



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

# **View from Germantown Advanced Scientific Computing Research**

Presented to the  
ASCAC

by

Barbara Helland  
Associate Director

September 22, 2019

# FY 2020 President's Budget Priorities

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**FY 2018 Enacted: \$6.260B**

**FY 2019 Enacted: \$6.585B**

**FY 2020 President's Request: \$5.546B**

## **Priorities:**

- Continue operations of all the national laboratories
- Focus on the development of foundational Artificial Intelligence (AI) and Machine Learning (ML) capabilities
- Continue exascale computing research for delivery in FY 2021
- Expand quantum computing and quantum information science efforts
- Provide sufficient funding to ensure robust cybersecurity program
- Focus on cutting edge, early stage research and development
- Maintain interagency and international partnerships

# FY 2020 Priority #1 Research Initiatives

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- Machine Learning/Artificial Intelligence
- Bio (security, materials, manufacturing)
- Quantum Information Science - includes quantum sensing, computing, networking, and isotope production
- Exascale Computing
- Microelectronics Innovation
- National Isotopes Strategy
- U.S. Fusion Program Acceleration

# FY 2020 Priority #1 Research Initiatives

Dollars in Thousands

Research Initiative	ASCR	BES	BER	FES	HEP	NP	Total
Machine Learning / Artificial Intelligence	36,000	10,000	3,000	7,000	15,000		<b>71,000</b>
Biosecurity			20,000				<b>20,000</b>
Quantum Information Science	51,161	52,503	12,000	7,520	38,308	7,000	<b>168,492</b>
Exascale Computing	463,735	26,000	10,000				<b>499,735</b>
Microelectronics		25,000					<b>25,000</b>
Isotope Development and Production for Research and Applications						47,500	<b>47,500</b>
U.S. Fusion Program Acceleration				4,000			<b>4,000</b>
<b>Total</b>	<b>550,896</b>	<b>113,503</b>	<b>45,000</b>	<b>18,520</b>	<b>53,308</b>	<b>54,500</b>	<b>835,727</b>



# House Appropriations Report

The Advanced Scientific Computing Research program develops and hosts some of the world's fastest computing and network capabilities to enable science and energy modeling, simulation, and research.

*Exascale Computing Project.*—The recommendation includes **\$188,735,000 for exascale activities.**

*High Performance Computing and Network Facilities.*—In addition to the long-term exascale initiative, the Committee supports continued upgrade and operation of the Leadership Computing Facilities at Argonne National Laboratory and Oak Ridge National Laboratory and of the High Performance Production Computing capabilities at Lawrence Berkeley National Laboratory. The recommendation **includes \$150,000,000 for the Argonne Leadership Computing Facility, \$225,000,000 for the Oak Ridge Leadership Computing Facility, and \$100,000,000 for the National Energy Research Scientific Computing Center at Lawrence Berkeley National**

Laboratory. Within available funds, the recommendation **includes \$10,000,000 for the Computational Science Graduate Fellowship program and \$90,000,000 to support necessary infrastructure upgrades and operations for ESnet.**

*Mathematical, Computational, and Computer Sciences Research.*— The Committee notes the importance of a strong research program in applied and computational mathematics to the Department's mission. Maintaining international leadership in high performance computing requires a long-term and sustained commitment to basic research in computing and computational sciences, including applied math, software development, networking science, and computing competency among scientific fields. Within available funds, the recommendation **includes not less than \$155,000,000 for Mathematical, Computational, and Computer Sciences Research.**

Within available funds, the recommendation **includes up to \$15,000,000 for research in memory advancements for accelerated architectures used to enhance Artificial Intelligence and Machine Learning.**

# Other House Language

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National Institutes of Health (NIH) are developing breakthroughs in health research, including drug discovery, brain research, diagnostic technologies, imaging, and other biomedical research areas. **The Department is encouraged to expand its relationships with NIH in order to work together more strategically to leverage the Department's research capabilities, including instrumentation, materials, modeling and simulation, and data science.** The facilities and equipment funded in this Act support application in many areas of biomedical research. The Department is directed to provide to the Committee not later than 90 days after enactment of this Act a plan that responds to the findings and recommendations in the Final Report of the Secretary of Energy Advisory Board Task Force on Biomedical Sciences. The plan shall include a reporting of successful collaborations between the Department and NIH to date and plans to expand on these efforts.

The Committee supports the Office of Science's coordinated and focused research program in quantum information science and technology. This emerging field of science promises to yield revolutionary new approaches to computing, sensing, and communication. **The recommendation includes funding for quantum information science research and establishment of National Quantum Information Science Research Centers.**

**The Committee appreciates the Department's focus on the development of foundational Artificial Intelligence and Machine Learning capabilities,** and the Committee directs the Department to apply those capabilities to the Department's mission.

# Senate Appropriations Report

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The Committee recommends \$1,029,000,000 for Advanced Scientific Computing Research.

The Committee recommends **\$188,735,000 for the Exascale Computing Project**. In addition, the Committee recommends **\$235,000,000 for the Oak Ridge Leadership Computing Facility, \$165,000,000 for the Argonne Leadership Computing Facility, \$115,000,000 for the National Energy Research Scientific Computing Center, and \$90,000,000 for ESnet**. The Committee recommends **\$42,000,000 for Research and Evaluation Prototypes, including \$12,000,000 for the Computational Sciences Graduate Fellowship**.

Maintaining international leadership in high performance computing requires a long term and sustained commitment to basic research in computing and computational sciences, including applied math, software development, networking science, and computing competency among scientific fields. The Committee is concerned that the Department is falling behind in its research capabilities and capacity, threatening continued U.S. leadership, and **therefore provides no less than \$160,000,000 for research**.

The Committee appreciates the Department's focus on the development of foundational Artificial Intelligence and Machine Learning capabilities, and the Committee directs the Office of Science to apply those capabilities to the Office of Science's mission with a focus on accelerating scientific discovery in its Scientific User Facilities and large experiments.

## Other Senate Language

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The Committee recommends **\$7,215,000,000 for Science, an increase of \$1,669,028,000** above the budget request. The recommendation includes \$188,000,000 for program direction.

*Distinguished Scientist Program.*-The Committee recommends \$4,000,000 to support the Department's Distinguished Scientist Program, as authorized in section 5011 of Public Law 110-69 to promote scientific and academic excellence through collaborations between institutions of higher education and national laboratories to be funded from across all Office of Science programs.

*Quantum Information Science.*-The Committee supports the Office of Science's coordinated and focused research program in quantum information science to support the Department's science, energy, and national security missions, as authorized in sections 401 and 402 of Public Law 115-368, the National Quantum Initiative.

This industry of the future promises to yield revolutionary new approaches to computing, sensing, communication, data security, and metrology, as well as our understanding of the universe, and accordingly **the Committee recommends \$195,000,000 across the Office of Science programs to advance early-stage fundamental research in this field of science, including \$120,000,000 for activities authorized in section 401 and \$75,000,000 for the establishment of up to five National Quantum Information Science Research Centers authorized in section 402.** To the greatest extent practical, this effort shall be undertaken in coordination with the National Science Foundation and the National Institute of Standards and Technology.

