U.S. DEPARTMENT OF ENERGY | Office of Science

Advanced Scientific Computing Research

Presented to the

Advanced Scientific Computing Advisory Committee

by

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Associate Director

September 17, 2018

Office of Science FY 2019 Appropriations

	FY 2018	FY 2019			
	Enacted Approp.	President's Request	House Mark	Senate Mark	Enacted Approp.
Office Of Science					
Advanced scientific computing research	810,000	899,010	914,500	980,000	935,500
Basic energy sciences..	2,090,000	1,850,000	2,129,233	2,193,400	2,166,000
Biological and environmental research...............................	673,000	500,000	673,000	715,000	705,000
Fusion energy sciences..	532,111	340,000	590,000	425,000	564,000
High energy physics..	908,000	770,000	1,004,510	1,010,000	980,000
Nuclear physics...	684,000	600,000	690,000	710,000	690,000
Workforce Development for Teachers and Scientists	19,500	19,000	19,500	24,500	22,500
Science laboratories infrastructure.......................................	257,292	126,852	290,147	302,100	232,890
Safeguards and security..	103,000	106,110	106,110	106,000	106,110
Program direction...	183,000	180,000	183,000	184,000	183,000
Total, Office Of Science...	**6,259,903**	**5,390,972**	**6,600,000**	**6,650,000**	**6,585,000**

ASCR FY 2019 Budget Status

($K)

	FY 2017	FY 2018		FY 2019		
	Enacted Approp.	President's Request	Enacted Approp.	Request	Conference	Conference vs.FY18 enacted
Mathematical, Computational, and Computer Sciences Research	107,121	100,668	113,522	141,099	125,873	+9.350
SBIR/STTR	10,271	11,261	4,301	5,532	4,768	+354
Total, Mathematical, Computational, and Computer Sciences Research	117,392	111,929	117,823	146,631	130,641	+9,704
High Performance Computing and Network Facilities	352,446	398,773	469,760	500,887	551,452	+84,692
SBIR/STTR	13,162	14,728	17,417	18,786	20,701	+3,398
Total, High Performance Computing and Network Facilities	365,608	413,501	487,177	519,673	572,153	+88,090
Exascale Computing						
17-SC-20 Office of Science Exascale Computing Project (SC-ECP)	164,000	196,580	205,000	232,706	232,706	+27,706
Total, Advanced Scientific Computing Research	**647,000**	**722,010**	**810,000**	**899,010**	**935,500**	**+125,500**
Computational Sciences Workforce Programs, with WDTS (non-add)	*(10,000)*	*(10,000)*	*(10,000)*	*(10,000)*	*...*	*...*
Exascale Computing Crosscut (non-add)	*(164,000)*	*(346,580)*	*(377,500)*	*(472,706)*	*472,706*	*+95,206*

The following is the only direction provided for ASCR.
Within available funds, the agreement provides $140,000,000 for the Argonne Leadership Computing Facility, $200,000,000 for the Oak Ridge Leadership Computing Facility, $105,000,000 for the National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory, $10,000,000 for the Computational Sciences Graduate Fellowship program, and $85,000,000 for ESnet. The agreement provided $75,667,000 for Computational Partnerships (SciDAC). Within funds for SciDAC, up to $13,000,000 is to support work on artificial intelligence and big data focused on the development of algorithms and methods to identify new ways of extracting information generated at the Office of Science's large user facilities of validating the use of machine learning in the Office of Science's program's scientific simulations. This is the only funding recommended within the Office of Science that shall be available for this work. The Department is directed to provide to the Committees on Appropriations of both Houses of Congress not later than 90 days after the enactment of this Act a briefing on its plan for implementing this artificial intelligence and big data initiative.

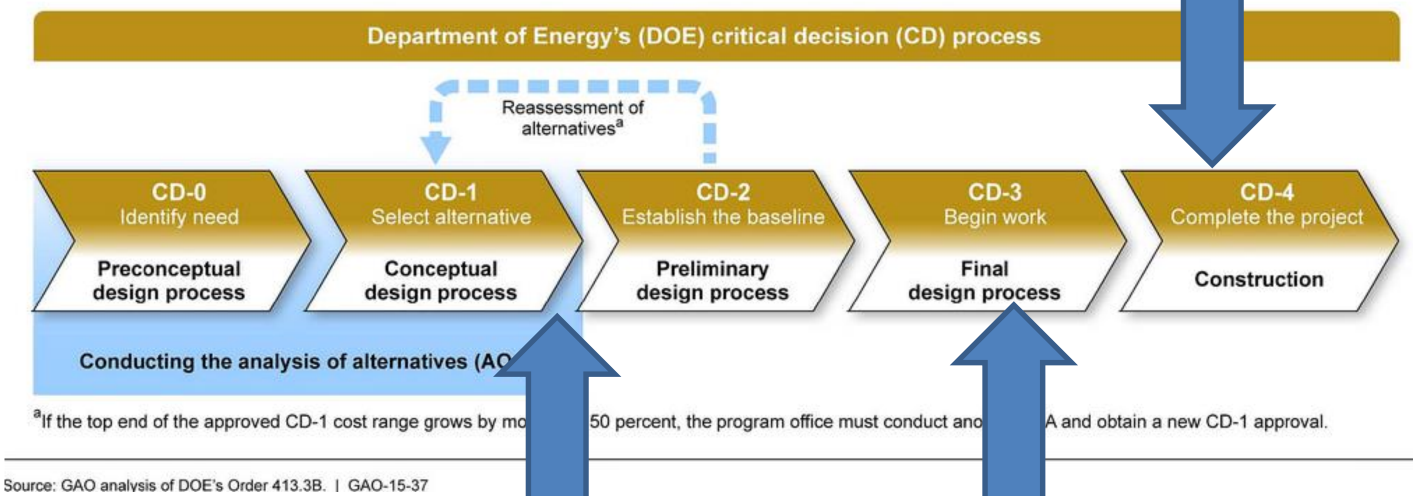
FACILITIES

Independent Project Reviews

- **2017**
  - November 7-9: ALCF-3 rebaseline review; Approval January 18, 2018
  - November 28-29: OLCF-5 CD1; Approval January 18, 2018
- **2018**
  - January 9-11: ECP annual review
  - June 26-28: ESnet CD1/3A review; Approval August 3
  - August 7-8: NERSC-9 CD2/3 review; Approval September 6
  - August 22-23: OLCF-5 CD3A review; Approval September 13
  - November 27-29: ALCF-3 annual review
  - December: OLCF-4 CD4 review
- **2019**
  - August: ESnet CD2/3 review

ASCR Project Status

Achieved in FY2015
OLCF-4 CD 2-3



Achieved in FY2018
Esnet -- CD 1-3A
OLCF-5 – CD 1-3A

Achieved in FY2018
NERSC- 9 – CD 2-3
ALCF-3 – CD 2-3 –A-21

ORNL Summit System Overview

System Performance

- Peak of 200 Petaflops (FP_{64}) for modeling & simulation
- Peak of 3.3 ExaOps (FP_{16}) for data analytics and artificial intelligence

The system includes

- 4,608 nodes
- Dual-rail Mellanox EDR InfiniBand network
- 250 PB IBM file system transferring data at 2.5 TB/s

Each node has

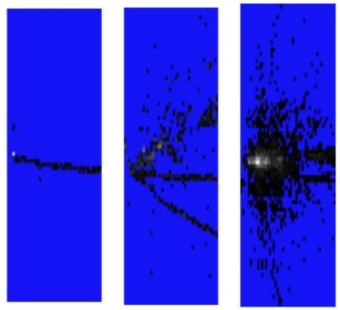
- 2 IBM POWER9 processors
- 6 NVIDIA Tesla V100 GPUs
- 608 GB of fast memory

  (96 GB HBM2 + 512 GB DDR4)
- 1.6 TB of NV memory

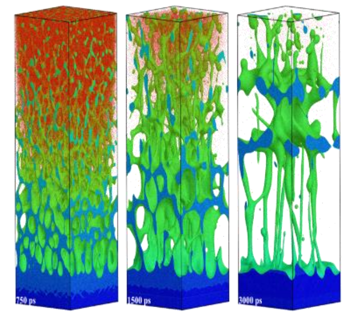
OLCF 2017/18 Science Highlights

HPC Neural Networks

Researchers are using the OLCF and an evolutionary algorithm, MENNDL, to generate deep neural networks that can classify high-energy physics data and improve the efficiencies of measurements. This approach eliminates much of the time-intensive, trial-and-error tuning traditionally required of machine learning and match or exceed the performance of handcrafted artificial intelligence systems.



An image generated from neutrino scattering data captured by the MINERvA detector at FermiLab.



Homogenous boiling (a phase explosion): Liquid superheated to ~90% of the spinodal temperature rapidly decomposes into vapor and liquid droplets.

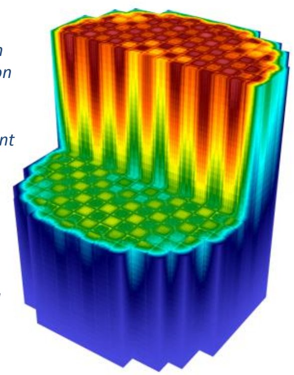
Advancing Materials

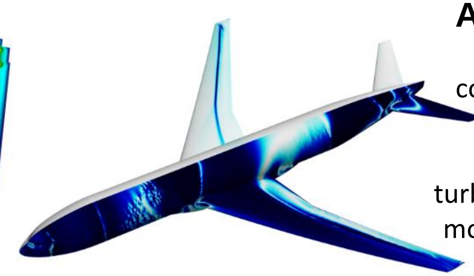
Reseachers used OLCF to gain insights into laser interactions with metal surfaces. By using a combination of virtual and real-world experiments, the team is gaining a fundamental understanding of the mechanisms for material-lasers interactions. Lasers allow researchers to manipulate materials on atomic and subatomic levels, leading to new materials and a host of other applications.

Predictive Power

Using the OLCF and data supplied by two Consortium for Advanced Simulation of Light Water Reactors (CASL) members—TVA and the Westinghouse Electric Company— ORNL carried out the largest time-dependent simulation of a nuclear power plant to date confirming engineers' predictions related to the safe and reliable operation of Watts Bar Unit 2 .

Distribution of the fission product Xenon-135, an important marker for predicting reactor behavior, in the WB2 reactor core during startup.





