Welcome to today’s ACM TechTalk, “The Exascale Computing Project and the Future of HPC.” The presentation starts at the top of the hour and lasts 60 minutes. Audio and video will automatically play throughout the event. On the bottom panel you’ll find a number of widgets, including Twitter and Sharing apps.

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The U.S. Department of Energy
Exascale Computing Project

Douglas B. Kothe (Oak Ridge National Laboratory)
Director, Exascale Computing Project (ECP)
kophe@ornl.gov

Association for Computing Machinery (ACM) Tech Talk
April 30, 2019
ACM Highlights

• Learning Center tools for professional development: http://learning.acm.org
  • The Safari Learning Platform featuring the entire Safari collection of nearly 50,000 technical books, video courses, O’Reilly conference videos, learning paths, tutorials, case studies
  • 1,800+ Skillsoft courses, 4,800+ online books, and 30,000+ task-based short videos for software professionals covering programming, data management, DevOps, cybersecurity, networking, project management, and more; including training toward top vendor certifications such as AWS, CEH, Cisco, CISSP, CompTIA, Oracle, RedHat, PMI.
  • 1,200+ books from Elsevier on the ScienceDirect platform (including Morgan Kaufmann and Syngress titles)
  • TechTalks from thought leaders and top practitioners
  • Podcast interviews with innovators, entrepreneurs, and award winners

• Popular publications:
  • Flagship Communications of the ACM (CACM) magazine: http://cacm.acm.org
  • ACM Queue magazine for practitioners: http://queue.acm.org

• The ACM Code of Ethics, a set of principles and guidelines designed to help computing professionals make ethically responsible decisions in professional practice: https://ethics.acm.org

• ACM Digital Library, the world’s most comprehensive database of computing literature: http://dl.acm.org

• International conferences that draw leading experts on a broad spectrum of computing topics: http://www.acm.org/conferences

• Prestigious awards, including the ACM A.M. Turing and ACM Prize in Computing: http://awards.acm.org

• And much more... http://www.acm.org.
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Talk Back

• Tweet your favorite quotes from today’s presentation with hashtag #ACMLearning

• Submit questions and comments via Twitter to @acmeducation – we’re reading them!

• The ACM Discourse Page is available for post-talk discussion – https://on.acm.org
The U.S. Department of Energy
Exascale Computing Project

Douglas B. Kothe (Oak Ridge National Laboratory)
Director, Exascale Computing Project (ECP)
kothe@ornl.gov

Association for Computing Machinery (ACM) Tech Talk
April 30, 2019
The Exascale Computing Project (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.
DOE Exascale Program: The Exascale Computing Initiative (ECI)

Three Major Components of the ECI

Exascale Computing Project (ECP)

- **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

Selected program office application development (BER, BES, NNSA)

Exascale system procurement projects & facilities
- ALCF-3 (Aurora)
- OLCF-5 (Frontier)
- ASC ATS-4 (El Capitan)
What is a “capable” exascale computing ecosystem?

**Hardware**
- At least two diverse system architectures
- Delivers 50x the performance of today’s 20 petaflop systems and 5x the performance of Summit, Oak Ridge National Laboratory’s supercomputer—i.e., allows at least a quintillion floating point operations per second
- Functions with sufficient resiliency: an average fault rate of ≤1 per week

**Software**
- Includes a software stack that meets the needs of a broad spectrum of applications and workloads

**Applications**
- Supports a wide range of applications that deliver high-fidelity solutions in less time to problems of greater complexity

_Exascale means real capability improvement in the science we can do, and how fast we can do it_
Why high performance computing is hard, and getting harder

- Applications need to find more and more concurrency to keep up.
- Moving data becoming increasingly costly relative to computation.
- I/O, vis, analysis becoming major bottlenecks
- Hardware landscape getting more diverse, future architectures have more uncertainty.
- New programming models are being developed to supplement traditional MPI+X approaches:
  - On-node: OCCA, Kokkos, RAJA, OpenACC, OpenCL, Swift
  - Inter-node: Legion, UPC++, Global Arrays

Preparing applications for new architectures can be difficult and time-consuming, working together and learning from each other is crucial
ECP by the Numbers

A seven-year, $1.7 B R&D effort that launched in 2016

- 7 YEARS
- $1.7B

- 6 CORE DOE LABS
  - Six core DOE National Laboratories: Argonne, Lawrence Berkeley, Lawrence Livermore, Oak Ridge, Sandia, Los Alamos
    - Staff from most of the 17 DOE national laboratories take part in the project

- 3 FOCUS AREAS
  - Three technical focus areas: Hardware and Integration, Software Technology, Application Development supported by a Project Management Office

- 100 R&D TEAMS
- 1000 RESEARCHERS

More than 100 top-notch R&D teams

Hundreds of consequential milestones delivered on schedule and within budget since project inception
Vision: Exascale Computing Project (ECP) Lifts all U.S. High Performance Computing to a New Trajectory

ECP enables all future U.S. HPC systems to be on this roadmap.

Today’s HPC roadmap achieves capable exascale 2027.

ECP benefits will also flow down to commodity computing.
Department of Energy (DOE) Roadmap to Exascale Systems
An impressive, productive lineup of *accelerated node* systems supporting DOE’s mission

<table>
<thead>
<tr>
<th>Pre-Exascale Systems [Aggregate Linpack (Rmax) = 323 PF]</th>
<th>First U.S. Exascale Systems</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>2012</strong></td>
<td><strong>2016</strong></td>
</tr>
<tr>
<td>Titan (9)</td>
<td>ORNL IBM/AMD/NVIDIA</td>
</tr>
<tr>
<td>Mira (21)</td>
<td>ANL IBM BG/Q</td>
</tr>
<tr>
<td>LBNL Cray/Intel Xeon/KNL</td>
<td>Cori (12)</td>
</tr>
<tr>
<td>Sequoia (10)</td>
<td>LLNL IBM BG/Q</td>
</tr>
<tr>
<td>LANL/SNL Cray/Intel Xeon/KNL</td>
<td>LLNL TBD</td>
</tr>
</tbody>
</table>

First U.S. Exascale Systems:
- Sierra (2)  
- FLX (TBD)  
- El Capitan (TBD)
The Summit System @ ORNL
#1 on Top 500

**System Performance**
- Peak of 200 Petaflops (FP\textsubscript{64}) for modeling & simulation
- Peak of 3.3 ExaOps (FP\textsubscript{16}) for data analytics and artificial intelligence
- Max power 13 MW

**The system includes**
- 4,608 nodes
- Dual-rail Mellanox EDR InfiniBand network
- 250 PB IBM file system transferring data at 2.5 TB/s

**Each node has**
- 2 IBM POWER9 processors
- 6 NVIDIA Tesla V100 GPUs
- 608 GB of fast memory (96 GB HBM2 + 512 GB DDR4)
- 1.6 TB of NV memory
## System specifications

