Update on the Exascale Computing Project (ECP)

Paul Messina, ECP Director

HPC User Forum
Santa Fe, New Mexico
April 18, 2017
ECP Aims to Transform the HPC Ecosystem and Make Major Contributions to the Nation

Develop applications to tackle a broad spectrum of mission critical problems of unprecedented complexity

Contribute to the economic competitiveness of the nation

Support national security

Collaborate with vendors to develop a software stack that is both exascale-capable and usable on industrial and academic scale systems

Partner with vendors to develop computer architectures that support exascale applications

Train a next-generation workforce of computational scientists, engineers, and computer scientists

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ECP is a Collaboration Among Six Labs

- ECP project draws from the Nation’s 6 premier computing national laboratories
- An MOA for ECP was signed by each Laboratory Director defining roles and responsibilities
- Project team has decades of experience advancing HPC and deploying first generation HPC systems
- Leadership team expertise spans all ECP activity areas
Four Key Technical Challenges Must be Addressed by the ECP to Deliver Capable Exascale Computing

• Parallelism a thousand-fold greater than today’s systems
• Memory and storage efficiencies consistent with increased computational rates and data movement requirements
• Reliability that enables system adaptation and recovery from faults in much more complex system components and designs
• Energy consumption beyond current industry roadmaps, which would be prohibitively expensive at this scale
What Has Not Changed?

• Scope: ECP’s work encompasses
  – applications,
  – system software,
  – hardware technologies and architectures, and
  – workforce development to meet scientific and national security mission needs.

• The project is executed with a holistic co-design and integration approach
ECP Has Formulated a Holistic Approach That Uses Co-Design and Integration to Achieve Capable Exascale

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<td>Scalable software stack</td>
<td>Hardware technology elements</td>
<td>Integrated exascale supercomputers</td>
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- Correctness
- Visualization
- Data Analysis
- Applications
- Co-Design
- Programming models, development environment, and runtimes
- Math libraries and Frameworks
- Tools
- System software, resource management, threading, scheduling, monitoring, and control
- Memory and Burst buffer
- Data management I/O and file system
- Node OS, runtimes

![Diagram showing the holistic approach and components of the Exascale Computing Project](image)
The New ECP Plan of Record

• A 7-year project that follows the **holistic/co-design** approach, that runs through 2023 (including 12 months of schedule contingency)

• Enable an initial exascale system based on **advanced architecture** 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 supercomputing facilities
What Is a **Capable** Exascale Computing System?

- 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.
Transition to Higher Trajectory with Advanced Architecture

- First exascale advanced architecture system
- Capable exascale systems
- Holistic project required to be on this elevated trajectory

Evolution of today’s architectures is on this trajectory

5X to 10X increase in computing capability from 2017 to 2027.
### Capable Exascale System Applications Will Deliver Broad Coverage of 6 Strategic Pillars

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- Nuclear fission and fusion reactor materials design
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- High-efficiency, low-emission combustion engine and gas turbine design
- Carbon capture and sequestration scaleup
- 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
Enabling GAMESS for Exascale Computing in Chemistry & Materials
Heterogeneous Catalysis on Mesoporous Silica Nanoparticles (MSN)

- MSN: highly effective and selective heterogeneous catalysts for a wide variety of important reactions
- MSN selectivity is provided by “gatekeeper” groups (red arrows) that allow only desired reactants A to enter the pore, keeping undesirable species B from entering the pore
- Presence of solvent adds complexity: Accurate electronic structure calculations are needed to deduce the reaction mechanisms, and to design even more effective catalysts
- Narrow pores (3-5 nm) create a diffusion problem that can prevent product molecules from exiting the pore, hence the reaction dynamics must be studied on a sufficiently realistic cross section of the pore
- Adequate representation of the MSN pore requires ~10-100K thousands of atoms with a reasonable basis set; reliably modeling an entire system involves >1M basis functions
- Understanding the reaction mechanism and dynamics of the system(s) is beyond the scope of current hardware and software – requiring capable exascale
High Performance, Multidisciplinary Simulations for Regional Scale Earthquake Hazard and Risk Assessments

- Ability to accurately simulate the complex processes associated with major earthquakes will become a reality with capable exascale.
- Simulations offer a transformational approach to earthquake hazard and risk assessments.
- Dramatically increase our understanding of earthquake processes.
- Provide improved estimates of the ground motions that can be expected in future earthquakes.
- Time snapshots (map view looking at the surface of the earth) of a simulation of a rupturing earthquake fault and propagation seismic waves.
Exascale Predictive Wind Plant Flow Physics Modeling
Understanding Complex Flow Physics of Whole Wind Plants