*Artificial Intelligence and Machine Learning.*-**The Committee recommends \$71,000,000 for Artificial Intelligence and Machine Learning across the following Office of Science Programs:** Advanced Scientific Computing Research, Basic Energy Sciences, Biological and Environmental Research, Fusion Energy Sciences, and High Energy Physics. As the stewards of the leadership computing facilities, **the Committee expects Advanced Scientific Computing Research to take a lead role in the Department's artificial intelligence and machine learning activities.**

# ASCR FY 2020 President's Request in thousands

	FY 2018	FY 2019	FY 2020		
	Enacted Approp.	Enact	Request	House Mark	Senate Mark
<b>Mathematical, Computational, and Computer Sciences Research</b>					
Applied Mathematics	34,104	28,206	41,500		
<i>Artificial Intelligence and Big Data (Non Add)</i>	(...)	(...)	(14,281)		
Computer Science	29,508	22,000	38,700		
<i>Artificial Intelligence and Big Data (Non Add)</i>	(6,402)	(2,000)	(9,719)		
<i>Quantum Information Science</i>	...	(3,000)	(5,000)		
Computational Partnerships	49,910	75,667	60,959		
<i>Artificial Intelligence and Big Data (Non Add)</i>	(3,500)	(13,000)	(12,000)		
<i>Quantum Information Science</i>	(6,349)	(16,214)	(16,708)		
SBIR/STTR	4,301	4,768	5,347		
<b>Total, Mathematical, Computational, and Computer Sciences Research</b>	<b>117,823</b>	<b>130,641</b>	<b>146,506</b>	<b>155,000</b>	<b>168,944</b>
<b>High Performance Computing and Network Facilities</b>					
High Performance Production Computing (NERSC)	94,000	104,000	85,000	100,000	115,000
Leadership Computing Facility at ANL (ALCF)	110,000	140,000	150,000	150,000	165,000
<i>Exascale</i>	(...)	(100,000)	(150,000)	(150,000)	(150,000)
Leadership Computing Facility at ORNL (OLCF)	162,500	199,000	210,000	225,000	235,000
<i>Exascale</i>	(62,500)	(100,000)	(125,000)	(125,000)	(125,000)
Total, Leadership Computing Facilities	272,500	339,000	360,000	375,000	400,000
Research and Evaluation Prototypes	24,260	24,452	39,453	25,620	42,000
<i>CSGF</i>	(10,000)	(10,000)	(10,000)	(10,000)	(12,000)
<i>Quantum Information Science</i>	(14,260)	(14,452)	(29,453)	(15,620)	(30,000)
High Performance Network Facilities and Testbeds (ESnet)	79,000	84,000	80,000	90,000	90,000
SBIR/STTR	17,417	20,701	21,194	22,185	24,321
<b>Total, High Performance Computing and Network Facilities</b>	<b>487,177</b>	<b>572,153</b>	<b>585,647</b>	<b>612,805</b>	<b>671,321</b>
<b>Exascale Computing</b>					
17-SC-20 Office of Science Exascale Computing Project (SC-ECP)	205,000	232,706	188,735	188,735	188,735
<b>Total, Advanced Scientific Computing Research</b>	<b>647,000</b>	<b>935,500</b>	<b>920,888</b>	<b>956,540</b>	<b>1,029,000</b>

# DOE's Artificial Intelligence and Technology Office

Colleagues,

Since its founding, DOE has had a profoundly positive impact on people's lives.

Nowhere does our potential impact show more promise than in the fusing of DOE's unmatched supercomputing capabilities with artificial intelligence (AI) technologies and applying them across the Department's core missions and beyond.

That is why I am pleased to announce that today, I am formally establishing DOE's Artificial Intelligence and Technology Office (AITO).

AITO will report directly to the Under Secretary for Science, and it will serve as the Department's hub for coordinating our efforts as a world-leading enterprise in the development, delivery, and adoption of AI.

AITO will add strength to fulfilling our vital missions in applied energy, basic and applied science and national security while aligning AI-related efforts across our various programs and labs, building on our current investments, and breaking new ground in innovation and technology.

Even more importantly, it will enable us to positively impact people's lives as we have never done before.

Today, the mission begins for the Artificial Intelligence and Technology Office and we look forward to the exciting work they will be doing for the Department and the Nation.

Secretary Rick Perry (9/6/2019)



# Quantum Center Request for Information (RFI)

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To gather community input on the topic areas, organization, requirements, review criteria, and assessment processes to be described in this FOA, ASCR, BES, and HEP issued a joint Federal Register notice constituting a combined Notice of Intent (NOI) and Request for Information (RFI) on May 20<sup>th</sup>, 2019. Comment period closed on July 5<sup>th</sup>, 2019.

## Results:

- 38 distinct comments received (43 total, 5 duplicates or updates)
- Published here except for 1 confidential response

<https://www.regulations.gov/docket?D=DOE-HQ-2019-0025>

- Labs: Ames, ANL, BNL, FNAL, LBNL, ORNL, PNNL, SNL, SLAC
- Universities: Caltech, Cornell, CU-Boulder, CUNY, Georgia Tech, Harvard, MIT, Princeton, Purdue, SBU, SUNY Albany, UCalgary, UC-Berkeley, UCSB, UChicago, UHouston, UIUC, UMD, URochester, UWashington [in NQN], UWisconsin, Yale
- Companies: Casting Analysis Corp., Centeva, Entanglement Inc., Global Foundries, Google, IBM, Intel, Lockheed Martin, Microsoft, Perspecta Labs, SC Solutions

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- Companies: Casting Analysis Corp., Centeva, Entanglement Inc., Global Foundries, Google, IBM, Intel, Lockheed Martin, Microsoft, Perspecta Labs, SC Solutions

We expect the Quantum Center Funding Opportunity Announcement to be released shortly after DOE receives its FY 2020 appropriations with decisions made by early summer

# NQI Advisory Committee

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## Executive Order 13885, August 30, 2019:

**Section 1. *Establishment.*** The National Quantum Initiative Advisory Committee (Committee) is hereby established. The Committee shall consist of the Director of the Office of Science and Technology Policy or the Director's designee (Director) and not more than 22 members appointed by the Secretary of Energy (Secretary). Committee members shall represent industry, universities, Federal laboratories, and other Federal Government agencies. Committee members must be qualified to provide advice and information on quantum information science and technology research, development, demonstrations, standards, education, technology transfers, commercial application, and national security economic concerns. The Director shall serve as a Co-Chair of the Committee. The Secretary shall designate at least one of the Committee members to serve as Co-Chair with the Director.

**Sec. 2. *Functions.*** (a) The Committee shall advise the Secretary and the Subcommittee on Quantum Information Science of the National Science and Technology Council (Subcommittee) and make recommendations to the Secretary to consider when reviewing and revising the National Quantum Initiative Program (Program) established pursuant to section 101 of the Act. The Committee shall also carry out all responsibilities set forth in section 104 of the Act.

# Nominations for NQIAC

- Request for Information published at <https://www.federalregister.gov/documents/2019/09/11/2019-19640/establishment-of-the-national-quantum-initiative-advisory-committee>
- Nominations are open to all individuals without regard to race, color, religion, sex, national origin, age, mental or physical handicap, marital status, or sexual orientation. The Secretary and the Director also encourage geographic diversity in the composition of the Committee.
- A nomination package should include the following information for each nominee: (1) A letter of nomination stating the name, affiliation, and contact information for the nominee, the basis for the nomination (*i.e.*, what specific attributes recommend him/her for service in this capacity), and the nominee's field(s) of experience; (2) a biographical sketch of the nominee and a copy of his/her curriculum vitae; and (3) the name, return address, email address, and daytime telephone number at which the nominator can be contacted.

All nomination information should be provided in a single, complete package by midnight Eastern Time on October 4, 2019. Interested applicants should send their nomination package to [NQIAC@science.doe.gov](mailto:NQIAC@science.doe.gov).

**Announcement Call Scope:**

Research and development of quantum communication network technologies to support emerging distributed quantum information Science (QIS) applications. The new quantum networks will have the following features:

- Enable the distributions QIS applications using diverse types of qubits;(superconducting qubits, microwave qubits, trapped ions qubits, etc.);
- Leverage existing all-optical telecommunication technologies, standards, and fiber transmission systems;
- Use hybrid CV/DV (continuous variable/Discrete Variable) quantum encoding schemes to handle different types of entanglements including squeezed states;

**Application requirements:**

- Open to all DOE laboratories
- DOE laboratories can include universities and sub-contractors
- One application per Lab
- No LOIs or pre- applications
- Funding level: \$800k/year for 4 years
- Selection by peer-review only ( Review Panel Used)

# STATISTICS

## [Preproposals/Letters of Intent], Full Applications, and Proposed Awards

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- **Preproposals/Letters of Intent Statistics:**
  - N/A
- **[Preproposal/Letter of Intent] review [if applicable]:**
  - N/A
- **Proposal Submissions Statistics:**
  - 9 Lab submissions (7 projects)
  - 4 University sub-Awards, 2 Lab Collaborative Projects
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- **Recommended Award Statistics: (70 % success)**
  - 5 Awards for FY 2019 funding.
  - Quantum Repeaters: 2, Quantum Edge Node: 1, Q-MAN: 1
  - 5 Different Labs (4 SC Labs, 1 NNSA), 4 University Sub-Awards
  - Women Awards:0