- Peak performance of 125 petaflops for modeling and simulation
- Memory: 1.38 petabytes
- 8,640 Central Processing Units (CPUs)
- 17,280 Graphics Processing Units (GPUs)
- Power consumption: 11 megawatts

## Each node has

- 2 IBM POWER9 processors
- 4 NVIDIA Tesla V100 GPUs
- 320 GiB of fast memory
  - 256 GiB DDR4
  - 64 GiB HBM2
- 1.6 TB of NVMe memory

## The system includes

- 4,320 nodes
- 2:1 tapered Mellanox EDR InfiniBand tree topology (50% global bandwidth) with dual-port HCA per node
- 154 PB IBM Spectrum Scale file system with 1.54 TB/s R/W bandwidth

---

**Sierra supports LLNL’s national security mission and ability to advance science in the public interest**
ECP Organization

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**Lori Diachin**, LLNL
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Kim Milburn, Finance Officer
Susan Ochs, Partnerships
Michael Johnson, Legal
and Points of Contacts at the Core Laboratories

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**Laboratory Operations Task Force (LOTF)**

**Laboratory Operations**

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**ECP Organization**
ECP Industry Council

Mission

Meet to provide advice and feedback to the ECP Director on:
• ECP project scope and strategic direction
• Technical approaches
• Progress on milestones and accomplishments
• Industrial requirements
• Impact on industrial competitiveness

Membership

Executives of U.S. companies (generally VPs of R&D, CTOs, CIOs) for whom HPC is a critical research and production tool
Executives of U.S. independent software vendors (ISVs)

DOE projects and programs historically fall short in executing mutually beneficial collaborations with industry. ECP is committed to working closely with industry: we believe it will make us both better.
ECP Industry Council Member Organizations
ECP Work Breakdown Structure (WBS)

Key leaders at WBS Level 1, 2, 3

Exascale Computing Project
2.0
Kothe (ORNL)

Project Management
2.1
Boudwin (ORNL)

Project Planning and Management
2.1.1
Boudwin (ORNL)

Project Controls and Risk Management
2.1.2
Middlebrook (ORNL)

Business Management
2.1.3
Hulsey (ORNL)

Procurement Management
2.1.4
Besancenez (ORNL)

Information Technology and Quality Management
2.1.5
Collins (ORNL)

Communications and Outreach
2.1.6
Bernhardt (ORNL)

Application Development
2.2
Siegel (ANL)

Chemistry and Materials Applications
2.2.1
Deslippe (LBL)

Energy Applications
2.2.2
Evans (ORNL)

Earth and Space Science Applications
2.2.3
Dubey (ANL)

Data Analytics and Optimization Applications
2.2.4
Hart (SNL)

National Security Applications
2.2.5
Francois (LANL)

Co-Design
2.2.6
Colella (LBL)

Software Technology
2.3
Heroux (SNL)

Programming Models and Runtimes
2.3.1
Thakur (ANL)

Development Tools
2.3.2
Vetter (ORNL)

Mathematical Libraries
2.3.3
McInnes (ANL)

Data and Visualization
2.3.4
Ahrens (LANL)

Software Ecosystem and Delivery
2.3.5
Munson (ANL)

NNSA Software Technologies
2.3.6
Neely (ANL)

Hardware and Integration
2.4
Quinn (LLNL)

PathForward
2.4.1
de Supinski (LLNL)

Hardware Evaluation
2.4.2
Hammond (SNL)

Application Integration at Facilities
2.4.3
Hill (ORNL)

Software Deployment at Facilities
2.4.4
Montoya (LANL)

Facility Resource Utilization
2.4.5
White (ORNL)

Training and Productivity
2.4.6
Barker (ORNL)

ECP would fail without its world-class Principal Investigators (PIs) leading the 100+ WBS Level 4 projects responsible for executing ECP’s RD&D activities.
The three technical areas in ECP have the necessary components to meet national goals.

Foster application development
Ease of use
Diverse architectures
HPC leadership

Performant mission and science applications @ scale

Application Development (AD)
Develop and enhance the predictive capability of applications critical to the DOE

Software Technology (ST)
Produce expanded and vertically integrated software stack to achieve full potential of exascale computing

Hardware and Integration (HI)
Integrated delivery of ECP products on targeted systems at leading DOE computing facilities

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

80+ unique software products spanning programming models and run times, math libraries, data and visualization

6 vendors supported by PathForward focused on memory, node, connectivity advancements; deployment to facilities
The three technical areas in ECP have the necessary components to address these challenges and meet national goals.

Performant mission and science applications @ scale

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6 vendors supported by PathForward focused on memory, node, connectivity advancements; deployment to facilities
Goal
Develop and enhance the predictive capability of applications critical to DOE across science, energy, and national security mission space

Targeted development of requirements-based methods
Integration of software and hardware via co-design methodologies
Systematic improvement of exascale readiness and utilization
Demonstration and assessment of effective software integration

Chemistry and Materials  Earth and Space Science  Energy  Data Analytics and Optimization  National Security  Co-Design
Hardware realities are forcing new thinking of algorithmic implementations and the move to new algorithms

**Algorithmic Implementations**
- Reduced communication/data movement
  - Sparse linear algebra, Linpack, etc.
- Much greater locality awareness
  - Likely must be exposed by programming model
- Much higher cost of global synchronization
  - Favor maxim asynchrony where physics allows
- Value to mixed precision where possible
  - Huge role in AI, harder to pin down for PDEs
- Fault resilience?
  - Likely handled outside of applications

**New Algorithms**
- Adopting Monte Carlo vs. Deterministic approaches
- Exchanging on-the-fly recomputation vs. data table lookup (e.g. neutron cross sections)
- Moving to higher-order methods (e.g. CFD)
- Particle algorithms that favor collecting similar events together rather than parallelism though individual histories
<table>
<thead>
<tr>
<th>National security</th>
<th>Energy security</th>
<th>Economic security</th>
<th>Scientific discovery</th>
<th>Earth system</th>
<th>Health care</th>
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<tr>
<td>Stockpile stewardship</td>
<td>Turbine wind plant efficiency</td>
<td>Additive manufacturing of qualifiable metal parts</td>
<td>Find, predict, and control materials and properties</td>
<td>Accurate regional impact assessments in Earth system models</td>
<td>Accelerate and translate cancer research</td>
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<tr>
<td>Next-generation electromagnetics simulation of hostile environment and virtual flight testing for hypersonic re-entry vehicles</td>
<td>High-efficiency, low-emission combustion engine and gas turbine design</td>
<td>Reliable and efficient planning of the power grid</td>
<td>Cosmological probe of the standard model of particle physics</td>
<td>Stress-resistant crop analysis and catalytic conversion of biomass-derived alcohols</td>
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<td>Materials design for extreme environments of nuclear fission and fusion reactors</td>
<td>Seismic hazard risk assessment</td>
<td>Validate fundamental laws of nature</td>
<td>Metagenomics for analysis of biogeochemical cycles, climate change, environmental remediation</td>
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<td>Design and commercialization of Small Modular Reactors</td>
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<td>Demystify origin of chemical elements</td>
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<td>Subsurface use for carbon capture, petroleum extraction, waste disposal</td>
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<td>Light source-enabled analysis of protein and molecular structure and design</td>
<td>Whole-device model of magnetically confined fusion plasmas</td>
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<td>Scale-up of clean fossil fuel combustion</td>
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<td>Biofuel catalyst design</td>
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## Application Co-Design

