Update on the Exascale Computing Project

Paul Messina, ECP Director

Stephen Lee, ECP Deputy Director

ASCAC Meeting, Washington, DC

American Geophysical Union
December 20, 2016



ECP aims to transform the HPC ecosystem and make major contributions to the nation

- Develop applications that will tackle a broad spectrum of mission critical problems of unprecedented complexity with unprecedented performance
- Contribute to the economic competitiveness of the nation
- Support national security
- Develop a software stack, in collaboration with vendors, that is exascale-capable and is usable on smaller systems by industry and academia
- Train a large cadre of computational scientists, engineers, and computer scientists who will be an asset to the nation long after the end of ECP
- Partner with vendors to develop computer architectures that support exascale applications
- Revitalize the US HPC vendor industry
- Demonstrate the value of comprehensive co-design

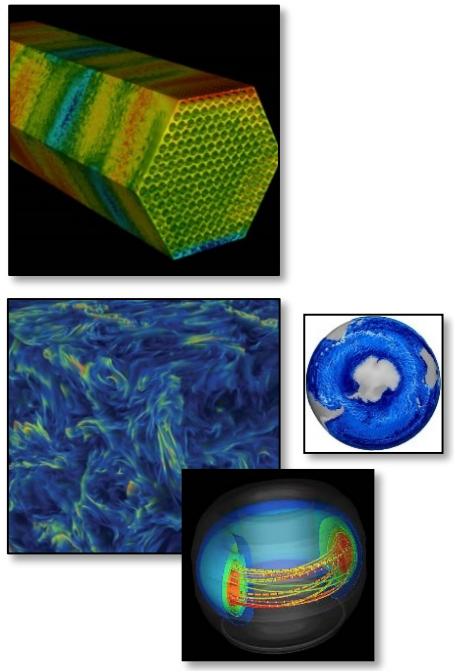
ECP EXASCALE COMPUTING PROJECT

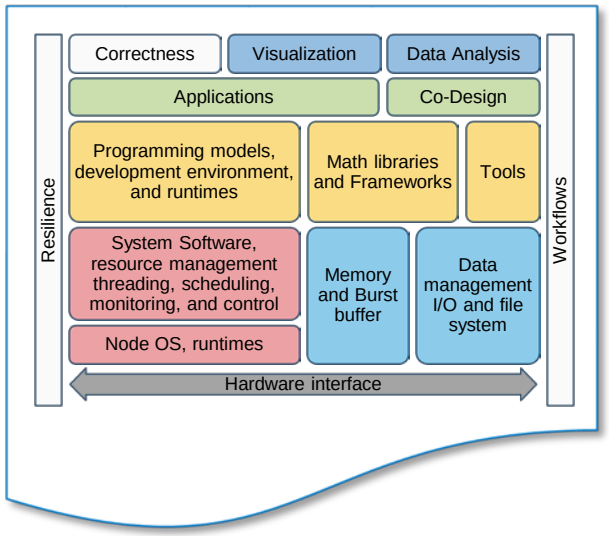
Exascale Computing Project Goals

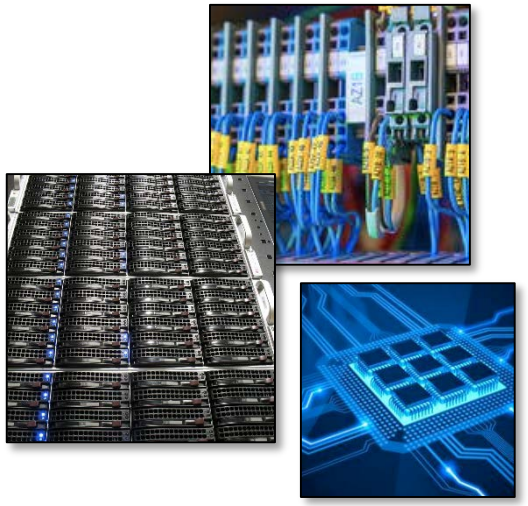
Develop scientific, engineering, and large-data applications that exploit the emerging, exascale-era computational trends caused by the end of Dennard scaling and Moore's law	Create software that makes exascale systems usable by a wide variety of scientists and engineers across a range of applications	Enable by 2021 and 2023 at least two diverse computing platforms with up to 50× more computational capability than today's 20 PF systems, within a similar size, cost, and power footprint	Help ensure continued American leadership in architecture, software and applications to support scientific discovery, energy assurance, stockpile stewardship, and nonproliferation programs and policies
Foster application development	Ease of use	Rich exascale ecosystem	US HPC leadership

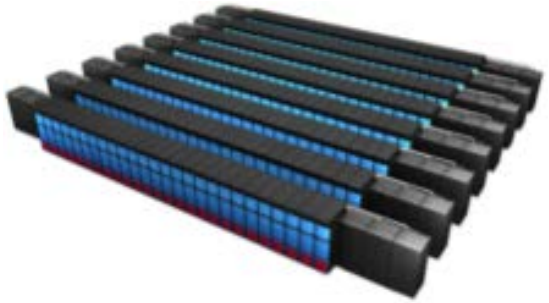
ECP has formulated a holistic approach that uses co-design and integration to achieve capable exascale

Application Development	Software Technology	Hardware Technology	Exascale Systems
Science and mission applications	Scalable and productive software stack	Hardware technology elements	Integrated exascale supercomputers









ECP's work encompasses applications, system software, hardware technologies and architectures, and workforce development

What is a *capable* exascale computing system?

