Advanced Scientific Computing Research

Presented to the

High Energy Physics Advisory Panel

by

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Outline

- FY 2018
- FY2021 -2023 -- Exascale
- FY2025 and beyond Moore's Law

FY 2019 SC Budget Request

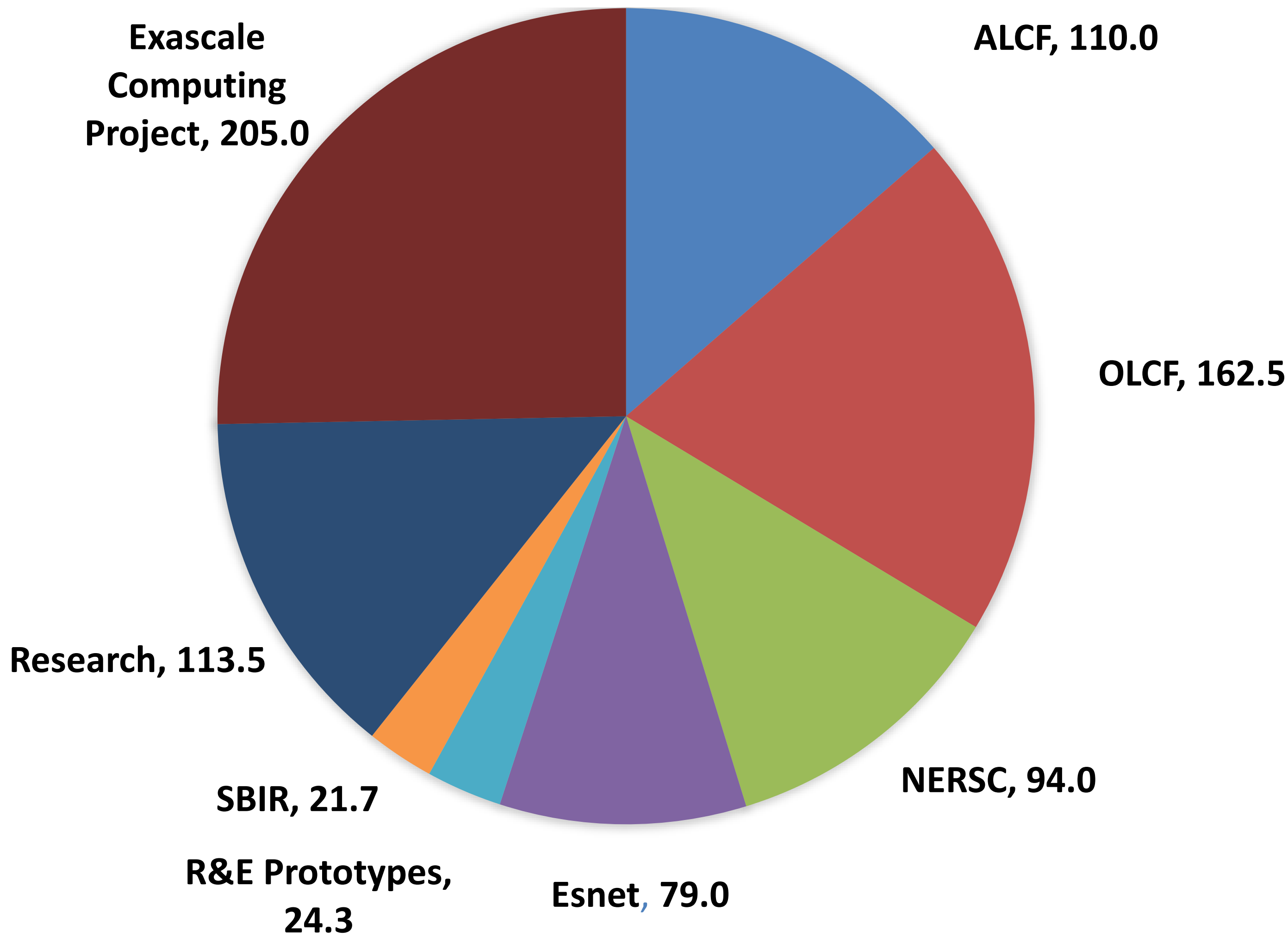
(Dollars in Thousands)

	FY 2017		FY 2018		FY 2019				
	Enacted Approp.	Current Approp.	Annualized CR [b]	Enacted Approp.	President's Request	President's Request vs. FY 2018 Enacted		President's Request vs. FY 2017 Enacted	
ASCR……	647,000	626,559	642,606	810,000	899,010	89,010	11.0%	252,010	39.0%
BES……	1,871,500	1,812,113	1,858,791	2,090,000	1,850,000	-240,000	-11.5%	-21,500	-1.1%
BER……	612,000	588,826	607,844	673,000	500,000	-173,000	-25.7%	-112,000	-18.3%
FES……	380,000	368,119	377,419	532,111	340,000	-192,111	-36.1%	-40,000	-10.5%
HEP……	825,000	802,849	819,397	908,000	770,000	-138,000	-15.2%	-55,000	-6.7%
NP……	622,000	604,473	617,776	684,000	600,000	-84,000	-12.3%	-22,000	-3.5%
WDTS……	19,500	19,500	19,368	19,500	19,000	-500	-2.6%	-500	-2.6%
SLI……	130,000	130,000	129,117	257,292	126,852	-130,440	-50.7%	-3,148	-2.4%
S&S……	103,000	103,000	102,301	103,000	106,110	3,110	3.0%	3,110	3.0%
PD……	182,000	182,000	180,764	183,000	180,000	-3,000	-1.6%	-2,000	-1.1%
SBIR/STTR (SC)……	……	154,561	……	……	……	……	……	……	……
Subtotal, Science……	5,392,000	5,392,000	5,355,383	6,259,903	5,390,972	-868,931	-13.9%	-1,028	0.0%
SBIR/STTR (DOE)……	……	90,813	……	……	……	……	……	……	……
Rescission of PY Bal [a] ……	-1,028	-1,028	-1,021	……	……	……	……	1,028	-100.0%
Total, Science……	**5,390,972**	**5,481,785**	**5,354,362**	**6,259,903**	**5,390,972**	**-868,931**	**-13.9%**	**……**	**……**

[a] *Rescission of PY funds in the amount -$239K for FY12 and older; -$239K for FY13; and -$550K for FY14 - FY16.*

[b] *FY 2018 Annualized CR column is based on the FY 2017 Enacted minus a 0.6791% reduction totaling $36.617M*

FY 2018 ASCR Budget: $810M



Installation Nearing Completion

- **Hardware installation completed in March**
- **Continuing to stabilize nodes, disks, and network**
- **In Dec., accepted 1,080 of 4,608 nodes to port codes**
- **OLCF is working with IBM, NVIDIA, Red Hat, and Mellanox to stabilize and debug system software**

