U.S. DEPARTMENT OF ENERGY | Office of Science

Advanced Scientific Computing Research

Presented to the

Advanced Scientific Computing Advisory Committee

by

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Associate Director

December 20, 2017

ASCR FY 2018 President's Request
(in thousands)

	FY 2016	FY 2017	FY 2018		
	Approp	Approp.	President's Request	House Mark	Senate Mark
Mathematical, Computational, and Computer Sciences Research					
Applied Mathematics	49,229	29,229	30,104	34,104	34,104
Computer Science	56,848	29,296	29,296	32,608	32,608
Computational Partnerships (SciDAC)	47,918	32,596	41,268	45,268	46,395
Next Generation Networking for Science	19,000	16,000	...	...	...
SBIR/STTR	6,181	10,271	11,261	4,242	4,285
Total, Mathematical, Computational, and Computer Sciences Research	179,995	117,392	111,929	116,222	117,392
High Performance Computing and Network Facilities					
High Performance Production Computing (NERSC)	86,000	92,145	80,000	92,000	94,000
Leadership Computing Facilities					
Leadership Computing Facility at ANL (ALCF)	77,000	80,000	100,000	100,000	100,000
Exascale	*(...)*	*(...)*	*(100,000)*	*(100,000)*	*(100,000)*
Leadership Computing Facility at ORNL (OLCF)	104,317	110,000	149,321	112,000	150,000
Exascale	*(...)*	*(...)*	*(50,000)*	*(...)*	*(50,000)*
Total, Leadership Computing Facilities	181,317	190,000	249,321	212,000	250,000
Research and Evaluation Prototypes	121,471	25,301	24,452	24,452	24,559
CSGF	*(10,000)*	*(10,000)*	*(10,000)*	*(10,000)*	*(10,000)*
High Performance Network Facilities and Testbeds (ESnet)	38,000	45,000	45,000	65,000	79,000
SBIR/STTR	15,036	13,162	14,728	14,526	14,049
Total, High Performance Computing and Network Facilities	441,824	365,608	413,501	407,978	461,608
Exascale Computing					
17-SC-20 Office of Science Exascale Computing Project (SC-ECP)	157,894	164,000	196,580	170,000	184,000
Total, Advanced Scientific Computing Research	**621,000**	**647,000**	**722,010**	**694,200**	**763,000**
Computational Sciences Workforce Programs, with WDTS (non-add)	*(10,000)*	*(10,000)*	*(10,000)*	*(10,000)*	*(10,000)*
Exascale Computing Crosscut (non-add)	*(157,894)*	*(164,000)*	*(346,580)*	*(282,000)*	*(334,000)*

Staffing Changes

- **Bill Harrod has accepted a new job at IARPA, starting January 8, 2018**
- **Steven Lee is currently the Acting Director for the Research Division**
- **Christine Chalk is currently the Acting Director for the Facilities Division**

Early Career Research Program FOA Released

- **Eligibility**
  - No more than ten (10) years can have passed between the year the Principal Investigator's Ph.D. was awarded and the year that the FOA was issued. For the present competition, those who received doctorates no earlier than 2007 are eligible.
  - University: The Principal Investigator must be an untenured Assistant Professor on the tenure track or an untenured Associate Professor on the tenure track at a U.S. academic institution as of the deadline for the application.
  - Lab: The Principal Investigator must be a full-time, permanent, non-postdoctoral national laboratory employee as of the deadline for the proposal.
- **Key Dates**
  - Monday, December 18, 2017: University and Laboratory Funding Opportunity Announcements released
  - 2018
    - Thursday, January 25: Pre-applications due at 5:00 PM EST
    - Tuesday, February 27: Encourage/Discourage notification process completed
    - Wednesday, April 4: Final Proposals due at 5:00 PM EST
    - Thursday, May 31: Internal SC Selection Process complete