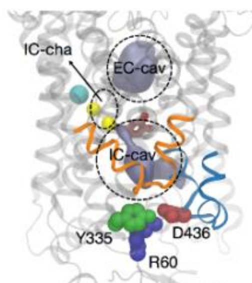
Simulation of a physical wind tunnel airplane model (the NASA Common Research Model), commonly used for CFD benchmarking and analysis.

Advancing Competitiveness

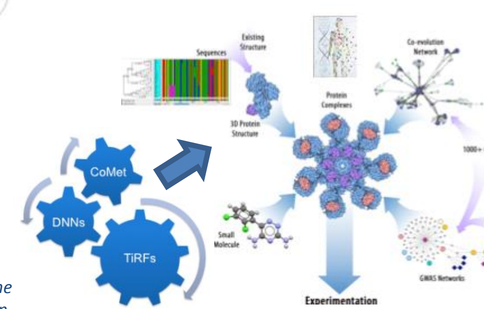
Boeing used OLCF to develop a new computational methodology that more accurately represents the input uncertainty for Spalart–Allmaras turbulence model, reduces the statistical model dimensions, and captures the full 3D dynamics of the problem while reducing computational requirements by 95.5%. Faster/better analysis reduces time-to-solution, accelerating aircraft design time and reducing costs.

Addiction and Disease

Dopamine is critical to signals in the nervous system linked to motor movements, learning, and habit formation. To develop drug therapies for addiction and disease, researchers need to understand the dopamine transporter (DAT). Researchers used OLCF to simulate the cascade of molecular interactions that activate DAT and uncovered pathways important to DAT function.



Detailed dynamic model of the dopamine transporter protein.



Entering the Exascale Era

CoMet bioinformatics application for comparative genomics used OLCF to find sets of genes that are related to a trait or disease in a population 5 orders of magnitude faster than previous state-of-art codes - achieving 2.3 ExaOps with mixed precision

Five Gordon Bell Finalists Credit Summit Supercomputer

Five Summit users are among the finalists for the prestigious Gordon Bell Prize, one of the top annual honors in supercomputing. The finalists—representing Oak Ridge, Lawrence Berkeley, and Lawrence Livermore National Laboratories and the University of Tokyo—leveraged Summit's unprecedented computational capabilities to tackle a broad range of science challenges and produced innovations in machine learning, data science, and traditional modeling and simulation to maximize application performance. The Gordon Bell Prize winner will be announced at SC18 in Dallas in November. Finalists include:

- An ORNL team led by computational systems biologist Dan Jacobson and OLCF computational scientist Wayne Joubert that developed a genomics algorithm capable of using mixed-precision arithmetic to attain exascale speeds.
- A team from the University of Tokyo led by associate professor Tsuyoshi Ichimura that applied AI and mixed-precision arithmetic to accelerate the simulation of earthquake physics in urban environments.
- A Lawrence Berkeley National Laboratory-led collaboration that trained a deep neural network to identify extreme weather patterns from high-resolution climate simulations.
- An ORNL team led by data scientist Robert Patton that scaled a deep learning technique on Summit to produce intelligent software that can automatically identify materials' atomic-level information from electron microscopy data.
- A LBNL and Lawrence Livermore National Laboratory team led by physicists André Walker-Loud and Pavlos Vranas that developed improved algorithms to help scientists predict the lifetime of neutrons and answer fundamental questions about the universe.

PI(s)/Facility Lead(s): Dan Jacobson, ORNL; Tsuyoshi Ichimura, Univ. Tokyo; Prabhat, LBNL; Robert Patton, ORNL; André Walker-Loud and Pavlos Vranas, LBNL and LLNL
ASCR Program/Facility: Summit Early Science
ASCR PM: Christine Chalk

ALCF AURORA ESP DATA & LEARNING PROJECTS

The Aurora Early Science Program (ESP) is designed to prepare key applications for the novel architecture and scale of the exascale supercomputer, and solidify libraries and infrastructure to pave the way for production applications to run on the system.

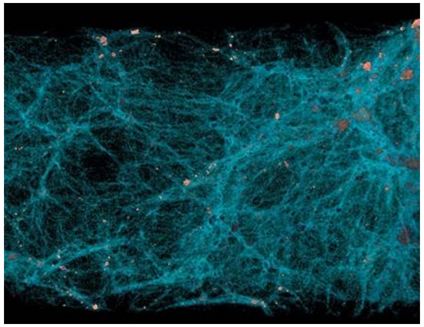
In addition to fostering application readiness for the future supercomputer, the ESP allows researchers to pursue innovative computational science projects not possible on today's leadership-class supercomputers.

Ten data and learning projects were selected to support the ALCF's new paradigm for scientific computing, which expands on traditional simulation-based research to include data science and machine learning approaches. The second call was open from January 10 - April 8, 2018.

The PI-led project teams consist of core developers of the application, domain science experts, and an ALCF postdoctoral appointee funded for each project. The teams will receive hands-on assistance to port and optimize their applications for the new architecture using systems available today and early Aurora hardware when it is available.

ALCF AURORA ESP DATA PROJECTS

Amanda Randles, Duke University and ORNL



Salman Habib, Argonne

Simulating and Learning in the ATLAS Detector at the Exascale
James Proudfoot, Argonne National Laboratory
This project prepares Aurora for effective use in the search for new physics by examining petabytes of data from the ATLAS experiment.

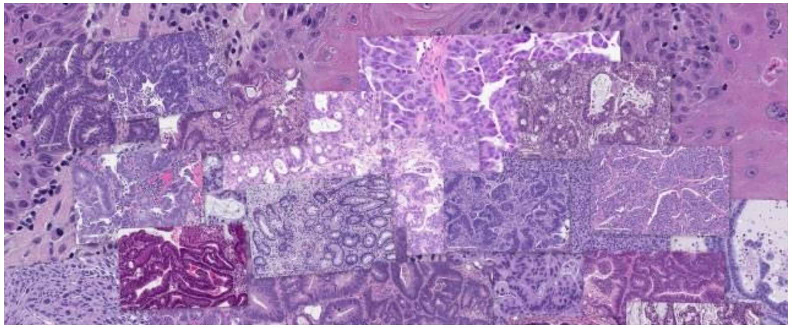
Dark Sky Mining
Salman Habib, Argonne National Laboratory
This project will connect some of the world's most detailed cosmological simulations with data obtained from the Large Synoptic Survey Telescope to usher in a new era of cosmological inference targeted at scientific breakthroughs.

Extreme-Scale In-Situ Visualization and Analysis of Fluid-Structure-Interaction Simulations
Amanda Randles, Duke University and Oak Ridge National Laboratory
This project advances our understanding of the role biological parameters play in determining tumor cell trajectory in the circulatory system.

Exascale Computational Catalysis
David Bross, Argonne National Laboratory
This project will facilitate and accelerate the quantitative description of crucial gas-phase and coupled heterogeneous catalyst/gas-phase chemical systems through the development of data-driven tools.

Data Analytics and Machine Learning for Exascale Computational Fluid Dynamics
Ken Jansen, University of Colorado Boulder
This project will develop data analytics and machine learning techniques that greatly enhance the value of flow simulations through extraction of meaningful dynamics information.

ALCF AURORA ESP LEARNING PROJECTS



Rick Stevens, Argonne

Virtual Drug Response Prediction
Rick Stevens, Argonne National Laboratory
This project enables billions of virtual cancer drugs to be screened singly and in numerous combinations, while predicting their effects on tumor cells.

Machine Learning for Lattice Quantum Chromodynamics
William Detmold, Massachusetts Institute of Technology
This project couples machine learning and simulations to determine possible interactions between nuclei and a large class of dark matter candidate particles.

Many-Body Perturbation Theory Meets Machine Learning to Discover Singlet Fission Materials
Noa Marom, Carnegie Mellon University
Supercomputers have been guiding materials discovery for the creation of more efficient organic solar cells. By combining quantum-mechanical simulations with machine learning and data science, this project will harness exascale power to revolutionize the process of photovoltaic design and advance physical understanding of singlet fission.

Accelerated Deep Learning Discovery in Fusion Energy Science
William Tang, Princeton Plasma Physics Laboratory
This project seeks to expand modern neural net software to make strides toward validated prediction and associated mitigation of large-scale disruptions in burning plasmas.

Enabling Connectomics at Exascale to Facilitate Discoveries in Neuroscience
Nicola Ferrier, Argonne National Laboratory
This project will develop a computational pipeline to extract brain-image-derived mappings of neurons and their connections from massive electron microscope datasets.

ALCF 2017/18 Science Highlights

Customize materials properties

A research team led by the University of Southern California is using ALCF supercomputers to understand how they can use light to create changes in the atomic structure of sheet-like materials, e.g., turning an electrical insulator into a conductor.. This ability would drastically reduce the time and cost required to manufacture semiconductors and extend their use to novel applications, like flexible electronics

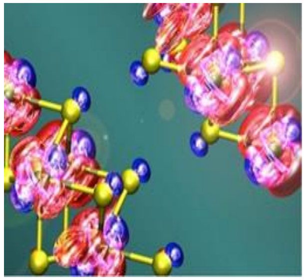
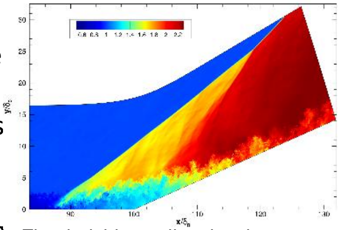


Image courtesy of Hiroyuki Kumazoe, University of Southern California

Supersonic turbulence flows

The military is seeking ever-faster aircraft, plane that can fly five times the speed of sound. Supersonic speeds bring many design challenges e.g. unsteady air-flow patterns can generate aircraft panel-damaging shock waves. J. Poggie, Purdue University with AFRL collaborators, using ALCF resources, are modeling unsteady flow patterns and strategies for preventing or eliminating them.



The dark blue-yellow border indicates a separation shock and the yellow-red border indicates a reattachment shock.