A capable exascale computing system requires an entire computational ecosystem that:

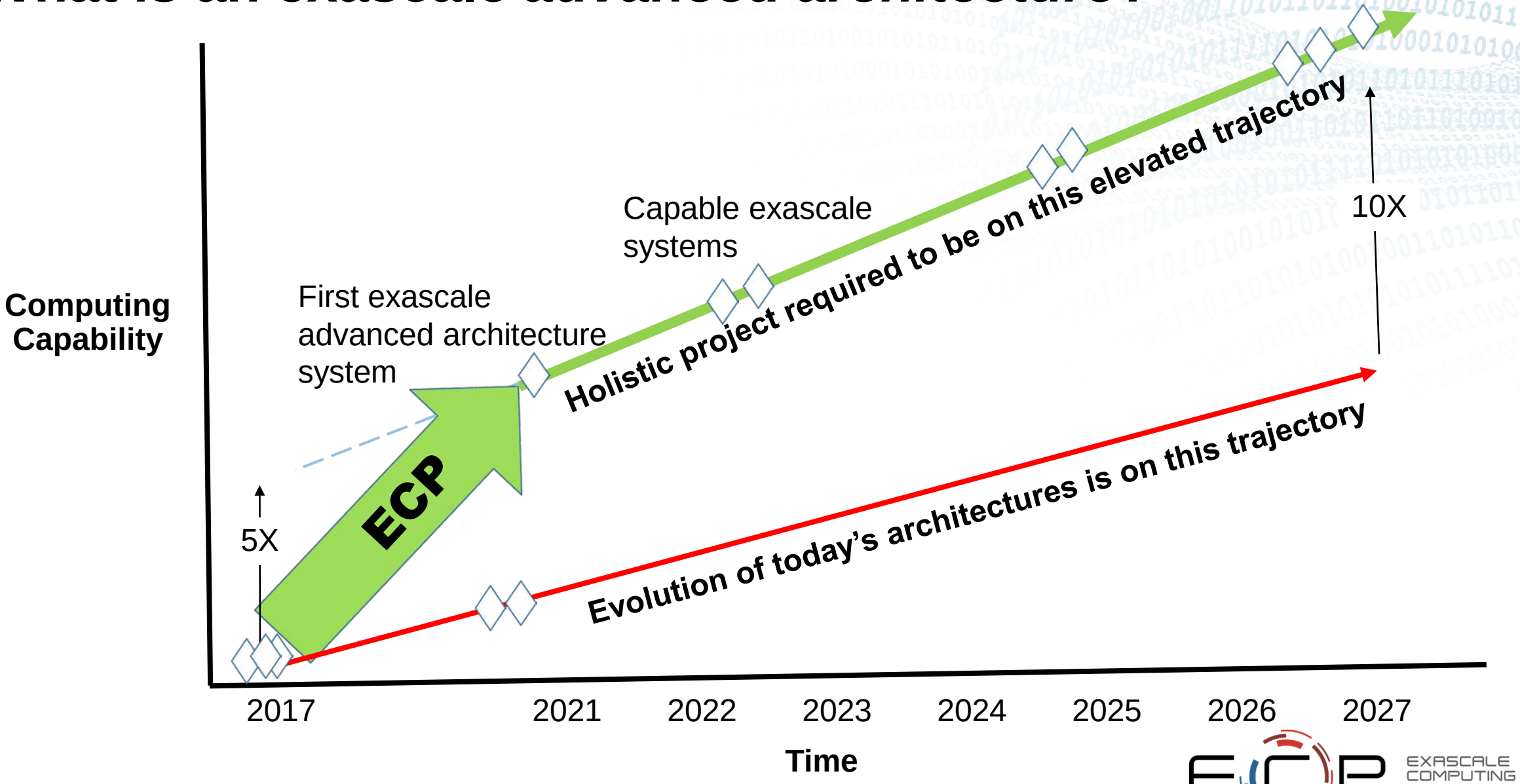
- Delivers 50× the performance of today's 20 PF systems, supporting applications that deliver high-fidelity solutions in less time and address problems of greater complexity
- Operates in a power envelope of 20–30 MW
- Is sufficiently resilient (perceived fault rate: ≤1/week)
- Includes a software stack that supports a broad spectrum of applications and workloads

This ecosystem will be developed using a co-design approach to deliver new software, applications, platforms, and computational science capabilities at heretofore unseen scale

The ECP Plan of Record

- A 7-year project that follows the *holistic/co-design* approach, which runs through 2023 (including 12 months of schedule contingency)
  - To meet the ECP goals
- Enable an initial exascale system based on *advanced architecture* and delivered in 2021
- Enable *capable exascale* systems, based on ECP R&D, delivered in 2022 and deployed in 2023 as part of an NNSA and SC facility upgrades
- Acquisition of the exascale systems is outside of the ECP scope, will be carried out by DOE-SC and NNSA-ASC facilities

What is an exascale *advanced architecture*?