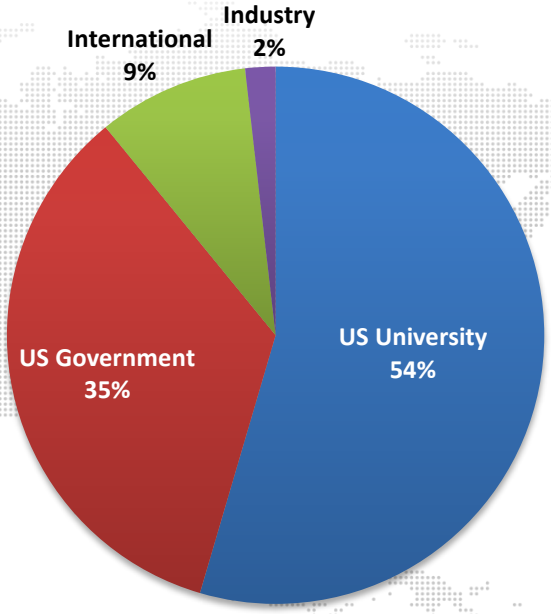
Anticipated FY2018 Research Funding Opportunity Announcements

- **Exploratory Research for Extreme-Scale Science (EXPRESS): Quantum Computing Application Teams (QCATS)**
- **Quantum Testbed Pathfinder**
- **Quantum Testbeds for Science**
- **Mathematical Multifaceted Integrated Capability Centers (MMICCs)**
- **Uncertainty Quantification for Enabling Extreme-Scale Science**

2018 INCITE award statistics

- Request for Information helped attract new projects
- Call closed June 23th, 2017
- Total requests of more than **15 billion core-hours**
- Awards of 5.95 billion core-hours for CY 2018
- **55 projects awarded of which 22 are renewals**

PIs by Affiliation (Awards)



Acceptance rates

34% of nonrenewal submittals and 91% of renewals

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

2018 submissions statistics, by system

	Total	Titan	Mira	Theta
Number of projects submitted (new and renewal)	121	57	39	25
Average Project Request		96.0M	141.8M	39.2M
Median Project Request		90.5M	99M	22.0M
Total Hours requested (core-hrs in CY2018)	15.3B	7.10B	7.09B	1.10B

* Total of 121 INCITE submissions (many of the projects requested time on a combination of Mira, Theta and Titan)
* Theta core-hours reported are in “Theta native core-hours”

2018 award statistics, by system

	Titan	Mira	Theta
Number of projects*	31	27	14
Average Project	70.1M	125.2M	27.9M
Median Project	80M	100M	12.3M
Total Awards (core-hrs in CY2018)	2.18B	3.38B	0.39B

* Total of 55 INCITE projects (many of the projects received time on a combination of Mira, Theta and Titan)
* Theta core-hours reported are in “Theta native core-hours”