Breakthroughs in Protein Structure and Design

Mini-proteins are the most promising candidates for therapeutics. Computer-guided design of synthetic mini-proteins with targeted properties is a grand challenge in structural biology. ALCF staff collaborated with David Baker, U. Washington, and with the Howard Hughes Medical Institute to generate more than 200 designs that were validated via nuclear magnetic resonance

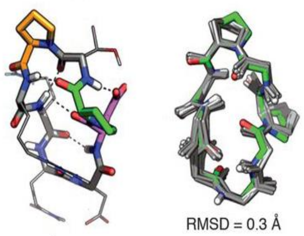
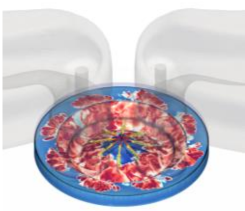


Image from Hosseinzadeh et al., Science 358, 1461–1466 (2017)

Reducing Engine Emissions

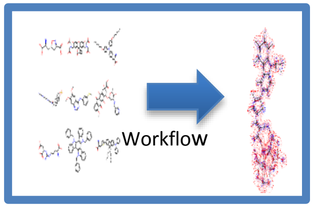
In 2017, transportation consumed over 15 billion barrels of oil and accounted for 23% of CO_2 generated. A 1% improvement in engine efficiency can save billions of gallons of fuel annually. ANL and Aramco, simulated over 2,000 engine designs on Mira, reducing design time from months to weeks, and producing simulation with more than 100 million cells - the largest engine simulation ever performed.



High-fidelity calculation of a heavy-duty Cummins engine fueled with a straight-run gasoline by ASC.

Molecular Engineering of Solar-Powered Windows

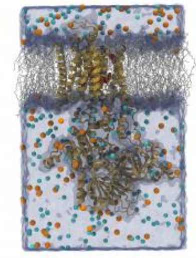
40% of total energy usage in the USA comes from buildings. Dye-sensitized solar cells (DSCs) have a desirable cost-efficiency tradeoff and can aid in the design of energy-efficient buildings. J. M. Cole, Cambridge University team, using ALCF resources, evaluated candidate molecules, created rules to describe optically active molecules, and discovered a new class of DSCs based on interaction between sulfur and carbon atoms.



Molecules from journal publications, J. M. Cole *et al*, *ACS Appl. Mater. Interfaces,* **2017**, *9* (31),25952

Molecular Machines for Drug Design

Membrane transport proteins are a unique class of large-molecule biological systems that play a major role in the dynamics of cell function, because some of them can function like little pumps. The processes by which membrane proteins accomplish these feats are little understood. Prof. Roux and team, using ALCF resources have significantly gained understanding of their dynamics, which could lead to the design of drugs that affect specific functions.



Brian Radak, University of Chicago; data courtesy of Huan Rui, University of Chicago)

NERSC 9 Upgrade Project

NERSC-9 Project will acquire and deploy an HPC system for Office of Science user community.

The project includes:

- **Facility upgrade for power and cooling**
- **System acquisition**
- **SC application and user readiness**

Mission Need (CD-0) signed August 2015

- **Increase computational capabilities** over Edison, at least 16x on a set of representative DOE applications
- **Demonstrate exascale era-technologies** and enable user community to continue to transition to advanced energy-efficient architectures
- **Support data analysis** from experimental and observational facilities and support new science initiatives

NERSC-9 Project History and Update

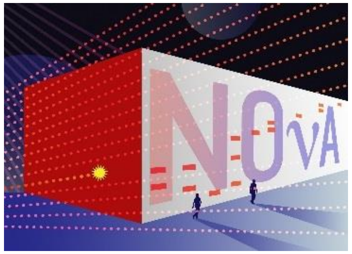
History

- **CD-0 Mission Need (Aug 2015)**
- **CD 1/3a to release RFP (May 2016)**
- **Change in procurement strategy (Sep 2017)**
  - Vendor technology roadmap changed significantly
  - Other vendors who responded to RFP would not commit to original responses
  - NERSC withdrew from RFP
- **NERSC-9 to be purchased off NERSC-8 contract**

Update

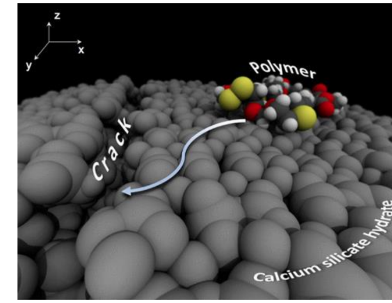
- **Time delay allowed NERSC upgrade project to take advantage of recent technology growth in machine learning and increased user demand for data and machine learning capabilities**
- **CD 2/3 (Approve performance baseline and start of construction) IPR held August 2018 at Berkeley National Lab**
- **CD 2/3 signed September 6, 2018**

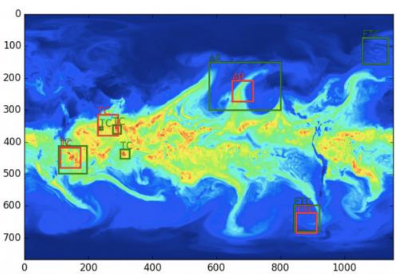
NERSC Supports High-impact SC Mission Science



Evidence for Anti-neutrino oscillation NOvA neutrino experiment in partnership with SciDAC-4, HEPCloud used NERSC resources to perform the largest-scale analysis ever to support evidence of antineutrino oscillation. *Phys. Rev. D (2018)*

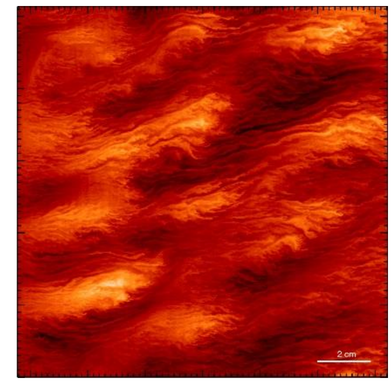
Self Healing Cement
Glezakou, (*PNNL).* DFT calculations on NERSC reveal atomic origins of self-healing function in cement; *ACS Appl. Mater. Interfaces* (Dec. 2017)

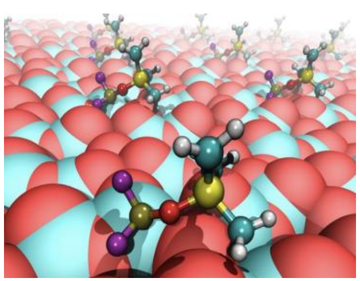




15 Pflop Deep Learning for Weather *Prabhat (NERSC, LBL)* DL tool developed and run at NERSC provides climate scientists ability to identify extreme weather events in huge simulations. *SC 17 Proceedings.*

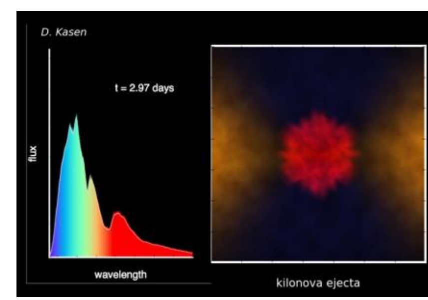
Mysterious Plasma Flows
C. Holland (*UCSD*) Simulations reveal electron energy transport key to a mysterious self-organized flow of fusion plasmas and predict rotation profile systems; *Nuc. Fusion* (May 2017)





Better Batteries
D. Abraham (*ANL*) Simulations reveal 'pickling' process can make better Li-ion batteries*; J. Phys. Chem* (April 2018*)*

Origin of Heavy Elements
D. Kasen (*LBL*). Experimental observations were found to be consistent with NERSC simulations for an event 1000 times brighter than a classical nova. *Nature, ApJ Letters, Science* (2017)



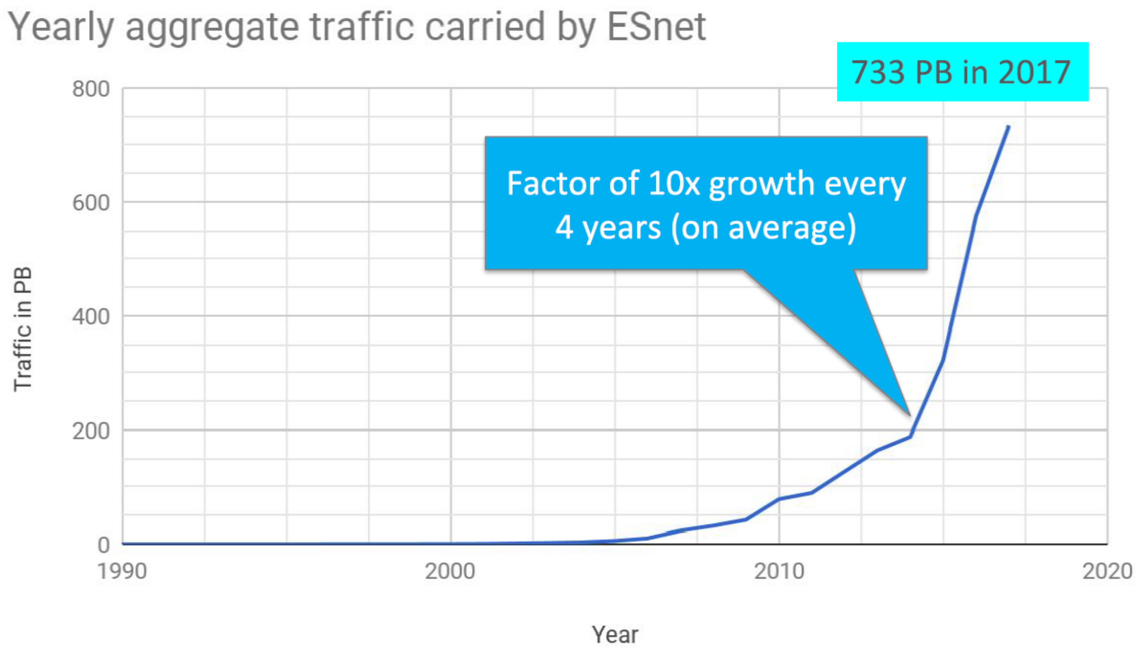
ESnet6 Upgrade Project: Mission Needs

Network capacity must expand to satisfy exponential growth of science data.