• Must advance fundamental understanding of flow physics governing whole wind plant performance: wake formation, complex terrain impacts, turbine-turbine interaction effects
• Greater use of U.S. wind resources for electric power generation (~30% of total) will have profound societal and economic impact: strengthening energy security and reducing greenhouse-gas emissions
• Wide-scale deployment of wind energy on the grid without subsidies is hampered by significant plant-level energy losses by turbine-turbine interactions in complex terrains
• Current methods for modeling wind plant performance are not reliable design tools due to insufficient model fidelity and inadequate treatment of key phenomena
• Exascale-enabled predictive simulations of wind plants composed of \(O(100)\) multi-MW wind turbines sited within a 10 km x 10 km area with complex terrains will provide validated "ground truth" foundation for new turbine design models, wind plant siting, operational controls and reliably integrating wind energy into the grid
Optimizing Stochastic Grid Dynamics at Exascale

Intermittent renewable sources, electric vehicles, and smart loads will vastly change the behavior of the electric power grid and impose new stochastics and dynamics that the grid is not designed for nor can easily accommodate.

- Optimizing such a stochastic and dynamic grid with sufficient reliability and efficiency is a monumental challenge.
- Not solving this problem appropriately or accurately could result in either significantly higher energy cost, or decreased reliability inclusive of more blackouts, or both.
- Power grid data are clearly showing the trend towards dynamics that cannot be ignored and would invalidate the quasi-steady-state assumption used today for both emergency and normal operation.
- The increased uncertainty and dynamics severely strains the analytical workflow that is currently used to obtain the cheapest energy mix at a given level of reliability.
- The current practice is to keep the uncertainty, dynamics and optimization analysis separate, and then to make up for the error by allowing for larger operating margins.
- The cost of these margins is estimated by various sources to be in $5-15B per year for the entire United States.
- The ECP grid dynamics application can result in the best achievable bounds on these errors and thus resulting in potentially billions of dollars a year in savings.

PI: Zhenyu (Henry) Huang (PNNL)
Exascale Deep Learning Enabled Precision Medicine for Cancer
CANDLE accelerates solutions toward three top cancer challenges

- Focus on building a scalable deep neural network code called the CANcer Distributed Learning Environment (CANDLE)
- CANDLE addresses three top challenges of the National Cancer Institute:
  1. Understanding the molecular basis of key protein interactions
  2. Developing predictive models for drug response, and automating the analysis
  3. Extraction of information from millions of cancer patient records to determine optimal cancer treatment strategies
ECP Co-Design Centers

• A Co-Design Center for Online Data Analysis and Reduction at the Exascale (CODAR)
  – **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 (AMReX)
  – **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

• Combinatorial Methods for Enabling Exascale Applications (ExaGraph)
  – **Motif(s)**: Graph traversals; graph matching; graph coloring; graph clustering, including clique enumeration, parallel branch-and-bound, graph partitioning
  – Develop methods and techniques for efficient implementation of key combinatorial (graph) algorithms that play a critical enabling role in numerous scientific applications. The irregular memory access nature of these algorithms makes them difficult algorithmic kernels to implement on parallel systems
Exascale Proxy Applications Suite

Objectives and Scope

- Assemble and curate a proxy app suite composed of proxies developed by other ECP projects that represent the most important features (especially performance) of exascale applications.
- Improve the quality of proxies created by ECP and maximize the benefit received from their use. Set standards for documentation, build and test systems, performance models and evaluations, etc.
- Collect requirements from app teams. Assess gaps between ECP applications and proxy app suite. Ensure proxy suite covers app motifs/requirements.
- Coordinate use of proxy apps in the co-design process. Connect consumers to producers. Promote success stories and correct misuse of proxies.

Links to Other ECP Projects

- **Application Assessment Project**: Cooperatively assess and quantitatively compare applications and proxy apps.
- **Design Space Evaluation Team**: Will need proxies specially adapted for hardware simulators.
- **Path Forward Vendors**: Evaluate needs and provides proxies & support. Review proxy app usage and results.
- **Application Development Projects & Co-Design Centers**: Producers of proxy apps. Close the loop with lessons learned from proxies.
- **Software Technology Projects**: Consumers of proxy apps. Use proxies to understand app requirements and to test and evaluate proposed ST offerings.