Facility Project Reviews

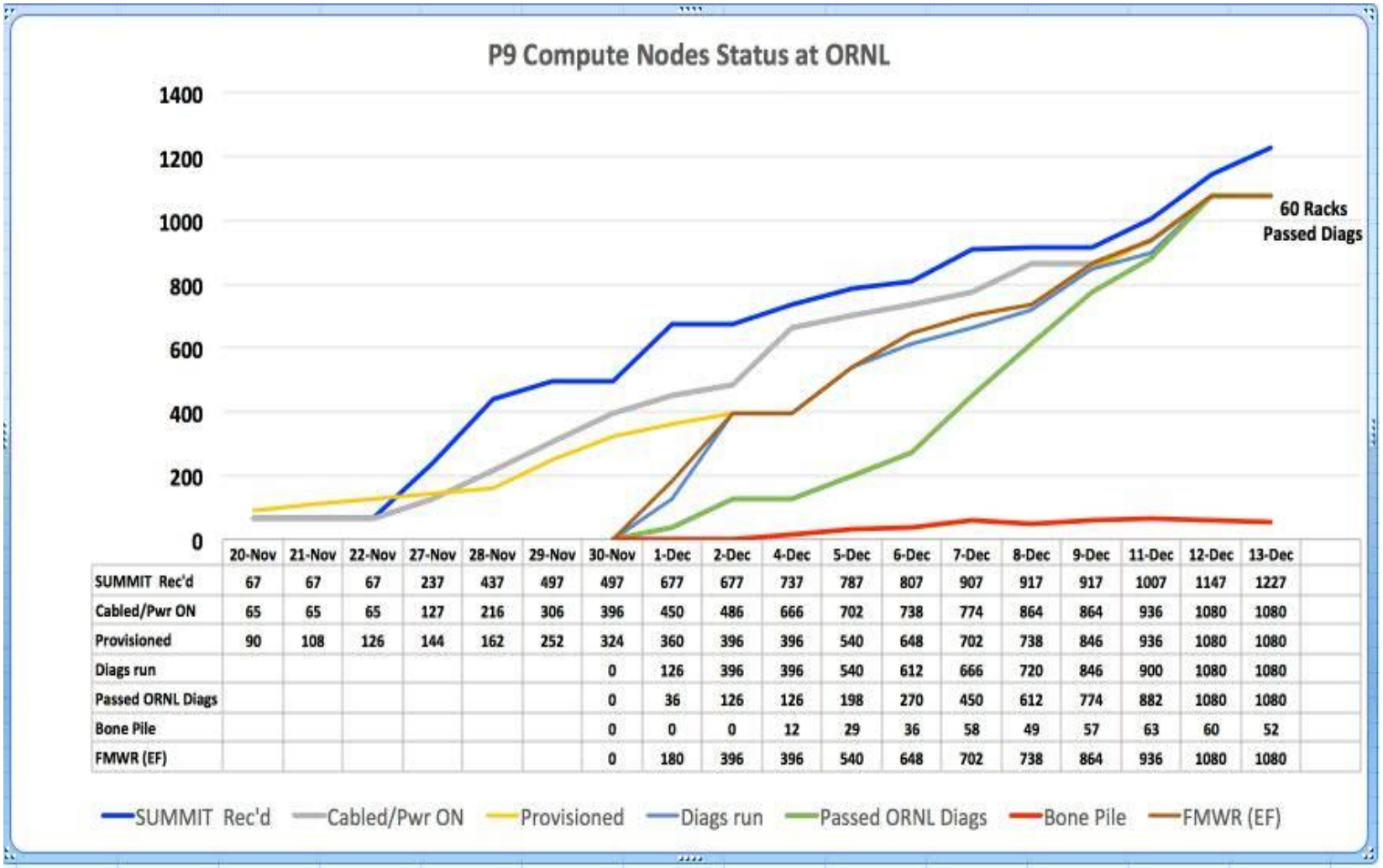
- **Conducted**
  - November 7-9, 2017, ALCF-3 Re-baseline review; panel recommended approval
  - November 28-29, 2017, OLCF-5 CD-1 review; panel recommended approval
- **Anticipated in 2018**
  - ESAAB for to approve ALCF-3 Re-baseline and OLCF-5 CD-1 in January.
  - CD 1/3A IPR and approval for ESnet-6
  - CD-2/3 IPR and approval for NERSC-9 site prep
  - CD-2/3 IPR for NERSC-9
  - CD-2/3 IPR for OLCF-5
  - CD 2/3 IPR for ESnet-6

Summit Begins at OLCF

Summit Schedule	
Start of Installation	7/2017
Installation Complete	2/2018
System Acceptance	9/2018
Early Science	10/2018
INCITE Allocations	1/2019