# Recommended Selections

PI Name	DOE Lab/ + partner institutions	Proposal Title	FY 2019 Funding Levels	Total Award
<b>Peters, Nicholas</b>	<b>ORNL (Lead Institution)</b> • U. Arizona (subcontract)	Towards Hybrid Continuous/Discrete Variable All-Optical Quantum Repeaters for Quantum-Classical Coexistence in Optical Fiber Networks	\$800,000	\$3,200,000
<b>Figueroa B.Eden</b>	<b>BNL (Lead Institution)</b> • NJIT (subcontractor)	Inter-campus network enabled by atomic quantum repeater nodes	\$1,450,000	\$2,950,000
<b>Pena, Cristian</b>	<b>FNAL (Lead Institution)</b> • Northwestern U (subcontractor) • Caltech (Subcontractor) • ANL (Collaborator)	Illinois-Express Quantum Network	\$800,000	\$3,200,000
<b>Eichenfield, Matt</b>	<b>SNL (Lead Institution)</b>	Quantum Transduction and Buffering Between Microwave Quantum Information Systems and Flying Optical Photons In Fibers	\$1,200,000	\$2,550,000
<b>Nanni, Emilio</b>	<b>SLAC (Lead Institution)</b>	Integrated Platform for Quantum Photonic Networks	\$450,000	\$1,800,000
<b>Total</b>			<b>\$4,700,000</b>	<b>\$13,700,000</b>



**ASCR Funding Opportunity Announcement**  
**ACCELERATED RESEARCH IN QUANTUM COMPUTING (ARQC)**  
**DE-FOA-0002081 and LAB 19-2081**

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## FOA Scope:

- Basic research foundations in quantum algorithms and in quantum computer science. It is expected that the proposed teams will describe processes by which the results, capabilities and resources of the QATs and QCATs will be incorporated into a robust core basic research agenda.
- Mechanisms for taking on cross-cutting algorithmic and computer science challenges across quantum computing topics for DOE and SC relevant application-specific research.
- Tools and resources to facilitate the use of diverse hardware technologies and architectures.
- Mechanisms for providing a bridge between QIS and classical applied mathematics and computer science communities.
- Plans for engaging and interacting with (as appropriate) the DOE-supported QIS community.

QATs and QCATs are quantum computing programs within ASCR research division. The current 5 QAT and QCAT projects are high-risk, high reward projects with a shorter timeline (3-4 years).

## Application requirements:

- Eligible Institutions: All types of applicants are eligible to apply, except FFRDC Contractors, and nonprofit organizations described in section 501(c)(4) of the Internal Revenue Code of 1986 that engaged in lobbying activities after December 31, 1995. DOE National Laboratories and other Federal agencies are not eligible to receive financial assistance awards under the FOA. They are eligible to apply to the companion lab announcement (LAB 19-2081).
- Scope of award: award size: \$250,000K to \$2.5M/year, up to 5 year awards
- An individual may participate in no more than two applications and may be the Team Director on no more than one application. An institution may be the Lead Institution on no more than one application. There is no limitation on the number of applications in which an institution may participate.
- Letters of intent were required.
- The review was conducted online with 12 reviewers who are leading experts in computer science, applied mathematics and quantum computing. An onsite review panel was convened with 5 of the reviewers on July 23<sup>rd</sup>, 2019 to discuss the proposals.

# STATISTICS

## Letters of Intent, Full Applications, and Proposed Awards

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- **Letters of Intent Statistics:**
  - 18 letters of intent were received.
  - 56 institutions and 22 states are represented
- **Letter of Intent review:**
  - 38 of the institutions who submitted letters of intent submitted full proposals.
- **Proposal Statistics:**
  - 60 full proposals which made up 14 distinct collaborative proposals were received. 3 were out of scope and declined without review.
- **Recommended Award Statistics: 23 awards that make up 3 collaborative projects are recommended (27% success)**
  - Total funding to be awarded under the FOA and the companion lab program announcement: \$45M, FY19 funding: \$9M
  - 1 project on quantum algorithms, 2 projects on quantum computing software stack.
  - 1 (33%) university-led; 2 (67%) lab-led; 0% of collaborative projects led by women.
  - 6 states
  - 4 institutions selected for award have not previously been awarded by my quantum computing programs.



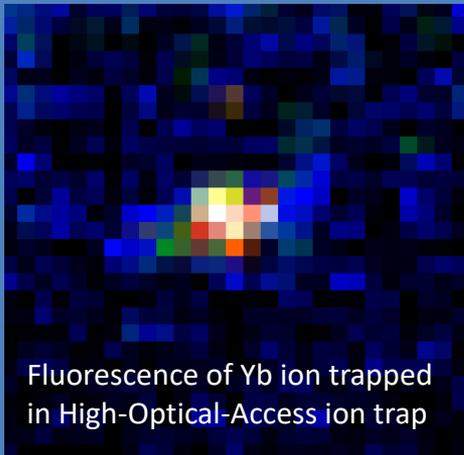
# Recommended Selections

PI Name	Institution	Proposal Title	Recommended FY 2019 Funding \$	Total Award
Ojas Parekh	SNL	Fundamental Algorithmic Research for Quantum Computing (FAR-QC)	\$3.70M	\$18.75M
Bert de Jong	LBNL	Advancing Integrated Development Environments for Quantum Computing through Fundamental Research (AIDE-QC)	\$3.50M	\$17.50M
Brian Clader	Johns Hopkins APL	Tough Errors Are no Match (TEAM): Optimizing the quantum compiler for noise resilience	\$1.80M	\$9.00M



# Quantum Testbed Update, Sept. 2019

## QSCOUT: Quantum Scientific Open User Testbed (SNL)



Expected advantages:

- Identical qubits
- No idle errors
- Low gate errors ( $< 10^{-3}$ )
- Low crosstalk
- All-to-all connectivity
- Reconfigurable in software

- Subsystems are complete, system integration is underway, **first ion trapped!**
- Next steps: optimize trap fields, trap multiple ions, perform and characterize single and two-qubit gates

## AQT: the Advanced Quantum Testbed (LBNL)



- 1 mW dilution fridge with capacity to control up to 128 qubits operational at 9 mK
- Cryogenic package designed and modeled to reduce classical crosstalk to  $< -40$  dB
- **High-coherence quantum processors being optimized**

- Qubit count in Gen 1 testbeds will be lower than industry offerings (5 ions, 8 transmons) but they will be **fully transparent** and give users **access to all levels of control (i.e., the full software stack)**
- **Early science projects include exploration of approaches for high-fidelity entangling gates, implementation of novel characterization techniques, applications of ternary quantum logic ("qutrits"), and error-aware compilation**
- Superusers with science projects suitable for testbed commissioning should contact project PIs (P. Maunz, I. Siddiqi)



# Using Roofline to Characterize Tensor Flow on GPUs

## Scientific Achievement

Created a methodology for analyzing the execution of GPU Tensor Core-accelerated AI/Deep Learning applications using Roofline.

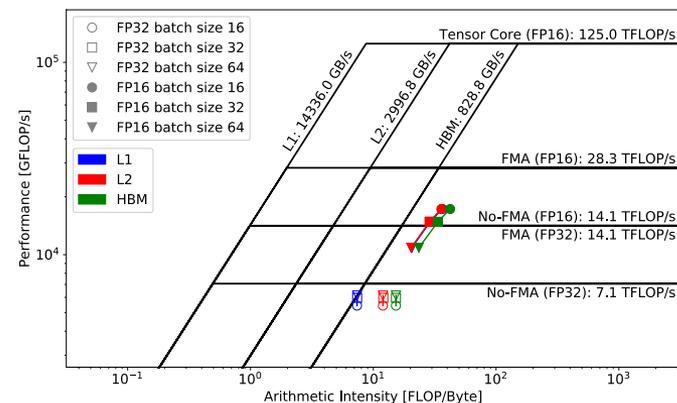
## Significance and Impact

This work enables Roofline-based analysis of NVIDIA Tensor Core accelerated AI/Deep Learning Applications including quantitative assessments of TensorFlow performance on NVIDIA Volta GPUs.

