Quadrennial Technology Review 2015

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U.S. DEPARTMENT OF ENERGY

Quadrennial Technology Review 2015

High Performance Computing Capabilities and Resource Allocations

Chapter 9: Enabling Capabilities for Science and Energy

High Performance Computing Capabilities

The Department of Energy (DOE) laboratories integrate high performance computing (HPC) capabilities into their energy, science, and national security missions. Within the Office of Science (DOE-SC), HPC systems are classified as either leadership-class machines, reserved for computational challenges requiring massive parallelization, or production-class machines, used for computational problems that do not require the unique capabilities of the leadership-class machines. The two DOE-SC-supported computers in Table 1, Titan and Mira, are classified as leadership-class machines. The relative ranking of the top supercomputers in the world is updated twice annually as part of the Top 500 list (www.top500.org).[1] Computational performance for each system is determined using the LINPACK Benchmark, which measures the speed with which the computer

Table 1 The top 10 supercomputers in the world as of November 2015. The computers supported by the DOE are listed in **bold**.

Ranking	Name	Computing performance (PFlops)	Research facility/university/company	Country	Year entering service
1	Tianhe-2	33.9	National Super Computer Center (Guangzhou)	China	2013
2	**Titan**	**17.6**	**Oak Ridge National Laboratory**	**US**	**2012**
3	**Sequoia**	**17.2**	**Lawrence Livermore National Laboratory**	**US**	**2011**
4	K computer	10.5	RIKEN Advanced Institute for Computational Science (AICS)	Japan	2011
5	**Mira**	**8.6**	**Argonne National Laboratory**	**US**	**2012**
6	**Trinity**	**8.1**	**Los Alamos National Laboratory/ Sandia National Laboratories**	**US**	**2015**
7	Piz Daint	6.3	Swiss National Supercomputing Centre (CSCS)	Switzerland	2012
8	Hazel Hen	5.6	Hochstleistungsrechenzentrum (HLRS)	Germany	2014
9	Shaheen II	5.5	King Abdullah University of Science and Technology (KAUST)	Saudi Arabia	2015
10	Stampede	5.2	Texas Advanced Computing Center	US	2012

solves a dense system of linear equations. Because this task is included in many simulations, the LINPACK benchmark has achieved wide acceptance as a measure of computational performance. However, it is generally recognized that LINPACK does not capture all of the operations involved in advanced simulation and should not be considered to be an absolute measure of system performance.

The DOE hosts substantial high performance computing capacity at its national laboratories that is utilized in a manner similar to the DOE-SC production-class machines described above. These machines are typically easier to use than the massively-parallel leadership class machines listed in Table 1. A list of DOE machines ranked between 12 and 300 in the world is given in Table 2.

Table 2 High performance computers supported by the Department of Energy that are ranked between 12 and 300 in the world at the time of publication of the current Top 500 list (November 2015).

Ranking	Name	Computing Performance (PFlops)	Research Facility	Year Entering Service
12	Vulcan	4.293	Lawrence Livermore National Laboratory	2012
27	Cascade	2.539	Pacific Northwest National Laboratory	2013
40	Edison	1.654	Lawrence Berkeley National Laboratory	2014
65[3]	Cielo	1.110	Los Alamos National Laboratory	2011
72[4]	Hopper	1.054	Lawrence Berkeley National Laboratory	2010
106	Zin	0.773	Lawrence Livermore National Laboratory	2011
120	Cetus	0.715	Argonne National Laboratory	2012
142	Gaea C2	0.565	NOAA/Oak Ridge National Laboratory (Administered by Oak Ridge for NOAA)	2011
161	Sky Bridge	0.533	Sandia National Laboratories	2015
170	Falcon	0.511	Idaho National Laboratory	2014
212	Red Sky	0.433	Sandia National Laboratories/National Renewable Energy Laboratory	2010
232	HPCEE	0.413	National Energy Technology Laboratory	2012
271	Vesta	0.358	Argonne National Laboratory	2012
281	Cab	0.347	Lawrence Livermore National Laboratory	2012
282	Luna	0.347	Los Alamos National Laboratory	2011
295	Pecos	0.337	Sandia National Laboratories	2012

Allocation Mechanisms

Computational time at the DOE-SC Office of Advanced Scientific Computing Research (SC-ASCR) scientific user facilities is allocated on a competitive basis. This occurs through multiple mechanisms. At the two leadership computing facilities, time is allocated through three programs: the ASCR Leadership Computing Challenge (ALCC), the Innovative & Novel Computational Impact on Theory & Experiment (INCITE) program, and director's discretionary (DD) awards. ALCC awards account for 30% of the time at these facilities, while INCITE accounts for 60% of the time. Director's discretionary awards account for the remaining 10%.

Because NERSC exists to provide capacity computing for Office of Science programs, the distribution of time is different from the leadership facilities. At NERSC, 80% of the computational time is reserved for the Energy Research Computing Allocations Process (ERCAP). ERCAP supports the computational needs of the 6 Office of Science programs and the SBIR/STTR program. This program typically supports 600-700 projects, but with individual allocations less than those seen in ALCC or INCITE. 10% of the time at NERSC is reserved for ALCC, and 10% for Director's Discretionary awards.