Feature	Titan	Summit
Application Performance	Baseline	5-10x Titan
Nodes	18,688	~4,600
Node performance	1.4 TF	> 40 TF
Memory per Node	32 GB DDR3 + 6 GB GDDR5	512 GB DDR4 + 96 GB HBM
NV memory per Node	0	1600 GB
System Interconnect	Gemini (6.4 GB/s)	Dual Rail EDR-IB (23 GB/s)
Interconnect Topology	3D Torus	Non-blocking Fat Tree
Processors	1 AMD Opteron™ 1 NVIDIA Kepler™	2 IBM POWER9™ 6 NVIDIA Volta™
File System	32 PB, 1 TB/s, Lustre®	250 PB, 2.5 TB/s, GPFS™

Summit Update



	20-Nov	21-Nov	22-Nov	27-Nov	28-Nov	29-Nov	30-Nov	1-Dec	2-Dec	4-Dec	5-Dec	6-Dec	7-Dec	8-Dec	9-Dec	11-Dec	12-Dec	13-Dec
SUMMIT Rec'd	67	67	67	237	437	497	497	677	677	737	787	807	907	917	917	1007	1147	1227
Cabled/Pwr ON	65	65	65	127	216	306	396	450	486	666	702	738	774	864	864	936	1080	1080
Provisioned	90	108	126	144	162	252	324	360	396	396	540	648	702	738	846	936	1080	1080
Diags run							0	126	396	396	540	612	666	720	846	900	1080	1080
Passed ORNL Diags							0	36	126	126	198	270	450	612	774	882	1080	1080
Bone Pile							0	0	0	12	29	36	58	49	57	63	60	52
FMWR (EF)							0	180	396	396	540	648	702	738	864	936	1080	1080

Components of the DOE Exascale Program

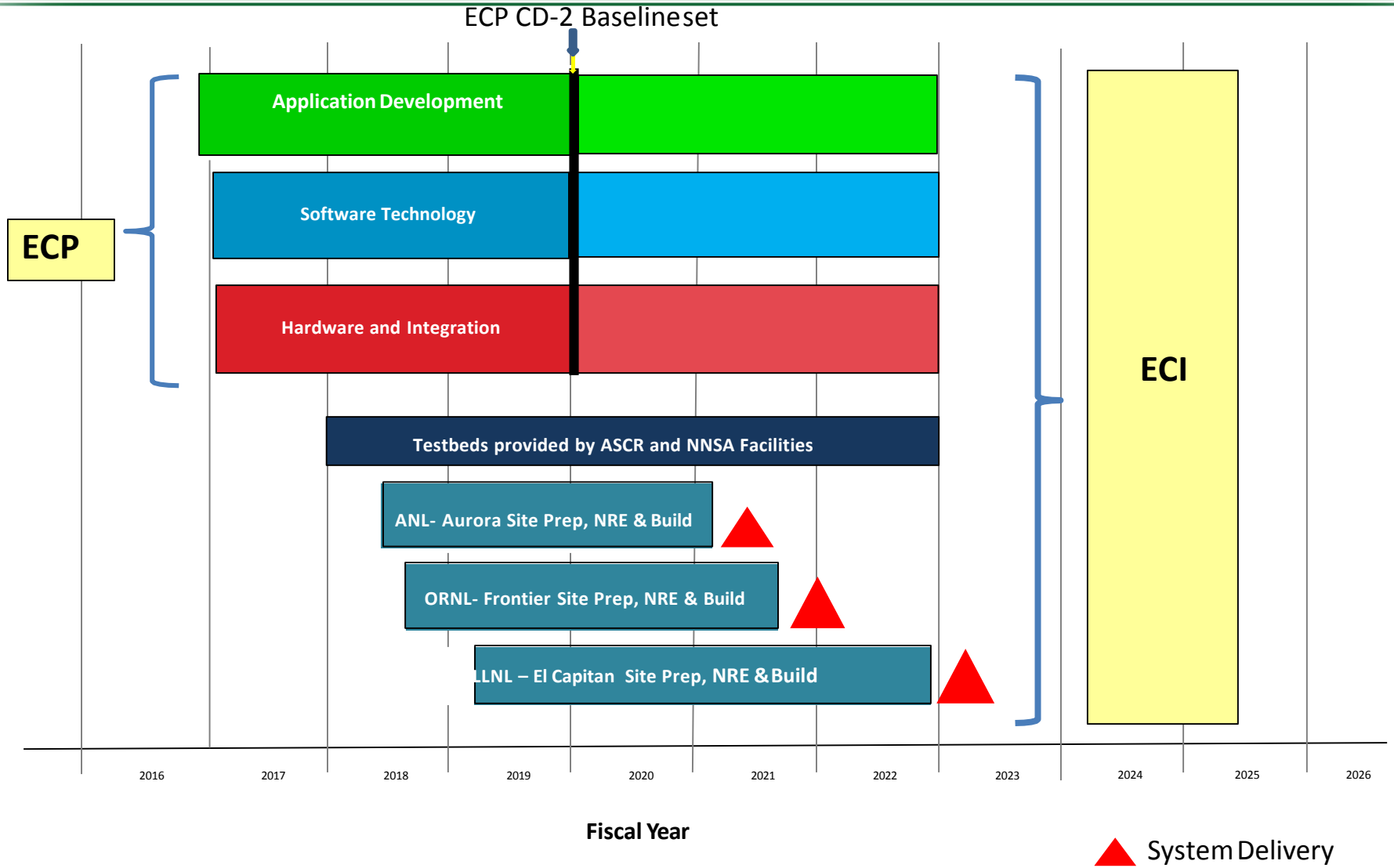
- **Exascale Computing Initiative (ECI)**
  - The ECI was initiated in FY 2016 to support research, development and computer system procurements to deliver an exascale (10^{18} ops/sec) computing capability by the early to mid-2020s.
  - It is a partnership between SC and NNSA, addressing science and 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.