Early Results

- **FLASH – AMR code widely used by astrophysics community**
  - Summit "fundamentally changes the potential science impact" by enabling large-network simulations of 160+ nuclear species that ***could not run on Titan.***
- **QMCPACK – accurate quantum mechanics-based simulation of materials, including High-T_c superconductors**
  - Current release version getting ~50x performance over Titan; 3.7x increase in complexity or scale of the materials computable in the same time to solution.
  - Weak-scaled QMCPACK to 1,024 nodes
- **XGC – PIC code capable to model the tokamak fusion plasma edge**
  - Summit enables new science in XGC by allowing the electron time step to be realistically small for ITER edge plasma, which ***is not possible with Titan***
  - 32 Summit nodes is 3x faster than 192 nodes of Titan; weak-scaled XGC to 1,024 nodes.
- **HACC – high-resolution, hybrid cosmology code**
  - Explore new regimes of baryonic physics in cosmological simulations on Summit.
  - Short-range solver 6.7x faster than Titan; Weak-scaled to 1,024 nodes and strong-scaled to 512 nodes.

Power limitations are driving fundamental changes to architectures

- ***We are reaching minimum size limits on transistors.***
  - Current processors can no longer increase performance by increasing frequency and reducing voltage
  - Increasing transistor count (Moore's Law) drives ***apparent*** performance through increasing the number of cores which requires more complex programming
- **Current industry trends more suited for textual data analytics than scientific computing**
- **Doing nothing will result in decreasing performance for application codes.**
- **Consequently, buying off-the-shelf could lead to platforms incapable of running complex codes at the scale required.**

Technology Challenge	Hardware Mitigation	Application Impact
Flat or decreasing processing unit (core) speeds	Dramatically increased CPU core count to track Moore's Law	First fundamental change in programming model in decades
Memory speed and capacity improvements lag far behind compute speed improvements	Multiple levels/types of memory in a CPU	Explicit management of memory placement/motion
Complex CPU designs too power-hungry to scale to exascale	Heterogeneous architectures with specialized processing units	Must coordinate both how and where specific computations are executed

National Strategic Computing Initiative
Executive Order Signed July 29, 2015

There are three lead agencies for NSCI: the Department of Energy (DOE), the Department of Defense (DOD), and the National Science Foundation (NSF).

- The DOE Office of Science and DOE National Nuclear Security Administration will execute a joint program focused on advanced simulation through a capable exascale computing program emphasizing sustained performance on mission relevant applications and on analytic computing to support its missions and post-Moore's Law HPC capability.
- NSF will play a central role in scientific discovery advances, the broader HPC ecosystem for scientific discovery, and workforce development.
- DOD will focus on data analytic computing to support its mission.

These responsibilities leverage the historical roles each of the lead agencies have played in pushing the frontiers of high-performance computing, and will keep the nation on the forefront of this strategically important field. The lead agencies will also work with the foundational research and development agencies and the deployment agencies to support the objectives of the NSCI to address the wide variety of needs across the Federal Government.

Components of the DOE Exascale Program

- **Exascale Computing Initiative (ECI)**
  - The ECI was initiated in FY 2016 to support research, development and computer system procurements to deliver an exascale (10^{18} ops/sec) computing capability by the early to mid-2020s.
  - It is a partnership between SC and NNSA, addressing science and national security missions.
  - *In the FY2018 President's Budget request, ECI includes the SC/ASCR and NNSA/ASC facility investments in site preparations and non-recurring engineering activities needed for delivery of early to mid-2020s exascale systems.*
  - **Exascale Computing Project (ECP)**
    - Beginning in FY 2017, the ASCR ECI funding was transitioned to the DOE project (ECP), which is managed according to the principles of DOE Order 413.3B.
    - The ECP subprogram in ASCR (SC-ECP) includes only support for research and development activities in applications, and in partnership with NNSA, investments in software and hardware technology and co-design required for the design of capable exascale computers .
    - The NNSA/ASC Advanced Technology Development and Mitigation (ATDM) program supports the development of applications and, in collaboration with SC/ASCR, investments in software and hardware technology and co-design required for the design of exascale capable computers.

ECI FUNDING

By Appropriation and Program ($K)

	FY 2017 Enacted	FY 2019 Request	FY 2019 Request vs FY 2017 Enacted
Office of Science (SC) Advanced Scientific Computing Research (ACSR)			
SC-Exascale Computing Project (SC-ECP, 17-SC-20)	$164,000	$232,706	+$68,706
ECP Focus Area 1: Applications	*$97,000*	*$120,706*	+$23,706
ECP Focus Area 2: Software	*$37,000*	*$62,000*	+$25,000
ECP Focus Area 3: Hardware	*$30,000*	*$50,000*	+$20,000
Argonne Leadership Computing Facility (ALCF)	$0	$140,000	+$140,000
Oak Ridge Leadership Computing Facility (OLCF)	$0	$100,000	+$100,000
Total, SC Exascale[1]	**$164,000**	**$472,706**	**+$308,706**
National Nuclear Security Agency (NNSA) Advanced Simulation and Computing (ASC)			
Advanced Technology Development & Mitigation (ATDM)	$95,299	$95,073	-$226
ECP Focus Area 1: Applications	*$23,000*	*$30,000*	*+$7,000*
ECP Focus Area 2: Software	*$37,299*	*$35,073*	*-$2,226*
ECP Focus Area 3: Hardware	*$25,000*	*$0*	*-$25,000*
ECI Stockpile Applications	*$10,000*	*$11,000*	*+1,000*
ECI Advanced Architecture System & Software	*$0*	*$19,000*	*+$19,000*
Exascale Class Facility Modernization (18-D-680)	$0	$23,000	+$23,000
Exascale Class Computer Cooling Equipment (18-D-670)	$0	$24,000	+$24,000
Exascale System	$0	$21,000	+$21,000
Total, NNSA Exascale[2]	**$95,299**	**$163,073**	**+$67,774**
Total, ECI	**$259,299**	**$635,779**	**+$376,480**

[1] The SC-ECP project was initiated in FY 2017 to prepare the LCFs for deployment of at least one exascale system included in ECI. Only a portion of the OLCF funds are shown because they are also operating Summit which is a 200 PF pre-exascale system; funding for the ALCF is primarily focused on the delivery of the exascale system. BES investments in computational materials and chemistry applications are also included in ECI but not shown on the table for FY 2017 and beyond.

[2] The FY 2019 request includes $47M to construct cooling equipment and support infrastructure to prepare for deployment of pre-exascale and exascale systems at LANL and LLNL, respectively.