Reaching the Elevated Trajectory will require Advanced and Innovative Architectures

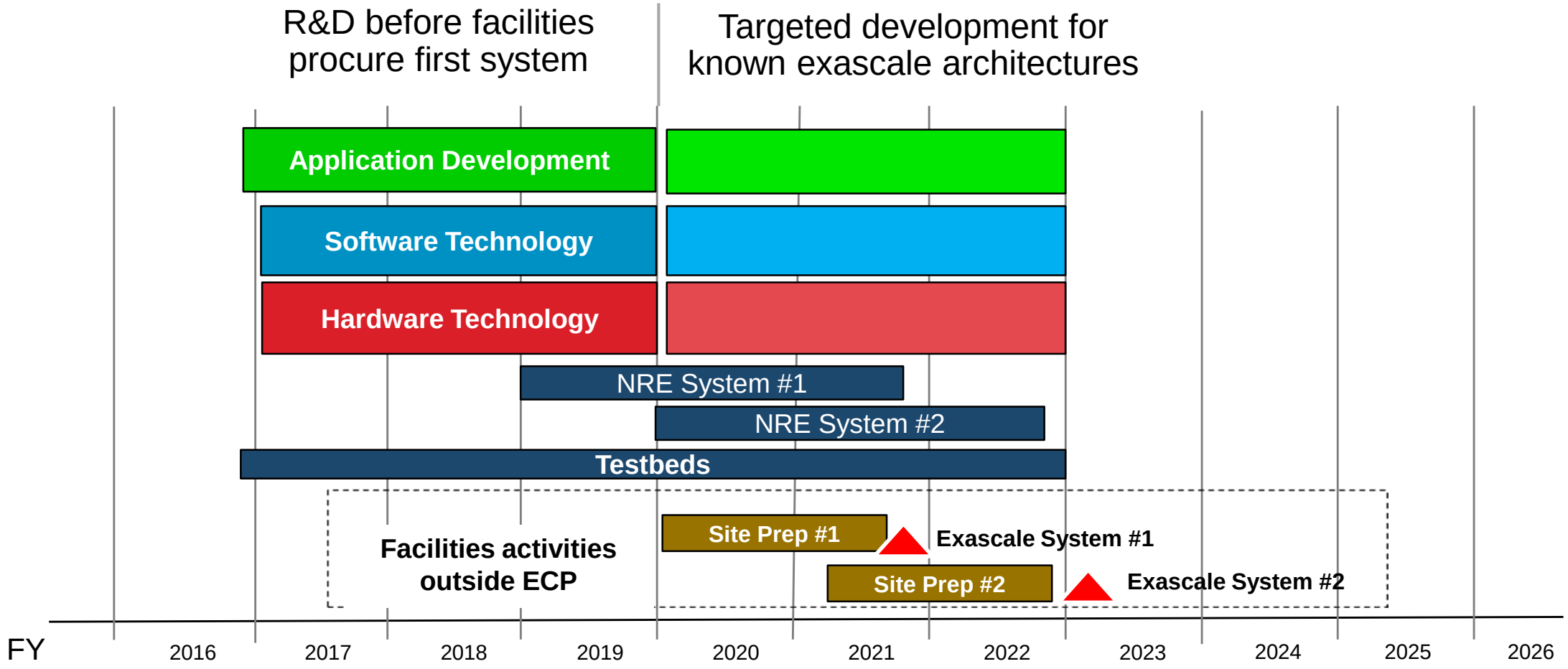
In order to reach the elevated trajectory, advanced architectures must be developed that make a big leap in:

- Parallelism
- Memory and Storage
- Reliability
- Energy Consumption

The exascale advanced architecture developments benefit all future U.S. systems on the higher trajectory

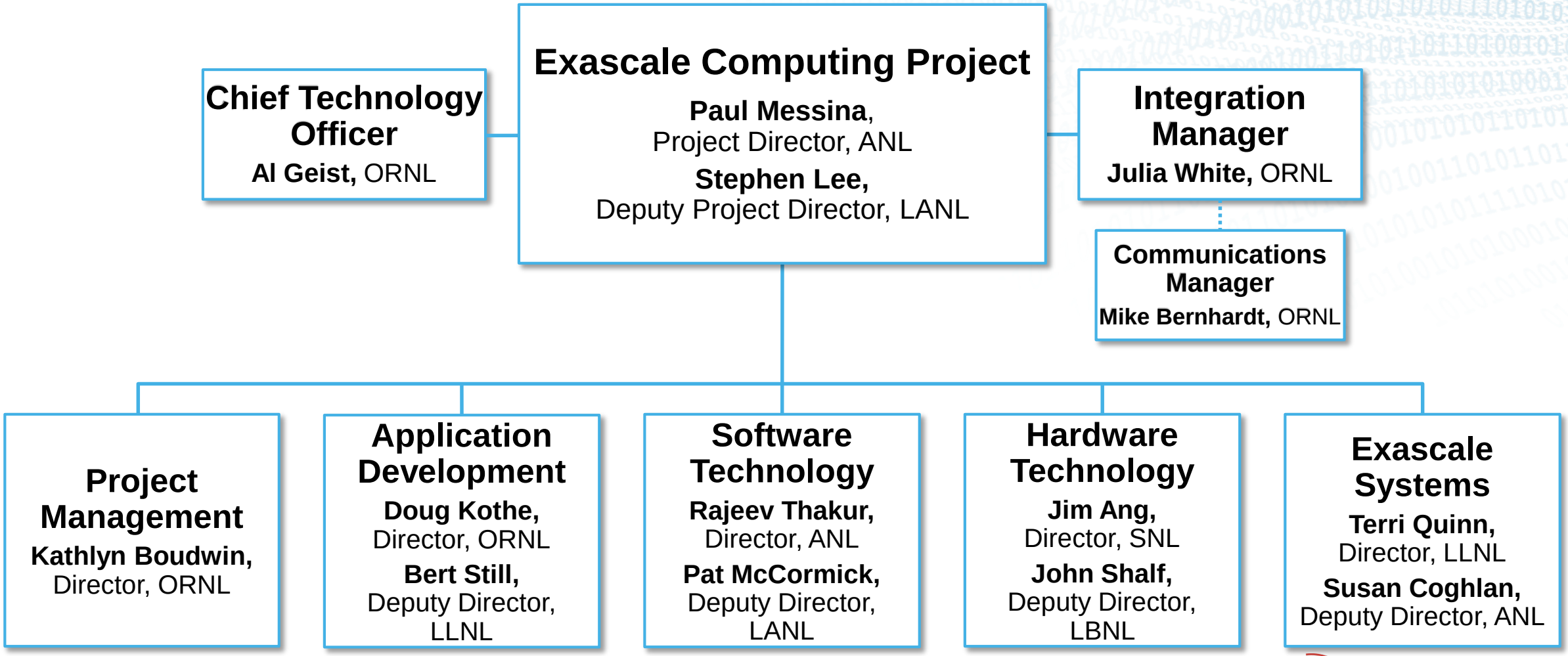
In addition, the exascale advanced architecture will need to solve emerging data science and machine learning problems in addition to the traditional modeling and simulations applications.

