOW | Cenaero | TOTAL
Westinghouse | SpiralGen | CASCADE TECHNOLOGIES
ROLLS ROYCE | leidos | TECH-X | Vestas
brewer science | Shell | GM | GENERAL ATOMICS | STINGER GHAFFARIAN TECHNOLOGIES
DENSO Crafting the Core | Cummins
TRI ALPHA ENERGY THE POWER OF INGENUITY
GT | DASSAULT SYSTEMES | NAVISTAR | achatesPOWER Fundamentally Better Engines
CRAY | CAT | United Technologies | RogueWave SOFTWARE Accelerating Great Code
saudi aramco | GLOBALFOUNDRIES | CloudPharmaceuticals | IBM
CONVERGENT SCIENCE
DELPHI

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ACCOLADES FROM INDUSTRY PARTNERS

"Working with Argonne researchers has provided us access to the HPC facilities and their expertise in spray and combustion modeling. Through this HPC study, we have learned more about model settings that have improved our simulation practices at Caterpillar," said **Marcus Weber, team leader at Caterpillar, Inc.**

Where it once took two to three months to get the level of predictions for which we were striving for, now takes only one to two weeks given the power and precision of Mira," said **Umesh Paliath, a mechanical engineer at GE Global Research.**

"The implementation of an improved load-balancing algorithm called METIS has enabled the effective use of ALCF computing resources for engine simulations. METIS is now available in the CONVERGE code so that other original equipment manufacturers can also realize the benefits," said **Keith J. Richards, vice-president and co-founder of Convergent Science, Inc.**