ECP Strategic Goals and Outcome

- **Deliver mission results with exascale-ready applications, addressing currently intractable exascale challenge problems of strategic importance and national interest**
- **Deliver a sustainable software product suite required by exascale applications and platforms, sustainable into the future**
- **Deploy integrated ECP products on targeted systems at DOE HPC Facilities (pre-exascale and exascale)**
- **Transition PathForward results into Facility NRE to enhance capabilities of delivered exascale systems**
- ***Outcome: accelerated delivery of a capable exascale computing ecosystem***
  - *Capable*: wide range of applications effectively use the exascale systems, addressing DOE mission needs
  - *Exascale*: applications perform at least 50x of today’s systems
  - *Ecosystem*: all methods and tools required for efficient and effective use of exascale systems

ECP Focus Areas

Application Development

The Application Development effort develops and enhances the predictive capability of applications critical to the DOE, including the science, energy, and national security mission space. The scope of the AD focus area includes

- targeted development of requirements-based models, algorithms, and methods,
- integration of appropriate software and hardware via co-design methodologies,
- systematic improvement of exascale system readiness and utilization, and
- demonstration and assessment of effective software integration.

Software Technology

Software Technology spans low-level operational software to high-level applications software development environments, including the software infrastructure to support large data management and data science for the DOE SC and NNSA computational science and national security activities at exascale. Projects will have:

- line of sight to application's efforts
- inclusion of a Software Development Kit to enhance the drive for collaboration, and
- delivery of specific software products across this focus area.

Hardware and Integration

This focus area is centered on the integrated delivery of specific outcomes (ECP Key Performance Parameters, or KPPs) and products (e.g., science as enabled by applications, software, and hardware innovations) on targeted systems at leading DOE computing facilities. Areas include:

- PathForward
- Hardware Evaluation
- Application Integration at Facilities
- Software Deployment at Facilities
- Facility Resource Utilization
- Training and Productivity

ECP Structure and Leadership

Possessing the requisite skills, experience, and resources to focus on product delivery

- **Structure: recent changes to the WBS structure needed to increase ECP focus on *product delivery* and “steady state” execution post-startup**
  - **AD** changed from programmatic to a domain-based structure for more effective leadership and project management by domain science experts.
  - **ST** consolidated and streamlined, with aggressive movement into a critical *product development* stage after its initial R&D stage and line of sight of ST products to applications.
  - **HI** [formerly Hardware Technology (HT)] required expanded scope to more proactively and directly integrate - *including a formal handoff of ECP products and technologies*- with DOE HPC facilities.
- **Leadership: size and complexity of ECP warranted a more empowered extended leadership team (ELT)**
  - **L2 leads**: strategic thinkers - integrating their technical area within the larger US exascale ecosystem; influential relative to the technical community and within ECP; can represent full ECP scope in a compelling manner
  - **L3 leads**: technical leaders for sub-projects within their element, providing technical oversight and management; serve as Control Account Managers for their element
  - **ELT** (SLT+L3s): now involved in most leadership discussions, with SLT decisions based on informed-input from ELT

Other key ECP leaders: ~100 L4 subproject PIs from 16 Labs, 6 companies, numerous universities

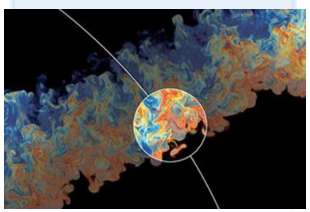
ECP Application Development (AD)

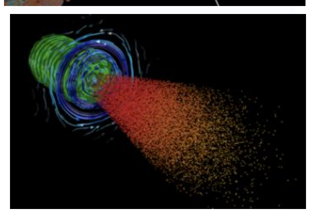
Chemistry and Materials Applications	Describes underlying properties of matter needed to optimize and control the design of new materials and energy technologies
Energy Applications	Model and simulation of existing and future technologies for the efficient and responsible production of energy to meet the growing needs of the U.S.
Earth and Space Science Applications	Spans fundamental scientific questions from the origin of the universe and chemical elements to planetary processes and interactions affecting life and longevity
Data Analytics and Optimization Applications	Applications partially based on modern data analysis and machine learning techniques rather than strictly on approximate solutions to equations that state fundamental physical principles or reduced semi-empirical models
National Security Applications	Stewardship of the US nuclear stockpile and assessment of future threats; related physics and engineering modeling and scientific inquiries consistent with that mission space
Co-Design	Focused on crosscutting algorithmic methods that capture the most common patterns of computation and communication in ECP applications

ECP Applications Target National Problems

National security

- Next-generation, full-system stockpile stewardship codes
- Reentry-vehicle-environment simulation
- Multi-physics science simulations of high-energy density physics conditions





Energy security

- Turbine wind plant efficiency
- Design and commercialization of SMRs
- Nuclear fission and fusion reactor materials design
- Subsurface use for carbon capture, petroleum extraction, waste disposal
- High-efficiency, low-emission combustion engine and gas turbine design
- Scale up of clean fossil fuel combustion
- Biofuel catalyst design

Economic security

- Additive manufacturing of qualifiable metal parts
- Urban planning
- Reliable and efficient planning of the power grid
- Seismic hazard risk assessment

Scientific discovery

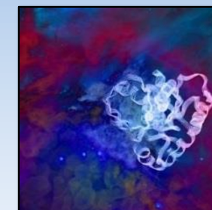
- Cosmological probe of the standard model of particle physics
- Validate fundamental laws of nature
- Plasma wakefield accelerator design
- Light source-enabled analysis of protein and molecular structure and design
- Find, predict, and control materials and properties
- Predict and control stable ITER operational performance
- Demystify origin of chemical elements

Earth system

- Accurate regional impact assessments in Earth system models
- Stress-resistant crop analysis and catalytic conversion of biomass-derived alcohols
- Metagenomics for analysis of biogeochemical cycles, climate change, environmental remediation

Health care

- Accelerate and translate cancer research



ECP Software: Productive, Sustainable Ecosystem

Goal

Build a comprehensive, coherent software stack that enables application developers to productively write highly parallel applications that effectively target diverse exascale architectures

- Extend current technologies to exascale where possible
- Perform R&D required for new approaches when necessary
- Guide, and complement, and integrate with vendor efforts
- Develop and deploy high-quality and robust software products

56 WBS L4 subprojects executing RD&D

233 L4 subproject (P6) milestones delivered in FY17 (out of 249 planned)

426 L4 subproject (P6) milestones planned in FY18-19

Software Development Kits (SDKs): A Key ST Design Feature

An important delivery vehicle for software products with a direct line of sight to AD applications