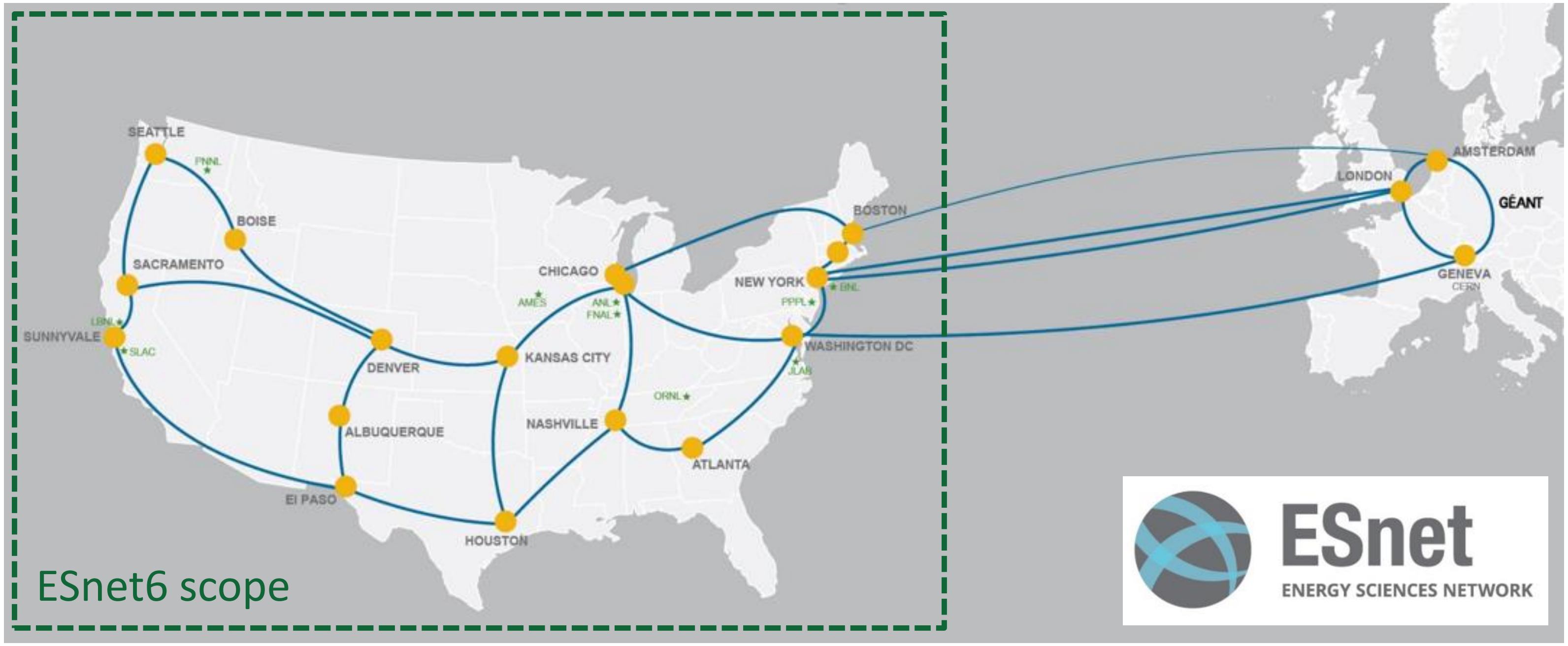
Network equipment is at end-of-life, and must be replaced to sustain reliability and cyber-resiliency.

Network operational flexibility must improve if we are to create services to open new scientific opportunities.

Research workflows of growing complexity require automation and programmability of network services – major innovations.



The ESnet6 project will acquire and deploy a greenfield high performance network on unlit dark fiber – a strategic investment for DOE.



- This approach provides long term stability and the autonomy to execute a novel programmable network architecture.
- The architecture is based on a scalable and resilient "switching core" coupled to a flexible and dynamic "services edge."
- Early finish date is Q1 FY 2023.
- ESnet will be fully operational throughout the ESnet6 project.
- The project does not include the transatlantic links (just renewed).

2018 ALCC Allocation Highlights

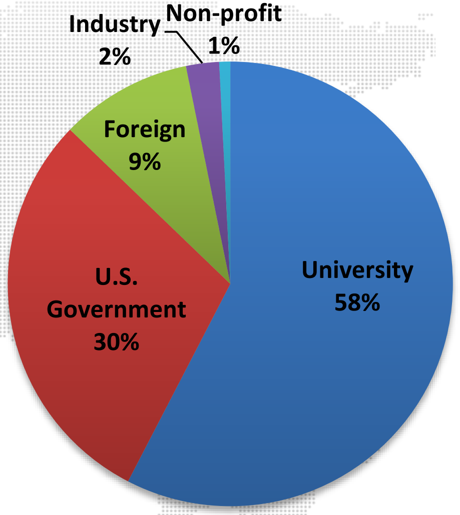
		Time in node-hours			
System	**Facility**	**Requested**	**Available**	**Allocated**	**Number of Projects**
Mira	**ALCF**	**2,226 M**	**1,178 M**	**1,178 M**	**14**
Theta	**ALCF**	**1,181 M**	**346 M**	**345 M**	**7**
Titan	**OLCF**	**2,136 M**	**730 M**	**730 M**	**14**
Cori	**NERSC**	**2,115 M**	**600 M**	**600 M**	**12**
Edison	**NERSC**	**479 M**	**200 M**	**200 M**	**4**

- 67 proposals received in response to the 2018 open call.
- Awarded 3,052 M node-hours to 33 proposals.
- ALCC utilizes 20% of the computational resources on five machines at ASCR's HPC user facilities.
- No hours were held back for off-cycle proposals.
- Successful proposals included the top priority requests from ASCR, BER, BES, EE, EERE, FES, HEP, NE, NNSA, and NP.

2019 INCITE Submission Statistics

- Annual INCITE call for new proposals closed June 22nd, 2018
- 125 new and renewal submissions were received
- LCF resources are more than 2x oversubscribed
- Awards will be made on Summit and Titan (OLCF) and Theta and Mira (ALCF) for CY2019

PIs by Affiliation (Proposals)



Awards Announcements

Public announcement of the 2019 INCITE Awards will happen the week of November 12th (to coincide with SC18)

Contact information
Judith C. Hill, INCITE Manager
hilljc@DOEleadershipcomputing.org

RESEARCH

ASCR Applied Mathematics
FY18 Renewals for Lab Base Math projects (12)

Title	Lead PI	Institution
Scalable Algorithms for Space-Time Indexed Optimization of Complex Systems	Mihai Anitescu	ANL
Automatic Differentiation for Heterogeneous Applications & Architectures	Paul Hovland	ANL
NORDEx: Nonlinear Optimization for Robust Design of Experiments	Sven Leyffer	ANL
Extending PETSc's Composable Hierarchical Nested Solvers	Lois McInnes Mark Adams	ANL LBNL
Stochastic Hybrid Models & Algorithms for Fluids	John Bell	LBNL
Parallel Primitives for Randomized Algorithms on Sparse Data	Aydin Buluc	LBNL
Simulation-Driven High-Order Mesh Adaptivity	Tzanio Kolev	LLNL
Multilevel Methods, Numerical Upscaling & Space-Time AMR	Panayot Vassilevski	LLNL
Uncertainty Quantification for Complex Systems described by Stochastic PDEs	Alexandre Tartakovsky	PNNL
Tensor Decompositions for Data-Driven Applications	Tamara Kolda	SNL
Primal-Dual Mesh Optimization with Mathematical Foundations	Scott Mitchell	SNL
Non-Invasive Semi-Structured Multigrid Methods on Advanced Architectures	Ray Tuminaro	SNL

Lab Base Math Portfolio sustains foundational research projects in PDEs, Multiphysics modeling & simulation, Optimization, Multigrid methods, & Computational mathematics.

2018 Mathematical Multifaceted Integrated Capability Centers
LAB 18-1900, DE-FOA-0001900

MMICCs Purpose: Basic research that address fundamental mathematical challenges within the DOE mission & from a perspective that requires new integrated efforts across multiple mathematical, statistical, and computational disciplines.

Emphasis: MMICC proposals should

- Advance multifaceted, integrated mathematics that appropriately spans novel formulations, discretizations, algorithm development, data analysis, uncertainty quantification, optimization, and other mathematical & statistical approaches
- Address mathematical problems with clear relevance & significant impact to DOE
- Actively engage in community building events to rapidly disseminate scientific advances & maintain clear channels of communication to the DOE user community

Number of full proposals submitted: 19

Project awards: 2

AEOLUS – Advances in Experimental Design, Optimal Control, & Learning for Uncertain Complex Systems (Project Director: Omar Ghattas / Karen Willcox)

UT-Austin (Lead), ORNL, BNL. Texas A&M and MIT supported in subawards.

PhILMs – Collaboratory on Mathematics & Physics-Informed Learning Machines for Multiscale & Multiphysics Problems (Project Director: George Karniadakis)

PNNL (Lead), SNL, Brown, Stanford, UC Santa Barbara. MIT supported in subaward.

MACSER: Multifaceted Mathematics for Rare, High Impact Events in Complex Energy and Environment Systems

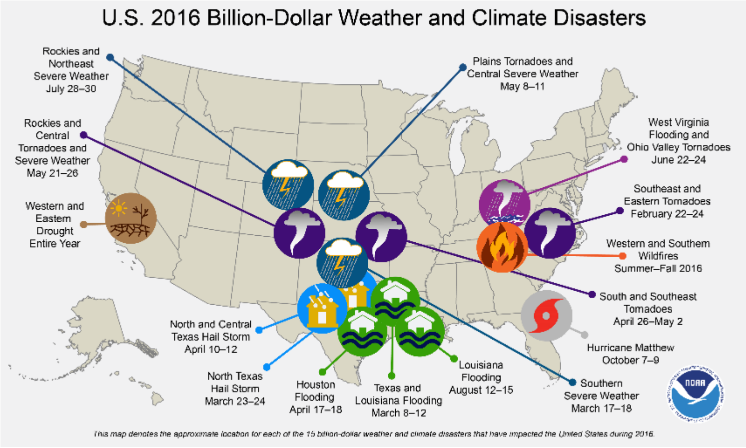
Project Director: Mihai Anitescu, Argonne National Laboratory

Purpose

- Quantify -- by taking a holistic view -- the occurrence and features of rare, high-impact events; and design and optimize energy systems that withstand and recover from such events.
- Address the mathematical and computational complexities of extreme space-time statistics of environmental events and the impact on analyzing, planning, and operating the energy infrastructure.

Integrated Novel Mathematics Research

- *Statistics of rare space-time events* that characterize distributions of extremes and efficiently sample from them.
- *Novel formulations for optimization under uncertainty* that best balance worst-case and probabilistic energy systems requirements.
- *Advanced optimization algorithms* that employ model reduction and decomposition to address the feature and rare-event complexities.