Develop efficient exascale libraries that address computational motifs common to multiple application projects

<table>
<thead>
<tr>
<th>Project</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CODAR</td>
<td>Advance understanding of the constraints, mappings, and configuration choices that determine interactions of applications, data analysis and reduction, and exascale platforms</td>
</tr>
<tr>
<td>COPA</td>
<td>Create co-designed numerical recipes for particle-based methods that meet application team requirements within design space of STs and subject to constraints of exascale platforms</td>
</tr>
<tr>
<td>AMReX</td>
<td>Build framework to support development of block-structured adaptive mesh refinement algorithms for solving systems of partial differential equations on exascale architectures</td>
</tr>
<tr>
<td>CEED</td>
<td>Develop next-generation discretization software and algorithms that will enable a wide range of finite element applications to run efficiently on future hardware</td>
</tr>
<tr>
<td>ExaGraph</td>
<td>Develop methods and techniques for efficient implementation of key combinatorial (graph) algorithms</td>
</tr>
<tr>
<td>ExaLearn</td>
<td>Target learning methods to aid application and experimental facility workflows: deep neural networks (RNNs, CNNs, GANs), kernel &amp; tensor methods, decision trees, ensemble methods, graph models, reinforcement learning</td>
</tr>
<tr>
<td>Proxy Apps</td>
<td>Improve the quality of proxy applications created by ECP and maximize the benefit received from their use. Maintain and distribute ECP Proxy App Suite.</td>
</tr>
</tbody>
</table>
Center for Efficient Exascale Discretizations (CEED)
Co-Design of unstructured mesh, FE-based PDE discretizations

Goal
- Develop algorithms and software to enable more efficient HPC simulations in a wide range of PDE-based science applications.
- Focus on next-generation discretization methods: high-order finite elements on general unstructured grids.
- Target high performance on a variety of hardware: CPU, GPU, A21 in a flexible and user-friendly way.

Approach
- Performance-enabling math foundation: high-order operator decomposition
- Fast kernels: CEED benchmarks, combine expertise, engage community
- Library integration: high-level API (MFEM, Nek5000), low-level API (libCEED)
- Application engagement: liaisons, CEED miniapps (Nekbone, Laghos)
- Collaborate with ECP/ST, broader community (SciDAC, xSDK, deal.ii, …)
- High-order software ecosystem: operator format, FMS, matrix-free solvers

PI: Tzanio Kolev (LLNL)
CEED is targeting several ECP applications

- Compressible flow (MARBL)
- Climate (E3SM)
- Modular Nuclear Reactors (ExaSMR)
- Wind Energy (ExaWind)
- Urban systems (Urban)
- Additive Manufacturing (ExaAM)
- Magnetic Fusion (WDMApp)
- Subsurface (GEOS)
- Combustion (Nek5000)

PI: Tzanio Kolev (LLNL)
ECP’s Adaptive Mesh Refinement Co-Design Center: AMReX

- Develop and deploy software to support block-structured adaptive mesh refinement on exascale architectures
  - Core AMR functionality
  - Particles coupled to AMR meshes
  - Embedded boundary (EB) representation of complex geometry
  - Linear solvers
  - Supports two modalities of use
    - Library support for AMR
    - Framework for constructing AMR applications

- Provide direct support to ECP applications that need AMR for their application

- Evaluate software technologies and integrate with AMReX when appropriate

- Interact with hardware technologies / vendors

PI: John Bell (LBNL)
ECP’s Co-Design Center for Online Data Analysis and Reduction
CODAR

Traditional approach: Compute...output...analyze [offline]
Write simulation output to secondary storage; read back for analysis
Decimate in time when simulation output rate exceeds output rate of computer

New approach: Online data analysis and reduction
Co-optimize simulation, analysis, reduction for performance and information output
Substitute CPU cycles for I/O, via online data (de)compression and/or online data analysis

Provide the right information at the right time and place to accelerate discovery!

**Goal:** Replace the activities in HPC workflow that have been mediated through file I/O with in-situ methods / workflows. Data reduction, analysis, code coupling, aggregation (e.g. parameter studies).

**Cross-cutting tools:**
- Workflow setup, manager (Cheetah, Savanna); Data coupler (ADIOS-SST); Compression methods (MGARD, FTK, SZ), compression checker (Z-checker)
- Performance tools (TAU, Chimbuco, SOSFlow)

PI: Ian Foster (ANL)
**Goal:** Develop algorithms and software for particle methods,

**Cross-cutting capabilities:**
- Specialized solvers for quantum molecular dynamics (Progress / BML).
- Performance-portable libraries for classical particle methods in MD, PDE (Cabana).
- FFT-based Poisson solvers for long-range forces.

**Technical approach:**
- High-level C++ APIs, plus a Fortran interface (Cabana).
- Leverage existing / planned FFT software.
- Extensive use of miniapps / proxy apps as part of the development process.

PI: Sue Mniszewski (LANL) recently replacing Tim Germann (LANL), who is taking on a larger role in ECP
ECP’s Co-Design Center for Machine Learning: ExaLearn
Bringing together experts from 8 DOE Laboratories

• AI has the potential to accelerate scientific discovery or enable prediction in areas currently too complex for direct simulation (ML for HPC and HPC for ML)

• AI use cases of interest to ECP:
  – *Classification and regression*, including but not limited to image classification and analysis, e.g. scientific data output from DOE experimental facilities or from national security programs.
  – *Surrogate models* in high-fidelity and multiscale simulations, including uncertainty quantification and error estimation.
  – *Structure-to-function relationships*, including genome-to-phenome, the prediction of materials performance based on atomistic structures, or the prediction of performance margins based on manufacturing data.
  – *Control systems*, e.g., for wind plants, nuclear power plants, experimental steering and autonomous vehicles.
  – *Inverse problems* and optimization. This area would include, for example, inverse imaging and materials design.

