The Exascale Computing Project

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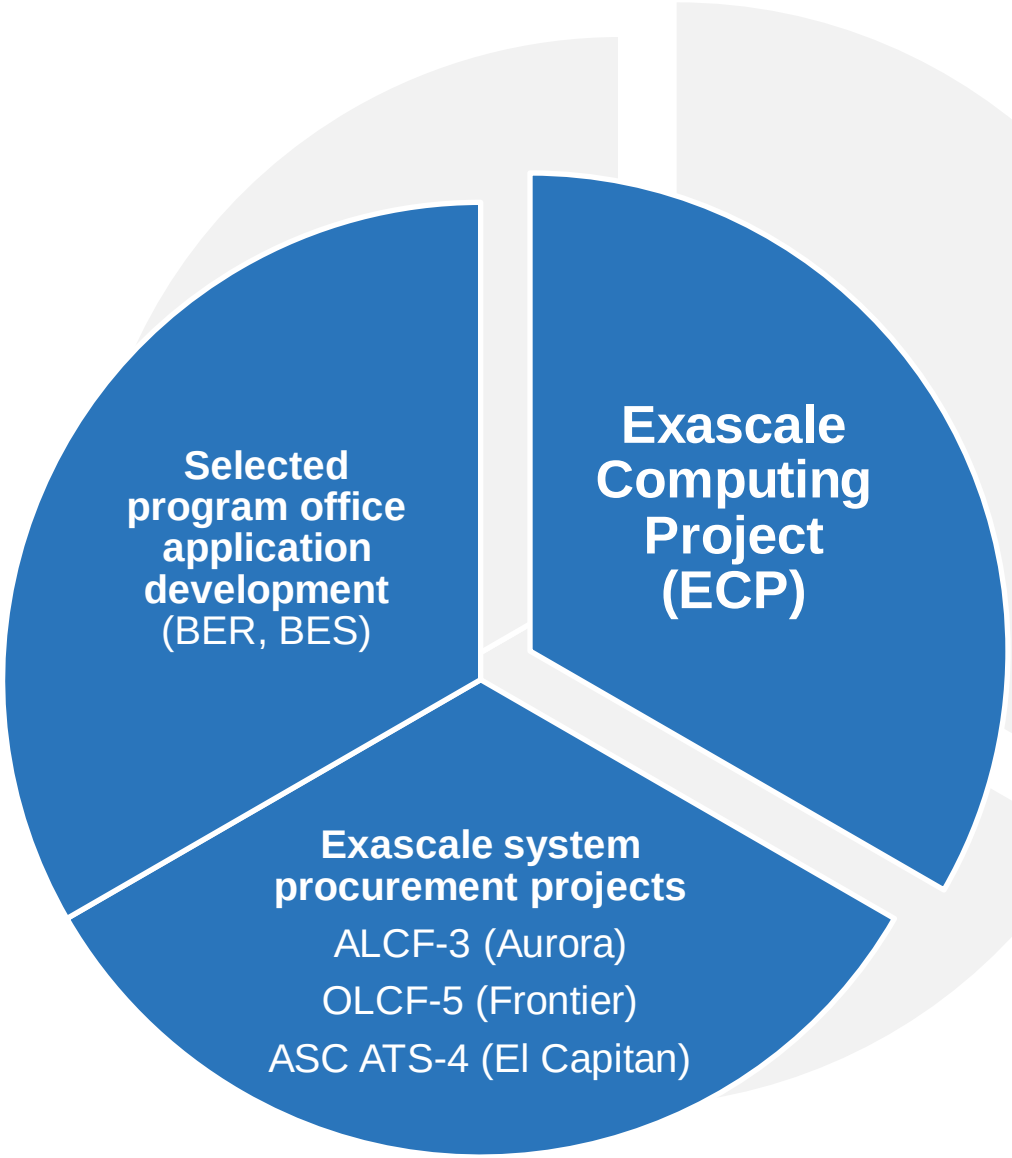
DOE Exascale Program: The Exascale Computing Initiative (ECI)



Three Major Components of the ECI

ECI partners

US DOE Office of Science (SC) and National Nuclear Security Administration (NNSA)

ECI mission

Accelerate R&D, acquisition, and deployment to deliver exascale computing capability to DOE national labs by the early- to mid-2020s

ECI focus

Delivery of an enduring and capable exascale computing capability for use by a wide range of applications of importance to DOE and the US

ECP enables US revolutions in technology development; scientific discovery; healthcare; energy, economic, and national security

ECP mission

Develop exascale-ready applications and solutions that address currently intractable problems of strategic importance and national interest.

Create and deploy an expanded and vertically integrated software stack on DOE HPC exascale and pre-exascale systems, defining the enduring US exascale ecosystem.

Deliver **US HPC vendor technology advances and deploy ECP products** to DOE HPC pre-exascale and exascale systems.

ECP vision

Deliver **exascale simulation and data science innovations and solutions to national problems** that enhance US economic competitiveness, change our quality of life, and strengthen our national security.