High-level ECP technical project schedule

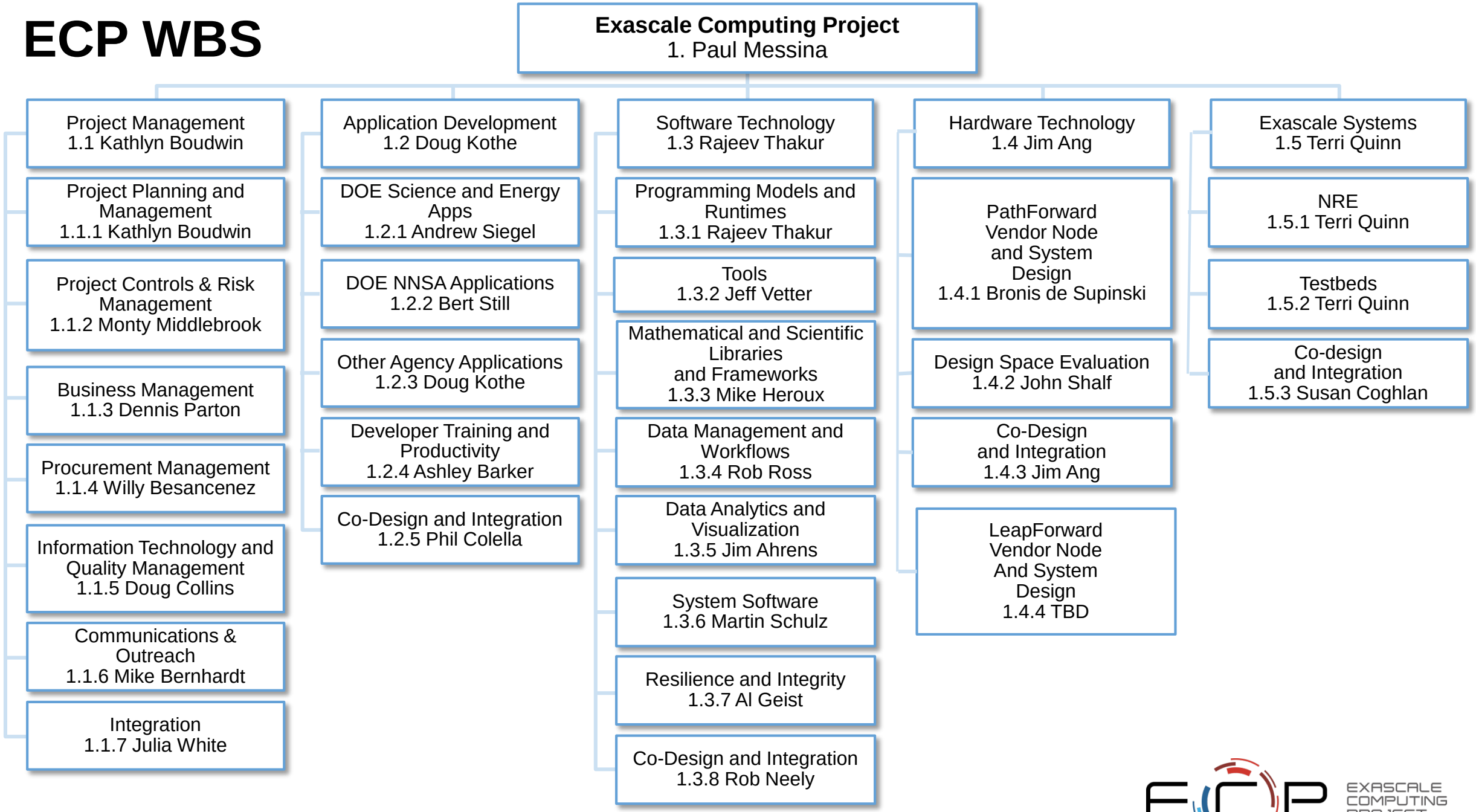


ECP leadership team

Staff from 6 national laboratories, with combined experience of >300 years



ECP WBS


Exascale Computing Project
1. Paul Messina
Project Management
1.1 Kathlyn Boudwin
Project Planning and Management
1.1.1 Kathlyn Boudwin
Project Controls & Risk Management
1.1.2 Monty Middlebrook
Business Management
1.1.3 Dennis Parton
Procurement Management
1.1.4 Willy Besancenez
Information Technology and Quality Management
1.1.5 Doug Collins
Communications & Outreach
1.1.6 Mike Bernhardt
Integration
1.1.7 Julia White
Application Development
1.2 Doug Kothe
DOE Science and Energy Apps
1.2.1 Andrew Siegel
DOE NNSA Applications
1.2.2 Bert Still
Other Agency Applications
1.2.3 Doug Kothe
Developer Training and Productivity
1.2.4 Ashley Barker
Co-Design and Integration
1.2.5 Phil Colella
Software Technology
1.3 Rajeev Thakur
Programming Models and Runtimes
1.3.1 Rajeev Thakur
Tools
1.3.2 Jeff Vetter
Mathematical and Scientific Libraries and Frameworks
1.3.3 Mike Heroux
Data Management and Workflows
1.3.4 Rob Ross
Data Analytics and Visualization
1.3.5 Jim Ahrens
System Software
1.3.6 Martin Schulz
Resilience and Integrity
1.3.7 Al Geist
Co-Design and Integration
1.3.8 Rob Neely
Hardware Technology
1.4 Jim Ang
PathForward Vendor Node and System Design
1.4.1 Bronis de Supinski
Design Space Evaluation
1.4.2 John Shalf
Co-Design and Integration
1.4.3 Jim Ang
LeapForward Vendor Node And System Design
1.4.4 TBD
Exascale Systems
1.5 Terri Quinn
NRE
1.5.1 Terri Quinn
Testbeds
1.5.2 Terri Quinn
Co-design and Integration
1.5.3 Susan Coghlan

ECP application, co-design center, and software project awards



EXASCALE COMPUTING PROJECT

NEWS RELEASE

The Exascale Computing Project Awards $34 Million for Software Development

OAK RIDGE, Tenn., Nov. 10, 2016 – The Department of Energy's Exascale Co
(ECP) today announced the selection of 35 software development proposals
research and academic organizations.

The awards for the first year of funding total $34 million and cover many co
software stack for exascale systems, including programming models and run
mathematical libraries and frameworks, tools, lower-level system software,
and I/O, as well as in situ visualization and data analysis.

EXASCALE COMPUTING PROJECT

NEWS RELEASE

The Exascale Computing Project Announces $48 Million to Establish Four Exascale Co-Design Centers