ECP software projects

Each project to define (at least 2) release vectors

More projects ⟷ Fewer projects

SDKs
Reusable software libraries embedded in applications; cohesive/interdependent libraries released as sets modeled on xSDK

- Regular coordinated releases
- Hierarchical collection built on Spack
- Products may belong to >1 SDK based on dependences
- Establish community policies for library development
- Apply Continuous Integration and other robust testing practices

Math SDK
Tools SDK
PM&RT SDK
DataViz SDK
Facility SDK

OpenHPC
Potential exit strategy for binary distributions

- Target similar software to existing OpenHPC stack
- Develop super-scalable release targeting higher end systems

Direct2Facility
Platform-specific software in support of a specified 2021–2023 exascale system

- Software **exclusively** supporting a specific platform
- System software, some tools and runtimes

Assume all releases are delivered as “build from source” via Spack – at least initially

Focus on ensuring that software compiles robustly on all platforms of interest to ECP (including testbeds)

ECP Hardware and Integration: Delivery of integrated ECP/DOE facility products

Goal
A capable exascale computing ecosystem made possible by integrating ECP applications, software and hardware innovations within DOE facilities

- Innovative supercomputer architectures for competitive exascale system designs
- Accelerated application readiness through collaboration with the facilities
- A well integrated and continuously tested exascale software ecosystem deployed at DOE facilities through collaboration with facilities
- Training on key ECP technologies, help in accelerating the software development cycle and in optimizing the productivity of application and software developers

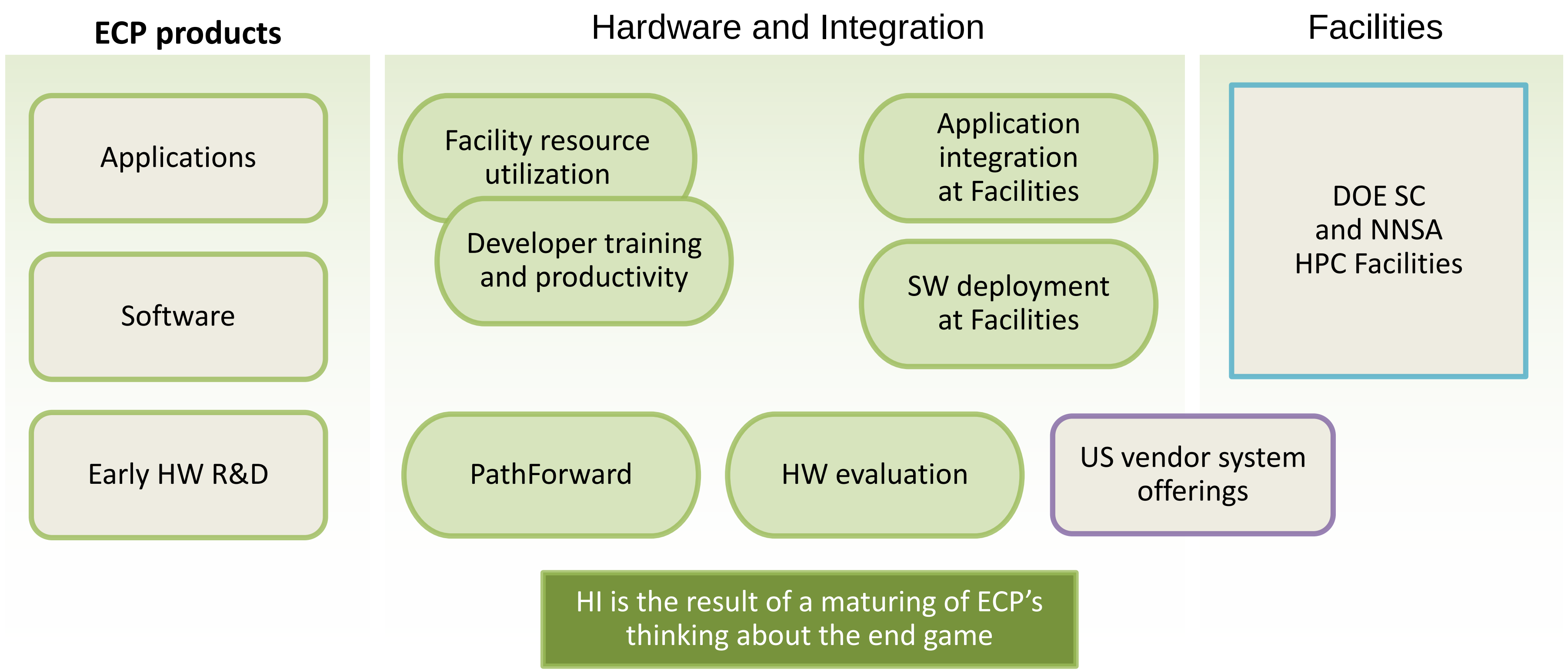
20 WBS L4 subprojects executing RD&D

47 L4 subproject (P6) milestones delivered in FY17 (of 47 milestones planned)

284 L4 subproject (P6) milestones planned in FY18-19 (6 of 284 completed as of 11/30)

HI: Designed to Enable Integration of ECP's products into HPC Environments at the Facilities

ECP will demonstrate meeting objectives on Facility resources



PathForward

Funds 6 US HPC companies to accelerate hardware technologies to maximize the energy efficiency and overall performance of future supercomputers

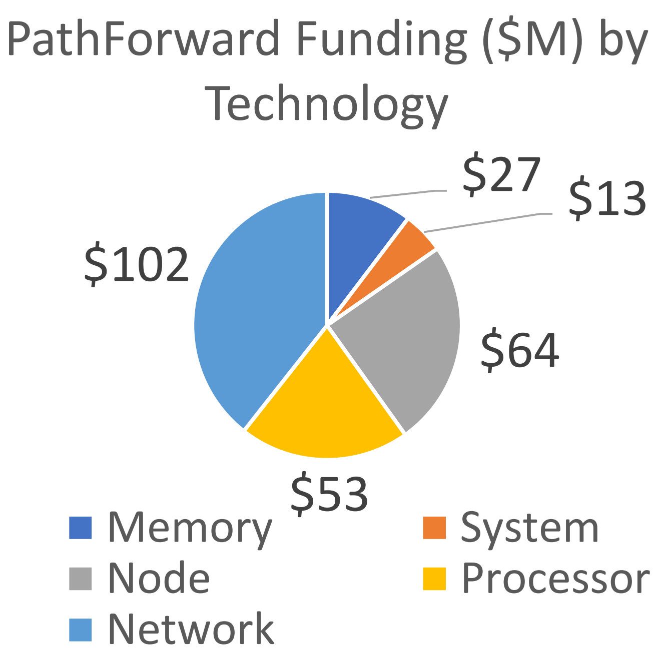
- **Objective – Critical hardware R&D to enable at least two diverse and viable exascale system designs in the ECP timeframe**
- **3-year program ending in 2020**
- **Total value of the R&D is $430M**
- **DOE provides $258M and the companies provide additional funding amounting to at least 40 percent of their total project cost**