Location of the 15 weather events in 2016 with more than $1B in damages, a large part due to energy infrastructure damage (NOAA).

Long-Term DOE Impact

- Leads to development of new mathematics at the intersection of multiple mathematical sub-domains.
- Addresses a broad class of applications for complex energy systems.
    - Limiting the probability of cascading failures such as the 2003 blackout.
    - Planning an energy infrastructure that is robust & resilient to rare weather events.

U.S. DEPARTMENT OF ENERGY

<u>Team</u>: Argonne National Lab (Lead), Pacific Northwest National Lab, Lawrence Livermore National Lab, Univ of Wisconsin, Univ of Chicago, Ohio State Univ

Optimization-based coupling provides new paradigm for efficient multiphysics simulations

Scientific Achievement

Developed, analyzed and demonstrated a new, optimization-based coupling approach for multiphysics applications.

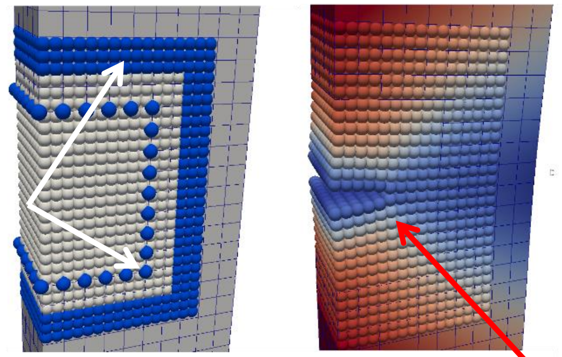
Significance and Impact

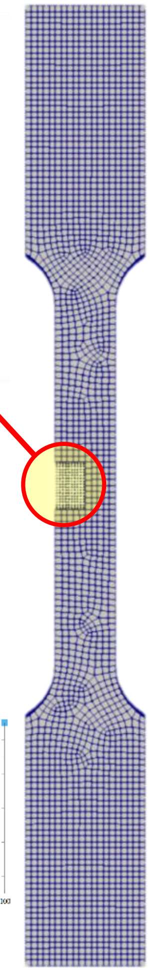
- **Combines the efficiency** of local, PDE models with the accuracy of computationally expensive nonlocal models.
- **Mathematically rigorous**: provably stable, admits formal error analysis.
- **Applicable in multiple contexts**: particles + FEM, FEM+FV, which enables code reuse for new applications.

Research Details

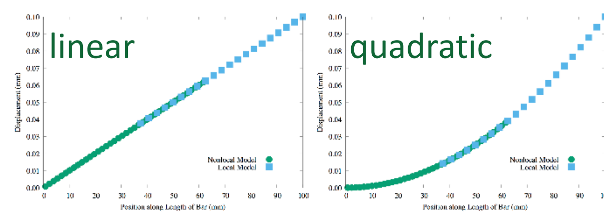
- Existing methods blend energy, force or material properties, creating “hybrid” materials with unphysical artifacts.
- We keep material models independent and couple them by minimizing the misfit of their states using virtual controls.
- This divide-and-conquer approach eliminates ghost forces and is consistent for all polynomial orders.

Virtual controls





Crack simulation in a tensile bar using an optimization-based coupling of elasticity and peridynamics. The latter is applied only in a small region where the crack develops. Implementation uses Sandia’s agile component codes Peridigm (peridynamics), Albany (elasticity) and Rol (optimization).



Demonstration of polynomial consistency for linear and quadratic displacement fields

D’Elia, Bochev, Littlewood, Perego, Optimization-based coupling of local and nonlocal models: Applications to peridynamics. Handbook of Nonlocal Continuum Mechanics for Materials and Structures, Springer Verlag, 2017

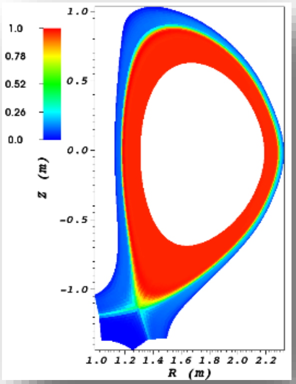
High-resolution methods in complex geometries enable accurate & robust simulations of fusion reactor edge plasmas

Objectives

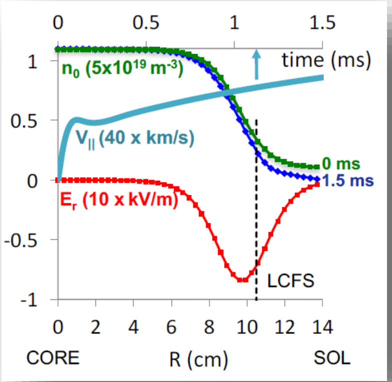
- Develop high-resolution discretization and solution methods for continuum kinetic systems, addressing
  - High phase space dimensionality, conservation, strong anisotropy, positivity, multiple fast time scales
  - Complex geometries such as those defined by the magnetic field in fusion edge plasma applications
- Approach: Development of a systematic formalism and implementation in the COGENT testbed code as part of a multidisciplinary collaboration with FES

Impact

- Facilitate the use of high-resolution discretizations for simulation models involving coordinate mappings
- Enable accurate, efficient and robust numerical simulation of fusion reactor edge plasmas for the design and optimization of experiments
- Provide a complementary, noise-free continuum alternative to particle-based approaches for solving kinetic systems



Edge plasma geometry (General Atomics DIII-D experiment)

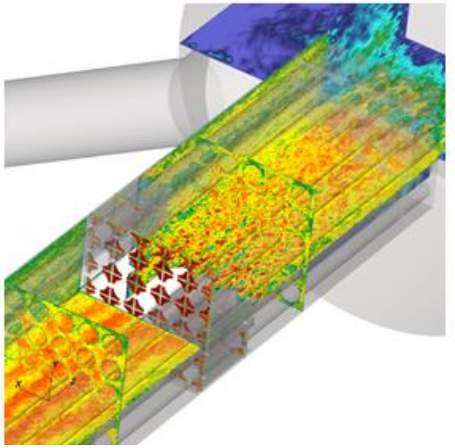


Plasma profiles (n_0, $v_{||}$) spanning the magnetic separatrix (LCFS) including self-consistent electric field (E_r) computed from a continuum kinetic model

Recent Highlights and Accomplishments

- Algorithm and COGENT development
  - New, discretely divergence-free, high-order, mapped-grid, finite-volume approach developed for a gyrokinetic system
  - Implicit-explicit time integration developed and successfully applied to address fast collisional time scales
- FES collaborators utilized COGENT for physics investigations presented at APS-DPP (11/2016)
- COGENT enabled the first ever, self-consistent solution of a continuum gyrokinetic system in edge geometry across the magnetic separatrix (figures at left)
- COGENT provides the edge plasma component of the Advanced Tokamak Modeling SciDAC-3 FES Partnership and two pending SciDAC-4 FES partnership applications

High-order methods enable high-performance multiphysics simulations for DOE applications



Problem

- Nonlinear multiscale interactions govern much of the physics in the energy sector: turbulence, heat transfer, combustion, MHD, semiconductors, ion channels, and advanced materials design require accurate simulation techniques.

Solution

- Nek5000/NekCEM (Gordon Bell Prize and R&D 100 Award winning codes) provide efficient high-order methods with enhanced stability, performance, geometric flexibility, scalable implementations, and multilevel solvers.
- Full support of analysis tools for the application-scientist, more than just a PDE solver.
- New algorithmic approaches focus on overlapping grids, compressible flow, particle transport with two-way coupling, robust preconditioners, level-set formulation for premixed combustion, monotonicity preserving schemes, nonlinear steady and unsteady drift-diffusion solver, magneto-electric effects, quantum density matrix formalism – ***all developed to run on millions of cores.***

Impact

- Major impact in DOE scientific computing mission areas including nuclear, combustion, ocean, wind, and solar power.
- Over 320 users in academia, laboratories, and industry, including collaborations with AREVA, Westinghouse, Kairos, Nuscale, TerraPower, GE, NRG (Netherlands); ORNL, LLNL, INL; ETH Zurich, KTH Sweden, U. Miami, U. Florida, U. Minnesota, U. Illinois, and National Taiwan U.
- Central role in other DOE projects: ECP projects (CEED, SMR, Urban, combustion), PSAAP-II, NEAMS, and NE High-Impact Project (HIP).

ASCR Computer Science
FY18 Awards

Scientific Data Management, Analysis and Visualization

4 Projects @ Total $5,796K spread over 3 years

- **Scientific Data Services - Autonomous Data Management on Exascale Infrastructure**
  Lead: LBNL (Kesheng (John) Wu)
- **In Situ Visual Analytics Technologies for Extreme Scale Combustion Simulations**
  Leads: UC Davis (Kwan-Liu Ma), Sandia (Jacqueline Chen)
- **Science Capsule**
  Lead: LBNL (Lavanya Ramakrishnan)
- **Extreme Scale, Distributed Data Management**
  Lead: BNL (Eric Lancon)

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  Lead: LBNL (Lavanya Ramakrishnan)
- **Extreme Scale, Distributed Data Management**
  Lead: BNL (Eric Lancon)

Characterizing Faults, Errors, and Failures in Extreme-Scale Systems

Scientific Achievement

Developed an understanding of faults, errors and failures in DOE supercomputers

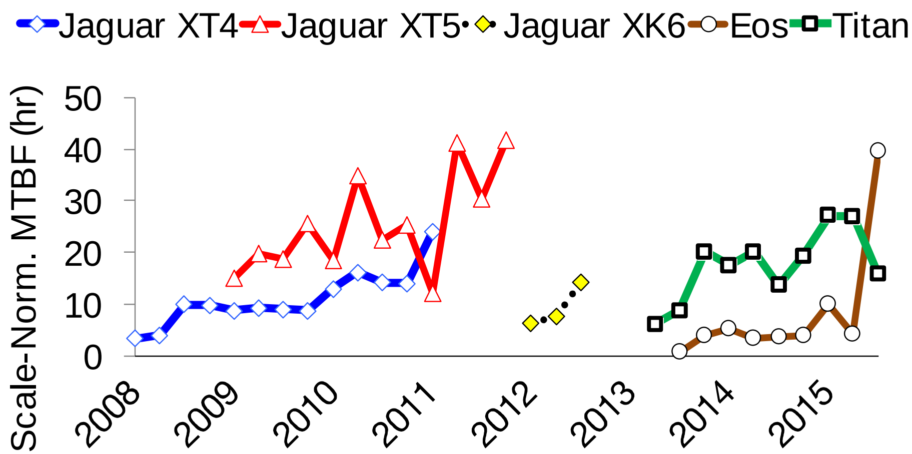
Significance and Impact

Created new insights that can be applied to improve the efficiency of DOE's current and future supercomputers

