Observations on the Evolution of HPC for Science and Industry

Paul Messina

Director of Science
Argonne Leadership Computing Facility
Argonne National Laboratory

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Outline

- Evolution of HPC systems
- Evolution of scientific applications due to capability increases
- Software is infrastructure
- Co-design
- Industry and HPC
- Training
- Summary
Past Transitions in HPC Architectures

Anyone can build a fast CPU. The trick is to build a fast system. Seymour Cray

Serial to HPC serial (1960-1975)
- Memory access was a bottleneck

Serial to vector (1975-1985)
- Fujitsu, Convex vectorizing compilers, later others, were very helpful

Vector to parallel (1985-1995)
- Programming models: message passing, threads
- I/O becomes an even bigger bottleneck than on serial systems

Parallel to highly parallel (1995-2010)
- MPI
- Beowulf clusters
- Evolutionary architectures
- Funding for transitioning applications to highly parallel architectures, 3-D
- Funding for specific technologies, hardware and software (Pathforward)
N-body Simulation of Evolution of Universe

J. Salmon (Caltech), M. Warren (LANL)

1992 Gordon Bell Prize for performance (5 Gflops on Intel Touchstone Delta):
Simulation of 9 million gravitating stars by parallelizing a tree code
How to Build a Beowulf
A Guide to the Implementation and Application of PC Clusters

Thomas L. Sterling
John Salmon
Donald J. Becker
Daniel F. Savarese

Publication Date: March 1999

Performance Prize: Simulating the motion of 322,000,000 self-gravitating particles on ASCI Red

Price-performance Prize: Galaxy formation following 10,000,000 self-gravitating particles on a Beowulf cluster of 16 PCs that cost $50,000.
The Outer Rim Simulation: Shown is a zoom-in to small scales, the largest image shows the full simulation. These snapshots are taken when the Universe was 2.7 billion years old, 25% into the simulation time.

The Outer Rim Simulation -- Salman Habib, Argonne

• Largest cosmology simulation ever performed: 3 times larger than the largest high-resolution simulation worldwide, 15 times larger than the largest simulation carried out in the US

• Evolves 1.1 trillion particles through cosmic time in a 4225 Mpc volume on ANL’s Mira, 25% complete

• Simulation will resolve important questions about the paradigm of structure formation

• Galaxy catalogs will be generated from the simulation and served to the cosmology community via PDACS, a portal for serving cosmological simulations currently developed by ANL/Fermilab/NERSC, funded in part by DOE/HEP

• Simulation results extremely valuable for ongoing and upcoming DOE funded sky surveys, such as the Dark Energy Survey and the Large Synoptic Survey Telescope
Cosmology

1992 Salmon, Warren: 9 million gravitating stars, 5 GF (Intel Delta)

1997 Salmon et al: 322 million gravitating stars, 430 GF (ASCI Red)

2012 Habib et al: 3.6 trillion particles, 14 PF = 14,000,000 GF (Sequoia)
  - 69% of peak speed on Mira: Argonne’s IBM BG/Q (786,432 cores)
    • 90% parallel efficiency

Not a stunt: the code is used for science runs on Argonne’s Mira with 1.1 trillion particles: “The Outer Rim Simulation”, the largest cosmology simulation yet performed.
  - 4.25 Gpc domain, 10,240^3 grid
  - 1.07 trillion particles
  - 12 billion years
Major Scientific User Facilities at Argonne National Laboratory

Advanced Photon Source

Argonne Tandem Linear Accelerator System

Center for Nanoscale Materials

Argonne Leadership Computing Facility

Electron Microscopy Center
The DOE Leadership Computing Facility
Centers at Argonne and Oak Ridge

- Mission: Provide the computational and data science resources required to solve the most important scientific & engineering problems in the world.
- Established by DOE High-End Computing Revitalization Act of 2004

- Highly competitive user allocation programs (INCITE, ALCC).
- Projects receive 10-100x more hours than at other generally available centers.
- LCF centers partner with users to enable science & engineering breakthroughs (Liaisons, Catalysts).
## Titan and Mira