ASCR Leadership Computing Challenge (ALCC)

ALCC provides single-year allocations to research that either contributes directly to the DOE missions in energy, science, environmental management, and stockpile stewardship, or broadens the community of researchers capable of using leadership computing resources. This can include both DOE-supported research and relevant research supported through other public and private funding sources.

The review process is managed by the Office of Advanced Scientific Computing Research (SC-ASCR) within the DOE-SC. Because the program is intended to cover the entire DOE mission, priority areas are developed jointly with relevant DOE offices, including Energy Efficiency and Renewable Energy (DOE-EERE), Nuclear Energy, Fossil Energy, Environmental Management, and all DOE-SC offices. During the 2015 review cycle, the following areas were prioritized:

- Advancing energy efficiency and the clean energy agenda
- Ensuring nuclear reactor safety and effective environmental management of nuclear waste
- Enabling mesoscale materials science
- Enabling and performing predictive simulation of chemical processes
- Simulating the Dark Universe, Understanding the High Energy Higgs sector, Lattice Gauge theories probing beyond the Standard Model and other topics of importance to the DOE High Energy Physics Program
- Enabling Lattice QCD, other simulations of low energy nuclear physics, or simulations of nuclear astrophysics problems. Problems relevant to experimental research programs at DOE Nuclear Physics facilities are of particular interest
- Advancing a robust predictive understanding and capability across scales and systems for Climate Science
- Advancing Earth Science, Environmental Science, and Subsurface Technology particularly as relates to energy resources, the carbon cycle and sequestration, and environmental management
- Developing new solutions for Big Data intersections with leadership computing
- Broadening the community of researchers capable of using next generation leadership computing resources
- Exploring new frontiers in physical, biological, and computational science

ALCC awards are single-year awards determined by peer review from scientists across the academic, industrial, and federal research communities, as well as input from relevant DOE programs. Awards are made through an annual review cycle, with additional hours reserved for urgent projects that may emerge between annual review cycles. In 2015, 43 awards were made for a total of three billion processor hours. While Table 9.3 in QTR, Chapter 9, *Enabling Capabilities for Science and Energy* indicates awards made with specific relevance to energy technology, a complete list of supported projects is included in Tables 3 and 4.

Table 3 2015 ALCC Awards in Climate Science, Computational Fluid Dynamics, Nuclear Engineering, and Materials Science

Science Area	Project Title	Institution
Climate Science	Delivering the Department of Energy's Next-Generation High Resolution Earth System Model	ORNL
	Cloud-System Simulations with a Multiscale Nonhydrostatic Global Atmospheric Model	LBNL
Computational Fluid Dynamics (CFD)	Credible Predictive Simulation Capabilities for Advanced Clean Energy Technology Development through Uncertainty Quantification	ALPEMI Consulting, LLC
	Advancing Internal Combustion Engine Simulations using Sensitivity Analysis	ANL
	System-level LES of High-efficiency Gas Turbine Combustors to Advance Low-emission Combustion Technology	GE Co.
	Computational Design of Novel Multiscale Concrete Rheometers	NIST
	Chombo-Crunch: Modeling Pore Scale Reactive Transport Processes Associated with Carbon Sequestration	LBNL
	Large Eddy Simulation and Direct Numerical Simulation of Fluid Induced Loads on Reactor Vessel Internals	Westinghouse Electric Corp.
	Multi-Scale Modeling of Rotating Stall & Geometric Optimization	Dresser-Rand, Inc.
	Large-Eddy Simulation of Turbine Internal Cooling Passages	GE, Inc.
	Simulating Multiphase Heat Transfer in a Novel Receiver for Concentrating Solar Power (CSP) Plants	UC Boulder
	Validation of RAP/HRRR for the Wind Forecast Improvement Project II	NOAA
Nuclear Engineering	Delivering Advanced Modeling & Simulation for Nuclear Energy Applications	ORNL
	High-fidelity Computations of Fuel Assemblies Subjected to Seismic Loads	GWU
	Toward a Longer-life Core: Thermal-hydraulic CFD Simulations of Deformed Fuel Assemblies	ANL
Materials Science	Anomalous Density Properties and Ion Solvation in Liquid Water: A Path-Integral Ab Initio Study	Princeton University
	Predictive Modeling of Functional Nanoporous Materials	University of Minnesota
	Computational Design of Interfaces for Photovoltaics	Tulane University
	Understanding Helium-Hydrogen Plasma Mediated Tungsten Surface Response to Predict Fusion Plasma Facing Component Performance in ITER	University of Tennessee
	First Principles Large Scale Simulations of Interfaces for Energy Conversion and Storage	University of Chicago
	Prediction of Morphology and Charge-transfer Properties in Bulk Material and at Donor/Acceptor Interfaces of Thin-film Organic Photovoltaic Cells	UCLA
	PT-symmetric Quantum Mechanics for Real-time Electron Transport Simulations	GWU
	Introducing Carriers and Control Polaronic States in Energy-related Complex Solids	University of Colorado Boulder
	Large Scale Ab-initio Simulation of Crystalline Defects in Mg-alloys	Caltech