OAK RIDGE, Tenn., Nov. 11, 2016 – The Department of Energy's Exascale Computing Project (ECP) today
announced that it has selected four co-design centers as part of a 4 year, $48 million funding award. The first
year is funded at $12 million, and is to be allocated evenly among the four award recipients.

The ECP is responsible for the planning, execution, and delivery of technologies necessary for a capable
exascale ecosystem to support the nation's exascale imperative including software,
and early testbed platforms.

EXASCALE COMPUTING PROJECT

NEWS RELEASE

For Immediate Distribution

The Exascale Computing Project (ECP) Announces $39.8 million in First-Round Application Development Award

OAK RIDGE, Tenn., Sept. 07, 2016 – The Department of Energy's Exascale Computi
(ECP) today announced its first round of funding with the selection of 15 applicatio
development proposals for full funding and seven proposals for seed funding, repr
teams from 45 research and academic organizations.

The awards, totaling $39.8 million, target advanced modeling and simulation solut
specific challenges supporting key DOE missions in science, clean energy and natio
as well as collaborations such as the Precision Medicine Initiative with the Nation
Health's National Cancer Institute.

EXASCALE COMPUTING PROJECT

ECP Mission Need Defines the Application Strategy

Support DOE science *and* energy missions	Meet national security needs	Key science and technology challenges to be addressed with exascale
• Discover and characterize next-generation **materials** • Systematically understand and improve **chemical processes** • Analyze the extremely large datasets resulting from the next generation of **particle physics** experiments • Extract knowledge from **systems-biology** studies of the microbiome • Advance **applied energy** technologies (e.g., whole-device models of plasma-based fusion systems)	• Stockpile Stewardship Annual Assessment and Significant Finding Investigations • Robust uncertainty quantification (UQ) techniques in support of lifetime extension programs • Understanding evolving nuclear threats posed by adversaries and in developing policies to mitigate these threats	• Materials discovery and design • Climate science • Nuclear energy • Combustion science • Large-data applications • Fusion energy • National security • Additive manufacturing • Many others!