• Areas in need of research
  – Data quality and statistics
  – Learning algorithms
  – Physics-Informed AI
  – Verification and Validation
  – Performance and scalability
  – Workflow and deployment

**Expected Work Product: A Toolset That . . .**

• Has a line-of-sight to exascale computing, e.g. through using exascale platforms directly, or providing essential components to an exascale workflow
• Does not replicate capabilities easily obtainable from existing, widely-available packages
• Builds in domain knowledge where possible “Physics”-based ML and AI
• Quantifies uncertainty in predictive capacity
• Is interpretable
• Is reproducible
• Tracks provenance

PI: Frank Alexander (BNL)
Machine Learning in the Light Source Workflow

Beam Line Control and Data Acquisition (DAQ)
- DAQ
- Data TB/s
- ML to control the beam line parameters
- ML at DAQ to control data as it is acquired
- ML to design light source beam lines

Local Systems
- Compressor Nodes
- Network Monitoring and Fast Feedback
- Online Monitoring and Fast Feedback
- Data
- Model
- ML for data compression (e.g., hit finding). Use models learned remotely.
- ML for fast analysis at the experimental facility. Uses models learned remotely.

Network
- Model
- 10 GB/s - 1Tb/s
- ML networks for image classification, feature detection, and solving inverse problems (how to change experiment parameters to get desired experiment result)

Remote Exascale HPC
- Exascale Supercomputer
- Data
- Model
- Model
- Model
- Simulate experiments, beam line control, and diffraction images at scale to create data for training

PI: Frank Alexander (BNL)
Exascale apps can deliver transformative products and solutions

**ExaWind**

**Turbine Wind Plant Efficiency**
(Mike Sprague, NREL)

- Harden wind plant design and layout against energy loss susceptibility
- Increase penetration of wind energy

*Challenges*: linear solver perf in strong scale limit; manipulation of large meshes; overset of structured & unstructured grids; communication-avoiding linear solvers

**ExaAM**

**Additive Manufacturing (AM) of Qualifiable Metal Parts**
(John Turner, ORNL)

- Accelerate the widespread adoption of AM by enabling routine fabrication of qualifiable metal parts

*Challenges*: capturing unresolved physics; multi-grid linear solver performance; coupled physics

**EQSIM**

**Earthquake Hazard Risk Assessment**
(David McCallen, LBNL)

- Replace conservative and costly earthquake retrofits with safe purpose-fit retrofits and designs

*Challenges*: full waveform inversion algorithms
Eqsim: Understanding and predicting earthquake phenomenon

Site ground motions

Vertical motion

Horizontal motion

Surface waves

Body waves

Site

Path

Source

Ground motions tend to be very site specific

PI: David McCallen (LBNL)
EQSIM: The Exascale “Big Lift” – regional ground motion simulations at engineering frequencies

- Pipelines
- Long-span Bridges
- Tall Buildings
- Low-rise Buildings and Industrial Facilities
- Energy System Components
- Nuclear Power Equipment

Exascale objective

Range of historical ground motion simulations

Doubling the frequency resolution = 16X computational effort!

PI: David McCallen (LBNL)
EQSIM: Advancing geophysics and infrastructure applications

**EQSIM**

- **Earthquake Hazard**
- **Earthquake Risk**

**SW4** – 4th order finite difference geophysics code for wave propagation

**NEVADA & MSESSI** – finite deformation, inelastic Finite Element codes for structures and soils

Weak Coupling

Strong Coupling

PI: David McCallen (LBNL)
• RAJA is a C++ abstraction layer developed at LLNL.

• Same C++ source code for OpenMP and CUDA backends
  – Machine specific options in a policy file

• Coding complexity similar to OpenMP

• Currently running on the Sierra GPU machine at LLNL with low overhead

• August-2018: 1,024 nodes of Sierra, 4,096 GPUs, 6.9 Hz, giving an overall performance (Figure or Merit) improvement of 24.2
Exascale apps can deliver transformative products and solutions

**MFIX-Exa**

Scale-up of Clean Fossil Fuel Combustion
(Madhava Syamlal, NETL)

- Commercial-scale demonstration of transformational energy technologies – curbing CO₂ emissions at fossil fuel power plants by 2030

*Challenges:* load balancing; strong scaling thru transients

**GAMESS**

Biofuel Catalyst Design
(Mark Gordon, Ames)

- Design more robust and selective catalysts orders of magnitude more efficient at temperatures hundreds of degrees lower

*Challenges:* weak scaling of overall problem; on-node performance of molecular fragments

**EXAALT**

Materials for Extreme Environments
(Danny Perez, LANL)

- Simultaneously address time, length, and accuracy requirements for predictive microstructural evolution of materials

*Challenges:* SNAP kernel efficiency on accelerators; efficiency of DFTB application on accelerators
### ExaSMR

**Design and Commercialization of Small Modular Reactors**  
(Steve Hamilton, ORNL)

- Virtual test reactor for advanced designs via experimental-quality simulations of reactor behavior

**Challenges:** existing GPU-based MC algorithms require rework for hardware less performant for latency-bound algorithms with thread divergence; performance portability with OCCA & OpenACC not achievable; insufficient node memory for adequate CFD + MC coupling

### Subsurface

**Carbon Capture, Fossil Fuel Extraction, Waste Disposal**  
(Carl Steefel, LBNL)

- Reliably guide safe long-term consequential decisions about storage, sequestration, and exploration

**Challenges:** performance of Lagrangian geomechanics; adequacy of Lagrangian crack mechanics) + Eulerian (reaction, advection, diffusion) models; parallel HDF5 for coupling

### QMCPACK

**Materials for Extreme Environments**  
(Paul Kent, ORNL)

- Find, predict and control materials and properties at the quantum level with unprecedented accuracy for the design novel materials that rely on metal to insulator transitions for high performance electronics, sensing, storage

**Challenges:** minimizing on-node memory usage; parallel on-node performance of Markov-chain Monte Carlo
Efficient Monte Carlo on accelerator–based architectures

**Challenge**: Monte Carlo neutron particle transport is a stochastic method

- Not amenable to single kernel optimization – no “high cost” kernel to optimize
- Independent random walks are not readily amenable to SIMT algorithms
- Sampling data (interaction cross sections) are:
  - randomly accessed
  - characterized by detailed structure
  - in standard applications consist of large point-wise representations (>1 – 5 GB per temperature point)

Distribution of history lengths in SMR core

PI: Steve Hamilton (ORNL)
The Monte Carlo algorithm maps well to GPUs after changing from a history-based to an event-based algorithm

- Reduce thread divergence – change from history- to event-based algorithm
- Flatten algorithms to reduce kernel size; smaller kernels = higher occupancy
- Partition events based on fuel and non-fuel regions
- Debuted first comprehensive windowed multipole library for nuclear data (with temp correction)
- MC performance on Summit ~16x that achieved on Titan for the same algorithm
  - Significantly out-pacing gains in machine theoretical peak (7x on LINPACK)
- Overall MC performance has progressed from 15M to 600M particles/s!