Table 4 2015 ALCC Awards in Molecular Biophysics, Nuclear Physics, High Energy Physics, Fusion and Plasma Energy, and Computer And Data Science

Science Area	Project Title	Institution
Molecular Biophysics	Developing Hyper-catalytic Enzymes for Renewable Energy	ORNL
	Molecular Dynamics Studies of Biomass Degradation in Biofuel Production	UIUC
Nuclear Physics	Probing Novel Physics using Nucleon Matrix Elements	LANL
	Multi-Neutron Forces from QCD	MIT
	In Search of the Elusive Glue of Quantum Chromodynamics	Jefferson Laboratory
	Three-dimensional Simulations of Core-collapse Supernovae from High-mass Progenitor Stars	ORNL
High Energy Physics	Hadronic Light-by-light Scattering Contribution to the Muon Anomalous Magnetic Moment from Lattice QCD with Chiral Fermions	University of Connecticut
	Cosmic Frontier Computational End-station	ANL
	An End-Station for Intensity and Energy Frontier Experiments and Calculations	ANL
Fusion and Plasma Energy	Modeling RF-induced Sheath E	Tech-X Corp.
	Dynamics of Magnetic Fields in High-Energy-Density Plasmas from Fusion to Astrophysics	Princeton University
	Validation Simulations of Macroscopic Burning-plasma Dynamics	Tech-X Corp.
Computer and Data Science	Hobbes: Operating System and Runtime Research for Extreme Scale	SNL
	Performance Analysis, Modeling and Scaling of HPC Applications and Tools	LLNL
	XPRESS Program Environment Testing at Scale	SNL
	Exploring Quantum Optimizers via Classical Supercomputing	USC
	Enabling Next-Generation Light Source Data Analysis through Massive Parallelism	LBNL
	Demonstration of the Scalability of Programming Environments By Simulating Multi-Scale Applications	Leidos, Inc.
	Portable Application Development for Next Generation Supercomputer Architectures	ORNL

Innovative & Novel Computational Impact on Theory & Experiment (INCITE)

INCITE is the primary means by which the larger scientific community gains access to the DOE-SC leadership-class computers, Titan and Mira. The INCITE program is specifically targeted towards the most intensive computational challenges that fully utilize the capabilities of leadership class computing. These include problems that address "grand challenges" in science and engineering regardless of discipline or relevance to the DOE missions (see the QTR 2015 report, Section 9.6.1). The INCITE program awards approximately 5.8 billion core hours annually based on peer review of the proposals. In opening the leadership class facilities to both DOE and non-DOE research areas, INCITE is acting in accordance with the Department of Energy High-End Computing Revitalization Act of 2004,[2] which directs the DOE to provide the entire scientific community with access to leadership computing capabilities.

In addition to being open to all science and engineering disciplines, INCITE differs in scope from ALCC. INCITE allocations are significantly larger than ALCC allocations. For the 2015 ALCC allocations listed in Tables 3 and 4, the 1-year allocations ranged from 5 to 175 million processor hours, with an average of 67 million hours. The 2015 INCITE projects ranged from 13 to 280 million processor hours per year over the three year life of the projects, with an average of 104 million processor hours per year. The projects are also expected to be massively parallel simulations, using 20% or more of the processors of a leadership-class computer for a single run. This is done to ensure that these resources are available for projects that can most effectively use these capabilities. The INCITE process includes a review of the computational readiness of any project, designed to ensure that the code is ready to take advantage of the massively parallel architecture of the platform, as well as additional capabilities such as Titan's graphics processing unit (GPU) accelerators.

A complete list of the 2015 INCITE projects is included in Tables 5 and 6. The projects are organized by scientific and engineering disciplines: biology, biological sciences, chemistry, computer science, earth science, engineering, materials science, and physics.

The important role the INCITE program plays in fulfilling the DOE energy mission is seen in multiple projects. For example, research in advanced materials for energy applications include modeling new materials for lithium-air batteries (ANL) and simulating heterogeneous interfaces in solar cells (University of Chicago). Simulations of chemical processes within energy systems include the simulation of turbulent combustion that could enable fuel-flexible gas turbines (SNL). Computational fluid dynamics at the leadership-class computing scale is being used to simulate a range of engineering systems, including energy-efficient aircraft (University of Colorado Boulder) and the design of advanced combustion turbines (GE, Inc.).

Leadership-class computing at the INCITE level is also used within the DOE science mission. Applications include climate research (SNL and UCAR), enabling computer science (ANL, LBNL, and BNL), and a broad range of physics simulations.

Finally, many science challenges outside of the DOE mission are being advanced through DOE leadership computing capabilities. Topics include the behavior of human skin (Temple University), energy conversion processes occurring within the cell (UIUC), simulation of the mechanics of sickle-cell anemia (Brown University), assessment of earthquake risk in the Los Angeles area (USC), and novel cancer therapies (HZDR).