Research Details

- Created a taxonomy of faults, errors and failures
- Analyzed and modeled faults, errors and failures in:
  - 5 Cray systems at the Oak Ridge Leadership Computing Facility: Jaguar XT4, Jaguar XT5, Jaguar XK6, Titan and Eos
  - Mira, the IBM Blue Gene/Q system at the Argonne Leadership Computing Facility
  - Linux clusters at the Livermore Computing facility
- Developed novel system log analysis software tools
- Applied Big Data analytics to system logs

inside HPC: Characterizing Faults, Errors and Failures in Extreme-Scale Computing Systems. https://insidehpc.com/2018/08/characterizing-faults-errors-failures-extreme-scale-computing-systems/



$$\text{Scale-Normalized MTBF} = \frac{\text{MTBF}\times\text{Num of Nodes in the System}}{\text{Max Number of Nodes across all Systems}}$$

Scale-normalized mean-time between failures (MTBF) of each ORNL system over time (averaged quarterly): The MTBF can change significantly over time with often a non-monotonic trend. This makes it averaged over lifetime an unattractive choice as metric. For the largest system, Titan, it is 15 hours. However, it varied between 6 and 27 hours with the largest quarterly drop from 27 to 17 hours. Up to 30% wasted time spent in taking unnecessary checkpoints can be saved on systems such as Titan by dynamically adapting the checkpoint frequency to the current system reliability.

Work was performed at Oak Ridge National Laboratory (lead), Argonne National Laboratory, Lawrence Livermore National Laboratory, Northeastern University, Wayne State University, University of Tennessee, Knoxville, and University of North Texas.

UniviStor – Unified View of Heterogeneous HPC Storage

Scientific Accomplishment

Proactive Data Containers (PDC) project team at LBNL developed UniviStor, a data management service for integrating on-node memory, near-node storage, and system-wide storage layers. UniviStor achieved up to **46X** faster I/O performance than the state-of-the-art Lustre file system deployed on NERSC's Cori system.

Significance and Impact

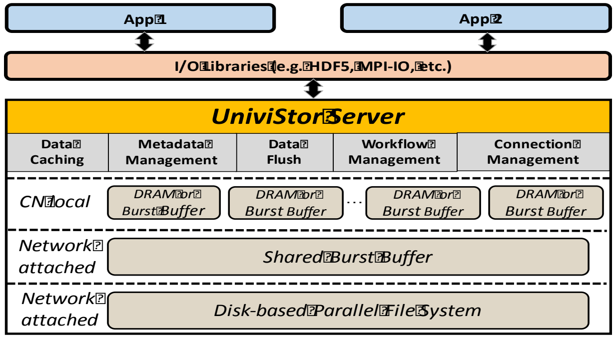
Exascale storage architectures are adding new layers of heterogeneous storage devices. Existing storage management solutions require users to explicitly move data between different storage layers. The unified view of storage service in UniviStor uses existing I/O library APIs, such as HDF5 and MPI-IO, to reduce complexity and to optimize I/O performance.

Research Details

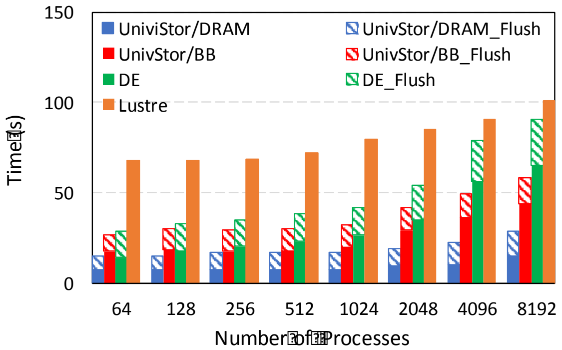
– Scalable metadata service to unify node-local, shared burst buffer, and file system storage as a single name-space

– Novel performance optimizations to place and move data judiciously using the heterogeneous storage devices

– Support for in situ analysis while data is close to analysis



An overview of UniviStor: UniviStor servers on each compute node (CN) maintain a unified namespace and handle data placement/movement on heterogeneous storage layers. Applications can transparently use UniviStor with parallel I/O libraries, e.g., HDF5 and MPI-IO, without requiring any changes to their code.



Performance of UniviStor: In supporting a plasma physics simulation and analysis, UniviStor outperforms Data Elevator and Lustre by up to **17X and 21X**, respectively.

- **T. Wang, S. Byna, B. Dong, and H. Tang, "UniviStor: Integrated Hierarchical and Distributed Storage for HPC", IEEE Cluster 2018**

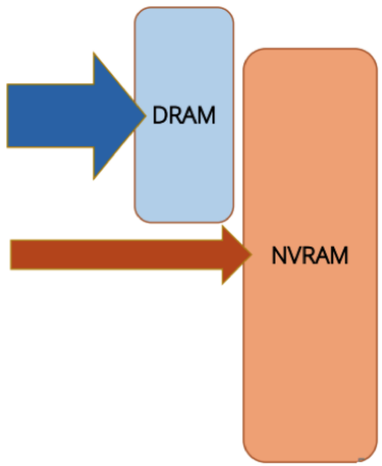
Improving A Supercomputer's Memory

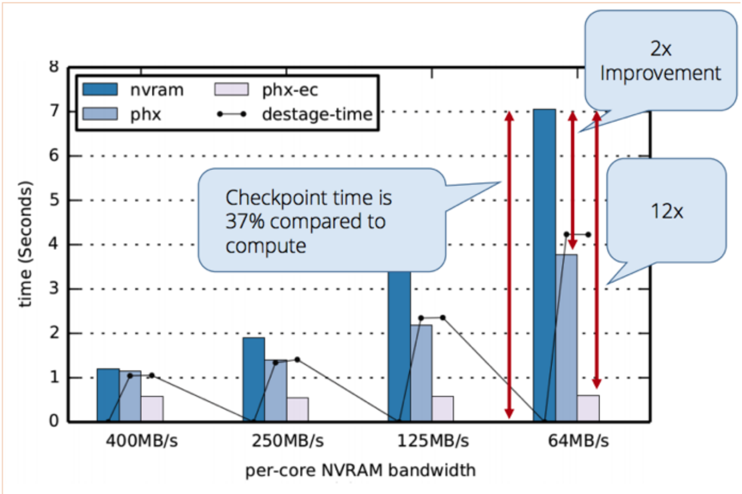
Significance and Impact

Traditional computer memory is volatile which means that it is subject to complete data loss in the event of a loss of power. Recently, computer architects have started to address this with NVRAM -- new technology that retains information in the presence of a power loss. However, NVRAM brings it's own challenges which must be solved before widespread adoption.

Scientific Achievement

Because NVRAM devices have limited bandwidth and slower access times than traditional memory devices (DRAM), care must be taken to retain performance or their usage is problematic. New research has solved this problem using a dual data path approach.





I/O data gets written to both local NVRAM and DRAM to exploit aggregate bandwidth of the devices. Data de-staging from DRAM to NVRAM ensures the bounded DRAM memory usage.

Research Details

- To address this, we have put forward Phoenix (PHX), an NVRAM-bandwidth aware object store for persistent objects. PHX achieves efficiency through use of memory-centric object interfaces and device access stack specialized for NVRAM.
- Furthermore, PHX minimizes the data movement overheads due to additional data copies, by using a cost model that considers device bandwidths, remote storage distance and energy costs.

P. Fernando, et al, *23rd Annual International Conf. on High Performance Computing, Data and Analytics (HiPC'16).*

In Situ Data Management (ISDM) Workshop

- **GOAL: This workshop seeks community input on the development of in situ capabilities for managing the execution and data flow among a wide variety of coordinated tasks for scientific computing.**

  The workshop considers ISDM beyond the traditional roles of accelerating simulation I/O and visualizing simulation results, to more broadly support future scientific computing needs. In particular, the convergence of simulation, data analysis, and artificial intelligence will require machine learning, data manipulation, creation of data products, assimilation of experimental and observational data, analysis across ensemble members, and, eventually the incorporation of tasks on non-von Neumann architecture.
- **Logistics**: January – February, 2019 in the DC area

Organizing Committee

Name	Affiliation	Role
Tom Peterka	ANL	Chair
Debbie Bard	NERSC	Organizer
Janine Bennett	SNL	Organizer
Wes Bethel	LBNL	Organizer
Ron Oldfield	SNL	Organizer
Line Pouchard	BNL	Organizer
Christine Sweeney	LANL	Organizer
Mathew Wolf	ORNL	Organizer
Laura Biven	DOE-ASCR	Program Manager

Enabling Global Adjoint Tomography at scale through next-generation I/O

Scientific Achievement

Most detailed 3-D model of Earth's interior showing the entire globe from the surface to the core–mantle boundary, a depth of 1,800 miles.

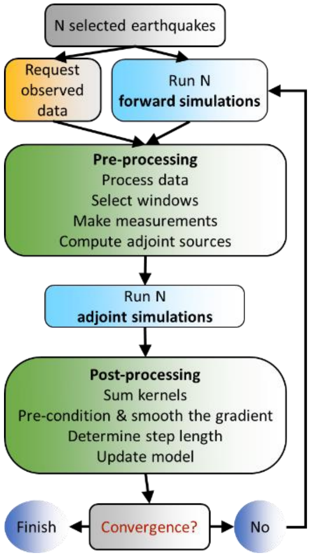
Significance and Impact

First global seismic model where no approximations were used to simulate how seismic waves travel through the Earth. The data sizes required for processing are challenging even for leadership computer facilities.