PI: Steve Hamilton (ORNL)
Exascale apps can deliver transformative products and solutions

ExaSGD

Reliable and Efficient Planning of the Power Grid
(Henry Huang, PNNL)

- Optimize power grid planning, operation, control and improve reliability and efficiency

Challenges: parallel performance of nonlinear optimization based on discrete algebraic equations and possible mixed-integer programming

Combustion-PELE

High-Efficiency, Low-Emission Combustion Engine Design
(Jackie Chen, SNL)

- Reduce or eliminate current cut-and-try approaches for combustion system design

Challenges: performance of chemistry ODE integration on accelerated architectures; linear solver performance for low-Mach algorithm; explicit LES/DNS algorithm not stable
Pele Code Design Overview

- Baseline algorithm design for multicomponent flow with stiff reactions, AMR
  - **PeleC**: Comparable advection, diffusion time scales, motivates IMEX-type scheme based on Spectral Deferred Corrections (SDC) with time-implicit chemistry
    - Robust highly efficient time-explicit Godunov-type upwind advection, simple centered diffusion
    - BDF-style implicit chemistry ODE integration, with sources that approximate the other processes
  - **PeleLM**: Acoustics filtered away analytically, but still want robust, time-explicit advection
    - Chemistry and diffusion are now time-implicit – iterative timestep simultaneously incorporates flow constraint (constant pressure), mutually coupled species/energy diffusion and chemistry. Entire system evolved stably on slower advection time scales across AMR grid hierarchy

- SDC-based iterative timestep – treats each process essentially independently, with accelerated iteration to couple everything together efficiently

- Robust baseline allows stable, well-behaved extensible time step
  - Switch 2nd order advection scheme with more accurate 4th order algorithm
  - Option for “destiffened” chemistry model that allows highly efficient time-explicit advance
  - Robust to other, potentially stiff, tightly coupled processes, such as sprays, radiation, soot, etc

PI: Jackie Chen (SNL)
## Exascale apps can deliver transformative products and solutions

<table>
<thead>
<tr>
<th>E3SM-MMF</th>
<th>NWChemEx</th>
<th>ExaBiome</th>
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<tbody>
<tr>
<td><strong>Accurate Regional Impact Assessment in Earth Systems</strong> (Mark Taylor, SNL)</td>
<td><strong>Catalytic Conversion of Biomass-Derived Alcohols</strong> (Thom Dunning, PNNL)</td>
<td><strong>Metagenomics for Analysis of Biogeochemical Cycles</strong> (Kathy Yelick, LBNL)</td>
</tr>
<tr>
<td>- Forecast water resources and severe weather with increased confidence; address food supply changes</td>
<td>- Develop new optimal catalysts while changing the current design processes that remain costly, time consuming, and dominated by trial-and-error</td>
<td>- Discover knowledge useful for environmental remediation and the manufacture of novel chemicals and medicines</td>
</tr>
</tbody>
</table>

*Challenges:* MMF approach for cloud-resolving model has large biases; adequacy of Fortran MPI+OpenMP for some architectures; Support for OpenMP and OpenACC

*Challenges:* computation of energy gradients for coupled-cluster implementation; on- and off-node performance

*Challenges:* Inability of message injection rates to keep up with core counts; efficient and performant implementation of UPC, UPC++, GASNet; GPU performance; I/O performance
E3SM-Multiscale Modeling Framework (MMF)
Cloud Resolving Climate Model for E3SM

- Develop capability to assess regional impacts of climate change on the water cycle that directly affect the US economy such as agriculture and energy production.

- Cloud resolving climate model is needed to reduce major systematic errors in climate simulations due to structural uncertainty in numerical treatments of convection – such as convective storm systems.

- Challenge: cloud resolving climate model using traditional approaches requires zettascale resources.

- E3SM “conventional” approach:
  - Run the E3SM model with a global cloud resolving atmosphere and eddy resolving ocean.
    - 3 km atmosphere/land (7B grid points) and 15-5 km ocean/ice (1B grid points)
    - Achieve throughput rate of 5 SYPD to perform climate simulation campaigns including a 500 year control simulation.
    - Detailed benchmarks on KNL and v100 GPUs show negligible speedups compared to conventional CPUs.
      - Low arithmetic intensity of most of the code; throughput requirements lead to strong scaling and low work per node.

- E3SM-MMF: Use a multiscale approach ideal for new architectures to achieve cloud resolving convection on Exascale.
  - Exascale will make “conventional” cloud resolving simulations routine for shorter simulations (process studies, weather prediction).
  - For cloud resolving climate simulations, we need fundamentally new approaches to take advantage of exascale resources.

PI: Mark Taylor (SNL)
Exascale apps can deliver transformative products and solutions

**ExaSky**

Cosmological Probe of the Standard Model of Particle Physics
(Salman Habib, ANL)

- Unravel key unknowns in the dynamics of the Universe: dark energy, dark matter, and inflation

*Challenges:* subgrid model accuracy; OpenMP performance on GPUs; file system stability and availability

**LatticeQCD**

Validate Fundamental Laws of Nature
(Andreas Kronfeld, FNAL)

- Correct light quark masses; properties of light nuclei from first principles; <1% uncertainty in simple quantities

*Challenges:* performance of critical slowing down; reducing network traffic to reduce system interconnect contention; strong scaling performance to mitigate reliance on checkpointing

**WarpX**

Plasma Wakefield Accelerator Design
(Jean-Luc Vay, LBNL)

- Virtual design of 100-stage 1 TeV collider; dramatically cut accelerator size and design cost

*Challenges:* scaling of Maxwell FFT-based solver; maintaining efficiency of large timestep algorithm; load balancing
| Exascale apps can deliver transformative products and solutions |
|------------------|------------------|------------------|------------------|
| **WDMApp** | **ExaStar** | **ExaFEL** | **CANDLE** |
| **High-Fidelity Whole Device Modeling of Magnetically Confined Fusion Plasmas** (Amitava Bhattacharjee, PPPL) | **Demystify Origin of Chemical Elements** (Dan Kasen, LBNL) | **Light Source-Enabled Analysis of Protein and Molecular Structure and Design** (Amadeo Perazzo, SLAC) | **Accelerate and Translate Cancer Research** (Rick Stevens, ANL) |
| • Prepare for ITER exps and increase ROI of validation data and understanding | • What is the origin of the elements? | • Process data without beam time loss | • Develop predictive preclinical models and accelerate diagnostic and targeted therapy through predicting mechanisms of RAS/RAF driven cancers |
| • Prepare for beyond-ITER devices | • How does matter behave at extreme densities? | • Determine nanoparticle size and shape changes | Challenges: increasing accelerator utilization for model search; effectively exploiting HP16; preparing for any data management or communication bottlenecks |
| Challenges: robust, accurate, and efficient code-coupling algorithm; reduction in memory and I/O usage | • What are the sources of gravity waves? | • Engineer functional properties in biology and materials science | **Challenges**: improving the strong scaling (one event processed over many cores) of compute-intensive algorithms (ray tracing, M-TIP) on accelerators |

**Exascale Computing Project**
## Exascale Application Development Challenges Overall

1. **Porting to accelerator-based architectures**
2. **Exposing additional parallelism**
3. **Coupling codes to create new multiphysics capability**
4. **Adopting new mathematical approaches**
5. **Algorithmic or model improvements**
6. **Leveraging optimized libraries**

ECP will intensify efforts to effectively exploit reduced precision representations of hardware-accelerated operations.
The three technical areas in ECP have the necessary components to address these challenges and meet national goals.