Risks and Challenges

- Proxies are too complex for simulators or HW design activity.
- Proxies fail to accurately represent parent apps.
- Proxy app authors unable or unwilling to meet quality and/or support standards.
- Full coverage of DOE workload/motifs produces a large and unwieldy suite.
- Proxy apps misused by consumers.
- Inability to balance agility and stability/quality of proxies.

Development Plan

- Release updated versions of the proxy app suite every six months. This cadence allows for improved coverage and changing needs while maintaining needed stability.
- Annually update guidance on quality standards. Increase rigor of standards.
- Meet with each application project at least quarterly to maintain a catalog of their requirements, proxies, and key questions for which they are seeking assistance.
- Publish annual proxy app producer report with requirements and assessment of proxies in comparison to parent apps.
- Publish annual proxy app consumer report with success stories, surveys of how proxy consumers are using proxies, and plans to satisfy any unmet needs.
IDEAS: Interoperable Design of Extreme-scale Application Software
- Project began in Sept 2014 as ASCR/BER partnership to improve application software productivity, quality, and sustainability

Resources: [https://ideas-productivity.org/resources](https://ideas-productivity.org/resources)

Highlights:
-Whats and HowTo docs: concise characterizations & best practices
  - What is CSE Software Testing?
  - What is Version Control?
  - What is Good Documentation?
  - How to Write Good Documentation
  - How to Add and Improve Testing in a CSE Software Project
  - How to do Version Control with Git in your CSE Project

Webinar series, 2016: Best Practices for HPC Software Developers
- What All Codes Should Do: Overview of Best Practices in HPC Software Development
- Developing, Configuring, Building, and Deploying HPC Software
- Distributed Version Control and Continuous Integration Testing
- Testing and Documenting your Code
- more topics …

IDEAS-ECP team: Catalysts for engaging ECP community on productivity issues
- Partnerships with ECP applications teams
  - Understand productivity bottlenecks and improve software practices
- Collaborate to curate, create, and disseminate software methodologies, processes, and tools that lead to improved scientific software
  - ECP software technologies projects, applications teams, co-design centers, broader community
  - Software Carpentry-type approach to training for extreme-scale software productivity topics
- Web-based hub for collaborative content development and delivery
  - Community-driven collection of resources to help improve scientific software productivity, quality, and sustainability

History and Accessibility

IDEAS-ECP – Advancing Software Productivity for Exascale Applications

Collaborators

• Software Challenges: Exploit massive on-node concurrency and handle disruptive architectural changes while working toward predictive simulations that couple physics, scales, analytics, and more
• Goals: Improve ECP developer productivity and software sustainability, as key aspects of increasing overall scientific productivity
• Strategy: In collaboration with ECP community:
  - Customize and curate methodologies for ECP app productivity & sustainability
  - Create an ECP Application Development Kit of customizable resources for improving scientific software development
  - Partner with ECP application teams on software improvements
  - Training and outreach in partnership with DOE computing facilities

First Year Plan

- MS1/Y1: Templates for Productivity and Sustainability Improvement Plans (PSIPs) and Progress Tracking Cards
  - Framework for software teams to identify, plan, and track improvements in productivity and sustainability
- MS2/Y2: Interviews with Phase-1 ECP applications teams
  - Understand current software practices, productivity challenges, preferred modes of collaboration, and needs for on-line ECP knowledge exchange
  - Determine prioritized needs for productivity improvement; initiate Phase-1 application partnerships
- MS3/Y1: Training and outreach to ECP community on productivity and sustainability
  - Develop and deliver tutorials, webinars, and web content

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SIAM CSE17 Conference (Feb 27-Mar 3, 2017)
Premier CSE Conference (largest SIAM meeting, over 1700 attendees)

- Invited tutorial: CSE Collaboration through Software: Improving Software Productivity and Sustainability
    - Why Effective Software Practices Are Essential for CSE Projects
    - An Introduction to Software Licensing
    - Better (Small) Scientific Software Teams
    - Improving Reproducibility through Better Software Practices
    - Testing of HPC Scientific Software