ECP Independent Project Review

- **Scheduled for January 9-11, 2018 in Oak Ridge**
- **In preparation for IPR**
  - **Independent Design Review of Preliminary Design Report held December 5, 2017** and found *"that the ECP has restructured and realigned their technical approach to reflect the changes to the project's scope, schedule and budget in order to meet the overall project goals and KPPs."*
  - **Red Team Review held December 6, 2017** and found *"the ECP management team to be highly skilled, experienced, and committed to the success of the Project. The technical approach is appropriate; supports the mission need; and is responsive to the recent baseline change."*
- **Charge Questions:**

1. Has the project satisfactorily addressed recommendations from the September 13-15, 2016Project Review?
2. Does the documentation, including the Preliminary Design Report and Preliminary Project Execution Plan (PPEP), describe the current ECP scope and plans with rigor appropriate for this stage of the project (pre CD-2)? Does the project document reflect an actionable tailoring strategy?
3. Is the risk-informed milestone-based plan, with its associated resources and contingencies, reasonable for ECP to meet its mission need and preliminary KPP?
4. Is the proposed baseline change reasonable and have the risks associated with the changes appropriately considered and documented.
5. Is the management team appropriately structured with the requisite skills, experience and resources and empowered to ensure success of the project?
6. Has the project negotiated an actionable engagement plan with the appropriate DOE SC and NNSA Computing facilities to ensure mutual success?
7. Is the project on track to meet its major milestones as identified in the PPEP?