## Research Details

- Collaboration between RAPIDS, NERSC, and NVIDIA
- Formulated methodology for using NVProf to analyze tensor-core accelerated applications using Roofline
- Used Roofline to analyze the forward and backward phases in TensorFlow as a function of FP16 and FP32.
- TensorFlow cannot sustain the theoretical 125TF/s due to a lack of locality and data permutation overheads.

Yang et al., "Hierarchical Roofline Analysis for GPUs: Accelerating Performance Optimization for the NERSC-9 Perlmutter System", CUG, 2019.



## TensorFlow (forward pass) on Volta V100

Results shown are relative to precision (32b and 16b tensor cores) and batch size (16,32,64). Although tensor cores deliver >2x performance, performance is far from theoretical 125TF/s



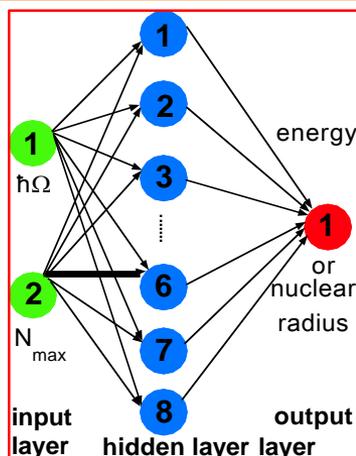
# Deep Learning for Nuclear Binding Energy and Radius

## Scientific Achievement

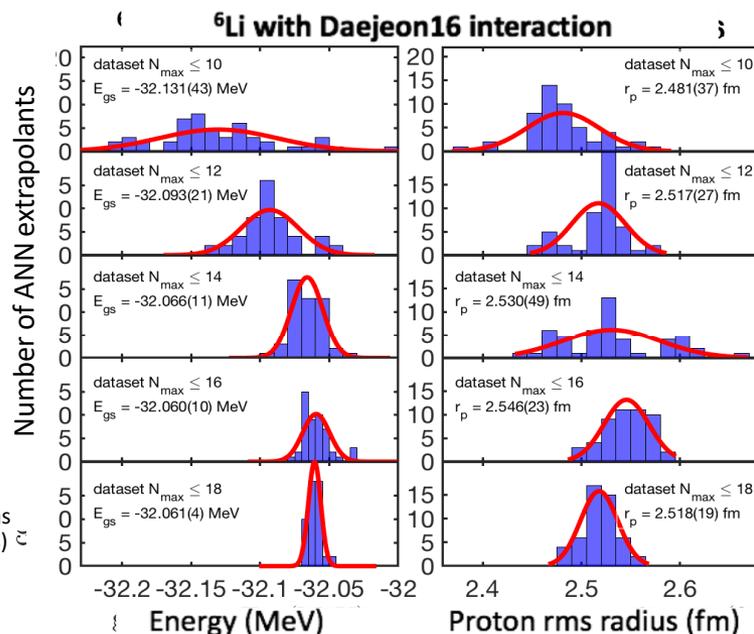
- Developed artificial neural networks (ANNs) for extending the application range of the *ab initio* No-Core Shell Model (NCSM)
- Demonstrated predictive power of ANNs for converged solutions of weakly converging simulations of the nuclear radius
- Provided a new paradigm for matching deep learning with results from high performance computing simulations

## Significance and Impact

- Guides experimental programs at DOE's rare isotope facilities
- Extends the predictive power of *ab initio* nuclear theory beyond the reach of current high performance computing simulations
- Establishes foundation for deep learning tools in nuclear theory useful for a wide range of applications



Neural network (above) used to successfully extrapolate the  ${}^6\text{Li}$  ground state energy and rms radius from modest basis spaces ( $N_{\text{max}}$  datasets) to extreme basis spaces achieving basis parameter independence (histograms of extrapolation ensembles in right figure).



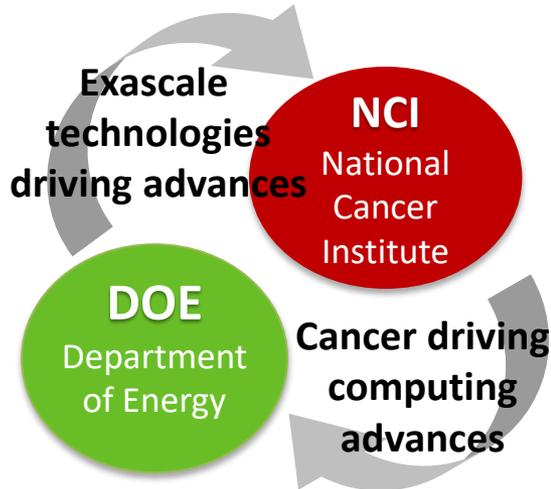
## Research Details

- Develop ANNs that extend the reach of high performance computing simulations of nuclei
- Predict properties of nuclei based on *ab initio* structure calculations in achievable basis spaces
- Produce accurate predictions of nuclear properties with quantified uncertainties using fundamental inter-nucleon interactions such as Daejeon16

# NCI-DOE Collaboration Update

The NCI/DOE Collaborations were formed to jointly accelerate NCI and DOE federal missions in precision oncology and high-performance computing (HPC).

The partnership is designed to push the frontiers of high performance computing through application to NCI's mission to improve understanding of cancer biology and its application to more effective cancer therapies.



Frederick National Lab for  
Cancer Research

# Conclusions from June, 2019 NCI-DOE partnership review

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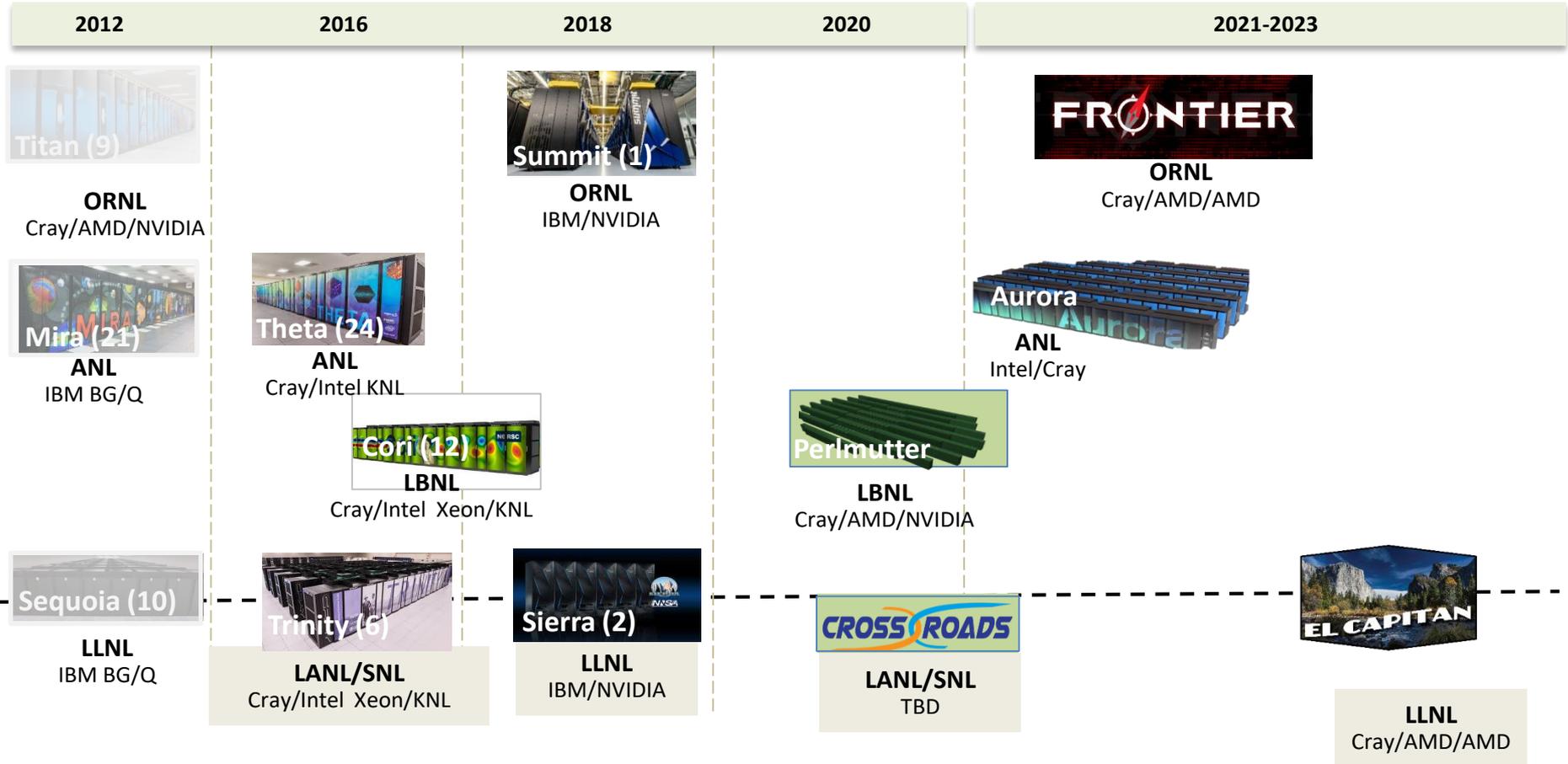
- Overall, the three pilots have developed impressively over the past three years.
- Each pilot is helping define the quality and type of data that are necessary to make progress
- Important work has been done across the pilots on uncertainty quantification. This is essential for the utility of knowledge extracted from data and for the predictive models in all pilots.
- We have learned that the problems are, if anything, more difficult and challenging than initially imagined.
- There is a sharpening and focusing of the aims for years 4 and 5 following the lessons learned from the existing pilots.
- While I have described the progress mostly through an NCI perspective, the tools and methodologies developed in the pilots have broad applicability to many machine learning problems. Beyond the developed methodologies, the scale of the problems tackled by the pilots is helping DOE define what architectures are needed at the exascale.