<table>
<thead>
<tr>
<th></th>
<th>INCITE Production Systems</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Cray XK7 “Titan”</td>
</tr>
<tr>
<td></td>
<td>IBM Blue Gene/Q “Mira”</td>
</tr>
<tr>
<td><strong>Node</strong></td>
<td>16-Core AMD 6274 Opteron + NVIDIA K20x (Kepler)</td>
</tr>
<tr>
<td></td>
<td>16-Core PowerPC A2</td>
</tr>
<tr>
<td><strong>Compute Nodes</strong></td>
<td>18,688 hybrid nodes</td>
</tr>
<tr>
<td></td>
<td>49,152 nodes</td>
</tr>
<tr>
<td><strong>Compute Node configuration</strong></td>
<td>16 x86_64 cores + 14 GPU</td>
</tr>
<tr>
<td></td>
<td>16 PPC64 Cores</td>
</tr>
<tr>
<td><strong>Aggregate Configuration</strong></td>
<td>299,008 x86 Cores</td>
</tr>
<tr>
<td></td>
<td>786,432 PPC64 Cores</td>
</tr>
<tr>
<td><strong>Memory/Node</strong></td>
<td>32 GB x86 + 6 GB K20x</td>
</tr>
<tr>
<td></td>
<td>16 GB RAM per node</td>
</tr>
<tr>
<td><strong>Memory/Core</strong></td>
<td>2 GB x86</td>
</tr>
<tr>
<td></td>
<td>1 GB</td>
</tr>
<tr>
<td><strong>Interconnect</strong></td>
<td>Gemini</td>
</tr>
<tr>
<td></td>
<td>5D Torus</td>
</tr>
<tr>
<td><strong>GPUs</strong></td>
<td>18,688 K20x Keplers</td>
</tr>
<tr>
<td></td>
<td>None</td>
</tr>
<tr>
<td><strong>Speed</strong></td>
<td>27 PF</td>
</tr>
<tr>
<td></td>
<td>10 PF</td>
</tr>
</tbody>
</table>
Argonne Leadership Computing Facility: People

- The people are as important as the hardware – probably more
- In addition to the usual support functions, we have:
  - **Catalyst Team**: Dedicated computational scientists who work with projects
  - **Performance Engineers**: serious optimization down to the core
  - **Visualization Team**: help understand the results
Three primary ways for access to LCF

Distribution of allocable hours

- Leadership-class computing
- 60% INCITE
  5.8 billion core-hours in CY2014
- Up to 30% ASCR Leadership Computing Challenge
- 10% Director’s Discretionary
- DOE/SC capability computing
Is INCITE right for you?

<table>
<thead>
<tr>
<th></th>
<th>Selecting an allocation program</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>INCITE</td>
</tr>
<tr>
<td>Eligible <em>regardless</em> of funding source or nationality</td>
<td>✔️</td>
</tr>
<tr>
<td>Require <em>tens of thousands</em> of cores for production jobs</td>
<td>✔️</td>
</tr>
<tr>
<td>Require up to <em>hundreds of millions</em> of core-hours for campaign</td>
<td>✔️</td>
</tr>
</tbody>
</table>
Innovative and Novel Computational Impact on Theory and Experiment

INCITE is an annual, peer-review allocation program that provides unprecedented computational and data science resources.

- 5.8 billion core-hours awarded for 2014 on the 27-petaflops Cray XK7 “Titan” and the 10-petaflops IBM BG/Q “Mira”
- Average award: 78 million core-hours on Titan and 88 million core-hours on Mira in 2014
- INCITE is open to any science domain
- INCITE seeks computationally intensive, large-scale research campaigns

Call for Proposals

The INCITE program seeks proposals for high-impact science and technology research challenges that require the power of the leadership-class systems. Allocations will be for calendar year 2015.