**Performant mission and science applications @ scale**

- **Foster application development**
- **Ease of use**
- **Diverse architectures**
- **HPC leadership**

### Application Development (AD)
Develop and enhance the predictive capability of applications critical to the DOE

### Software Technology (ST)
Produce expanded and vertically integrated software stack to achieve full potential of exascale computing

### Hardware and Integration (HI)
Integrated delivery of ECP products on targeted systems at leading DOE computing facilities

- 20+ applications ranging from national security, to energy, earth systems, economic security, materials, and data
- 80+ unique software products spanning programming models and run times, math libraries, data and visualization
- 6 vendors supported by PathForward focused on memory, node, connectivity advancements; deployment to facilities
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
ECP ST Software Ecosystem

Collaborators (with ECP HI)

ECP Applications  Facilities  Vendors  HPC Community

Software Ecosystem & Delivery

ECP Software Technology

Programming Models Runtimes

Development Tools

Mathematical Libraries

Data & Visualization
The Bottom Line for ECP Software Technology

- Next-generation **HPC technologies for 90 open source scientific software products**
- The performance potential of leadership computers in preparation for exascale
- **Software development kits (SDKs)** with turnkey installation and interoperability
- The **Extreme-scale Scientific Software Stack (E4S):**
  - Target: Comprehensive software environment for HPC scientific applications
  - Tested on growing collection of HPC platforms in preparation for Exascale systems
  - Managed complexity using SDKs as components
  - From-source builds for leadership environments
  - Pre-built containers for development, debugging and portability
- A commitment to software quality leveraging industry best practices
- A legacy to build upon for US security, science, industry and technology leadership
ECP investments in software technologies help ensure the exascale computers will be a success

**Programming Models & Runtimes**
- Enhance and get ready for exascale the widely used MPI and OpenMP programming models (hybrid programming models, deep memory copies)
- Development of performance portability tools (e.g. Kokkos and Raja)
- Support alternate models for potential benefits and risk mitigation: PGAS (UPC++/GASNet), task-based models (Legion, PaRSEC)
- Libraries for deep memory hierarchy and power management

**Development Tools**
- Continued, multifaceted capabilities in portable, open-source LLVM compiler ecosystem to support expected ECP architectures, including support for F18
- Performance analysis tools that accommodate new architectures, programming models, e.g., PAPI, Tau

**Math Libraries**
- Linear algebra, iterative linear solvers, direct linear solvers, integrators and nonlinear solvers, optimization, FFTs, etc
- Performance on new node architectures; extreme strong scalability
- Advanced algorithms for multi-physics, multiscale simulation and outer-loop analysis
- Increasing quality, interoperability, complementarity of math libraries

**Data and Visualization**
- I/O via the HDF5 API
- Insightful, memory-efficient in-situ visualization and analysis – Data reduction via scientific data compression
- Checkpoint restart

**Software Ecosystem**
- Develop features in Spack necessary to support all ST products in E4S, and the AD projects that adopt it
- Development of Spack stacks for reproducible turnkey deployment of large collections of software
- Optimization and interoperability of containers on HPC systems
- Regular E4S releases of the ST software stack and SDKs with regular integration of new ST products
Implementation of a new integer type for global integers in hypre

Scope and objectives

- Determine and document where code changes are required, and implement the new integer type
- Investigate the performance and memory usage of the new mixed-int hypre version in comparison to the 64-bit integer hypre version and the 32-bit version, where possible
- Summarize the results and make the implementation available to application code teams

Impact

- Linear systems are an important part of many application codes, and often make up a large portion of their execution times.
- Efficient linear solvers are crucial for ECP applications, and any improvements in performance and memory usage positively impact the applications.

Performance improvement of new capability

Weak scaling study:
Total runtimes in seconds for AMG-PCG using 1M points/core for 2 different 3D diffusion problems.
The new mixed-int capability performs about 20-25% better than the 64-int version while using less memory and solves larger problems than 32-int.

Project accomplishment

- Implemented a new integer type HYPRE_BigInt in hypre to reduce use of 64-bit integers for large problems and improve performance and memory use
- Investigated its performance and memory usage, and summarized the results and code changes in a document
- Generated a new hypre release: v. 2.16.0.

Deliverables
Hypre release v. 2.16.0 at https://github.com/hypre-space/hypre
ECP ST staff contribute to ISO and *de facto* standards groups: assuring sustainability through standards

<table>
<thead>
<tr>
<th>Standards Effort</th>
<th>ECP ST Participants</th>
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<tr>
<td>MPI Forum</td>
<td>15</td>
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<tr>
<td>OpenMP</td>
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<td>BLAS</td>
<td>6</td>
</tr>
<tr>
<td>C++</td>
<td>4</td>
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<tr>
<td>Fortran</td>
<td>4</td>
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<tr>
<td>OpenACC</td>
<td>3</td>
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<tr>
<td>LLVM</td>
<td>2</td>
</tr>
<tr>
<td>PowerAPI</td>
<td>1</td>
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<tr>
<td>VTK ARB</td>
<td>1</td>
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</tbody>
</table>

- **MPI/OpenMP**: Several key leadership positions
- Heavy involvement in all aspects.
- **C++**: Getting HPC requirements considered, contributing working code.
- **Fortran**: Flang front end for LLVM.
- **De facto**: Specific HPC efforts.
- **ARB**: Good model for SDKs.

*Architecture Review Board*
Many ECP ST products are available for broad community use

For example...

The exascale software ecosystem will be comprised of a wide array of software, all of which are expected to be used by DOE applications; a key ST effort is focused on developing turn-key installations for DOE Facilities through **software development toolkits** and the **Extreme Scale Scientific Software Stack (E4S)**.
Software Development Toolkits are a key delivery vehicle for ECP

• A collection of related software products (called packages) where coordination across package teams will improve usability and practices and foster community growth among teams that develop similar and complementary capabilities

• Attributes
  – Domain scope: Collection makes functional sense
  – Interaction model: How packages interact; compatible, complementary, interoperable
  – **Community policies**: Value statements; serve as criteria for membership
  – Meta-infrastructure: Encapsulates, invokes build of all packages (Spack), shared test suites
  – Coordinated plans: Inter-package planning. Does not replace autonomous package planning
  – Community outreach: Coordinated, combined tutorials, documentation, best practices

• Overarching goal: Unity in essentials, otherwise diversity
Extreme-Scale Scientific Software Development Kit (xSDK)

- **SW engineering**
  - Productivity tools.
  - Models, processes.

- **Libraries**
  - Solvers, etc.
  - Interoperable.

- **Frameworks & tools**
  - Doc generators.
  - Test, build framework.

