HPC Current Use and Practice: National Laboratories

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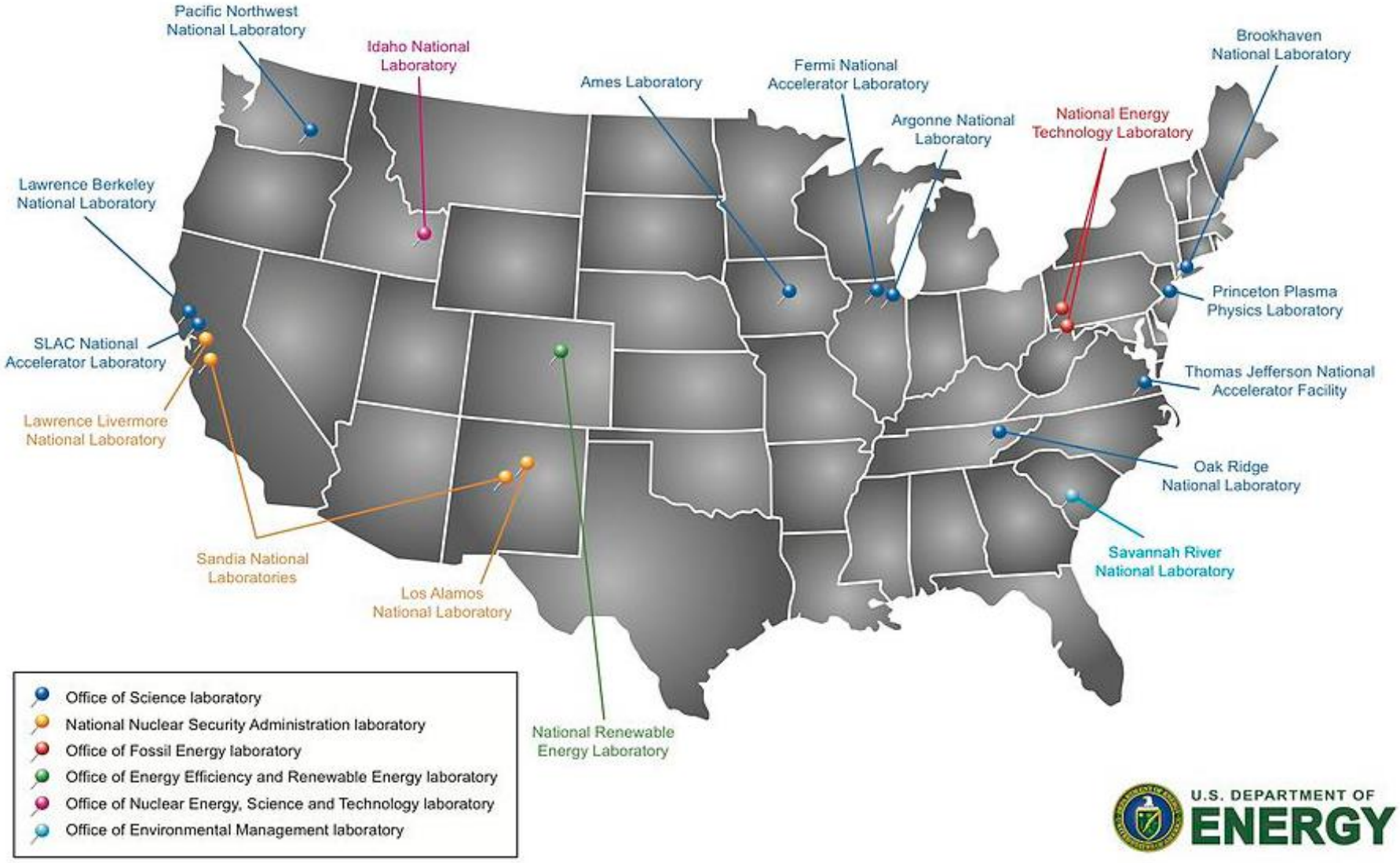
HPC is critical to all 17 DOE National Laboratories

Why HPC?

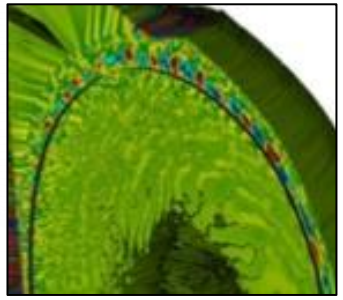
- Modeling & Simulation of complex systems
  - Weather
  - Earth systems
  - Cosmology
  - Energy
  - National Security
- Data analysis
  - Needle in haystack
  - Graph problems
  - Machine learning



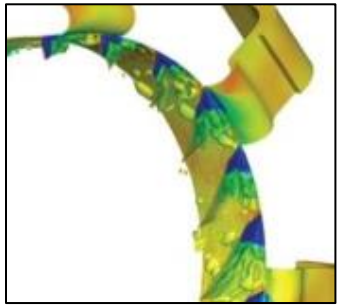
U.S. DEPARTMENT OF ENERGY

How do we use High Performance Computing

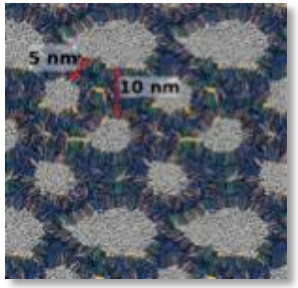
Fusion Energy
A Princeton Plasma Physics Laboratory team led by C.S. Chang was able to simulate and explain nonlinear coherent turbulence structures on the plasma edge in a fusion reactor by exploiting increased performance of the Titan architecture.