April 16 - June 27, 2014

Contact information
Julia C. White, INCITE Manager
whitejc@DOEleadershipcomputing.org
What is an advance in applications?
High Resolution Hurricane Studies

Greg Holland, NCAR

Sample results from simulation of 2005 hurricane season. These data are freely available to download from NCAR, useful for research on the role resolution plays in representation of individual weather events and on seasonal statistics.

Image: Strongest hurricane (not necessarily the same) produced per simulation at 36km, 12km and 4km resolution.
Examples of advances in applications

- Explain observed phenomena for the first time
- Guide design of new experiments or experimental facilities
- Predict phenomena
- Design new products, materials
- Not only due to increase in speed, memory
  - in almost every case new methods and algorithms contribute as much or more
Determining protein structures

Dramatic new capabilities through Rosetta

“Using the INCITE resources, we have been able to determine the structures of many proteins of biological interest using very sparse experimental data sets, design novel enzymes catalyzing new chemistries, and design small proteins which block influenza virus infection.” David Baker

Known Structure
Rosetta method is being tested on proteins of known Structure.

Unknown Structure on Minimal NMR Data
Large protein structures can now be computationally determined by incorporating backbone-only NMR data into Rosetta. (A) computationally (B) experimentally, Science 327, 1014 (2010).

Protein from low resolution electron structure data

Very large unsolved structures
A crystal structure of Spanish influenza hemagglutinin (trimer) bound to a computationally designed binder (green).
NDM-1, which stands for New Delhi metallo-beta-lactamase-1 is a gene (DNA code) carried by some bacteria. If a bacteria strain carries the NDM-1 gene it is resistant to nearly all antibiotics, including carbapenem antibiotics - also known as antibiotics of last resort.

A bacterium carrying the NDM-1 gene is the most powerful superbug around.

- Carbepenems are the most powerful antibiotics, used as a last resort for many bacterial infections, such as *E. coli* and *Klebsiella*. The NDM-1 gene makes the bacterium produce an enzyme that neutralizes the activity of carbapenem antibiotics.
### Protein-Ligand Interaction Simulations and Analysis

**Andrew Binkowski, Argonne National Laboratory**

<table>
<thead>
<tr>
<th>Science and Approach</th>
<th>Key Impact</th>
<th>ALCF Contributions</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Screen many compounds and feed into molecular dynamics simulations of the NDM-1 enzyme</td>
<td>• Reduce design time for drugs to fight drug-resistant infections from months or years to weeks</td>
<td>• ALCF integrated NAMD with an IBM PAMI version of charm++. This was the root of a 40% speedup. This impacts the current work.</td>
</tr>
<tr>
<td>• Identified the root cause of NDM-1’s effectiveness by determining the size and flexibility of the cavity</td>
<td>• Identify key flaw in current drug design – antibiotic design cannot just be bigger</td>
<td></td>
</tr>
<tr>
<td>• Determined exactly how NDM-1 breaks the antibiotic to render it ineffective</td>
<td>• Fight epidemics or weaponization of diseases by faster delivery of drug design</td>
<td></td>
</tr>
</tbody>
</table>

The gray is NDM-1’s structure, resolved by the Advanced Photon Source. Simulations revealed the very large cavity (dark gray) capable of binding a variety of known antibiotics (shown in colors). Once bound, the enzyme can cut the antibiotic, eliminating its efficiency.
# Combustion stability in complex engineering flows

**Lee Shunn, Cascade Technologies, US**

## Science and Accomplishments

- Self-excited, oscillatory combustion in rocket motors, scramjets and afterburners, utility boilers, and furnaces, can lead to intense pressure fluctuations and increased heat transfer to combustor surfaces. It can limit device performance, reduce efficiency, increase emissions, shorten service life, and cause structural damage.

- LES modeling capabilities developed during this award reproduce many of the flame stabilization patterns, burner interactions, and emissions signatures that are observed experimentally. This is enabling virtual testing of prototype pre-production combustor designs prior to full-load physical testing (see fig.).

## Key Impact

- Partnership with GE Energy to improve next generation low-NOx combustors

- Virtual testing of prototype combustor designs to predict emissions and operability.