Research Details

- To improve data movement and flexibility, the Adaptable Seismic Data Format (ASDF) was developed that leverages the Adaptable I/O System (ADIOS) parallel library.
- It allows for recording, reproducing, and analyzing data on large-scale supercomputers
- 1PB of data is produced in a single workflow step, which is fully processed later in another step.
- https://www.olcf.ornl.gov/2017/03/28/a-seismic-mapping-milestone

A



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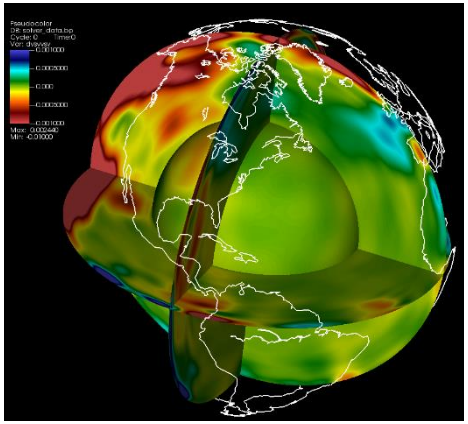


(A) Seismic Tomography workflow graph. The heavy computational steps are the Forward and Adjoint Simulations steps. They produce and consume the large data sets, respectively. ***(B)*** *A* visualization of the Earth's interior with unprecedented details from the seismic tomography process model, which maps the speeds of waves generated after earthquakes. *(Image Credit Dave Pugmire)*

Ebru Bozdag; Daniel Peter; Matthieu Lefebvre; Dimitri Komatitsch; Jeroen Tromp; Judith Hill; Norbert Podhorszki; David Pugmire. **Global adjoint tomography: first-generation model.** *Geophysical Journal International* 2016 207 (3): 1739-1766 https://doi.org/10.1093/gji/ggw356

New Unstructured Mesh Technologies are Being Developed for Fusion Applications

Scientific Achievement

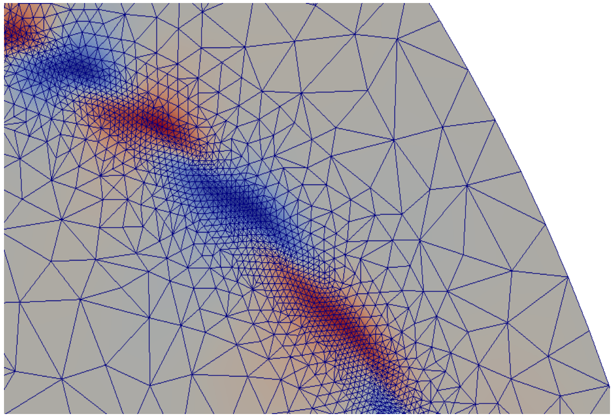
Advanced unstructured mesh technologies support several fusion simulation codes including core and edge plasma, wall interactions, and RF interactions

Significance and Impact

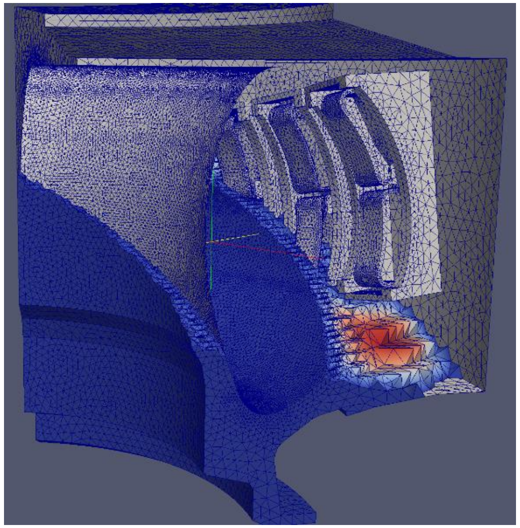
Unstructured mesh tools decrease model preparation time and increase results accuracy. Unstructured mesh based particle-in-cell well suited to effective execution on new systems.

Research Details

- Developing new mesh generation accounting for the geometry, physics and needs of the numerical methods used
- High-order conforming and nonconforming mesh adaptation that effectively captures the physics of interest via in-memory integration into codes
- Developing unstructured mesh based particle-in-cell methods that will perform well on current and near term architectures



Adapted mesh from ELM study



3D mesh for RF simulation

Work was performed at LRPI and LLNL
For more information contact Mark Shephard: shephard@rpi.edu

Quantum Algorithm Teams & Quantum Computing Application Teams

Purpose: Build on ASCR's fundamental science community to advance basic research in quantum algorithms and in quantum computer science (2015 ASCR Workshop on Quantum Computing for Science).

Emphasis: Interdisciplinary teams of QIS experts, applied mathematicians and computer scientists that adopt a methodical approach to fill in the missing elements in order to connect SC grand challenges to quantum computing hardware.

FY 2017 Quantum Algorithm Teams (QAT): 3 PROJECTS @ TOTAL $4M/YEAR (FY17-19):

Focus on Algorithms

Quantum Algorithms, Mathematics and Compilation Tools for Chemical Sciences.
Lead: LBNL (Bert de Jong), Collaborators: ANL, Harvard University. https://qat4chem.lbl.gov/overview

Heterogeneous Digital-Analog Quantum Dynamics Simulations. Lead: ORNL (Pavel Lougovski), Collaborator: University of Washington. https://hdaqds.ornl.gov/index.html

Quantum Algorithms from the Interplay of Simulation, Optimization, and Machine Learning. Lead: SNL (Ojas Parekh), Collaborators: LANL, CalTech, UMD. https://qoalas.sandia.gov/

FY2018 Quantum Computing Applications Teams (QCAT): 2 QCAT PROJECTS @ TOTAL $4M/YEAR (FY18-21):

Focus on Algorithms, Software Stack, V&V

Software Stack and Algorithms for Automating Quantum-Classical Computing. Lead: ORNL (Pavel Lougovski), Collaborators: Georgetown University, UMD, USC, Johns Hopkins University APL.

Optimization, Verification and Engineered Reliability of Quantum Computers. Lead: SNL (Mohan Sarovar), Collaborators: LANL, Dartmouth University.

ASCR Tools: Quantum Testbeds Pathfinder

Purpose: To provide decision support for future investments in quantum computing (QC) hardware and increase both breadth and depth of expertise in QC hardware in the DOE community.

Emphasis: Research in the relationship between device architecture and application performance, including development of meaningful metrics for evaluating device performance. Focus is on applications of QC relevant to the Office of Science.

FY 2017: DOE National Laboratory Announcement; 2 awards; total investment of $9.4M over 5 years:

- Advanced Quantum-Enabled Simulation (**LBNL**, LLNL, UC Berkeley)
- Methods and Interfaces for Quantum Acceleration of Scientific Applications (**ORNL**, IBM, IonQ, Georgia Tech, Virginia Tech)

FY 2018: DOE National Laboratory Announcement + companion FOA; 3 awards; total investment of $9.1M over 5 years:

- Quantum-hardware-focused Application Performance Benchmarks (**Virginia Tech**, Duke)
- Efficient and Reliable Mapping of Quantum Computations onto Realistic Architectures (U of Maryland)
- Quantum Performance Assessment (SNL)

ASCR Tools: Quantum Testbeds for Science

Purpose: To provide the research community with novel, early-stage quantum computing resources and advance our understanding of how to use these resources for advancing scientific discovery.

Motivation: Researchers will need low-level access to quantum computing devices, and even the ability to modify these devices, to experiment with different implementations of gates and circuits, explore programming models, and understand the practical consequences of device imperfections. (2017 Quantum Testbed Stakeholder Workshop Report)

Details: Quantum Testbed for Science (QTS) Laboratories will function as small collaborative research facilities that host experimental quantum computing resources on site, provide external researchers with access to and support in using these resources, and sponsor community engagement activities. Research performed at the QTS Laboratories will inform the design of next-generation devices, ensuring that tomorrow's quantum computers will be capable of running quantum algorithms in support of DOE's science and energy mission.

FY 2018: DOE National Laboratory Announcement; 2 awards; total investment of $56.3M over 5 years:

- Advanced Quantum Testbed (**LBNL**, MIT-LL): multiple novel superconducting qubit architectures
- Quantum Scientific Computing Open User Testbed (**SNL**): room-temperature and cryogenic trapped ion platforms

Both testbeds will give users access to low-level control parameters and complete information about their QC platforms. The testbeds are expected to be available to users by the end of FY 2019, and will be upgraded throughout the award term.

The First Simulation of an Atomic Nucleus on Quantum Cloud

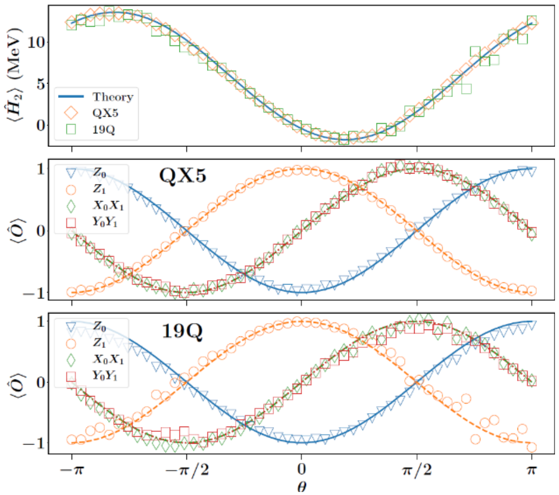
Significance: First application of quantum computers in nuclear physics and it opens the avenue for quantum computations of heavier nuclei via quantum cloud access

Highlight: Computed the binding energy of the deuteron (nucleus of ${}^2_1H$ – bound state of a proton and a neutron

Research Details:

- Implemented Variational Quantum Eigensolver (VQE) with a novel low-depth Unitary Couple Cluster (UCC) wavefunction ansatz
- Performed systematic error mitigation using hybrid quantum-classical data post processing
- Computed Deuteron's binding energy -2.28 MeV (True value - 2.22 MeV; 3% error)

E. F. Dumitrescu *et al.*, accepted in Phys. Rev. Lett. (April 2018) (PRL Editors' Suggestion) [arXiv:**1801.03897**]



Experimentally determined binding energies for the deuteron (top) and expectation values of the Pauli terms that enter the two-qubit deuteron Hamiltonian as determined on the IBM QX5 (center) and Rigetti 19Q (bottom) chips as a function of the variational parameter. Experimental (theoretical) results are denoted by symbols (lines).