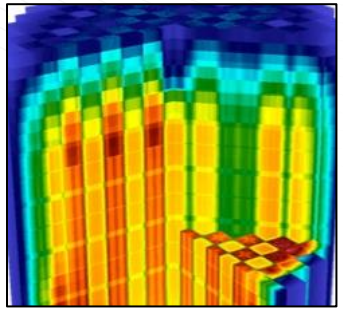


Turbomachinery
Ramgen Power Systems is using the Titan system to significantly reduce time to solution in the optimization of novel designs based on aerospace shock wave compression technology for gas compression systems, such as carbon dioxide compressors.

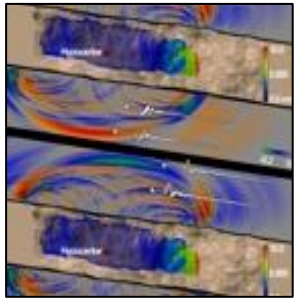


Molecular Science
Researchers at Procter & Gamble and Temple University used DOE's Titan to better understand the three-dimensional structure of skin's outermost barrier, the stratum corneum.

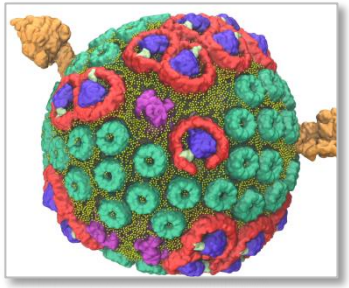




Nuclear Reactors
Center for the Advanced Simulation of Light water Reactors (CASL) investigators successfully performed full core physics power-up simulations of the Westinghouse AP1000 pressurized water reactor core using their Virtual Environment for Reactor Application code that has been designed on Titan architecture.



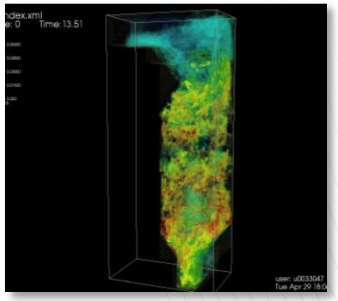
Earthquake Hazard Assessment
To better prepare California for large seismic events SCEC joint researchers have simulated earthquakes at high frequencies allowing structural engineers to conduct realistic physics-based probabilistic seismic hazard analyses.



Photosynthesis
A team from the University of Illinois at Urbana-Champaign used Titan to achieve a milestone in the field of biomolecular simulation, modeling a complete photo-synthetic organelle of the bacteria Rhodobacter sphaeroides in atomic detail. The project is the first of its kind.

Climate Science
Simulations on OLCF resources recreated the evolution of the climate state during the first half of the last deglaciation period allowing scientists to explain the mechanisms that triggered the last period of Southern Hemisphere warning and deglaciation.

Clean Coal Combustion
Researchers at the University of Utah and its Carbon Capture Multi-Disciplinary Simulation Center (CCMSC) are using Titan to improve modeling capabilities to enable petascale simulations to guide the design of next-generation oxy-coal boilers for clean electric energy.



Complex Materials
Using nearly 10 million core hours for the ultimate calculations, condensed matter theorists at Rutgers University, led by Prof. Gabriel Kotliar, predicted the electronic and magnetic structure of plutonium using leading-edge dynamical mean field theory and the Titan supercomputer.

Science • Energy • Industry • Security

What do our computers look like?

- Massively parallel systems
  - Millions of threads of execution
  - Advanced processors
    - Many-core and Heterogeneous
  - High speed interconnects
    - OmniPath™, InfiniBand, Aries™
  - Users run large jobs that can use every processor on the system
    - Demands extreme reliability & scalability
  - Large, fast data stores
    - Fast non-volatile memory
    - Parallel file systems
    - Archival storage

Lawrence Berkeley National Laboratory

Cori: Heterogeneous system with over 1,900 Intel Xeon and over 9,300 Xeon Phi processors. >30 PetaFLOPS

Oak Ridge National Laboratory

Titan: Heterogeneous system with 18,688 NVIDIA GPUs and 16-core AMD processors. 27 PetaFLOPS

Argonne National Laboratory

Mira: Homogeneous system with 49,152 processors, each with 16 cores. 10 PetaFLOPS

ESnet
ENERGY SCIENCES NETWORK

Esnet: 400 Gb/s network that links DOE laboratories and universities

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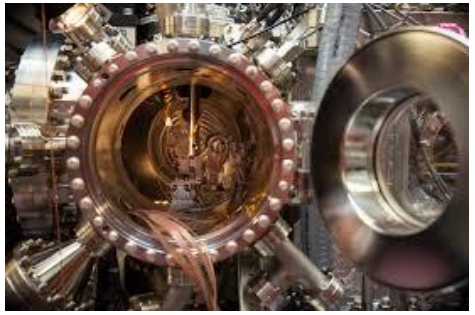
What are the types of workflows we support?