Table 5 Current INCITE Awards in Biology, Chemistry, Computer Science, Earth Science, and Engineering

Discipline	Title	Lead Institution	Processor Hours (M)
Biology & Biological Sciences	Designing O_2 Tolerant Hydrogenases	Stanford University	13
	Biological Sciences	Temple University	92
	Simulation of Fundamental Energy Conversion Processes in the Cell	UIUC	150
	Characterizing Large-Scale Structural Transitions in Membrane Transporters	UIUC	96
	Multiscale Simulations of Human Pathologies	Brown University	70
	Studies of Large Conformational Changes in Biomolecular Machines	University of Chicago	120
Chemistry	Towards Breakthroughs in Protein Structure Calculation and Design	University of Washington	80
	Catalyst Support Interactions	Stanford University	50
	DNS of Turbulent Combustion Towards Fuel-Flexible Gas Turbines and IC Engines	SNL	106
	First-Principles Simulations of High-Speed Combustion and Detonation	University of Chicago	150
	Computational Actinide Chemistry: Reliable Predictions and New Concepts	University of Alabama	150
	Large-scale Coupled-Cluster Calculations of Supramolecular Wires	Aarhus University	48
Computer Science	Dynamic and Adaptive Parallel Programming for Exascale Research	BNL	15
	Performance Evaluation and Analysis Consortium (PEAC) End Station	LBNL	90
	Scalable System Software for Parallel Programming	ANL	25
Earth Science	Accelerated Climate Modeling for Energy	SNL	190
	CESM Century-Scale Climate Experiments with a High-Resolution Atmosphere	UCAR	200
	Advancing Models for Multiphase Flow and Transport in Porous Medium System	Virginia Tech	60
	Frontiers in Planetary and Stellar Magnetism through High-Performance Computing	UCLA	83
	Global Adjoint Tomography	Princeton University	50
	High Frequency Ground Motion Simulation for Seismic Hazard Analysis	USC	167

Table 5 Current INCITE Awards in Biology, Chemistry, Computer Science, Earth Science, and Engineering, Continued

Discipline	Title	Lead Institution	Processor Hours (M)
Engineering	Adaptive Detached Eddy Simulation of a High Lift Wing with Active Flow Control	University of Colorado Boulder	70
	Direct Numerical Simulations and Robust Predictions of Cloud Cavitation Collapse	ETH Zürich	88
	DNS/LES of Complex Turbulent Flows	University of Minnesota	100
	High-Fidelity Simulations of Gas Turbine Stages with GPU Acceleration	GE Co.	40
	Large Eddy Simulations of Combustor Liner Flows	GE Co.	89
	Large-Eddy Simulation of the Bachalo-Johnson Flow, with Shock-Induced Separation	Boeing Co.	135
	Parameter Studies of Boussinesq Flows	LANL	44

Table 6 Current INCITE Awards in Materials Science and Physics

Discipline	Title	Lead Institution	Processor Hours (M)
Materials Science	Computational Spectroscopy of Heterogeneous Interfaces	University of Chicago	180
	Innovative Simulations of High-Temperature Superconductors	ORNL	60
	Non-covalent Bonding in Complex Molecular Systems with Quantum Monte Carlo	University College London	148
	Petascale Simulations of Self-Healing Nanomaterials	USC	180
	Predictive and Insightful Calculations of Energy Materials	ORNL	50
	Predictive Materials Modeling for Li-Air Battery Systems	ANL	50
	QMC Simulations Database for Predictive Theory and Modeling	UIUC	185
	Quantum Monte Carlo Simulations of Hydrogen and Water Ice	University of Cambridge	80
	Scalable First Principles Calculations for Materials at Finite Temperature	ORNL	150
	Simulation of Correlated Electrons for Superconducting Materials	UIUC	106
	SiO_2 Fracture: Chemomechanics with a Machine Learning Hybrid QM/MM Scheme	King's College London	125
	State-of-the Art Simulations of Liquid Phenomena	Iowa State University	200
	Nucleation and Growth of Colloidal Crystals Using Highly Scalable Monte Carlo	University of Michigan	55
	Reactive MD Simulations of Electrochemical Oxide Interfaces at Mesoscale	ANL	40
	Ab Initio Simulations of Carrier Transports in Organic and Inorganic Nanosystems	LBNL	25