- **Domain components**
  - Reacting flow, etc.
  - Reusable.

- **External software**
  - HDF5
  - BLAS

Notation: **A** → **B**: **A** can use **B** to provide functionality on behalf of **A**

**xSDK functionality, Dec 2017**
Tested on key machines at ALCF, NERSC, OLCF, also Linux, Mac OS X

- Alquimia
- PFLOTRAN
- PETSc
- hypre
- SUNDIALS
- MFEM
- SuperLU
- Trilinos
- More contributed libraries
- MAGMA
- Spack
- HDF5
- BLAS

**https://xsdk.info**

- More domain components
- More external software

**July 2018: Revisions of xSDK Community Policies**

https://xsdk.info/policies

- PFLOTRAN
- More domain components
xSDK Version 0.4.0: December 2018 (this is now)

https://xsdk.info

Each xSDK member package uses or can be used with one or more xSDK packages, and the connecting interface is regularly tested for regressions.

xSDK functionality, Dec 2018
Tested on key machines at ALCF, NERSC, OLCF, also Linux, Mac OS X

Impact: Improved code quality, usability, access, sustainability
Foundation for work on performance portability, deeper levels of package interoperability

December 2018
- 17 math libraries
- 2 domain components
- 16 mandatory xSDK community policies
- Spack xSDK installer

Domain components
- Reacting flow, etc.
- Reusable.

Libraries
- Solvers, etc.
- Interoperable.

Frameworks & tools
- Doc generators.
- Test, build framework.

SW engineering
- Productivity tools.
- Models, processes.

Extreme-Scale Scientific Software Development Kit (xSDK)
The planned ECP ST SDKs will span all technology areas
Extreme-Scale Scientific Software Stack – E4S

- **E4S**: A Spack-based distribution of ECP ST and related and dependent software tested for interoperability and portability to multiple architectures
- Provides distinction between SDK usability / general quality / community and deployment / testing goals
- Will leverage and enhance SDK interoperability thrust
- Oct: E4S 0.1 - 24 full, 24 partial release products
- Jan: E4S 0.2 - 37 full, 10 partial release products
- Current primary focus: Facilities deployment

Lead: Sameer Shende
(U Oregon)
E4S Full Release and Installed Packages

- Adios
- Bolt
- Caliper
- Darshan
- Gasnet
- GEOPM
- GlobalArrays
- Gotcha
- HDF5
- HPCToolkit
- Hypre
- Jupyter
- Kokkos
- Legion
- Libquo
- Magma
- MFEM
- MPICH
- OpenMPI
- PAPI
- Papyrus
- Parallel netCDF
- ParaView
- PETSc/TAO
- Program Database Toolkit (PDT)
- Qthreads
- Raja
- SCR
- Spack
- Strumpack
- Sundials
- SuperLU
- Swift/T
- SZ
- Tasmanian
- TAU
- Trilinos
- VTKm
- Umpire
- UnifyCR
- Veloc
- xSDK
- Zfp

Packages installed using Spack
Detailed Information about the software technology projects is available in the ECP ST Capability Assessment Report

• Products discussed here are presented with more detail and further citations.

• We classify ECP ST Products deployment as Broad, Moderate or Experimental.
  – Broad and Moderate Deployment is typical suitable for collaboration.
  – Web links are available for almost all products.
  – About 1/3 of ECP ST Products are available as part of the Extreme-scale Scientific Software Stack (E4S) http://e4s.io.

V 1.0 https://www.exascaleproject.org

V 1.5 https://github.com/E4S-Project/ECP-ST-CAR-PUBLIC/blob/master/ECP-ST-CAR.pdf
The three technical areas in ECP have the necessary components to address these challenges and meet national goals.

**Application Development (AD)**
- Develop and enhance the predictive capability of applications critical to the DOE.

**Software Technology (ST)**
- Produce expanded and vertically integrated software stack to achieve full potential of exascale computing.

**Hardware and Integration (HI)**
- Integrated delivery of ECP products on targeted systems at leading DOE computing facilities.

**Performant mission and science applications @ scale**
- Foster application development
- Ease of use
- Diverse architectures
- HPC leadership

20+ applications ranging from national security, to energy, earth systems, economic security, materials, and data.

80+ unique software products spanning programming models and run times, math libraries, data and visualization.

6 vendors supported by PathForward focused on memory, node, connectivity advancements: deployment to facilities.
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
ECP’s PathForward Vendor Hardware R&D Efforts Accelerate Hardware Technologies for Exascale Systems

PathForward began in 2017; builds upon the FastForward I & II and DesignForward I & II efforts

Total value of the work is ~$430M; DOE paid 60% of the price or $250+M

Examples of work funded include:

a) innovative memory architectures
b) higher-speed interconnects
c) improved system reliability
d) Innovations for increased parallelism - 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)
ECP’s PathForward project and ASCR Facility system acquisition projects work together to accelerate the delivery of exascale systems.

Accelerating hardware innovations

PathForward
6 Vendors
Each with multiple Work Packages

Productizing hardware innovations

Facility Non-Recurring Engineering (NRE) Contracts

NRE funds the development of technology (both hardware and software) that is:
1. Required to deliver the system and
2. Would not have been developed (or developed in time) by the vendor.

Exascale system deliveries (notional)

FY16   FY17   FY18   FY19   FY20   FY21   FY22   FY23
Application Integration at the Facilities Accelerates ECP AD’s Application Readiness on ASCR Facilities Exascale Architectures

**Approach:** Leverage DOE Facilities Application Readiness expertise (from OLCF CAAR, ALCF ESP, NERSC NESAP programs) by providing:

- Facility computational scientists and performance engineering expertise to AD teams
- Access to Facilities Vendor Centers of Excellences

Provide AD efforts with access to (1) Facilities Vendor COEs and (2) production/development computing resources via ECP allocation program (WBS 2.4.5)

Benefits of this Approach:

- Facilities benefit by having more applications prepared to run on their systems as soon as the system is ready
- ECP benefits by leveraging the Facilities’ successful application readiness efforts
Software Deployment at Facilities deploys ECP’s ST products to meet ECP application needs

- Project Goal: ECP software integrated with facility software and vendor software targeting application needs
- Establish and operate a Continuous Integration Testing infrastructure for automated testing across HPC sites
- Develop a Software Deployment pipeline that supports packaging, efficient deployment at multiple facilities, and allows for container deployment approaches

**Approach**

- Establish ongoing collaborations (via funded efforts) across Facilities that have historically been ad-hoc
- Define infrastructure and production-quality processes that will live beyond the lifetime of ECP and establish a long-lasting DOE software sustainability model
- Address unique site-specific deployment models while attempting to drive more commonality where it benefits the ECP user community
- Maximize cross-fertilization of ST technology across multiple sites, vendors, and open source offerings (e.g. OpenHPC)

ECP affords a first-ever opportunity to drive the major DOE HPC Facilities and software developers to establish, share, and leverage common practices that will be critical for post-ECP software sustainability
The central DOE GitLab managed by OSTI for the CI process will provide software centralization with cross-site build and run capabilities
ECP’s Flow of Software and Application Delivery and Deployment

HPC and scientific community

Communication and release: GitLab, openHPC, workshops, conferences, publications, . . .