ECP Applications Deliver Broad Coverage of Strategic Pillars

Initial selections consist of 15 application projects + 7 seed efforts

National Security

- Stockpile Stewardship

Energy Security

- Turbine Wind Plant Efficiency
- Design/Commercialization of SMRs
- Nuclear Fission and Fusion Reactor Materials Design
- Subsurface Use for Carbon Capture, Petro Extraction, Waste Disposal
- High-Efficiency, Low-Emission Combustion Engine and Gas Turbine Design
- Carbon Capture and Sequestration Scaleup (S)
- Biofuel Catalyst Design (S)

Economic Security

- Additive Manufacturing of Qualifiable Metal Parts
- Urban Planning (S)
- Reliable and Efficient Planning of the Power Grid (S)
- Seismic Hazard Risk Assessment (S)

Scientific Discovery

- Cosmological Probe of the Standard Model (SM) of Particle Physics
- Validate Fundamental Laws of Nature (SM)
- 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 (S)

Climate and Environmental Science

- Accurate Regional Impact Assessment of Climate Change
- Stress-Resistant Crop Analysis and Catalytic Conversion of Biomass-Derived Alcohols
- Metegenomics for Analysis of Biogeochemical Cycles, Climate Change, Environ Remediation (S)

Healthcare

- Accelerate and Translate Cancer Research

ECP EXASCALE COMPUTING PROJECT

Application Development: Partnerships

INDUSTRY
Intel
NVIDIA
Stone Ridge Technology

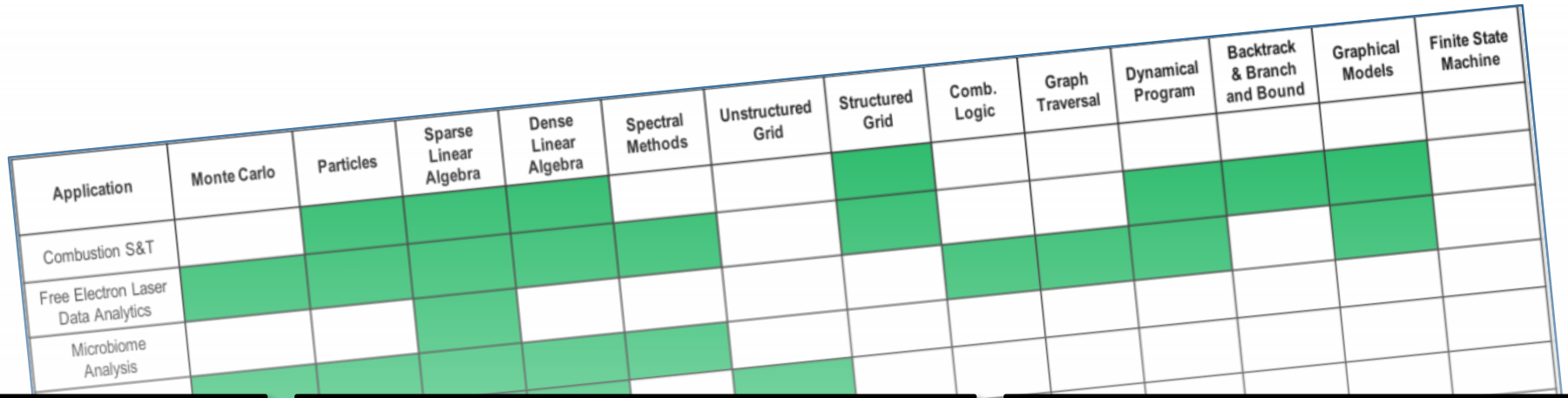
UNIVERSITY
College of William & Mary
Columbia University
University of Indiana
University of Utah
University of Illinois
University of Tennessee
Rutgers University
University of California, Irvine & Los Angeles
Colorado State University
University of Chicago
Virginia Tech.
University of Colorado

LABORATORY PARTNERSHIPS	
Ames	Argonne
Brookhaven	Fermi National Accelerator
Idaho	Oak Ridge
Los Alamos	Lawrence Berkeley
Lawrence Livermore	Pacific Northwest
National Renewable Energy Laboratory	Thomas Jefferson National Accelerator Facility
National Energy Technology Laboratory	Princeton Plasma Physics Laboratory
SLAC National Accelerator	Sandia

Meeting ECP Mission Need Application Requirements

- Current ECP application portfolio appropriately targets high-priority strategic problems in key DOE science, energy, national security programs
- Some application gaps remain relative to ECP Mission Need requirements
  - Data analytic computing (DAC) applications per the NSCI Strategic Plan
  - High priority applications for some NSCI deployment agencies (NASA, NOAA, DHS, FBI)
- ECP has not yet adequately targeted the talented U.S. computational science leadership in academia and industry
- A Request for Information (RFI) for candidate ECP application projects led by academia or industry is currently being drafted
  - Tentative release date of Jan 2017 with an informational videoconference scheduled shortly thereafter
  - Industry participation will adhere to standard DOE cost share requirements and IP provisions
  - A subset of RFI responses, determined by DOE, ECP, and external peer review, will be asked to submit full proposals, with final selection of 3-5 projects (sized initially with teams of 2-4 staff) by April 2017
- New Data Analytic Computing methods and applications are of particular interest, in addition to proposals to enhance the current ECP portfolio
  - Critical infrastructure, superfacility, supply chain, image/signal processing, in situ analytics
  - Machine/statistical learning, classification, streaming/graph analytics, discrete event, combinatorial optimization

Application Co-Design (CD)



Essential to ensure that applications effectively utilize exascale systems	Executed by several CD Centers focusing on a unique collection of algorithmic motifs invoked by ECP applications	Game-changing mechanism for delivering next-generation community products with broad application impact
• Pulls ST and HT developments into applications • Pushes application requirements into ST and HT RD&D • Evolved from best practice to an essential element of the development cycle	• Motif: algorithmic method that drives a common pattern of computation and communication • CD Centers must address all high priority motifs invoked by ECP applications, including not only the 7 “classical” motifs but also the additional 6 motifs identified to be associated with data science applications	• Evaluate, deploy, and integrate exascale hardware-savvy software designs and technologies for key crosscutting algorithmic motifs into applications