## ALCF Contributions

- Efficient parallel visualization for large datasets

- Troubleshooting compilation and memory issues in large-scale distributed applications

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**Temperature field in a Dry Low NOx (DLN) combustor.** Localized high-temperature regions in the outer burners lead to increased NOx production. Modifications to the upstream fuel delivery system result in a more uniform thermal field and reduced emissions at the same operating conditions. Original design (left) & improved design (right).
Lithium Air Battery
Jack Wells, Oak Ridge National Laboratory

<table>
<thead>
<tr>
<th>Science and Accomplishments</th>
<th>Key Impact</th>
<th>ALCF Contributions</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Study the use of polypropylene carbonate (PC) as a potential electrolyte</td>
<td>• Design a battery that weight-for-weight stores 10x the energy of lithium ion batteries</td>
<td>• Helped enable ensemble simulations with IBM and ANL researchers</td>
</tr>
<tr>
<td>• Simulations found that PC is not stable and chemical reactions decrease efficacy</td>
<td>• Increase the possibility of replacing gasoline vehicles with electric vehicles</td>
<td></td>
</tr>
<tr>
<td>• Simulations identified why these results had not been seen in experiment</td>
<td></td>
<td></td>
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<tr>
<td>• Excluded polypropylene carbonate as a viable candidate for Lithium/Air batteries</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Science and Accomplishments</th>
<th>Key Impact</th>
<th>ALCF Contributions</th>
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</thead>
</table>
| • Wind turbine noise increases as a fifth power of blade tip speed and presently limits the blade tip radius and hence the wind energy that the turbine can harness. As the size of wind turbines increases and cost reduction targets encourage lighter, more flexible structures, the ability to accurately predict and design for varying aero loads become increasingly important. | **Wind turbine:**  
• Predicting separated flow aerodynamics at a near-stall flow angle  
• Improved LES Wall-models to enable computational investigation of large span noise-reduction concepts. | • Two algebraic multi-grid flow solvers were tuned to improve the scaling and convergence of the pressure Poisson equation.  
• Creation of 3D animations to better understand flow and noise mechanisms. |
| • Large-eddy simulation (LES), through direct computation of flow separation and noise sources, improves predictive potential over RANS methods. |  
| • The GE team is leveraging the HPC capability to now demonstrate the industrial impact of high-fidelity numerical methods. |  
|  
| LES of the DU96 airfoil at Re = 1.5 million and flow angle of 10.3 degrees. Flow separating from the airfoil visualized by Q-criterion iso-surfaces colored by the vertical velocity. |
Improved prediction through use of different method

Separated flow near the trailing edge of a wind turbine airfoil
*Results from a Large Eddy Simulation of the DU96 airfoil at Reynolds number of 1.5 million and flow angle of 10.3 degrees. Flow separating from the airfoil visualized by Q-criterion iso-surfaces colored by the vertical velocity.

Significant improvement in wake prediction using LES based approach
*Results from a Large Eddy Simulation of a fan cascade blade
Software is Infrastructure

- **System software (OS, compilers, runtime systems, file systems, visualization, software tools) form an ecosystem**
  - Need to transition as much of it as possible to new systems

- **Application codes often have lifetimes spanning decades**
  - Across many generations of computer architectures and environments
  - Maintenance/transition to new systems
  - Continual enhancement to broaden scope of problems, increase fidelity of simulations

- **Yet funding to maintain and transition software is seldom available**
  - And Federal agencies are reluctant to commit to support for indefinite duration
  - Although maintenance of physical infrastructure is usually provided

- **Every so often it is necessary to start from scratch**
  - NWChem and MADNESS
  - HACC
  - NNSA-ASCI codes

- **Note: it is still possible for individual researchers to develop ground-breaking applications; sustaining them may become a group/community effort (e.g., NEK)**
A sample of codes with local expertise available at Argonne and Oak Ridge