  Slides and audio: https://doi.org/10.6084/m9.figshare.c.3704287

- Minisymposium and Minisymposterium: Software Productivity and Sustainability for CSE and Data Science
  - Organizers: D. Bernholdt, M. Heroux, D. Katz, A. Logg, L.C. McInnes
  - Slides for presentations: https://doi.org/10.6084/m9.figshare.c.3705946
    - 8 community presentations, including one from the IDEAS team
    - CSE Software Ecosystems: Critical Instruments of Scientific Discovery, L.C. McInnes
  - Posters: https://doi.org/10.6084/m9.figshare.c.3703771
    - 29 posters from the community, including several from members of IDEAS-ECP

- Plenary Presentation: Productive and Sustainable: More Effective CSE, M. Heroux
  - Slides and audio: https://doi.org/10.6084/m9.figshare.4728697

Productivity and Sustainability Improvement Planning Tools
Tools for helping a software team to increase software quality while decreasing the effort, time, and cost to develop, deploy, maintain, and extend software over its intended lifetime.

March 2017: Released PSIP templates & instructions: https://github.com/betterscientificsoftware/PSIP-Tools
Beginning Phase-1 interviews with ECP applications teams: Identify productivity bottlenecks and priorities.

- Slide 1: Document Project Practices Describes current practices and future plans.
- Slide 2: Set Goals Identifies practices ready for improvement.
- Slide 3: Workflows for Productivity and Sustainability Improvement Plans
  - Workflow 1: Documentation. Identify documentation needs.

Productivity and Sustainability Improvement Plan (PSIP): a lightweight iterative workflow to identify, plan, and improve selected practices of a software project.

Other practices: Source management system, documentation, software distribution, issue tracking, developer training, etc.
Argonne Training Program on Extreme-Scale Computing

extremecomputingtraining.anl.gov

What?
An intensive two-week program on HPC methodologies applicable to both current and future supercomputers.

Who?
Open to all doctoral students, postdocs, and scientists interested in conducting CS&E research on large-scale computers.

When?
July 30 - August 11, 2017

Where?
Q Center, St Charles, IL (USA)

# of Applicants
Call closed March 10. Reviewing 167 applicants from 95 institutions worldwide. Making final selections now. Expect to select up to 70 participants.
Conceptual ECP Software Stack

**Correctness**
- Programming Models, Development Environment, Runtime

**Visualization**
- Math Libraries & Frameworks

**Data Analysis**
- Tools

**Resilience**
- System Software, Resource Management, Threading, Scheduling, Monitoring and Control
- Node OS, Low-level Runtime

**Applications**
- Memory & Burst Buffer

**Co-Design**
- Data Management, I/O & File System

**Workflows**

**Hardware interfaces**
Current Set of ST Projects Mapped to Software Stack

Correctness
- VTK-m, ALPINE, Cinema

Visualization
- ALPINE, Cinema

Data Analysis
- ALPINE, Cinema

Applications
- VTK-m, ALPINE, Cinema

Co-Design
- ALPINE, Cinema

Math Libraries/Frameworks
- ScaLAPACK, DPLASMA, MAGMA, PETSc/TAO, Trilinos, xSDK, PEEKS, SuperLU, STRUMPACK, SUNDIALS, DTK, TASMANIAN, AMP, FleCSI, KokkosKernels, Agile Comp., DataProp, MFEM

Tools
- PAPI, HPCToolkit, Darshan, Perf.
- portability (ROSE, Autotuning, PROTEAS), TAU, Compilers (LLVM, Flang), Mitos, MemAxes, Caliper, AID, Quo, Perf. Anal.

Memory and Burst buffer
- Chkpt/Restart (VeloC, UNIFYCR), API and library for complex memory hierarchy (SICM)

Data Management, I/O and File System
- ExaHDF5, PnetCDF, ROMIO, ADIOS, Chkpt/Restart (VeloC, UNIFYCR), Compression (EZ, ZFP), I/O services, HXHIM, SIO
- Components, DataWarehouse

System Software, Resource Management
- Threading, Scheduling, Monitoring, and Control
- Argo Global OS, Qthreads, Flux, Spindle, BEE, Spack, Sonar

Node OS, low-level runtimes
- Argo OS enhancements, SNL OS project

Resilience
- Checkpoint/Restart (VeloC, UNIFYCR), FSEFI, Fault Modeling

Programming Models, Development Environment, and Runtimes
- MPI (MPICH, Open MPI), OpenMP, OpenACC, PGAS (UPC++, Global Arrays), Task-Based (PaRSEC, Legion, DARMA), RAJA, Kokkos, OMPTD, Power steering