ECP EXASCALE COMPUTING PROJECT

ECP Co-Design Centers

- **CODAR: A Co-Design Center for Online Data Analysis and Reduction at the Exascale**
  - Motifs: Online data analysis and reduction
  - Address growing disparity between simulation speeds and I/O rates rendering it infeasible for HPC and data analytic applications to perform offline analysis. Target common data analysis and reduction methods (e.g., feature and outlier detection, compression) and methods specific to particular data types and domains (e.g., particles, FEM)
- **Block-Structured AMR Co-Design Center**
  - Motifs: Structured Mesh, Block-Structured AMR, Particles
  - New block-structured AMR framework (AMReX) for systems of nonlinear PDEs, providing basis for temporal and spatial discretization strategy for DOE applications. Unified infrastructure to effectively utilize exascale and reduce computational cost and memory footprint while preserving local descriptions of physical processes in complex multi-physics algorithms
- **Center for Efficient Exascale Discretizations (CEED)**
  - Motifs: Unstructured Mesh, Spectral Methods, Finite Element (FE) Methods
  - Develop FE discretization libraries to enable unstructured PDE-based applications to take full advantage of exascale resources without the need to “reinvent the wheel” of complicated FE machinery on coming exascale hardware
- **Co-Design Center for Particle Applications (CoPA)**
  - Motif(s): Particles (involving particle-particle and particle-mesh interactions)
  - Focus on four sub-motifs: short-range particle-particle (e.g., MD and SPH), long-range particle-particle (e.g., electrostatic and gravitational), particle-in-cell (PIC), and additional sparse matrix and graph operations of linear-scaling quantum MD

Ongoing Training: Important for ECP Development Teams

- Training for ECP AD and ST project teams is crucial to keep them abreast of key emerging exascale technologies and productive in integrating them
  - Latest algorithms and methods, high performance libraries, memory and storage hierarchies, on-node and task-based parallelism, application portability, and software engineering design principles and best practices.
- ECP training project will offer both generic and focused training activities through topical workshops, deep-dives, hands-on hackathons, seminars, webinars, videos, and documentation
  - Leverage partnerships with the ASCR and NNSA facilities and complement their existing training programs
  - Model training events on previous facility events such as the ATPESC
  - Disseminate lessons learned, best practices, and other T&P materials to the ECP teams and to the general HPC community through the use of the ECP website.
- Early training activities have been focused on developing training and best practices for Agile software development tools and methodologies
- Near term training will focus on using the newly provisioned ECP testbed systems
- Training materials (documents, slides, videos) will be disseminated broadly whenever possible

Ensuring ECP Development Teams are Productive

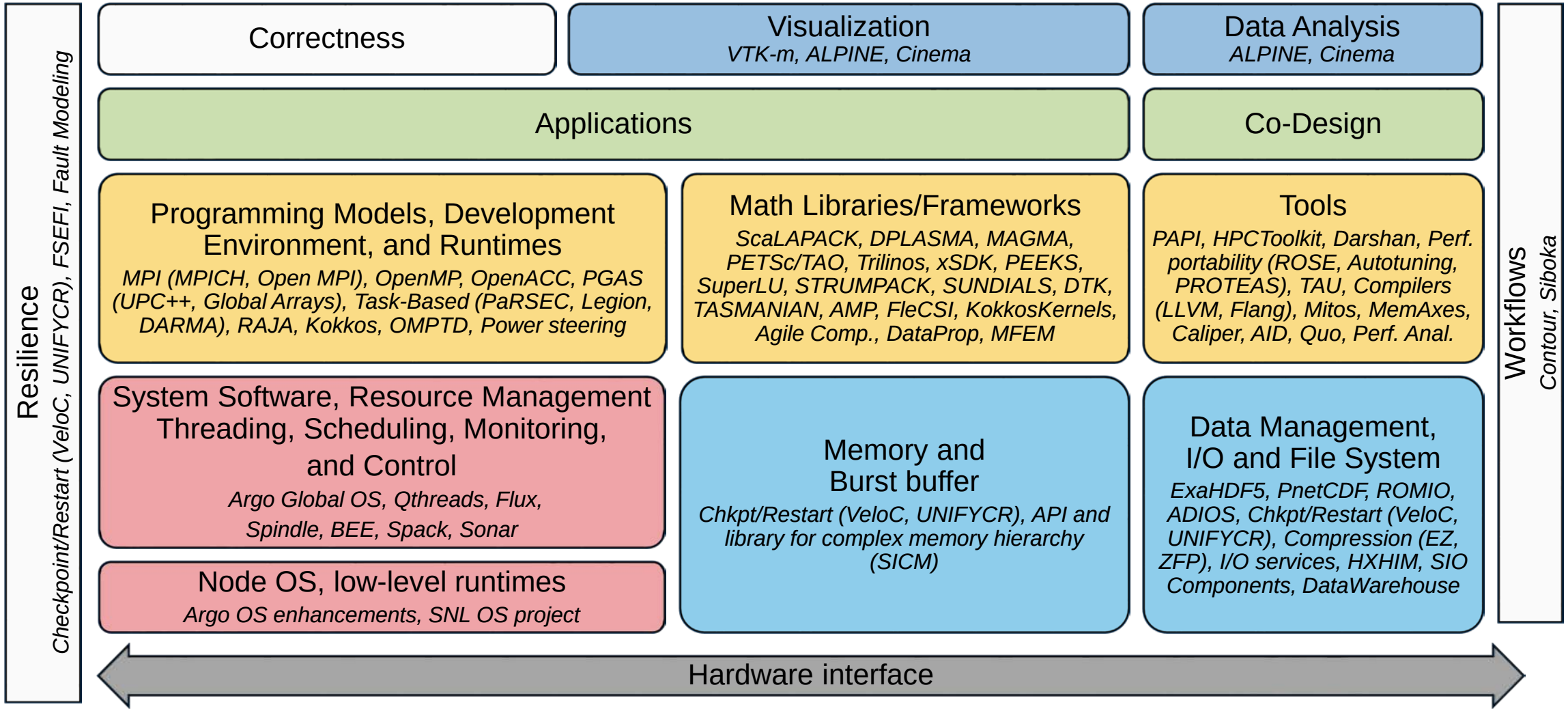
- ECP must assess, recommend, develop and/or deploy software engineering tools, methodologies, and/or processes for software development teams and to cultivate and disseminate software engineering best practices across the teams for improved scientific software development
- ECP is currently standing up a Productivity Project modeled in part on the recent ASCR IDEAS project
  - Includes participation from six DOE Labs and one University partner
- The productivity project team will first assess ECP AD and ST productivity needs and then address these needs through a combination of technical deep dives, implementation of software engineering tools, the development of “how to” documents, training, and one-on-one assistance.
- The productivity work will kick-off in January, 2017