<table>
<thead>
<tr>
<th>Application</th>
<th>Field</th>
<th>ALCF</th>
<th>OLCF</th>
</tr>
</thead>
<tbody>
<tr>
<td>FLASH</td>
<td>Astrophysics</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>MILC,CPS</td>
<td>LQCD</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Nek5000</td>
<td>Nuclear energy</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Rossetta</td>
<td>Protein structure</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>DCA++</td>
<td>Materials science</td>
<td>✓</td>
<td>✓</td>
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<tr>
<td>ANGFMC</td>
<td>Nuclear structure</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>NUCCOR</td>
<td>Nuclear structure</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Qbox</td>
<td>Chemistry</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>LAMMPS</td>
<td>Molecular dynamics</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>NWChem</td>
<td>Chemistry</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>GAMESS</td>
<td>Chemistry</td>
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<td>✓</td>
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<tr>
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<td>Earth Science</td>
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<td>✓</td>
</tr>
<tr>
<td>AWP-ODC</td>
<td>Earth Science</td>
<td>✓</td>
<td>✓</td>
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<tr>
<td>NAMD</td>
<td>Molecular dynamics</td>
<td>✓</td>
<td>✓</td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>Application</th>
<th>Field</th>
<th>ALCF</th>
<th>OLCF</th>
</tr>
</thead>
<tbody>
<tr>
<td>AVBP</td>
<td>Combustion</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>GTC,GTX</td>
<td>Fusion</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>IRMHD</td>
<td>Plasma</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>CPMD, CP2K</td>
<td>Molecular dynamics</td>
<td>✓</td>
<td>✓</td>
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<tr>
<td>CESM</td>
<td>Climate</td>
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<td>✓</td>
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<tr>
<td>CAM-SE</td>
<td>Climate</td>
<td>✓</td>
<td>✓</td>
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<tr>
<td>WRF</td>
<td>Climate</td>
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<td>✓</td>
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<tr>
<td>Amber</td>
<td>Molecular dynamics</td>
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<td>HACC</td>
<td>Cosmology</td>
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<tr>
<td>Falkon</td>
<td>Computer science/HTC</td>
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<td>✓</td>
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<tr>
<td>s3d</td>
<td>Combustion</td>
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<td>DENOVO</td>
<td>Nuclear energy</td>
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<td>LSMS</td>
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<tr>
<td>QMCPACK</td>
<td>Materials science</td>
<td>✓</td>
<td>✓</td>
</tr>
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</table>
HPC has made great strides

- Scientific computing has advanced dramatically during the last four decades, despite several upheavals in computer architectures.
  - The evolution of high-end computers in the next decade will again pose challenges as well as opportunities.

- Many applications are able to utilize today’s massive levels of parallelism
Advances do not happen for free

- In addition to operating computer facilities, substantial investments are needed to
  - enable the transition of widely used codes, programming frameworks, and libraries to new platforms
  - evolve application software to support the increased complexity of the problems that can be tackled by the more powerful systems
  - create a new multidisciplinary team to tackle an ambitious goal; e.g., co-design centers, NNSA ASCI Alliances, ASC PSAAPs

- Providing training on computational science and engineering to industrial and academic researchers is also quite important
Close involvement of applications experts in guiding the design of future hardware and software -- supplemented by funding to address development of key technologies and features -- has proven to be effective and will continue to be needed in the exascale era and beyond.

Conversely, new technologies and architectures will lead to new methods and algorithms.
DOE Exascale Co-design centers

- Exascale Co-design centers on application domains established by DOE Office of Science in 2011:
  - Simulation of combustion in turbulence
  - Materials in extreme environments
  - Simulation of advanced nuclear reactors
    - Industry advisors: companies that build nuclear reactors

- Plus data-intensive science partnerships started in 2014
Use of HPC by industry

- As we have seen at this conference, there is substantial and productive use of HPC by industry at PRACE and DOE LCF centers
  - And other centers worldwide
- This is not new: even in the 1980s some companies were using Crays and early parallel computers
- There are companies that use HPC but prefer not to reveal it
Some industrial partnerships (mostly INCITE projects)