# Department of Energy (DOE) Roadmap to Exascale Systems

An impressive, productive lineup of *accelerated node* systems supporting DOE's mission

Pre-Exascale Systems [Aggregate Linpack (Rmax) = 323 PF!]

First U.S. Exascale Systems



# Farewell, Titan

*A workhorse supercomputer for the scientific community retired August 1*

- After 7 years of operation, the OLCF decommissioned the Cray XK7 supercomputer on August 1, and disassembled the system for recycling.
- Titan represented a new generation of supercomputer with a revolutionary hybrid architecture that combined AMD 16-core Opteron CPUs and NVIDIA Kepler GPUs.
- In 2012, Titan debuted as No. 1 on the TOP500 list and remained among the top 10 of the world's fastest supercomputers until 2019.
- Through more than 26 billion core-hours of computing time, Titan has served hundreds of research teams working on today's most urgent scientific challenges.
- The OLCF is retrofitting the 20,000 square feet of data center space that housed Titan and its support systems to make room for the 2021 Frontier exascale system.



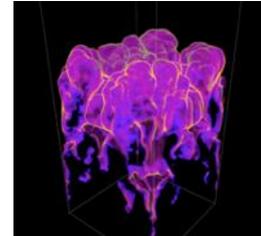


Using the OLCF's Cray XK7 Titan, researchers have contributed to the development of better biofuels, more efficient utility-scale gas turbines, and hazard maps for earthquake-prone regions. Research conducted on Titan has led to thousands of scientific journal articles enabled by OLCF systems and, more importantly, has contributed to a safer, more energy-secure future.



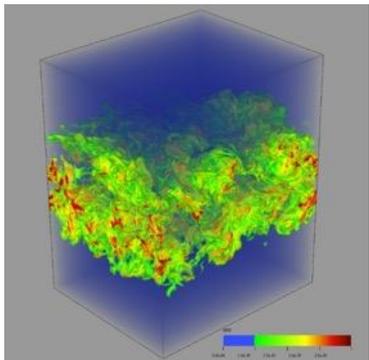
## Breaking down Biomass:

Using Titan, a team at ORNL developed simulations that help understand how to overcome an obstacle in ethanol production: lignin, a ubiquitous structural component of plants that blocks the enzymatic breakdown of biomass.



## Revealing Supernova Secrets:

An ORNL and University of Tennessee-led team has developed more realistic models of supernovas by leveraging Titan's GPUs to improve nuclear reaction networks, which are thought to play a central role in the star's explosion.



## Detailing Combustion:

Researchers from Sandia National Laboratories used Titan to increase the realism in fuel mixing simulations. The simulations are providing important benchmarks for combustion model development and validation.

**Deep Learning and AI:** Despite playing a leading role in traditional modeling and simulation, Titan also earned a reputation for solving large-scale problems in data science. For example, ORNL teams used Titan for training neural networks for robot navigation systems and to quickly generate custom neural networks with the same performance level as those created by humans. Researchers also used Titan to extract useful information from cancer pathology reports that may lead to a better understanding of the disease.

# Changes for ALCC 2020-2021

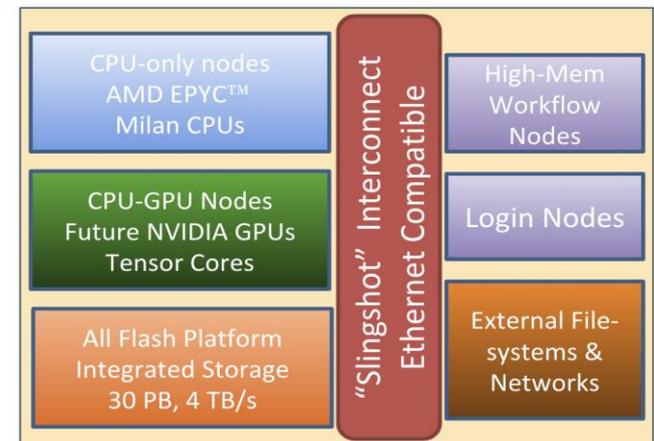
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- **New this year:**
  - Peernet is hosting the ALCC site. <https://science.osti.gov/ascr/ALCC>
  - a Letter of Intent (LOI) to streamline our process
    - The LOI is **REQUIRED** prior to proposal submission.
    - Proposers will be asked to identify project team members, an estimate of computer time to be requested, and an abstract.
    - There will be no feedback regarding the LOI submission
    - LOI submission site opens on October, 1, 2019 and will close on December 16, 2019
- Once the LOC call closes, information from the LOI will be uploaded to the ALCC proposal site so that PIs can begin submitting the rest of their proposals on **December 18, 2019**
- Deadline for ALCC proposal submissions will be **11:59 PM February 3, 2020**
- Available ALCC time: 6M node-hours on Summit, 5.9M node-hours on Theta, and 4.5M node-hours on Cori.

# NERSC's Next System: Optimized for Science



- Cray Shasta System providing 3-4x capability of Cori
- First NERSC system designed to meet needs of both large scale simulation and data analysis from experimental facilities
  - Includes both NVIDIA GPU-accelerated and AMD CPU-only nodes
  - Cray Slingshot high-performance network will support Terabit rate connections
  - Optimized data software stack enabling analytics and ML at scale
  - All-Flash filesystem for I/O acceleration
- Robust readiness program for simulation, data and learning applications and complex workflows
- Delivery in late 2020



# NESAP: Application Readiness for Perlmutter

**NESAP** is NERSC's Application Readiness Program for new Systems. Started with Cori; Continuing with Perlmutter.

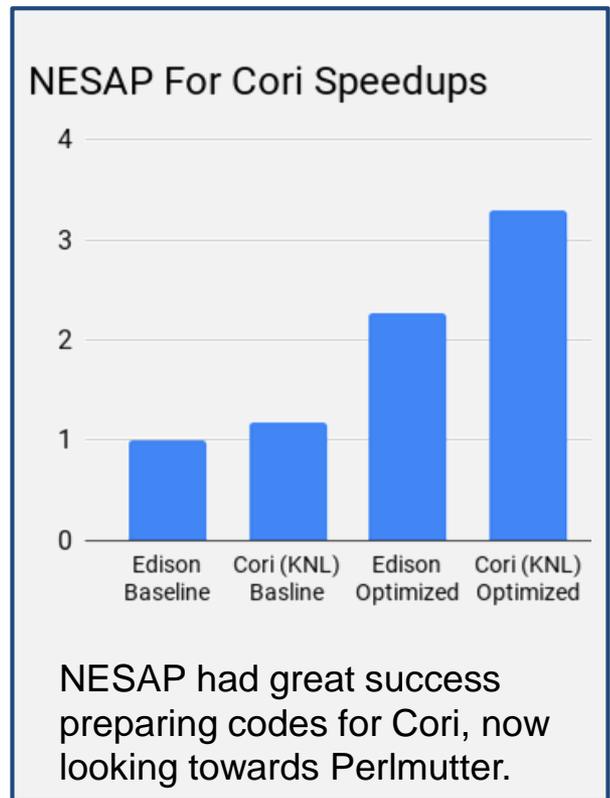
**Strategy:** Partner with application teams and vendors to optimize participating applications. Share lessons learned with with NERSC community via documentation and training.