Software Technology Summary

- ECP will build a comprehensive and coherent software stack that will enable application developers to productively write highly parallel applications that can portably target diverse exascale architectures

- ECP will accomplish this by extending current technologies to exascale where possible, performing R&D required to conceive of new approaches where necessary, coordinating with vendor efforts, and developing and deploying high-quality and robust software products

ST Projects (incl. ATDM) Mapped to Software Stack



Plan to involve additional Universities and Vendors

- The current set of Software Technology projects span 8 DOE national laboratories,15 universities, and 2 independent software vendors
- In FY17-18, we plan to issue additional solicitations for universities and vendors
- We plan to coordinate our activities with NSF to cover the broader university community through NSF
- ECP has formed an Industry Council. This group will also serve as an interface for engaging industrial users and software vendors.
- Small businesses: The solicitations in FY17-18 will include independent software vendors. DOE SBIR funding could also support software of interest to ECP.

Next Steps

- Over the next few months, we will undertake a **gap analysis** to identify what aspects of the software stack are missing in the portfolio, based on requirements of applications and DOE HPC facilities, and discussions with vendors

- Based on the results of the gap analysis, we will issue targeted RFIs/RFPs that will aim to close the identified gaps

Hardware Technology Overview

Objective: Fund R&D to design hardware that meets ECP's Targets for application performance, power efficiency, and resilience

Issue *PathForward and LeapForward* Hardware Architecture R&D contracts that deliver:

- Conceptual exascale node and system designs
- Analysis of performance improvement on conceptual system design
- Technology demonstrators to quantify performance gains over existing roadmaps
- Support for active industry engagement in ECP holistic co-design efforts

DOE labs engage to:

- Participate in evaluation and review of PathForward and LeapForward deliverables
- Lead Design Space Evaluation through Architectural Analysis, and Abstract Machine Models of PathForward/LeapForward designs for ECP's holistic co-design

Overarching Goals for PathForward

- Improve the quality and number of competitive offeror responses to the Capable Exascale Systems RFP
- Improve the offeror's confidence in the value and feasibility of aggressive advanced technology options that would be bid in response to the Capable Exascale Systems RFP
- Improve DOE confidence in technology performance benefit, programmability and ability to integrate into a credible system platform acquisition

PathForward Status

- LLNL is managing the procurement
- Competitive RFP released in June
- 14 PathForward proposals received in August
- 6 proposals selected for SOW negotiations of final Work Packages
  - As of Early December: The First Vendor SOW has completed the LLNL Procurement Review and is on to Livermore Field Office review, will need final review by NNSA/HQ
  - Two more Vendor SOWs are entering the LLNL Procurement Review
  - Final three are pending
- Firm Fixed Price contracts with milestone deliverables and payments
- DOE Advance IP Waivers for vendors that provide ≥ 40% cost share
- Project duration: 3 years
- Targeting Contract Awards in January 2017

This is a very exciting time for computing in the US

- Unique opportunity to do something special for the nation on a rapid time scale
- The advanced architecture system in 2021 affords the opportunity for
  - More rapid advancement and scaling of mission and science applications
  - More rapid advancement and scaling of an exascale software stack
  - Rapid investments in vendor technologies and software needed for 2021 and 2023 systems
  - More rapid progress in numerical methods and algorithms for advanced architectures
  - Strong leveraging of and broader engagement with US computing capability
- When ECP ends, we will have
  - Run meaningful applications at exascale in 2021, producing useful results
  - Prepared a full suite of mission and science applications for 2023 capable exascale systems
  - Demonstrated integrated software stack components at exascale
  - Invested in the engineering and development, and participated in acquisition and testing of 2023 capable exascale systems
  - Prepared industry and critical applications for a more diverse and sophisticated set of computing technologies, carrying US supercomputing well into the future

Thank you!

www.ExascaleProject.org