<table>
<thead>
<tr>
<th>Catalysis</th>
<th>Design innovation</th>
<th>Gasoline engine injector</th>
<th>Industrial fire suppression</th>
<th>Turbo machinery efficiency</th>
<th>Underhood cooling</th>
</tr>
</thead>
<tbody>
<tr>
<td>Demonstrated biomass as a viable, sustainable feedstock for hydrogen production for fuel cells; showed that nickel is a feasible catalytic alternative to platinum</td>
<td>Accelerating design of shock wave turbo compressors for carbon capture and sequestration</td>
<td>Optimization of injector hole pattern design for desired in-cylinder fuel-air mixture distributions (4-40x potential improvement in workflow throughput via 100s of ensemble simulations)</td>
<td>Developing high-fidelity modeling capability for fire growth and suppression; fire losses account for 30% of U.S. property loss costs</td>
<td>Simulated unsteady flow in turbo machinery, opening new opportunities for design innovation and efficiency improvements</td>
<td>Developed a new, efficient and automatic analytical cooling package optimization process leading to one of a kind design optimization of cooling systems</td>
</tr>
</tbody>
</table>

![Catalysis Image](image1)
![Design innovation Image](image2)
![Gasoline engine injector Image](image3)
![Industrial fire suppression Image](image4)
![Turbo machinery efficiency Image](image5)
![Underhood cooling Image](image6)
Some industrial partnerships (mostly INCITE projects)

<table>
<thead>
<tr>
<th>Boeing</th>
<th>P&amp;G</th>
<th>Ford</th>
<th>United Technologies Research Center</th>
<th>BOSCH</th>
<th>Smart Truck</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aircraft design</td>
<td>Consumer products</td>
<td>Engine cycle-to-cycle variation</td>
<td>Jet engine efficiency</td>
<td>Li-ion batteries</td>
<td>Long-haul truck fuel efficiency</td>
</tr>
</tbody>
</table>

- Simulating takeoff and landing scenarios improved a critical code for estimating characteristics of commercial aircraft, including lift, drag, and controllability.
- Leadership computing and molecular dynamics software advanced understanding of chemical processes that can limit product shelf life.
- Emerging model of engine cyclic variation will apply thousands of processors to a challenging problem.
- Accurate predictions of atomization of liquid fuel by aerodynamic forces enhance combustion stability, improve efficiency, and reduce emissions.
- New classes of solid inorganic Li-ion electrolytes could deliver high ionic and low electronic conductivity and good electrochemical stability.
- Simulations reduced by 50% the time to develop a unique system of add-on parts that increases fuel efficiency by 7–12%.
DOE-funded computer science and applied mathematics benefits IT industry

A few ASCR Technologies and the Companies that Use them

- **MPICH** – Message passing library
  "MPICH’s impact comes from the fact that since it is open source, portable, efficient, and solid, most computer vendors have chosen it as the foundation of the MPI implementation that they supply to their customers as part of their system software.” - Rusty Lusk, MPICH consortia
  "MPICH is critical to the development of the F135 engine, which will power America’s next-generation Joint Strike Fighter.” - Robert Barnhardt, VP, Pratt & Whitney

- **Fastbit** – Search algorithm for large-scale datasets
  "FastBit is at least 10 times, in many situations 100 times, faster than current commercial database technologies” – Senior Software Engineer, Yahoo!

- **OSCARS** - On-demand virtual network circuits
  "It used to take three months, 13 network engineers, 250 plus e-mails and 20 international conference calls to set up an inter-continental virtual circuit. With OSCARS and collaborative projects, we can establish this link in 10 minutes.” - Chin Guok, ESnet network engineer

- **perfSONAR** - network performance monitoring
  "These tools give us better visibility into the network, allowing us to troubleshoot performance issues quickly.” – Internet2 Network Performance Workshop participant

U.S. DEPARTMENT OF
Office of
Science

ASCAC March 26, 2012 22
But the number of companies that use computer simulation is a small fraction of the ones that could benefit from it