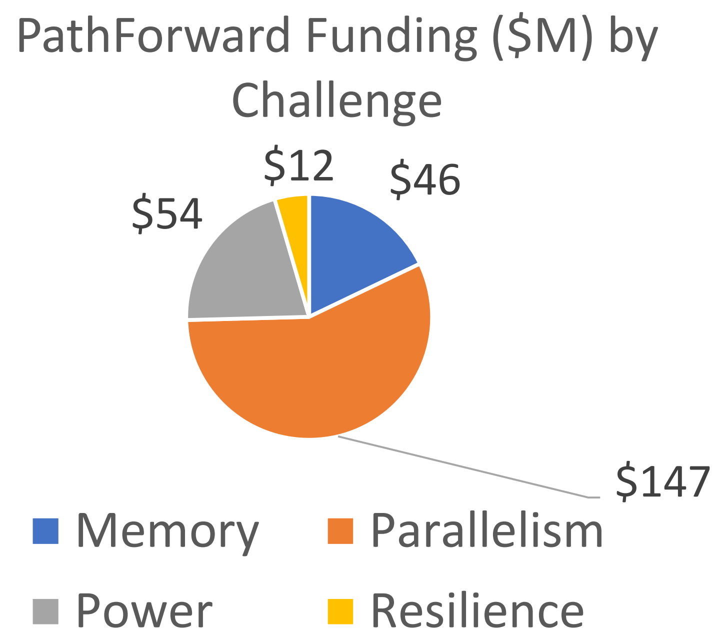
- Advanced Micro Devices (AMD)
- Cray Inc. (CRAY)
- Hewlett Packard Enterprise (HPE)
- International Business Machines (IBM)
- Intel Corp. (Intel)
- NVIDIA Corp. (NVIDIA)

Secretary Perry *"These awards will enable leading U.S. technology firms to marshal their formidable skills, expertise, and resources in the global race for the next stage in supercomputing—exascale-capable systems."*

PathForward R&D by technology and by challenge addressed

Note: costs are DOE's costs and do not include the vendor contributions





ASCR Facilities Engagement with ECP

- **Initial version of the ECP-Facility Engagement Framework scrutinized by the ECP Independent Project Review (IPR) committee in early Jan 2018**
  - recommended using a single engagement framework to develop specific facility plans
- **ECP and facilities subsequently held a 2-day meeting (Feb 22-23, 2018) to lay out a process for developing actionable plans (joint milestones) for FY18-19**
  - Identified mutually-beneficial activities & outcomes to be refined into key milestones and deliverables
- **Formal joint milestones currently being refined and reviewed for next revision of the ECP-Facility Engagement Plan**
- **What is included in the Engagement plan?**
  - Facilities help prepare a subset of ECP applications for future pre-exascale and exascale upgrades; ECP will provide some support for Post Docs and staff time
  - Facilities will work with ECP to provide a test beds and allocations for the software stack and applications use
  - Facilities and ECP will hold joint training programs and hackathons