Table 6 Current INCITE Awards in Materials Science and Physics, Continued

Discipline	Title	Lead Institution	Processor Hours (M)
Physics	Accelerator Modeling for Discovery	Fermilab	60
	Targeting Cancer with High Power Lasers	HZDR	57
	Approaching Exascale Models of Astrophysical Explosions	Stony Brook University	50
	Cosmic Reionization On Computers	Fermilab	74
	Petascale Simulation of Magnetorotational Core-Collapse Supernovae	Caltech	50
	Cosmological Simulations for Large-Scale Sky Surveys	ANL	160
	Quark Flavors and Conserved Charges at Finite Density in the QCD Phase Diagram	University of Houston	150
	Nuclear Structure and Nuclear Reactions	ISU	204
	Lattice QCD	Fermilab	280
	High-fidelity Simulation of Tokamak Edge Plasma Transport	PPPL	270
	Linkages Between Turbulence and Reconnection in Kinetic Plasmas	LANL	60
	Particle Acceleration in Shocks: From Astrophysics to Laboratory In Silico	LLNL	110
	Petascale Simulations of Laser Plasma Interaction Relevant to IFE	UCLA	90

Director's Discretionary Programs

Ten percent of the computational time on all SC-ASCR computers is reserved for director's discretionary programs, commonly referred to as DD. Time awarded under DD programs is intended to provide small allocations of computational time for 1-12 month periods, based on the decision of the facility. These projects typically include:

- Exploratory projects designed to demonstrate the potential for HPC to impact a particular science or technology area.
- Projects aimed at increasing the effectiveness of HPC systems, such as performance benchmarking, analysis, modeling and scaling studies. Visualization and data analytics for HPC are included in this category.
- Scaling studies for INCITE applications. The INCITE program is designed to support large jobs that use 20% or more of the processors in a given machine. This requires applicants to show that their code is genuinely capable of operating at this scale. Scaling studies are part of this process.
- Industrial Partnerships. The initial interaction with private sector users of HPC often occurs at the level of relatively small simulations. In many cases, the project grows into an ALCC or INCITE application, while in other cases, the response of the partners is to upgrade their own HPC capabilities.

Allocations to Private Sector Users for FY2015

A measure of the degree to which private companies are using DOE-supported computing resources to advance energy technology and other DOE priorities can obtained by examining the list of allocations for fiscal year 2015. Tables 7, 8, and 9 show the private sector allocations for OLCF, ALCF, and NERSC. These include ALCC, INCITE, ERCAP, and DD allocations. All allocations listed are for non-proprietary research projects designed to yield published scientific results, and the facilities do not charge for the computational time. Computational facilities are available on a cost-recovery basis to support proprietary research.

Table 7 A Complete List of Private Sector Supercomputer Allocations For FY2015 at the Oak Ridge Leadership Computing Facility (OLCF)

Company	Title	Hours Allocated (Millions)
Arkema, Inc.	High Performance Catalysts in Fluorination of Climate Impacting Fluorogases	2.0
Boeing Co.	Exploration Of New Computing Technology For Modeling High Lift Systems Of Commercial Aircraft	3.0
Robert Bosch GmbH	Safety in Numbers: Discovery of New Solid Li-ion Electrolytes	60.0
Caterpillar, Inc.	GPU Enhancement of Weld Distortion Prediction	10.5
FM Global, Inc.	CFD Modeling of Industrial Scale Fire Growth and Suppression	1.47
Ford Motor Co.	Cycle-to-Cycle Combustion Variation Modeling	1.47
	Simulating Cyclic Variability in Dilute Internal Combustion Engine Operation	17.5
GE Global Research	Tacoma Scalability for INCITE-sized problems	2.940
	Accelerating Design of Complex Fuel Injectors Through Petascale Computing	46.0
	Non-icing Surfaces for Cold Climate Wind Turbines	40.0
	Application of High Performance Computing for Simulating Cycle to Cycle Variation in Dual Fuel Combustion Engines	5.0
	TACOMA GPU Port (CFD Code Development)	1.5
	HIPSTAR-G-01 (CFD Code Development)	10.0
	Adjoint-Based Techniques for LES	3.0
General Motors Co.	Multi-Hole Injector Optimization for Spark-ignited Direct-Injection Gasoline Engines	16.47
Global Foundries US, Inc.	Density Functional Studies of Si/SiGe interface structures	5.88
HNULL, Inc.	Identify Organisms from a Stream of DNA Sequences	2.0
KatRisk, LLC	Worldwide Flood Maps	5.2
	The Cost of Global Climate Extremes	2.0
NVIDIA Corp.	Petascale Cross Correlation	2.0

Table 7 A Complete List of Private Sector Supercomputer Allocations For FY2015 at the Oak Ridge Leadership Computing Facility (OLCF), Continued

Company	Title	Hours Allocated (Millions)
Procter & Gamble Co.	Disruption of Lamellar Lipid Systems Induced by Small Molecule Permeants	8.0
	Assembling and Sustaining the 'Acid Mantle' of the Human Skin Barrier	75.0
	Can Supercomputing Help Mechanistic Understanding of a Novel Catalyst for a Strategic Raw Material?	3.0
Dresser-Rand, Inc.	Visualization of Tip Injection Phenomena in the near Stall Regime of Transonic Fan Stage	2.0
	Compressible Flow Turbomachinery Optimization: Numerical Tools Advancement	17.0
Rolls Royce, Inc.	HYDRA GPUs Architecture Migration Task I	1.0
Saudi Aramco Co.	GPU-Accelerated Large-Scale Basin and Reservoir Simulation	3.5
Tech-X Corp.	Tech-X High Performance Conjugate Gradient	3.0
	Extended Magnetohydrodynamic Simulations of Toroidal Fusion Plasmas	6.0
Total USA, Inc.	Advance computing for Geoscience applications	5.0
Tennessee Valley Authority	TVA CASL Test Stand - Evaluation of Lower Plenum Flow Anomaly using VERA/ Hydra-TH	1.0
United Technologies Research Center	Next Generation Turbulent Reactive Flow Simulation	10.0
	Towards Combustor Simulation Using Large Eddy Simulation and Graphical Processing Units	3.5
	High Fidelity Direct Numerical Simulation of Sprays for Realistic Injection Applications in Industry	1.0