***Collaborative effort between ORNL's QAT (P.Lougovski), QTP (R.Pooser) and NUCLEI SciDAC-4 (T.Papenbrock) teams**

Accelerating Applications of High-Performance Computing with Quantum Processing Units

Travis Humble
ASCR Early
Career Awardee

Goal

Accelerate existing scientific applications using quantum processors

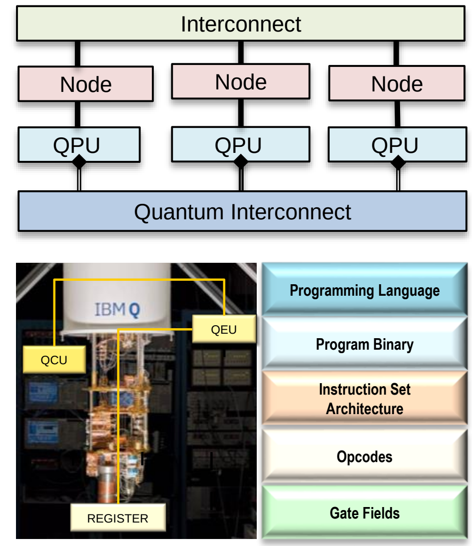
Significance and Impact

Development of long-term capabilities for the design and operation of quantum computing systems within DOE HPC facilities

Research Details

We design machine models that integrate quantum computing with modern HPC system principles. Performance expectations for proto-application codes are simulated using these models, and feedback from the simulations enables performance-driven co-design. Our machine models produce the input needed for processor development and programming abstractions.

Recent results have identified significant reductions in the energy consumption for quantum processing units (QPUs), while future work will emphasize resilient quantum computing in networked environments.



Accelerator architectures for quantum computing offer new opportunities in HPC system design. We evaluate performance with respect to machine models and language hierarchies.

"Quantum Accelerators for High-Performance Computing Systems," ICRC 2017
"Instruction Set Architectures for Quantum Processing Units," ISC 2017

This work was performed at Oak Ridge National Laboratory under the DOE ASCR Early Career Research program

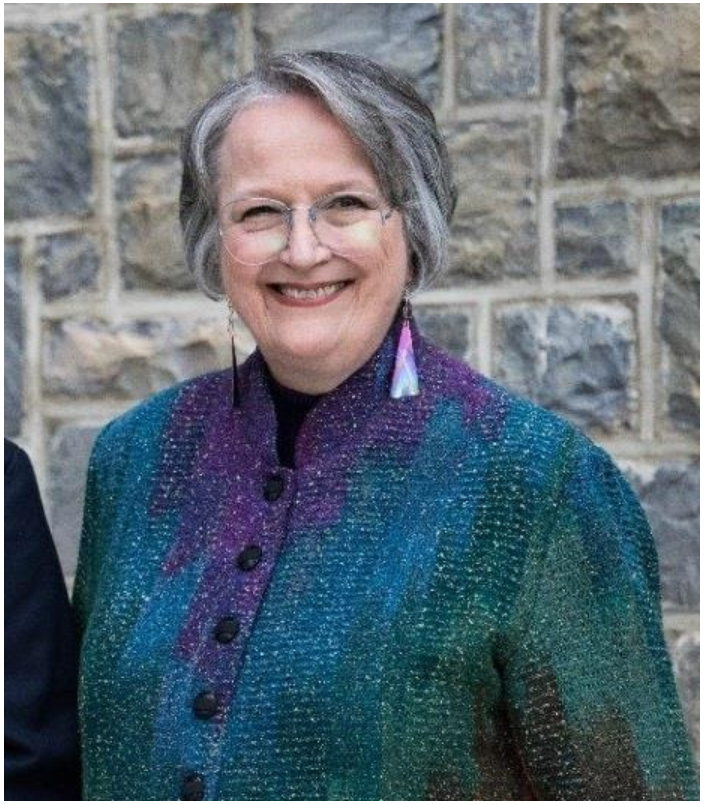
ASCR Staffing Changes

- **William Vandelinde will join ASCR on October 1, 2018 on detail from DOD. He will serve as the Acting Director of the Advanced Computing Technology Division**
- **Robinson Pino is currently the Acting Director for the Research Division**
- **Benjamin Brown is currently the Acting Director for the Facilities Division**

- **SC Approved Backfills**
  - Applied Math Program Manager – Currently interviewing candidates
  - NERSC Program Manager – will be posted soon

Virginia Tech Academy of Engineering Excellence

ASCR Computer Science Program Manager Dr. Lucy Nowell was recognized for meritorious lifetime achievements

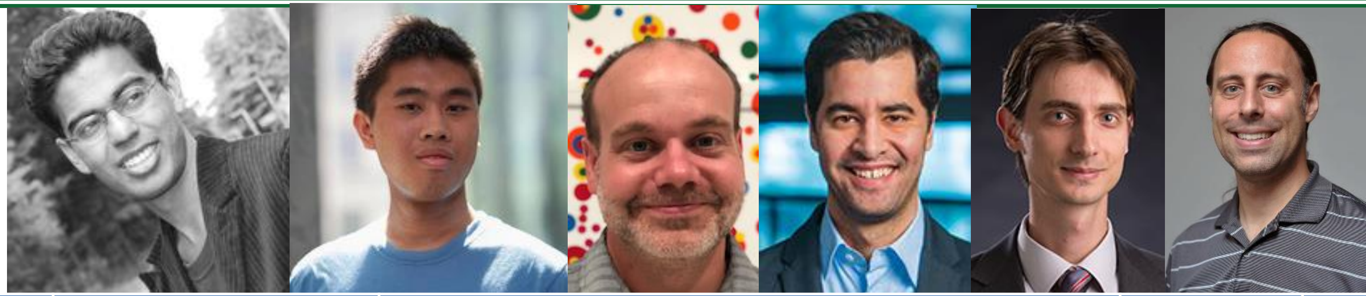


Dr Nowell was one of six new members inducted into the Virginia Tech's College of Engineering Academy of Engineering Excellence in 2018. The academy consists of 152 engineering alumni who have achieved exceptional career successes. Dr. Nowell earn her master's degree (1993) and Ph.D. (1998) in computer science at Virginia Tech.

"The alumni who are inducted into the academy are standouts in their respective careers, embodying the character and caliber of engineers we aspire to produce at Virginia Tech,"

Julia Ross, Paul and Dorothea Torgersen Dean of Engineering in the Virginia Tech College of Engineering

Awards – FY18 ASCR Early Career Research Program



Name	Institution	Title	Program	Topic Area
Prasanna Balaprakash PhD in 2009	Argonne National Laboratory	Scalable Data-Efficient Learning for Scientific Domains	Computer Science	Machine Learning
Julian Shun PhD: 2015	Massachusetts Institute of Technology	Portable Parallel Algorithms and Frameworks for Exascale Graph Analytics	Computer Science	Data & Visualization
Joshua Levine PhD: 2009	University of Arizona	Analyzing Multifaceted Scientific Data with Topological Analytics	Computer Science	Data & Visualization
Paris Perdikaris PhD: 2015	University of Pennsylvania	Probabilistic data fusion and physics-informed machine learning: A new paradigm for modeling under uncertainty, and its application to accelerating the discovery of new materials	Applied Math	Scalable Scientific Data Analysis
Omer San PhD: 2012	Oklahoma State University	Physics-reinforced machine learning for multiscale closure model discovery	Applied Math	Multiscale Mathematics
Eric Cyr PhD: 2008	Sandia National Laboratory	Parallel-in-Layer Methods for Extreme-Scale Machine Learning	Applied Math	Algorithms, Solvers, and Optimization

Daniela Ushizima (2015 Early Career Awardee)

Received 2017 LBNL Directors' Award for Outreach:

"For her selfless and tireless efforts as an exemplary ambassador of science and goodwill, engaging new and emerging scientists around the globe, and sharing knowledge that improves others' lives."

Over the course of several years, Dr. Ushizima's efforts of engagement have touched literally thousands of people around the world with a positive message of the value of science and technology, and in so doing, she has found new ways to apply technology to problems of significant societal benefit.

http://recognition.lbl.gov/laureates/

Jacqueline Chen (Sandia National Laboratory)

- Elected as Member of the National Academy of Engineering, Class of 2018: " For contributions to the computational simulation of turbulent reacting flows with complex chemistry."
- Elected Fellow of the Combustion Institute, Inaugural Class of 2018: "for groundbreaking direct numerical simulations elucidating the fundamental processes in turbulent flames in different modes of combustion"
- Recipient of Combustion Institute Bernard Lewis Gold Medal Award, 2018 for "exceptional skill in linking high performance computing and combustion research to deliver fundamental insights into turbulence-chemistry interactions" The Bernard Lewis Gold Medal is one of the highest awards of The Combustion Institute, presented biennially during the International Symposium on Combustion. Gold medals are bestowed to scientists whose major contributions have significantly advanced their fields of combustion science.
- Society of Women Engineers Achievement Award, 2018: "For pioneering research in computational combustion modeling; for harnessing the power of computers to advance the discipline; and for service both to science and the scientific community" This award is the highest honor given by the society and recognizes outstanding technical contributions for at least 20 years in engineering.

Secretarial Appreciation Award

In recognition of nearly 40 years of leadership in delivering high performance computing resources to address the Nation's science and engineering challenges across a wide array of disciplines and for critical contributions to the success of the Oak Ridge Leadership Computing Facility and sustained U.S. leadership in high performance computing and computational science.

Some ASCAC Agenda Details

- **ARTIFICIAL INTELLIGENCE AT THE EDGE R&D –** *Pete Beckman, ANL*
- **NATIONAL CANCER INITIATIVE UPDATE –** *Carolyn Lauzon, ASCR; Fred Streitz, LLNL; Martin Berzins***,** *ASCAC*
- **UPDATE ON THE EXASCALE COMPUTING PROJECT –** *Doug Kothe, ORNL and Mike Heroux, SNL*
- **EARLY CAREER: QUANTUM ACCERLERATED HIGH-PERFORMANCE COMPUTING --** *Travis Humble, ORNL*
- **EARLY CAREER: PREDICTIVE SCIENTIFIC SIMULATIONS FOR COMPLEX SYSTEMS --** *Emil Constantinescu, ANL*
- **PHOTONIC INTEGRATED SUBSYSTEMS FOR NEXT GENERATION LEADERSHIP CLASS HPC,** *Keren Bergman, ASCAC*
- **FUPDATE ON CURRENT CHARGES**
  - *Subcommittee Documenting ASCR Impacts – Paul Messina, ANL*
- **UPDATE ON SUMMIT:** *Buddy Bland, ORNL*
- **BASIC RESEARCH NEEDS FOR MICROELECTRONICS WORKSHOP –** *Andrew Schwartz, BES*