Relevant Pre-Exascale and Exascale Systems for ECP

Pre-Exascale Systems

2013 | 2016 | 2018 | 2020

Exascale Systems

2021-2023

Argonne
IBM BG/Q
Open

Argonne
Intel/Cray KNL
Open

ORNL
IBM/NVidia
P9/Volta
Open

NERSC-9

LBNL
TBD
Open

Argonne
Intel/Cray TBD
Open

ORNL
Cray/NVidia K20
Open

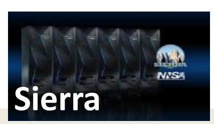
LBNL
Cray/Intel Xeon/KNL
Open

Frontier

ORNL
TBD
Open

LLNL
IBM BG/Q
Secure

LANL/SNL
Cray/Intel Xeon/KNL
Secure



LLNL
IBM/NVidia
P9/Volta
Secure

Crossroads

LANL/SNL
TBD
Secure

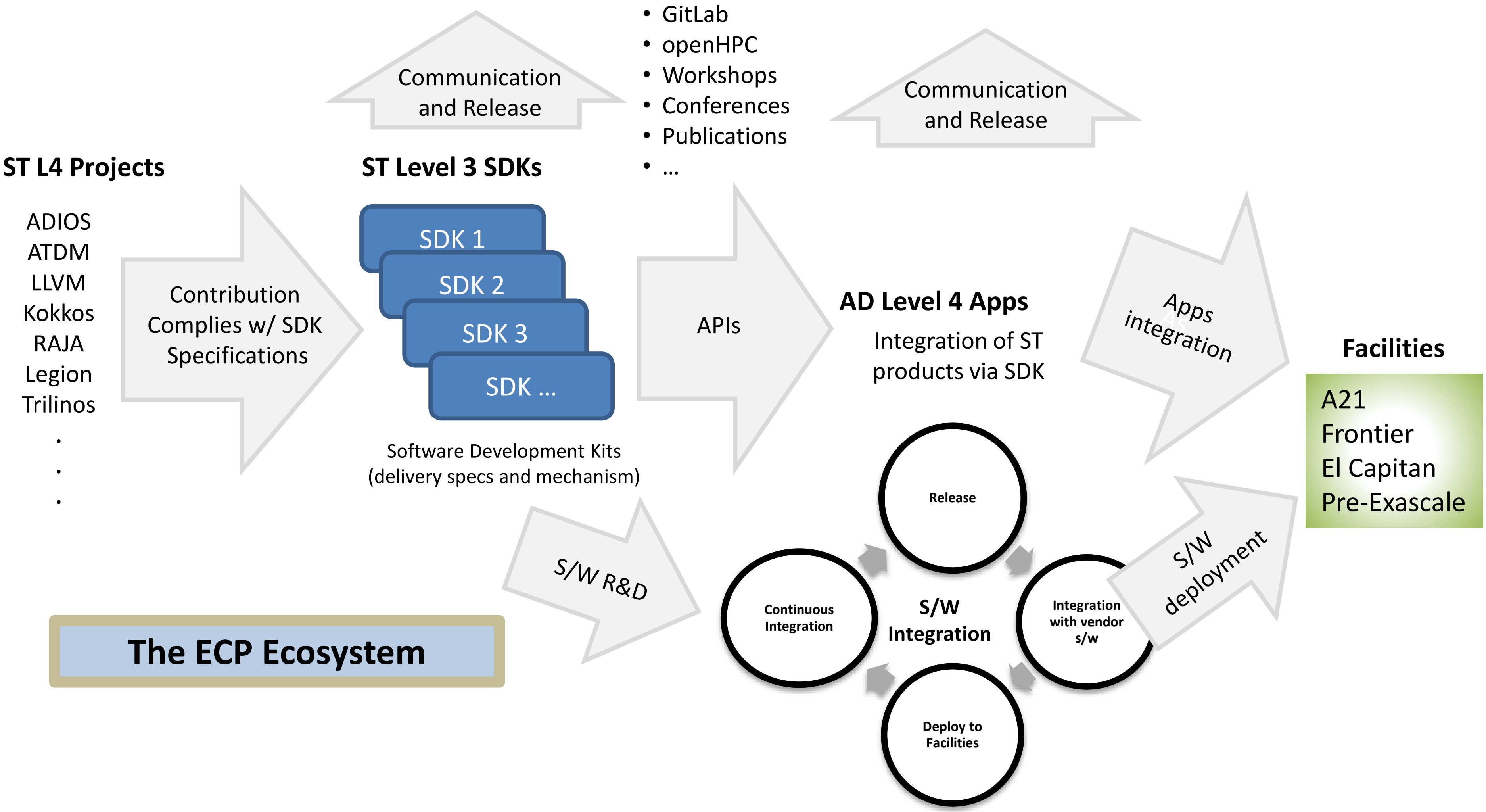
El Capitan

LLNL
TBD
Secure

ECI and SC Facilities

	Fiscal Year							
Exascale Computing Initiative	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**
Exascale Computing Project (ECP) Critical Decision Milestones	CD-0	CD1-CD3A		CD-2 CD-3				CD-4
ECP Applications		Apps Selected	AI CoDesign added	Apps Readiness	Performance for challenge prob		Early Science Runs	
ECP Software Technology		SW sel.	SW developed for apps needs	SW tuned for selected exascale system			SW updates as needed	
ECP Hardware and Integration			Integration with facilities and vendor partnerships					
Engagement Between Facilities and ECP			Application scaling and tuning on Leadership resources					
			SW productization and deployment at facilities					
			Joint training and assistance from vendor experts					
					testbeds	for A21 and Frontier		
SC Facilities	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**
ALCF (pre-exascale)			Theta (10 PF)					
ALCF (exascale)					Aurora NRE		Aurora (A21)	
NERSC (pre-exascale)			CORI (30 PF)					
NERSC 9 (pre-exascale)						NERSC-9 (TBD)		
OLCF (pre-exascale)		Titan (27 PF)						
OLCF (pre-exascale)					Summit (200 PF)			
OLCF-(exascale)					Frontier NRE		Frontier	

ECP Ecosystem

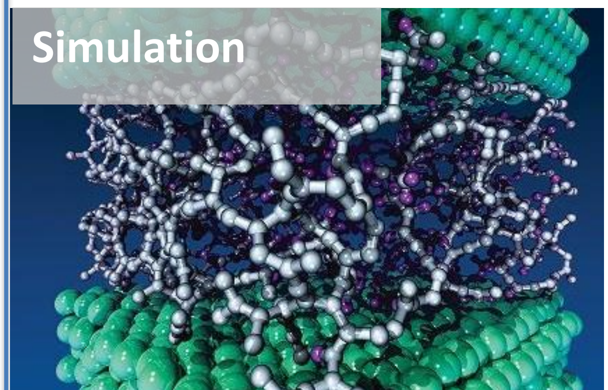


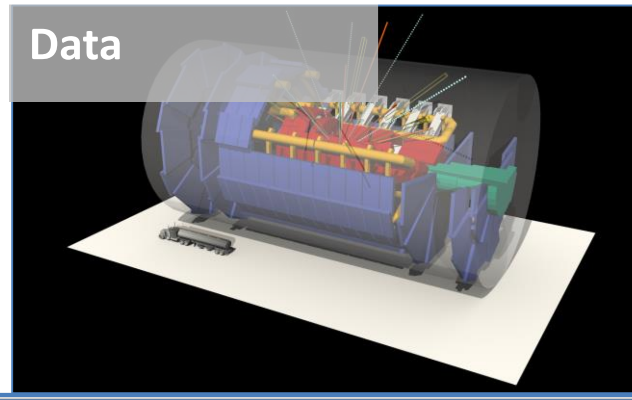
ALCF Aurora Exascale Supercomputer

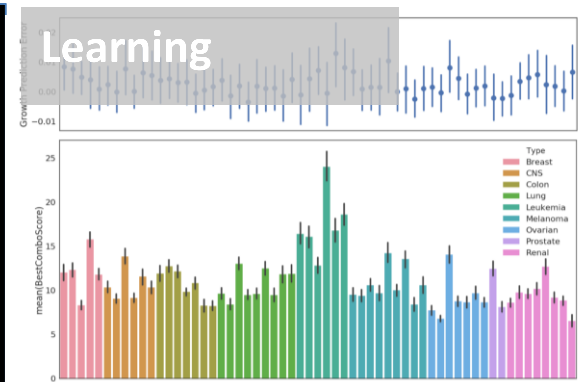
Intel supercomputer to be delivered in 2021

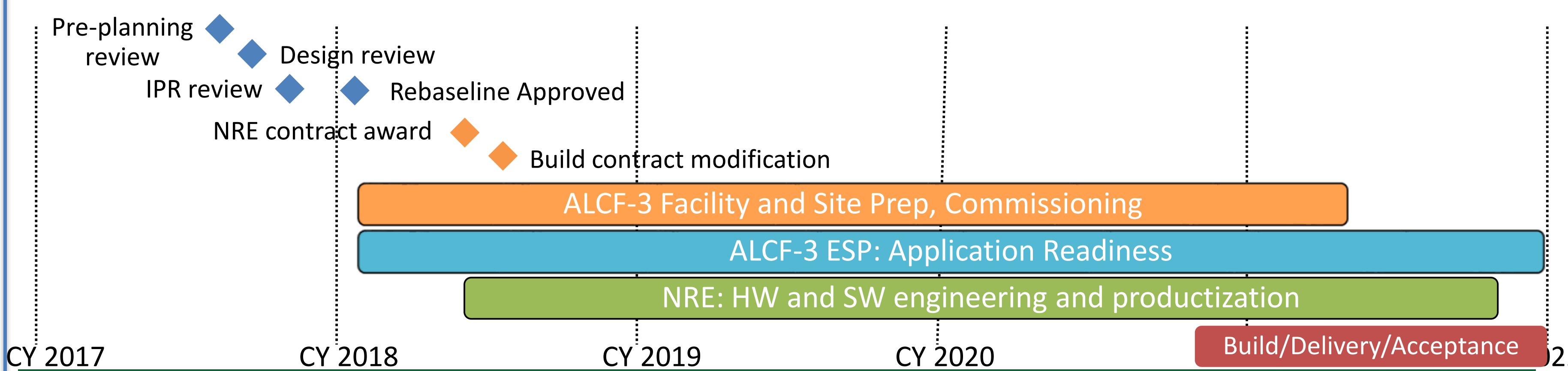
Over 1000 PF

Supporting the future of science









ALCF-3 Rebaseline Review

Design Review 9/20-21 Results

- “The system as presented is exciting with many novel technology choices that can change the way computing is done. The committee supports the bold strategy and innovation, which is required to meet the targets of exascale computing. The committee sees a credible path to success.”
- “The hardware choices/design within the node is extremely well thought through. Early projections suggest that the system will support a broad workload.”
- Rebaseline Independent Project Review recommended approval of the revised baseline. SC-ESAAB tentatively planned for January 18, 2018.