Table 8 A Complete List of Private Sector Supercomputer Allocations For FY2015 at the Argonne Leadership Computing Facility (ALCF)

Company	Title	Hours Allocated (Millions)
Boeing Co.	Simulation of a Shock-Boundary-Layer Interaction	2.0
Cascade Technologies, Inc.	Combustion Stability in Complex Engineering Flows	100
CERFACS	Evaluation of Mesoscale Atmospheric Model for Contrail Cirrus	9.0
	Upscaling Laws in Premixed Explosions	86
	Large scale Combustion Preparatory Access	10
Cloud Pharmaceuticals, Inc.	Inverse Design of Molecules and Drugs	2.0

Table 8 A Complete List of Private Sector Supercomputer Allocations For FY2015 at the Argonne Leadership Computing Facility (ALCF), Continued

Company	Title	Hours Allocated (Millions)
GE Global Research	Large Eddy Simulation of SFR Assembly Inlets	58
	Large Eddy Simulations of Combustor Liner Flows	75
	LES Simulation of Fan and Exhaust Aerodynamics & Acoustics for Propulsion Systems	5.5
	TACOMA Porting and Scaling Study	2.25
	Towards Petascale First-principles Simulations of Complex Two-phase Flow Systems	3.0
IBM Corp.	LAMMPS Performance Optimization	4.0
InterX, Inc.	A Comprehensive Survey of Molecular Interactions at Chemical Accuracy	3.0
Rolls-Royce Holdings plc	Hydra Test for INCITE Application	1.0
SGT, Inc.	Simulations of Ecosystem Carbon Dynamics in the Conterminous U.S.	2.5
Tech-X Corp.	Extended Magnetohydrodynamic Simulations for Burning Plasma Experiments	2.0
	Vorpal for Laser-Plasma Acceleration	0.2
Vestas Wind Systems	LES Investigation of Stability Enhanced Wake Losses on Large Wind Parks	12.5

Table 9 A Complete List of Private Sector Supercomputer Allocations For FY2015 at the National Energy Research Scientific Computing Center (NERSC)

Company	Title	Hours Allocated (Thousands)
ALPEMI Consulting, LLC	Performance Profiling and Assessment of MFIX Using Trilinos Linear Solvers Versus Using Native Linear Solvers	100
Continuum Dynamics Inc.	Advanced Methods for Predicting 3D Unsteady Flows Around Wind Turbine Blades	5
Combustion Research and Flow Technology, Inc.	Innovative Sub-Grid Scale Combustion Modeling for Gas Turbines	4,000
Dynaflow, Inc.	Multiscale Two-Phase Bubbly Flow Modeling	105
FAR-TECH Inc.	Interactive Real-time Analysis of Hybrid Kinetic-MHD Simulations with NIMROD	n/a
	Quasi-3D Model of an Electron Cyclotron Resonance Ion Source	11,500
	Integrated Modeling Tool for Electron-Beam Based Ion-Sources	20,000
General Atomics	Disruption and Disruption Mitigation Simulations	11,500
	ITER Plasma Response to ELM Stabilization Coils	425
	NIMROD Project: Extended Magnetohydrodynamic Modeling for Fusion Experiments	1,200
	Simulation of Magnetically Confined Fusion Plasmas	2,750

Table 9 A Complete List of Private Sector Supercomputer Allocations For FY2015 at the National Energy Research Scientific Computing Center (NERSC), Continued