**Resource Available to Teams:** NERSC Staff development effort and expertise, performance post-docs, access to vendor application engineers, hack-a-thons, early access to hardware

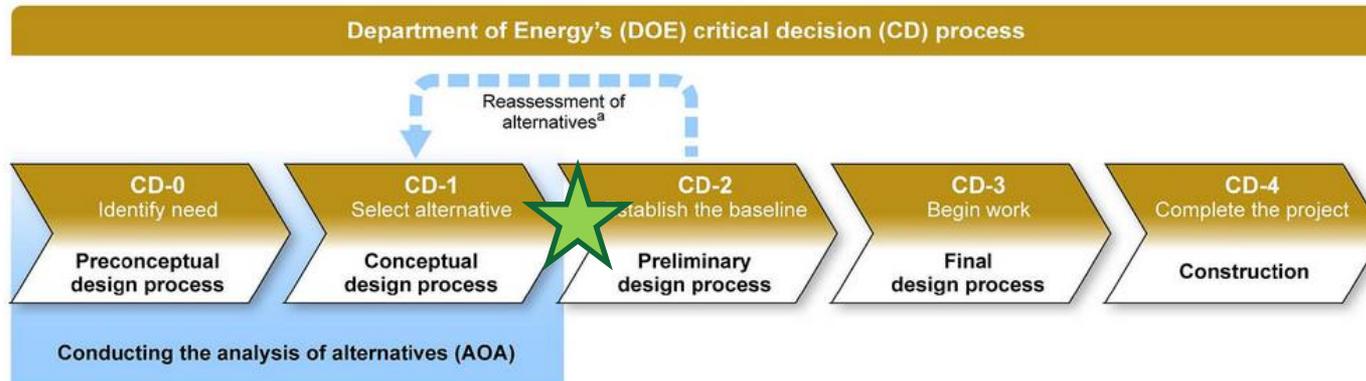
Simulation: 14 application teams  
Data: 9 applications  
Learning: 5 applications



Jack Deslippe  
Apps Performance Lead  
NESAP Lead



# ESnet6 Project Status



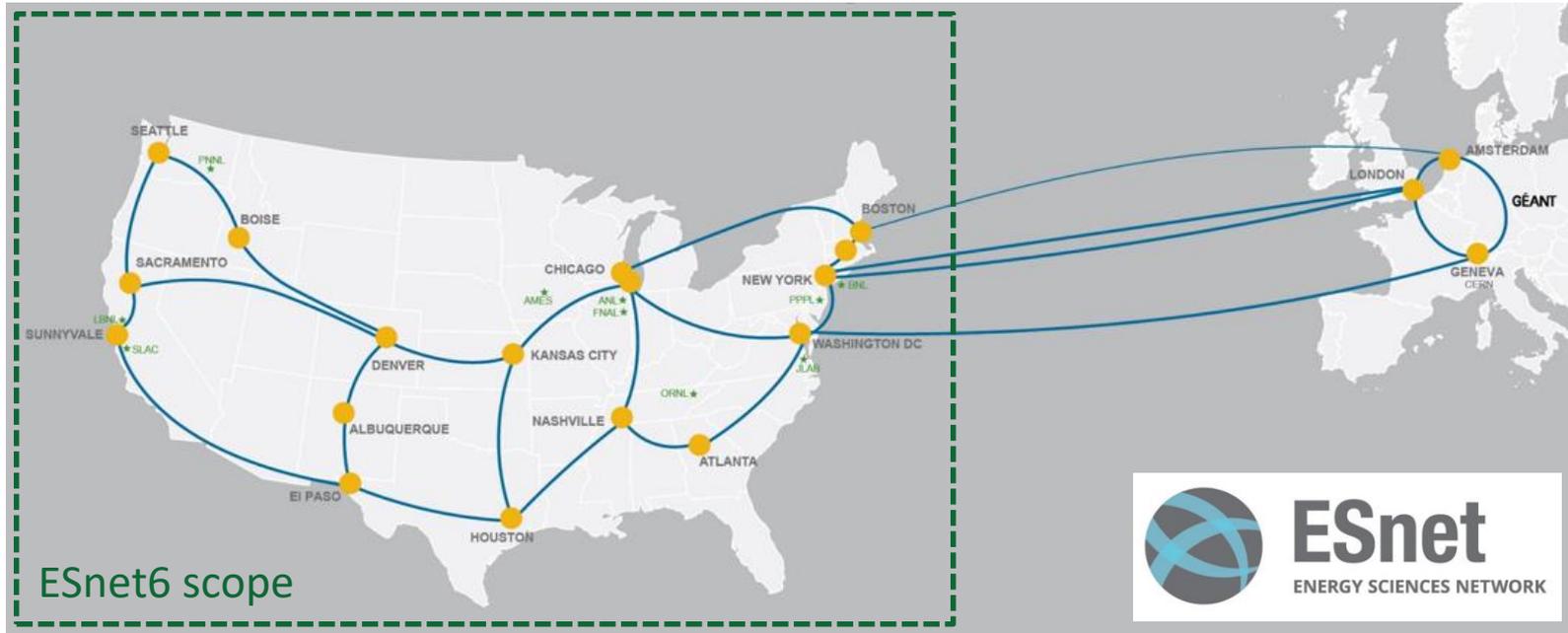
<sup>a</sup>If the top end of the approved CD-1 cost range grows by more than 50 percent, the program office must conduct another AOA and obtain a new CD-1 approval.

Source: GAO analysis of DOE's Order 413.3B. | GAO-15-37

- ✓ Dec. 2016: CD-0 (Mission Need) achieved
- ✓ Aug. 2018: CD-1/3a (Alternative Selection and Long Lead Procurement) achieved
- ✓ May 2019: successful Final Design Review
- Oct. 15-17 2019: LBNL Director's Review in preparation for CD-2/3
- Dec. 10-12 2019: SC Independent Project Review for CD-2/3
- Continuing to successfully execute essential Long Lead Procurements, in particular the optical system hardware, with planned build out in 1Q-3Q FY 2020



# 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 (renewed 2018).

# ESnet is a key partner in a newly awarded NSF project, FABRIC

The four year, \$20M project will build an “everywhere programmable” nationwide network R&D testbed



FABRIC is an **Adaptive Programmable Research Infrastructure** for **Computer Science** and **Science Applications**

**Motivation:** Enable the U.S. Research and Education network community to be at the forefront of technology and cybersecurity innovation for the next generation internet [integration of AI/ML tools, advanced sensors, IoT devices, ...].

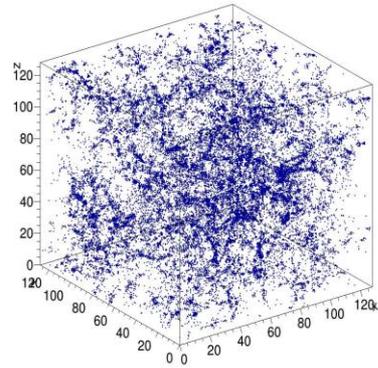
**Approach:** FABRIC will comprise integrated storage, computational, and network hardware nodes connected by dedicated high-speed optical links (100 Gbps to 1 Tbps).