- Traditional remote access for interactive or batch using ssh and mobile devices from around the world
- Grid access for data retrieval and job launch through proxy servers
- Data users storing information and serving it to known or unknown users
- Real-time analysis of data for experimental facilities
- Industrial users with open, proprietary, and export controlled data
- Combinations of multiple workflows



Remote Access using SSH or Mobile applications

- Our users come from around the country and overseas: ORNL - 50% Universities, 40% National Labs, 10% Industries
- Various centers use either traditional passwords or One-Time passwords (SecurID or CryptoCard) for authentication
- Users log on, prepare applications, submit batch jobs, and return later to see the results
- It is more and more common for users to use mobile apps to monitor and control workflows
- It is increasingly common for users to have more complex workflows
  - Users submit job to HPC system
    - System loads data from archive before job starts
    - Job launches on compute nodes
    - User(s) monitors and steers job
    - Submit job to analytics system, perhaps at a different site
    - Results visualized and stored in archive
    - Launch additional jobs
  - Requires credentials to authenticate at each phase
  - Credentials need long lifetime as some of these jobs take days or weeks to complete – often long wait times to start

Grid Access and Data Users

- Science Gateways and End stations
  - Communities work together to develop codes and prioritize work to be done
  - Data from simulations is published to community to analyze
- Community remotely finds, accesses, and analyzes data through portals
  - Users can select subsets of data on which to operate
  - Provides a suite of tools to analyze, visualize, and manipulate selected data
  - Download results to remote systems
- Authenticated or anonymous access

Examples

- **Earth Systems Grid**: Shares the results of climate observations and simulations for worldwide climate community analysis
- **QCD Consortium**: Thousands of researchers around the world work together to prioritize experiments, conduct simulations, analyze results, and collaborate on publications
- **Cosmology**: Simulations of the evolution of the universe produce datasets of many petabytes that can be used to compare to observational data

Real Time & High Throughput analysis of experiments

- Increasingly, modeling & simulation is required to analyze and understand the results of experiments and guide next steps
- Data must move in real-time, sometimes over the wide area. For example:
  - Experimental data moved from beam line to compute servers
  - Copy of raw data sent to archive
  - Simulation and analysis results sent back to the beam line as input for the next run, with a copy to the archive
  - Experimental and simulation results available to collaboration or public for analysis and publication
- Data from CERN in Geneva for the ATLAS project is collected and stored locally
- Duplicate copies are stored at several “mirror” sites for backup and analysis
- Thousands of jobs are run at sites around the world every day
  - Data is moved from mirror sites to analysis sites
  - Jobs are run and results returned to archive
- Science teams analyze results

Usability versus Security

- Science is an open endeavor
  - Many collaborators from around the world
    - How do you MFA4 authenticate users you never see?
  - Advances build upon earlier work
    - Must publish results, data, and methods
    - Must protect the data from modification
  - Likewise, we must protect proprietary, sensitive, and export controlled technology and results
- Certificate life
  - Users need long-lasting certificates as it can take weeks to months to run some workflows
  - But long lived certificates increase risk
- How long does it take to get an account?
  - Institutional user agreements, Principal Investigator agreements, Export control reviews, multi-factor authentication registration
  - It often takes 1-3 months to get users on a newly approved project
    - Too long considering many projects last less than a year and many users are students

What should we worry about in HPC security

- Attacks on high-profile systems
  - Titan gets about a million hits per day
- Who are our users – how do we know
  - Did a professor give the login token to grad student to run jobs?
- What are the users doing
  - How do we know if users are doing their science, or using the system for something else?
- Technology is making encryption less secure, undermining the basis for much of cyber security
  - Need techniques that are not subject to quantum computer attacks
- Data integrity
  - Do we know the answers are right and haven't been tampered with?
- Standards for establishing trust among domains
  - We have lots of tools for collaboration and sharing data, but often the cyber security experts won't allow them to be used
- Support for containerization and virtual machines
  - Users love them, but
  - How do you provide security patches for thousands of containers, with different software versions

Summary

- The science community has diverse needs with security postures ranging from open to export controlled
- Our collaborations are worldwide and require high-bandwidth connections that link computers, storage, experimental or observational facilities, and our users
- Technology is moving faster than cyber security solutions. We need to work with the cyber security community to find solutions that don’t hamper our ability to meet our mission

Acknowledgements

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