- And those that use HPC are an even smaller fraction
Obstacles to industrial use of HPC

- Industrial users are often users of application software, not developers
  - They cannot add missing modeling capabilities

- Commercial application codes are seldom (if ever) scaled to high levels because that takes a lot of effort and the market is small:
  - few industrial users have large systems
  - few use LCF-scale systems in other facilities

- Licensing of commercial codes by the number of cores leads to prohibitive cost on systems with a million or more cores

- Few companies have staff with expertise in computational science
Obstacles to industrial use of HPC

- Security of proprietary data and/or software installed in an facility used by many users
- For industrial users, proof-of-principle is not enough, need bulletproof software with “infinite” lifetime
  - How many HPC codes are bulletproof?
- Typical industry workflow is incompatible with typical turnaround time at LCFs
  - need to get consistently several turnarounds every 24 hours or less
- INCITE peer review of industrial proposals for time on LCFs may be negative because do not appear to be high-impact
  - Perhaps need to include economic impacts in evaluating
Industrial applications are complex

http://users.ece.gatech.edu/~mrichard/ExascaleComputingStudyReports/ECS_reports.htm

Based on table created by David Bailey, Lawrence Berkeley Laboratory
What approaches reduce the barriers?

- Work with the providers of the software that industry uses
- Provide a tier of facilities, not just the biggest
- Operate systems with familiar hardware and software
  - The IBM Blue Gene systems are excellent but rather different than x86 clusters
- Partner with the company
  - Effective, but not scalable
- Provide tailored training, including the equivalent of internships
- Tailored outreach
- MATLAB on steroids?
High Fidelity Engine Modeling
Doug Longman (ES), Sibendu Som (ES), Shashi Aithal (MCS), Marcus Weber (CAT), Tushar Shethaji (CAT), Peter Senecal (CSI), Keith Richards (CSI), Marta Garcia Martinez (ALCF)

- **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 Argonne and CAT

- **CELS Engagement**
  - LCRC: Identify 1000 core scaling bottlenecks, recommend approaches
  - LCRC+ESD+CAT: analyze results
  - ALCF+CSI: Discretionary Project to port CONVERGE to Blue Gene
The Virtual Engine Research Institute and Fuels Initiative

• A new Argonne effort that offers full range of services: test facilities, staff with expertise in relevant disciplines, access to clusters as well as Mira (if the project qualifies)
• Builds on similar but less comprehensive efforts
• Too early to tell whether it will be successful
The Argonne Training Program in Extreme-Scale Computing (ATPESC) provides training on the key skills, approaches, and tools necessary to design, implement, and execute Computational Science and Engineering (CS&E) applications on current high-end systems and the leadership-class systems expected to be available in 2017 and beyond.

The training features lectures by leading computer and computational scientists in the topics covered and extensive hands-on exercises on leadership-class computers.

High-level view of curriculum

- Computer architectures, mathematical models and numerical algorithms
- Programming methodologies that are effective across a variety of today’s supercomputers and that are expected to be applicable to exascale systems
- Software architecture, debugging and performance measurement tools, visualization
- Approaches to building community codes for HPC systems
- Methodologies and tools relevant for data-intensive and Big Data applications
Argonne Training Program on Extreme-Scale Computing: 2013 participants
Summary

- **Scientific computing has advanced due to many factors, including**
  - Multidisciplinary teams
  - Advances in algorithms and methods
  - Community codes
  - Software engineering
  - Oh yes, also from much more powerful computers

- **Computational science is now recognized as an important discipline**

- **Working with industry poses additional challenges but we can – and should – tackle them**
To do in your spare time

- Convince the world that software is infrastructure and that its maintenance and evolution requires long-term support
- And that computer science and mathematics research continues to be needed
- Educate the decision-makers who have money that it takes years and many person-years to develop application software that can tackle complex problems and be used by a community
- If you have time left: develop policies and technologies for creating and operating data archives with longevity appropriate to the application area and are affordable
Thank you!