Department of Energy (DOE) Roadmap to Exascale Systems

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

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

First U.S. Exascale Computers

2012	2016	2018	2020	2021-2023

ORNL
Cray/AMD/NVIDIA

ORNL
IBM/NVIDIA

ORNL
TBD

ANL
IBM BG/Q

ANL
Cray/Intel KNL

ANL
Intel/Cray

LBNL
Cray/Intel Xeon/KNL

LBNL
Cray/AMD/NVIDIA

LLNL
IBM BG/Q

LANL/SNL
Cray/Intel Xeon/KNL

LLNL
IBM/NVIDIA

LANL/SNL
TBD

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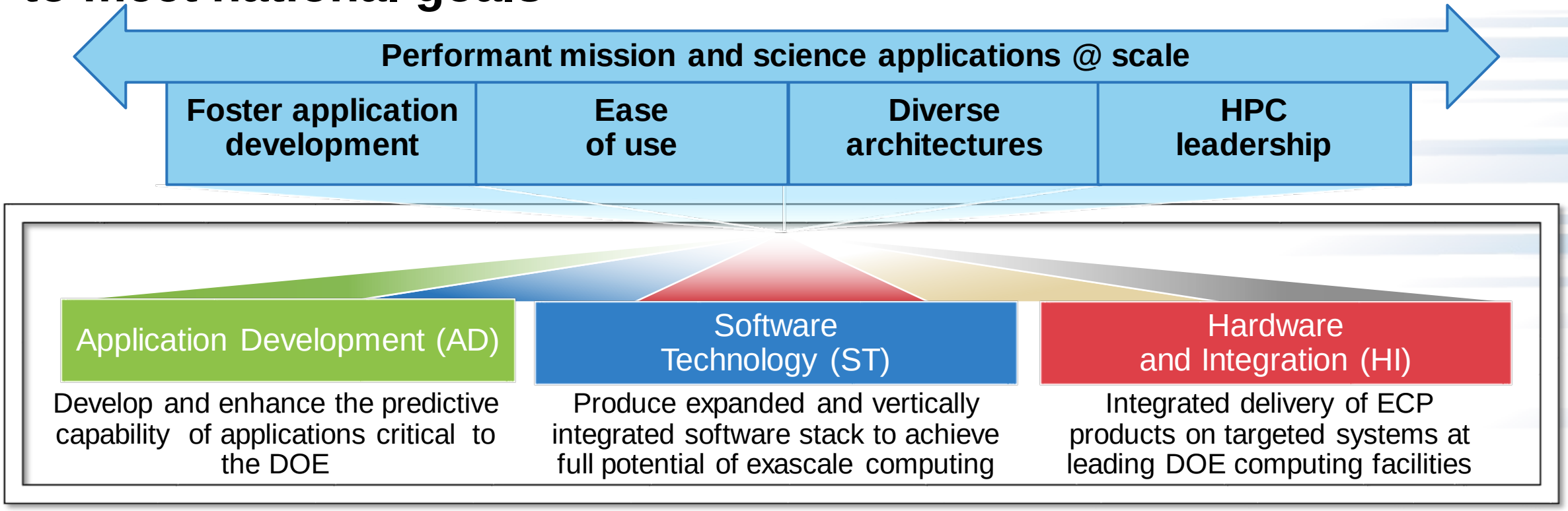
EXASCALE COMPUTING PROJECT

The three technical areas in ECP have the necessary components to meet national goals



25 applications ranging from national security, to energy, earth systems, economic security, materials, and data

89 unique software products spanning programming models and runtimes, math libraries, data and visualization

6 vendors supported by PathForward focused on memory, node, connectivity and reliability advancements; deployment to facilities

Back-up

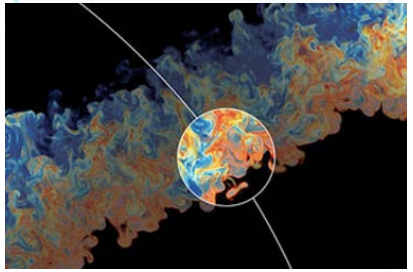
ECP applications target national problems in six areas

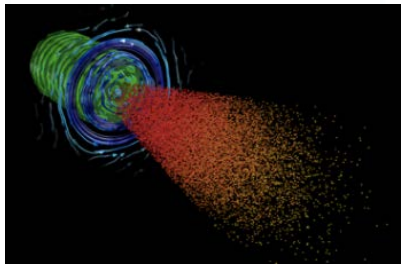
National security

Next-generation, 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

Software Development Kits Progress: Leadership in place, Spack packaging making rapid progress

ECP software projects

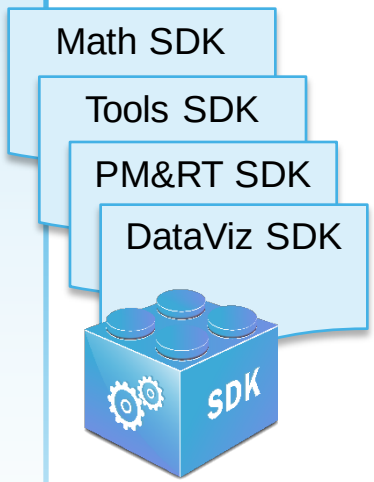
Each project to define (potentially ≥2) release vectors

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



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

SDK Leadership Team: Decades of Software Experience

- **Jim Willenbring – SDK Coordinator and Release Manager**
- **Sameer Shende – Programming Models & Runtimes**
- **Bart Miller – Development Tools**
- **Lois McInnes – Math Libraries**
- **Chuck Atkins - Data & Viz**

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

- Accelerate critical early hardware R&D leading to 3–5 viable exascale system designs for DOE Facilities
- 3-year program ending early in 2020
- Examples of work funded include:
  a) innovative memory architectures
  b) higher-speed interconnects
  c) improved system reliability
  d) approaches for increasing computing power without prohibitive increases in energy demand

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

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