**Possible future:** The award positions ESnet to create a federated NSF/DOE network R&D testbed in the future.

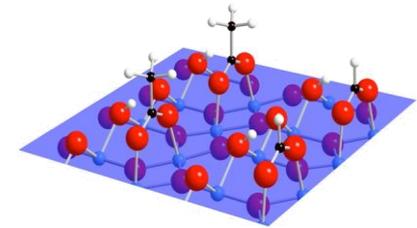


# NERSC Supports High-impact SC Mission Science

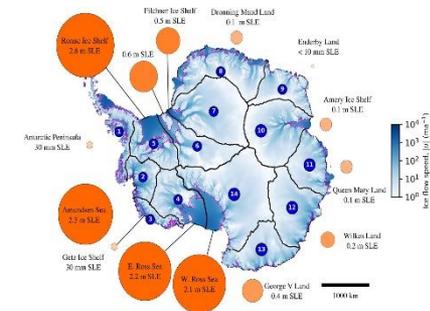
**Deep Learning for Cosmology**  
 Scientists from NERSC/LBNL, UC Berkeley, Cray & Intel ran the first science application of the TensorFlow framework at scale to predict cosmological parameters with unprecedented accuracy. *SC18*



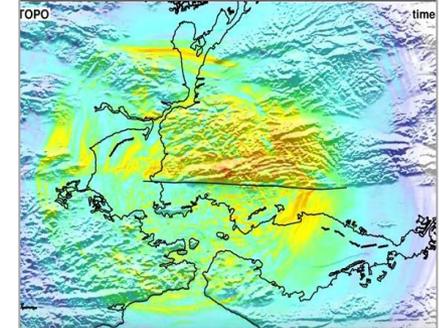
**Self-Cleaning Materials**  
 A Cornell-led team gained new insight into self-cleaning  $\text{TiO}_2$ , paving the way for commercialization of products for environmental remediation and self-sterilizing construction materials. *Science*, 2018.



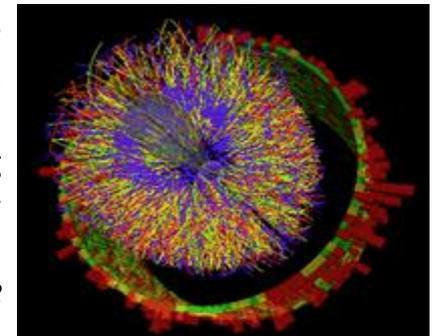
**Ice Sheet Vulnerability**  
 Using the DOE BISICLES ice sheet model researchers determined potential ice sheet loss in each of Antarctica's 14 sectors; *Geophysical Research Lett.*, 2019



**Earthquake Hazard & Risk**  
 Researchers from LBNL & LLNL simulated the impact of a major earthquake in the Bay Area at unprecedented resolution. The models predict how different building types would be affected. *Nat. Conf. Earthquake Eng.*, 2018.



**Nuclear Physics Pipeline**  
 NERSC helped the STAR experiment build a scalable, fault-tolerant data-processing pipeline, making PBs of raw data "physics ready." *J. Phys. Conference Series*, 2018



**Confining Fusion Plasmas**  
 The interaction of magnetic islands with high-temperature plasma was simulated in the geometry of a tokamak fusion reactor for the first time. (Chang, PPPL) *Phys. of Plasmas*, 2018



# ALCF 2018/19 Science Highlights

## Engineering Materials for Electronics

Future generation of portable electronics, including mobile sensors and wearable technology require both to be efficient in power consumption and size. This study addresses the problem of nano-fabrication by manipulating at the atomic scale transition metal layers, effectively sewing together atom-thick fabrics, to produce the building blocks for micro-electronic components.

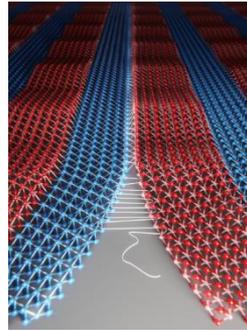


Image courtesy of Jiwoong Park (University of Chicago)

## Massive Star Explosions

The research team found that fully 3-D simulations of the outer layers of massive stars dramatically improved their ability to model observed behaviors. This work paves the way to use similar simulation methods to understand the behaviors of other kinds of massive stars.

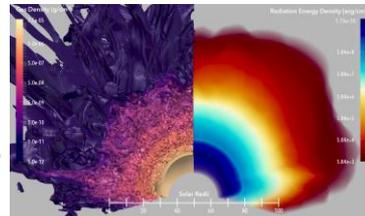


Image courtesy of Joe Insley (ALCF) & Yan-Fei Jiang (UCSB)

## Predicting Cancer Risk with Computational Electrodynamics

Early-stage cancer detection has been widely recognized as one of the most critical factors to successfully treat cancer and reduce mortality. Techniques from this project open the door for high-fidelity, high-throughput early-stage cancer screening. Seven different human cancers are now potential candidates for early detection with minimal false positives: lung, colon, ovarian, esophageal, pancreatic, thyroid, and prostate.

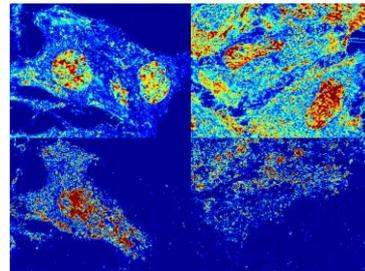


Figure 1 Reproduced from Figure 7 of *Nat. Commun.*, 10, 1652 (2019)

## Commercially Available Nuclear Fusion

TAE Technologies has built “Norman,” a \$100M advanced beam-driven field-reversed configuration plasma device, for experimental studies of the magnetic confinement of hot fusion plasmas. First principle simulations have been informing experimental behavior answering critical question to delivering fusion capability.

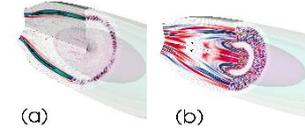


Image courtesy of Calvin Lau

## Ultra-intense Laser Light and Dense Plasmas Interaction

The success of petawatt ( $10^9$  watt) laser facilities presently under construction worldwide, which aim at understanding and controlling these promising particle and light sources, will rely on the strong coupling between experiments and large-scale simulations with particle-in-cell (PIC) codes. In this work, the team solved one of the major issues of the last decades in this research field, by shedding light on the coupling mechanisms at play in the interaction of ultra-intense laser pulses with dense plasmas.

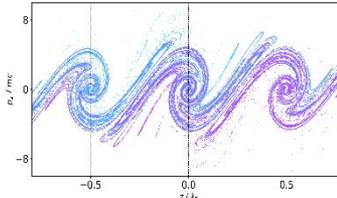


Image courtesy of G. Blaizot. Snapshot of the electron distribution phase space taken from PICSAR simulations .

## Accelerated Climate Modeling for Energy

Previous studies have not yielded consistent results regarding the impact of horizontal resolution on aspects of the global water cycle. Only by building a body of literature for different models can one get a sense for which behaviors are common and which are model-dependent. Given that small changes in the water cycle can have wide ranging societal and environmental impacts, accurate simulation and understanding of predicted changes continues to be a pursuit of the climate model community.

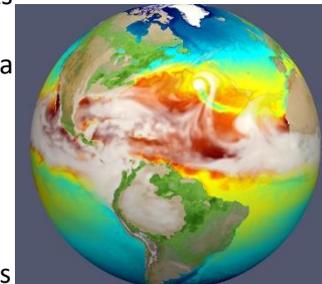


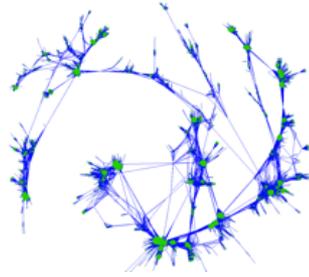
Image courtesy of Mark Taylor.



# OLCF 2018/19 Science Highlights

## Computing Genes

(Gordon Bell Prize winner) An ORNL team developed an algorithm to uncover networks of genes that contribute to complex traits, including diseases. Using mixed precision, the team attained a speedup on Summit of more than 20,000-fold over the previous state of the art, achieving a peak throughput of 2.36 exaops (the fastest science application ever reported).



*A visualization of a network showing correlations between genes in a population, which could be used to identify genetic markers linked to complex traits.*

## Engine Design

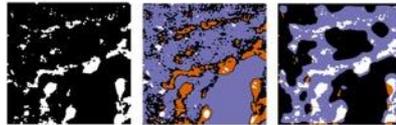
Pinnacle Engines performed simulations on Titan and Eos that revealed the importance of combining a swirling and tumbling motion of gas during combustion (called “swumble” mode), and the company is now building a prototype engine for testing based on this finding.