Company	Title	Hours Allocated (Thousands)
IBM Research - Almaden	Understanding the Nature of Atomic Scale Magnetism on Different Surfaces Using DFT	550
I.C. Gomes Consulting & Investment Inc.	Radioactive Beam Facilities and Isotope Production - Target, Shielding, Fragment Separators, Magnetic Spectrometers and Accelerator Studies	710
Intel Inc.	Massively Parallel Coupled Cluster Methods: Development and Applications	3,600
	Traleika Glacier X-Stack	10,000
Lodestar Corp.	Edge, SOL and Divertor Modeling	10
nanoPrecision Products Inc.	Robust Optimization of Optics	200
Optimal Solutions Inc.	Optimal Production Planning, Sourcing, Distribution and Routing for Complex Energy Intensive Manufacturing Companies Using High Performance Computing	15
QuantumScape Corp.	Development of Reactive MD Potentials for Energy Storage Materials	200
SciberQuest, Inc.	Petascale Kinetic Simulations in Laboratory and Space Plasmas	1,600
Saudi Arabia Basic Industries Corp.	Fundamental Investigation of Energy Materials Using DFT Calculations	1,800
Tech-X Corp	Modeling of Tokamak Plasmas with Large Scale Instabilities	2,750
	Improving Ion Source Antenna Lifetime for the Spallation Neutron Source	15
	Gyrotron Design and Evaluation using New Particle-in-Cell Capability	1,750
	Petawatt Lasers for Laser-Plasma Acceleration of Electrons	100
	Parallel Simulation of Electron Cooling Physics and Beam Transport	2,450
	NIMROD Project: Extended Magnetohydrodynamic Modeling for Fusion Experiments	1,000
	Modeling of Tokamak Plasmas with Large Scale Instabilities	2,500
Teraflux Corp.	Continuous Dynamic Grid Adaptation in Regional and Global Atmospheric Models	150
Trinum Research	Multiscale Hybrid Simulations of Plasma Systems	420
United Technologies Research Ctr.	High Fidelity Direct Numerical Simulation of Sprays for Realistic Injection Applications in Industry	230
Vertum Partners	Assessing Climate Change Effects on Wind Energy	4,250
Vorcat, Inc.	Development of Vorcat for HPC Cloud-based Complex Energy Applications	350
Woodruff Scientific LLC	CompactTorus Simulation	250
	Resistive MHD Simulations of Disruptions in ITER	80

Scientific Discovery through Advanced Computing (SciDAC)

The Scientific Discovery through Advanced Computing (SciDAC) program was initiated in 2001 as a partnership involving all of the DOE-SC program offices to dramatically accelerate progress in scientific computing in order to deliver breakthrough scientific results. The SciDAC program has two components: institutes and science partnerships. ASCR relies upon the SciDAC Institutes to connect basic research in applied mathematics and computer science to scientific challenges by forming the foundation to address commonalities in multiple and different SciDAC Partnerships. SciDAC Partnerships are targeted collaborations between scientists and applied mathematicians and computer scientists towards specific scientific challenges.

SciDAC institutes are designed to advance computational science by providing intellectual resources in applied mathematics and computer science, expertise in algorithms and methods, and scientific software tools to the scientific community. These resources can then be used to advance scientific discovery through modeling and simulation. The current iteration of the SciDAC program features four institutes, which are funded for FY2011-2015. While these institutes are led by individual Principle Investigators, their teams include researchers from six national laboratories, 23 universities, and one company. The current institutes are described below:

1. The Frameworks, Algorithms, and Scalable Technologies for Mathematics (FASTMath) Institute, led by Lawrence Livermore National Laboratory (LLNL), develops and deploys scalable mathematical algorithms and software tools for reliable simulation of complex physical phenomena. FASTMath provides capabilities in structured and unstructured meshing, linear and non-linear equation solvers, time integrators, variational inequality solvers, and eigensolvers. These capabilities are useful for a wide range of DOE science and energy problems, such as combustion science, climate, fusion, nuclear energy, subsurface science and engineering, and wind energy.
2. The Quantification of Uncertainty in Extreme Scale Computations (QUEST) Institute, led by Sandia National Laboratories, develops tools to quantify the uncertainty in large scale simulations. QUEST capabilities include proper characterization of the problem and the input space of available information; local and global sensitivity analysis; adaptive dimensionality and order reduction; forward and inverse propagation of uncertainty; handling of application code failures; missing data; and tolerance of faults in both the hardware/software combination, and in the models. Understanding the uncertainty in simulation results is critical to effectively using these results not only in scientific discovery, but in advanced engineering design.
3. The Institute for Sustained Performance, Energy, and Resilience (SUPER), led by Lawrence Berkeley National Laboratory, uses its expertise in compilers and other system tools, performance engineering, energy management, and resilience to ensure that DOE computational scientists can effectively use the capabilities of the DOE's high performance computers.
4. The Scalable Data Management, Analysis, and Visualization (SDAV) Institute, led by LBNL, develops tools for data management, data analysis, and data visualization for large-scale computing. These capabilities play a key role in ensuring that the results of scientific computing can be used effectively for both discovery science and advanced engineering.

SciDAC partnerships are designed to enable scientists to conduct complex scientific and engineering computations at a level of fidelity needed to simulate real-world conditions in targeted science application projects. SciDAC partnership projects are co-funded by SC-ASCR and other DOE-SC programs. Through these partnerships, SciDAC-supported researchers pursue computational solutions to challenging problems across the DOE-SC research areas. The FY2015 SciDAC projects are listed in Table 10.