Aurora programming guidelines

- **Nodes will have both high single thread core performance and the ability to get exceptional performance when there is concurrency of modest scale in the code**
- **Architecture optimized to support codes with sections of fine grain concurrency (~100 lines of code in a FOR loop e.g.) separated by serial sections**
  - Degree of fine grain concurrency (e.g. number of loop iterations) that will be needed to fully exploit the performance opportunities is moderate. (~1000 for most applications)
  - Independence of these loops is ideal but not required for correctness
  - No limit on the number of such loops; overhead of starting/ending loops is very low
- **Serial code (within an MPI rank) will execute very efficiently**
- **OpenMP 5 will likely contain the constructs necessary to guide the compiler to get optimal performance.**
- **The compute performance of the nodes will raise in a manner similar to the memory bandwidth**
- **The memory capacity will not grow as fast as the compute**
  - The memory will all be high performance alleviating some concerns of explicitly managing multievel memory & data movement
  - The memory in a node will be coherent
- **All compute will be first class citizens: equal access to all resources, memory and fabric etc.**
- **The fabric BW will be similar to the compute performance for local communication patterns**
  - Global communication BW will likely to not increase as fast as compute performance.

CORAL 2: Frontier and El Capitan

- **ORNL released the CORAL-2 RFP April 9, 2018**
  - Continues partnership between Argonne National Laboratory, Lawrence Livermore National Laboratory and Oak Ridge National Laboratory
  - Calls for non-recurring engineering activities and up to three exascale high performance computing systems

Laboratory	Description
ORNL	System delivered in 2021 and accepted in 2022 (ORNL system)
LLNL	System delivered in 2022 and accepted in 2023 (LLNL system)
ANL	Potential System delivered in 2022 and accepted in 2023 (ANL system)

- **Anticipated budget range for each system plus any associated NRE is $400M-$600M**
- **Proposals Due: May 24, 2018 by 5:00 pm Eastern Time**

Next Generation Archival Storage

Request for Information -

Secure | https://smallbusiness.ornl.gov/business-opportunities/request-information-doe-office-science-distributed-archival-storage-system

Apps | Visit ORNL | MyIDCare - Sign In | Imported From IE | Imported

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ORNL Small Business Opportunity

Return to Listings Page

Request for Information - DOE Office of Science Distributed Archival Storage System

Print this page

Type: Computer Equipment

Small Business Set–Aside: No

Estimated Value: TBD

NAICS Code: 334112 – Computer Storage Device Manufacturing

Expected Issue Date: TBD

Expected Award Date: TBD

Contact Name: Mitzi Bailey

Contact Email: baileymb@ornl.gov

ORNL, in conjunction with Lawrence Berkeley National Laboratory (LBNL), Argonne National Laboratory (ANL), and Brookhaven National Laboratory (BNL), is conducting a market survey that can assist with the evaluation of products and services that can provide the long-term storage requirements of data at these facilities. This RFI is forward-looking, for DOE Office of Science (SC) informational purposes only, and may not necessarily result in a subsequent solicitation. (Small business set-aside TBD).

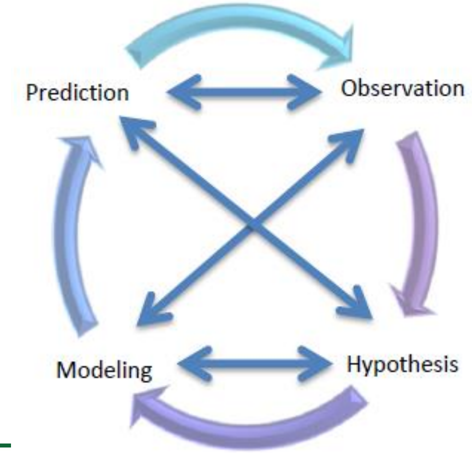
The RFI is posted on the Federal Business Opportunities (FedBizOpps) website at the following link:

RFI-DASS-032818

Last Updated: March 29, 2018 – 1:04 pm

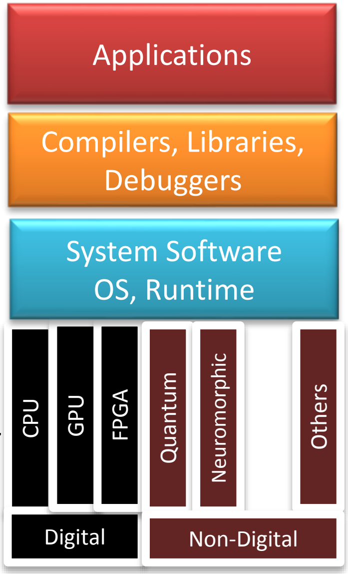
Scientific Machine Learning Workshop
Jan 30 to Feb 1, 2018

- **POC:** Steven Lee (steven.lee@science.doe.gov)
- **Co-organizers:** Mark Ainsworth (Brown) and Nathan Baker (PNNL)
- **Website**: https://www.orau.gov/ScientificML2018/
- **Purpose:** Define priority research directions for applied mathematics in scientific machine learning (ML). Identify the challenges and opportunities for increasing the rigor, robustness, and reliability of ML for DOE missions.
- **Read-ahead material:** A brief survey of topics in ML with relevance to DOE missions; an overview of relevant DOE ASCR capabilities.
- **Challenges and themes:** ML mathematical foundations, reliability & rigor, complexity, interpretability, probabilistic ML, applications, tools & techniques.
- **Participants:** ~100 participants, including plenary speakers, panel members, and observers
- **Position papers:** Intended to broaden community participantion; due Jan 5.
- **Final report due in Mar-Apr 2018.**



What Do We Mean by Extreme Heterogeneity?