ECI Timeline



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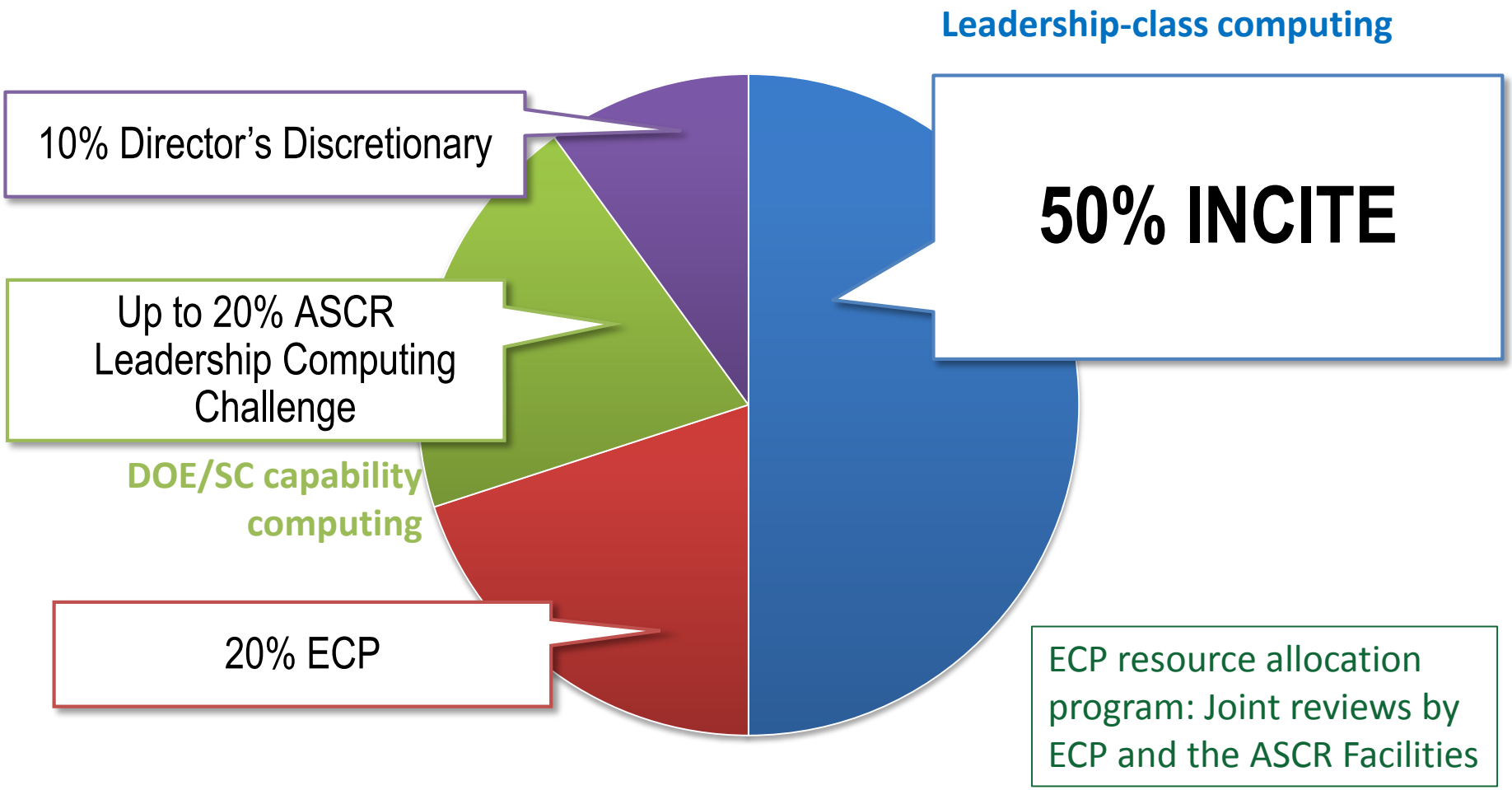
Components of ASCR's Current Allocation Policy

- **Facility directors will retain up to 10% of allocable hours to support pilot or startup projects, to support code scaling and for petascale computer science and performance metrics research.**
- **The majority of (60-80%) of available processor hours at NERSC will be for researchers working on SC-funded or SC relevant projects.**
  - NERSC issues Call for Proposals and Headquarters Program Management determines allocations
- **The majority (60-80%) of available processor hours on the Leadership Computing resources will be allocated through the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program.**
  - LCF Directors will be responsible for conducting joint reviews and select projects for their facility.
- **ASCR retains between 10-30% of resources at NERSC, ALCF and OLCF for the ASCR Leadership Computing Challenge**
  - ASCR issues Open Call for proposals, conducts reviews and selects projects
  - For projects critical to DOE Missions and to broaden HPC/LCF community