*To optimize design, Pinnacle Engines researchers simulated the engine's complex flow of air and fuel during combustion on Titan and Eos at ORNL.*

## Deep Learning and Microscopy

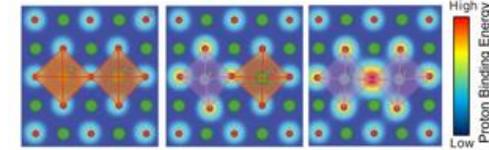
(Gordon Bell Prize finalist) An ORNL team used Summit to automatically create an optimal deep learning network tuned for scanning transmission electron microscopy data, an ability that could revolutionize how scientists manipulate materials at the atomic scale.



*An image showing defects (white) labelled by a human expert (left), defects labelled by a Fourier transform via the frequency spectrum (middle), and defects labelled by the optimal neural network (right).*

## Energy Storage

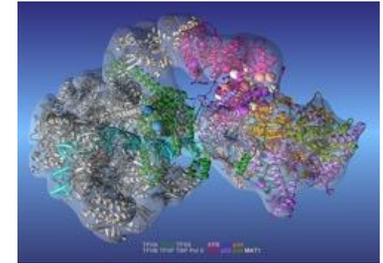
An ORNL team used Titan to develop a computational framework to analyze large datasets of ion-conducting solids and then used the framework to analyze a dataset of more than 80 different perovskite compositions to identify and optimize those with promising proton-conducting capabilities.



*Mitigating the interaction of lattice distortion and proton binding energy could help researchers improve the ionic conductivity of solid materials.*

## Genetic Disease

A team used Summit to develop an integrative model of the transcription preinitiation complex, a complex of proteins vital to gene expression, that could help scientists understand how mutations cause genetic diseases and thus inform the development of more effective treatments.



*Researchers used the new model to identify clusters of gene mutations, which helped them study the emergence of various genetic diseases.*

## Galactic Winds Demystified

Astrophysicists used Titan to create galactic wind simulations of the highest resolution ever performed, allowing researchers to explore in unprecedented detail how galactic winds affect the formation and evolution of galaxies.



*A galactic wind simulation, depicting the galactic disk comprised of interstellar gas and stars (red) and the outflows (blue).*

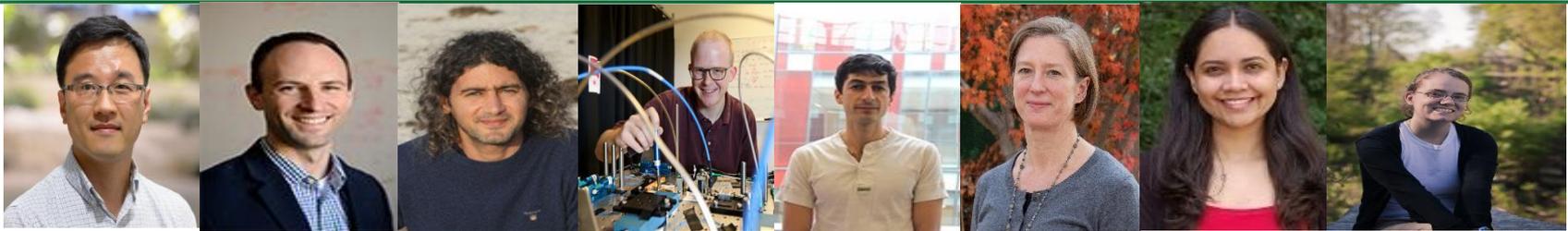


# Argonne ECP Workshop: Preparing for Exascale

- Over 170 attendees on September 17-19, 2019 learn about Aurora



# Awards – FY19 ASCR Early Career Research Program



Name	Institution	Title	Program
<b>Kibaek Kim</b>	Argonne National Laboratory (ANL)	Data-Driven Optimization under Uncertainty: Parallel Algorithms and Solver	Applied Mathematics
<b>Michael Shields</b>	Johns Hopkins University	Low-dimensional manifold learning for uncertainty quantification in complex multi-scale stochastic systems	Applied Mathematics
<b>Stratos Idreos</b>	Harvard University	Data Structure Alchemy	Computer Science
<b>Joe Lukens</b>	Oak Ridge National Laboratory (ORNL)	Scalable Architectures for Hybrid Quantum/Classical Networking	Computer Science
<b>Vladimir Manucharyan</b>	University of Maryland	Realization of a Quantum Slide Rule for 1+1 Dimensional Quantum Field Theories Using Josephson Superconducting Circuits	Computer Science
<b>Kathryn Mohror</b>	Lawrence Livermore National Laboratory (LLNL)	I/O Workload Characterization for Performance and Portability	Computer Science
<b>Cindy Rubio Gonzalez</b>	University of California, Davis	Towards Scalable Precision Tuning of Numerical Software	Computer Science
<b>Catherine Schuman</b>	Oak Ridge National Laboratory (ORNL)	Learning to Learn: Designing Novel Neuromorphic Algorithms with Machine Learning	Computer Science

# Presidential Early Career Award for Scientists and Engineers

highest honor bestowed by the US government on early-career researchers.



**Alvin Cheung**,  
University of  
California at  
Berkeley (Computer  
Science), “Using  
verified lifting to  
optimize legacy  
stencil codes”



**Henry Hoffman**,  
University of Chicago  
(Computer Science),  
“CALORIE: A constraint  
language and  
optimizing runtime for  
exascale power  
management”



**Lin Lin**, University of  
California at  
Berkeley (Applied  
Math), “Green’s  
function methods  
for multiphysics  
simulations”



**Victor Zavala**,  
University of  
Wisconsin at Madison  
(Applied Math),  
“Next-generation  
optimization under  
uncertainty:  
Structure-oriented  
algorithms”

## FY 2019 SIAM Fellows

### Recognizes ASCR leaders for exemplary research & outstanding service



**Mihai Anitescu**, Argonne National Laboratory, for his contributions to modeling, theory and the practice of optimization.



**Roger Ghanem**, University of Southern California, for his Seminal contributions to the mathematical foundations of uncertainty quantification methods



**Michael Heroux**, Sandia National Laboratories & St. Johns University, for his Research, leadership, and community building in software and algorithms for scientific and high-performance computing



## Two New AAAS Fellows sponsored by ASCR



**Dr. James Ricci** is a mathematician and Assistant Professor of Mathematics and Computer Science at Daemen College in Buffalo, New York, and last year, he served as the American Mathematical Society's Congressional Fellow where he advised on policy issues related to education, healthcare, workforce development, and data privacy.



**Dr. Michael W. Nestor** was Director of Neural Stem Cell Research and PI in the Laboratory of Human Stem Cell Neurophysiology at The Hussman Institute for Autism. He received his Ph.D. in Neuroscience from the University of Maryland, School of Medicine and completed a postdoctoral fellowship at the New York Stem Cell Foundation. Michael was also an NIH IRACDA Fellow at Rutgers University and a Venture Capital Consultant at the UMSOM Momentum Fund/Department of Technology Transfer.



# Some ASCAC Agenda Details

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- **VIEW FROM OSTP** – *Dr. Kelvin Droegemeier, Director of Office of Science and Technology Policy (OSTP)*
- **REPORT ON DATA FROM AI ROUNDTABLE** -- *Laura Biven, ASCR*
- **UPDATE ON MATHEMATICAL MULTIFACETED INTEGRATED CAPABILITY CENTERS** -- *Bill Spatz, ASCR*
- **REPORT FROM AI FOR SCIENCE TOWN HALL MEETINGS** -- *Jeff Nichols, ORNL; Rick Stevens, ANL; Kathy Yelick, LBNL*
- **REPORT ON THE IN-SITU DATA ANALYTICS WORKSHOP** – *Thomas Pertka, ANL*
- **THE DOE EXASCALE SYSTEMS** -- *Susan Coghlan, ANL and Justin Whitt, ORNL*
- **UPDATE ON THE EXASCALE COMPUTING PROJECT** – *Doug Kothe, ORNL and Lori Diachin, LLNL*
- **UPDATE ON CURRENT CHARGES**
  - *ASCR 40<sup>th</sup> Anniversary Accomplishments* – *Bruce Hendrickson, LLNL*
  - *Transitioning from Exascale project* – *Roscoe Giles, Boston University*
- **DIVERSITY AND INCLUSION IN THE OFFICE OF SCIENCE**– *Julie Carruthers, Office of Science*