Hardware interface
Co-Design in Action

• Design, implement, and demonstrate new prototype APIs to facilitate improved coordination between MPI and OpenMP runtimes for use of threads, message delivery, and rank/endpoint placement. (Due 12/31/2018)

• Execution Plan:
  – Interact with ECP AD teams to identify requirements about runtime coordination.
  – Interact with appropriate ECP ST teams to define coordination APIs for MPI and OpenMP (and other) runtimes.
  – Experiment and demonstrate the benefit running an ECP application or mini-application running on the ECP testbeds
Hardware Technology Activities

• PathForward: support DOE-vendor collaborative R&D activities required to develop exascale systems with at least two diverse architectural features; quote from RFP:
  – PathForward seeks solutions that will improve application performance and developer productivity while maximizing energy efficiency and reliability of exascale systems.

• Design Space Evaluation
  – Apply laboratory architectural analysis capabilities and Abstract Machine Models to PathForward designs to support ECP co-design interactions
PathForward Status

• Five PathForward Projects have received DOE/NNSA HQ’s fully signed and executed Coordination and Approval Document (CAP)
  – 4 contracts are fully signed
  – 1 is being routed for signatures by the LLNL Lab Director - Goldstein and his counterparts at the Vendors to fully execute these contracts – anticipated by COB April 14, 2017

• The last PathForward contract is at DOE/NNSA for approval

• The HT leadership team is developing a tiered communication plan to:
  – Introduce the PathForward projects to the rest of ECP, and
  – Establish high-quality co-design collaborations with interested lab-led ECP projects
## Design Space Evaluation: Technology Coverage Areas

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<td>Ray Bair</td>
<td>ROSS/CODES</td>
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<td><strong>LANL</strong></td>
<td>Jeff Kuehn</td>
<td>CoNCEPTual</td>
<td>Byfl</td>
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<td><strong>LBNL</strong></td>
<td>David Donofrio</td>
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<td>ExaSAT, Roofline Toolkit</td>
<td>Gem5, OpenSOC</td>
<td>Co-lead AMM v3</td>
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<td><strong>LLNL</strong></td>
<td>Robin Goldstone</td>
<td>LiME</td>
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<td><strong>ORNL</strong></td>
<td>Jeff Vetter</td>
<td>Blackcomb</td>
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<td><strong>PNNL</strong></td>
<td>Darren Kerbyson</td>
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<td><strong>SNL</strong></td>
<td>Rob Hoekstra</td>
<td>SST: VaultSimC, MemHierarchy</td>
<td>SST, Merlin, Ember, Firefly</td>
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<td>SST: Miranda, Ariel, Gem5</td>
<td>Co-lead AMM v3</td>
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</table>
ECP teams begin work on Office of Science systems via early access, ALCC awards, and testbeds

**Access to Office of Science Systems**

**NERSC’s Cori II**
- Cori II early access
  - Shared access with other users
  - Intel Xeon Phi (KNL) nodes
  - Through June 30, 2017

**OLCF’s Titan**
- 2016 ALCC Reserve Award to ECP
  - 13M Titan-core hours
  - March 30 to June 30, 2017
  - 10 AD, 6 ST, and 1 HT teams are getting access

**Access to testbeds supported with ECP funds**

**ALCF’s Theta**
- ECP allocation is 37+M hours on Theta for 2017
  - Intel Xeon Phi cpus
  - 3,624 nodes
  - 64 core processor per node

**OLCF’s Summitdev**
- ECP allocation is the equivalent of 18 nodes on Summitdev
  - Power 8+
  - NVIDIA Pascal GPGPUs
  - NVLINK1

ECP submitted an application to the 2017 ASCR Leadership Computing Challenge (ALCC) for time of Titan, Mira, Theta, Cori, and Edison
Communications and Outreach

- We have a website
  - www.ExascaleProject.org

- A newsletter *The ECP Update* has been launched
  - https://exascaleproject.org/newsletter/ecp-update-1/

- First PI meeting November 29 – December 1, 2016
  - 80+ PIs

- First Annual Meeting January 31 – February 2, 2017
  - 450+ participants
  - Focused on co-design and integration planning

- Industry Council established, first meeting March 6-7, 2017
800 Researchers
26 Application Development Projects
66 Software Development Projects
5 Co-Design Centers
Thank you!