Table 10 FY2015 SciDAC Projects

Office of Science Program	Project Title	Institution
Basic Energy Sciences	Advanced Modeling of Ions in Solutions, on Surfaces, and in Biological Environments	Princeton University
	Charge Transfer and Charge Transport in Photoactivated Systems: Developing Electron-Correlated Methods for Excited State Structure and Dynamics in the NWChem Software Suite	U. of Minnesota
	Discontinuous Methods for Accurate, Massively Parallel Quantum Molecular Dynamics: Lithium Ion Interface Dynamics From First Principles	LLNL
	OSCon -- Optimizing SuperConductor Transport Properties Through Large-Scale Simulation	ANL
	Scalable Computational Tools for Discovery and Design – Excited State Phenomena in Energy Materials	U. of Texas at Austin
	Simulating the Generation, Evolution, and Fate of Electronic Excitations in Molecular and Nanoscale Materials With First Principles Methods	LBNL
	Predictive Computing for Condensed Matter	UIUC
Biological and Environmental Research	Multiscale Methods for Accurate, Efficient, and Scale-Aware Models of the Earth System	LBNL
	Predicting Ice Sheet and Climate Evolution at Extreme Scales (PISCEES)	LANL/LBNL
Fusion Energy Science	Advanced Tokamak Modeling (AToM)	General Atomics
	Center for Edge Physics Simulation (EPSI)	PPPL
	Plasma Surface Interactions: Bridging from the Surface to the Micron Frontier through Leadership Class Computing	U. of Tennessee-Knoxville
High Energy Physics	Community Project for Accelerator Science and Simulation (ComPASS)	Fermilab
	Exascale Algorithms and Software for Lattice Field Theory	Fermilab
	Computing the Sky: Simulation and Analysis for Cosmological Surveys	ANL
	Optimizing HEP Data Management and Analysis Capabilities	Fermilab
Nuclear Physics	Computing Properties of Hadrons, Nuclei and Nuclear Matter from Quantum Chromodynamics	BNL
	Nuclear Computational Low-Energy Initiative (NUCLEI)	LANL
	A Multi-Scale Approach to Nuclear Structure and Reactions: Forming the Computational Bridge between Lattice QCD and Nonrelativistic Many-Body Theory (CalLAT)	U. of California-Berkeley

Endnotes

1. The Top 500 list is compiled by Erich Strohmaier (NERSC/LBNL), Jack Dongarra (University of Tennessee), Horst Simon (NERSC/LBNL) and Martin Meuer of Prometeus.
2. Public Law 108 - 423 - Department of Energy High-End Computing Revitalization Act of 2004. http://www.gpo.gov/fdsys/pkg/PLAW-108publ423/content-detail.html
3. Cielo, a NNSA-sponsored supercomputer located at Los Alamos National Laboratory, was officially retired in late 2015. It has been replaced by the Trinity supercomputer (see Table 1). This system is located at Los Alamos National Laboratory and managed and operated by Los Alamos National Laboratory and Sandia National Laboratories under the Alliance for Computing at Extreme Scale partnership.
4. Hopper, a production-class computer at the Office of Science's NERSC user facility, was officially retired in December 2015. Cori, the replacement for Hopper, is being delivered in two phases. The first phase became operational in late 2015, and the second phase is expected to be operational in mid-2016.

Acronyms

ALCC	ASCR Leadership Computing Challenge
ANL	Argonne National Laboratory
BNL	Brookhaven National Laboratory
Caltech	California Institute of Technology
CASL	Consortium for Advanced Simulation of Light Water Reactors
CERFACS	Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique
CESM	Community Earth System Model
CFD	Computational Fluid Dynamics
DD	Director's Discretion
DNS	Direct Numerical Simulation
ETH Zürich	Eidgenössische Technische Hochschule Zürich (Swiss Federal Institute of Technology Zürich)
ELM	Edge-localized mode
Fermilab	Fermi National Accelerator Laboratory
GPU	Graphics Processing Unit
GWU	George Washington University
HRRR	High-Resolution Rapid Refresh
HZDR	Helmoltz-Zentrum Dresden-Rossendorf
INCITE	Innovative & Novel Computational Impact on Theory & Experiment
ISU	Idaho State University

ITER	International Thermonuclear Experimental Reactor
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
LES	Large Eddy Simulation
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LLNL	Lawrence Livermore National Laboratory
MD	Molecular Dynamics
MIT	Massachusetts Institute of Technology
NERSC	National Energy Research Scientific Computing Center
NIMROD	Non-Ideal Magnetohydrodynamics with Rotation – Open Discussion
NIST	National Institute of Standards & Technology
NNSA	National Nuclear Security Administration
NOAA	National Oceanic and Atmospheric Administration
ORNL	Oak Ridge National Laboratory
PPPL	Princeton Plasma Physics Laboratory
QCD	Quantum Chromodynamics
QMC	Quantum Monte Carlo
QM/MM	Quantum Mechanics/Molecular Mechanics
RAP	Rapid Refresh
RF	Radio Frequency
SC-ASCR	Office of Advanced Scientific Computing Research
SGT	Stinger Ghaffarian Technologies, Inc.
SNL	Sandia National Laboratories
UCAR	University Corporation for Atmospheric Research
UCLA	University of California Los Angeles
UIUC	University of Illinois Urbana-Champaign
USC	University of Southern California