- **Exponentially Increasing Parallelism** (central challenge for ECP, but will be even worse)
  - **Trend**: *End of exponential clock frequency scaling (end of Dennard scaling)*
  - **Consequence:** *Exponentially increasing parallelism*
- **End of Lithography as Primary Driver for Technology Improvements**
  - **Trend:** *Tapering of lithography Scaling*
  - **Consequence:** *Many forms of heterogeneous acceleration (not just GPUs anymore)*
- **Data Movement Heterogeneity and Increasingly Hierarchical Machine Model**
  - **Trend:** *Moving data operands costs more than computation performed on them*
  - **Consequence:** *More heterogeneity in data movement performance and energy cost*
- **Performance Heterogeneity**
  - **Trend:** *Heterogeneous execution rates from contention and aggressive power management*
  - **Consequence:** *Extreme variability and heterogeneity in execution rates*
- **Diversity of Emerging Memory and Storage Technologies**
  - **Trend:** *Emerging memory technologies and stall in disk performance improvements*
  - **Consequence:** *Disruptive changes to our storage environment*
- **Increasingly Diverse User Requirements**
  - **Trend:** *Diverse and Complex and heterogeneous scientific workflows*
  - **Consequence:** *Complex mapping of heterogeneous workflows on heterogeneous systems.*



QATs & QCATs
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.

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.

NEW QCAT LAB PROGRAM ANNOUNCEMENT:
Algorithms, Software Stack, V&V

Pre-proposals due: May 16th, 2018
Proposals due: June 29th, 2018

https://science.energy.gov/~/media/grants/pdf/lab-announcements/2018/LAB_18-1898.pdf

3 QAT PROJECTS @ TOTAL $4M/YEAR:

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, VCU. https://qoalas.sandia.gov/

FY 2018: 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. Expands last year's program.

Emphasis: Research in the relationship between device architecture and application performance, including development of meaningful metrics for evaluating device performance.

Timeline & Proposals:

- A DOE National Laboratory Announcement and companion FOA were published on March 19, 2018.
- Preproposals/preapplications due on April 16, 2018.
- Full proposals due on May 14, 2018.

Anticipated Funding: $2M/year

FY 2018: 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.

Timeline & Proposals:

- A DOE National Laboratory Announcement was published on April 6, 2018.
- Preproposals due on May 14, 2018.
- Full proposals due on June 8, 2018.

Anticipated Funding: $9M/year

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**

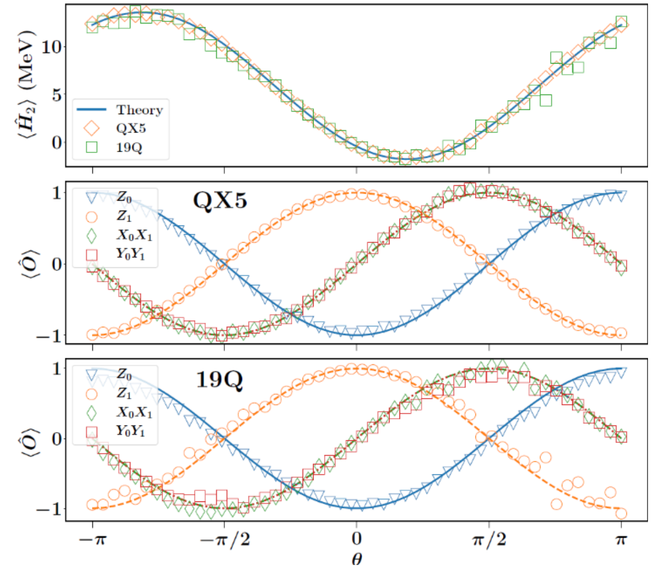
Highlight: Computed the binding energy of the deuteron (nucleus of ${}^{2}_{1}H$ – bound state of a proton and a neutron

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**]

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



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).

Towards Quantum Machine Learning with Tensor Networks

Scientific Achievement

Simulated quantum circuits inspired by tensor networks were trained to classify images of handwritten numerals.

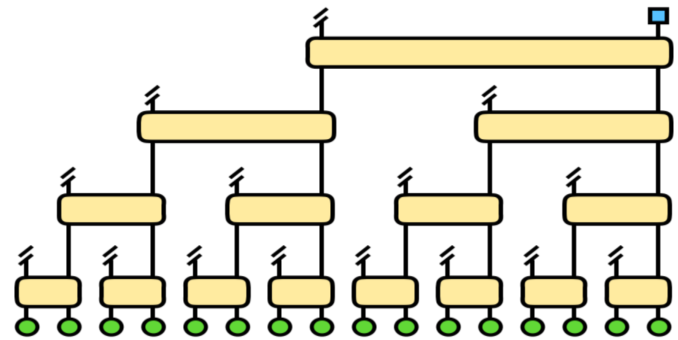
Significance and Impact

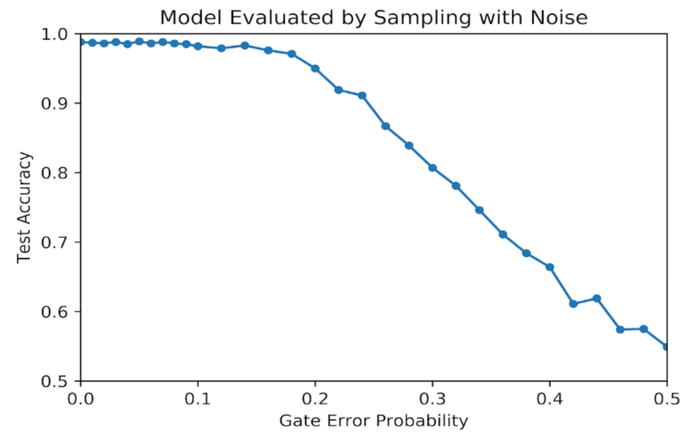
Quantum computing promises a fundamentally different set of capabilities than are available classically, and it is an open question how best to apply these emerging tools to the domain of machine learning. Circuits based on tensor networks present serious advantages for the small and noisy devices which will be available in near future.

Research Details

- Entire circuit, including model input, is easy to prepare and execute on near-term devices. Optimization is performed in a hybrid quantum/classical loop.
- For image classification, a number of qubits that is logarithmic in the dimension of the number of pixels is sufficient, and numerical simulations indicated a high level of resilience to noise.

Work was a collaboration between UC Berkeley (QAT PI: Birgitta Whaley) and The Flatiron Institute.





Above: A diagram of the circuit, where the input qubits are represented by green circles, unitary gates by yellow rectangles, unobserved outputs by hash marks, and the labeling output by a blue square.

Below: The accuracy of the model on a held out test set evaluated by a majority vote of 400 samples at various noise levels.

W. Huggins, P. Patel, K. B. Whaley, E. M. Stoudenmire, arXiv:1803.11537

- **Questions?**