New ECP-focused Allocation program: 2018 distribution of allocable hours

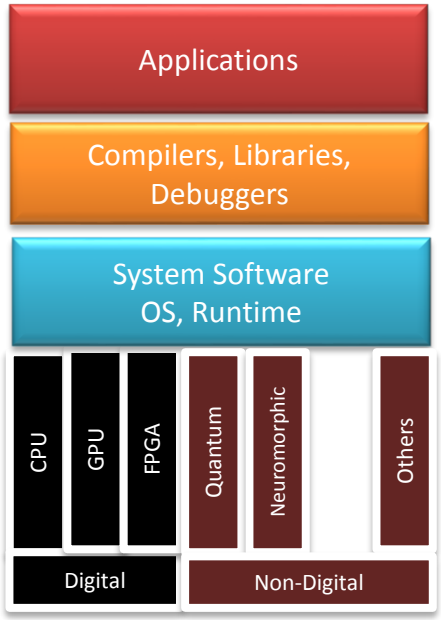


Workshop Update

Extreme Heterogeneity Workshop

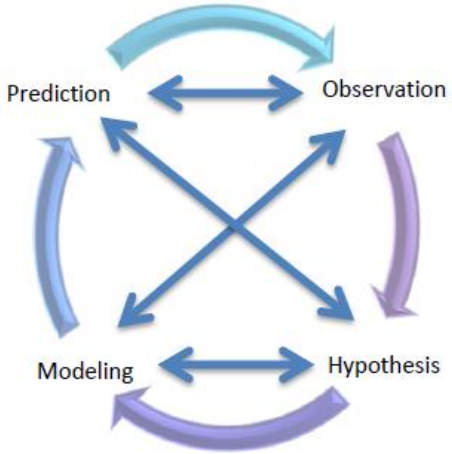
Jan. 23-25, 2018, in Gaithersburg, MD

- **POC: Lucy Nowell (Lucy.Nowell@science.doe.gov)**
- **Goal: Define challenges that extreme heterogeneity presents to the software stack and programming environment and identify related Computer Science priority research directions** that are essential to making extremely heterogeneous systems useful, usable and secure for science applications and DOE mission requirements in the 2025-2035 timeframe.
- 148 expected participants: DOE Labs, academia, & industry
- ~20 observers from DOE and other federal agencies (DoD, NSF, NASA)
- Pre-workshop report is being edited and will be posted by Jan. 1, 2018
- 105 white papers were received by the Dec. 4 deadline
  - After review, these resulted in 26 new invitations to Lab people and 20 to non-Lab people, including academics, industry and people from Europe and Japan.
- Agenda is being finalized, based in part on white paper content



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.**



Some Agenda Details

- **UPDATE ON THE EXASCALE COMPUTING PROJECT –** *Doug Kothe, ECP Director*
- **UPDATE ON CURRENT CHARGES**
  - *Committee of visitors – Susan Gregurick, ASCAC*
  - *Future Technologies – Vivek Sarkar, ASCAC*
- **SciDAC Institutes**
  - *RAPIDS/Computer Science Institute – Rob Ross, Argonne National Laboratory*
  - *FASTMATH/Applied Math Institute – Lori Diachin, Lawrence Livermore National Laboratory*
- **UPDATE on OSTI –** Brian Hitson, OSTI
- **USING FOREIGN HPC RESOURCES –** *Martin Berzins, ASCAC*
- **CORI DATA STRATEGY AND NESAP PROJECTS –** *Katie Antypas and Jack Deslippe, Lawrence Berkeley National Laboratory*

* Invited