Software projects
- ADIOS, ATDM, LLVM, Kokkos, RAJA, Legion, Trilinos, . . .

Contribution complies with SDK specifications

Software Development Kits (SDKs)
- SDK 1
- SDK 2
- SDK 3
- SDK ...

Applications
Integration of ST products via SDK
- APIs
- Release
- Integration with vendor software
- Software integration
- Continuous integration
- Deploy to Facilities

Apps integration

Systems
- Aurora
- Frontier
- El Capitan
- Pre-Exascale systems

Software deployment

Integration of ST products via SDK

Software R&D

Deploy to Facilities

Communication and release: GitLab, openHPC, workshops, conferences, publications, . . .
The ECP is on track to deliver a capable exascale computing ecosystem

### Applications
- 20+ application teams actively engaged in targeted development and capability enablement for 2+ years
- Apps have well-defined exascale challenge problem targets with associated “science work rate” goals
- Initial performance experiences on pre-exascale systems (Summit, Sierra) exceeding expectations

### Software Stack
- Over 80 software technology products being actively developed for next generation architectures
- Regular assessment of software stack products ensures line-of-sight to apps and HPC Facilities
- Plans for broad containerized delivery of products via SDKs and the E4S being executed

### Hardware & Integration
- Return on PathForward vendor hardware R&D element evident in recent exascale RFP responses
- Plans for deployment and continuous integration of SDKs into DOE HPC Facilities being executed
- Prioritized performance engineering of applications targeting first three exascale systems underway
ECP Acknowledgments
Department of Energy (DOE) Support and Leadership

• DOE Office of Science Advanced Scientific Computing Research (ASCR) Program
  • Barb Helland
    • ASCR Associate Director and ECP Program Manager

• DOE National Nuclear Security Administration (NNSA) Advanced Simulation and Computing (ASC) Program
  • Thuc Hoang
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  • Dan Hoag
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• Lawrence Livermore National Laboratory (LLNL) Site Office (LSO)
  • Sam Brinker
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For more information…

https://www.exascaleproject.org

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Questions?
**NVIDIA’s tesla v100**

- 5,120 CUDA cores (64 on each of 80 SMs)
- 640 NEW Tensor cores (8 on each of 80 SMs)
- 20MB SM RF | 16MB Cache | 16GB HBM2 @ 900 GB/s
- 300 GB/s NVLink
- 7.5 FP64 TFLOPS | 15 FP32 TFLOPS | 120 Tensor TFLOPS
- >27K of these on ORNL’s Summit system!
- Mixed precision matrix math 4x4 matrices

![Diagram of NVIDIA's tesla v100](image)

**Mixed precision matrix math 4x4 matrices**

\[ D = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix} + \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} \\ C_{21} & C_{22} & C_{23} & C_{24} \\ C_{31} & C_{32} & C_{33} & C_{34} \\ C_{41} & C_{42} & C_{43} & C_{44} \end{bmatrix} \]

\[ D = AB + C \]

<table>
<thead>
<tr>
<th>Type</th>
<th>Size</th>
<th>Range</th>
<th>( u = 2^{-l} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>half</td>
<td>16 bits</td>
<td>10(\pm5)</td>
<td>2(^{-11}) \approx 4.9 \times 10^{-4}</td>
</tr>
<tr>
<td>single</td>
<td>32 bits</td>
<td>10(\pm38)</td>
<td>2(^{-24}) \approx 6.0 \times 10^{-8}</td>
</tr>
<tr>
<td>double</td>
<td>64 bits</td>
<td>10(\pm308)</td>
<td>2(^{-53}) \approx 1.1 \times 10^{-16}</td>
</tr>
<tr>
<td>quadruple</td>
<td>128 bits</td>
<td>10(\pm4932)</td>
<td>2(^{-113}) \approx 9.6 \times 10^{-35}</td>
</tr>
</tbody>
</table>

- The M&S community must figure how to “cheat” and utilize mixed / reduced precisions
- Ex: Jack Dongarra shows he can get 4x FP64 peak for 64bit LU on V100 with iterative mixed precision (using GMRES!)
Principles for a Healthy ECP and Facilities Partnership

<table>
<thead>
<tr>
<th>Make it a win-win partnership</th>
<th>Leverage each others capacities</th>
<th>Align our plans to the extent that makes sense</th>
</tr>
</thead>
<tbody>
<tr>
<td>• ECP outputs are usable by and meet the needs of the Facilities</td>
<td>Two examples are:</td>
<td>• Two examples are:</td>
</tr>
<tr>
<td>• Facilities make available the expertise and resources needed by ECP</td>
<td>• ECP makes use of the Facilities’ application preparation programs for ECP applications</td>
<td>• Both are interested in improving software quality and ease of deployment within the Facilities’ HCP centers</td>
</tr>
<tr>
<td></td>
<td>• ECP’s early hardware R&amp;D investments improve the systems DOE Facilities are acquiring</td>
<td>• Both would like ECP applications to be ready to run on their exascale system</td>
</tr>
</tbody>
</table>
Essential to ensure that applications effectively utilize exascale systems

- Pulls software and hardware developments into applications
- Pushes application requirements into software and hardware RD&D
- Evolved from best practice to an essential element of the development cycle

CD Centers focus on a unique collection of algorithmic motifs invoked by ECP applications

- 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

Game-changing mechanism for delivering next-generation community products with broad application impact

- Evaluate, deploy, and integrate exascale hardware-savvy software designs and technologies for key crosscutting algorithmic motifs into applications
- An appropriate nexus for reduced precision?
E3SM: Energy Exascale Earth System Model

• Global Earth System Model
• Atmosphere, Land, Ocean and Ice component models
• 8 DOE labs, 12 university subcontracts, 53 FTEs spread over 87 individuals
• Development driven by DOE Office of Scientific Mission interests: Energy/water issues looking out 40 years
• Key computational goal: Ensure E3SM will run well on upcoming DOE pre-exascale and exascale computers
• E3SM is open source / open development
  – Website: www.e3sm.org
  – Github: https://github.com/E3SM-Project
  – DOE Science youtube channel: https://www.youtube.com/channel/UC_rhpi0lBeD1U-6nD2zvIBA

PI: David Bader (LLNL)
We work on products applications need now and into the future

**Key themes:**
- Exploration/development of new algorithms/software for emerging HPC capabilities:
- High-concurrency node architectures and advanced memory & storage technologies.
- Enabling access and use via standard APIs.

**Software categories:**
- The next generation of well-known and widely used HPC products (e.g., MPICH, OpenMPI, PETSc)
- Some lesser used but known products that address key new requirements (e.g., Kokkos, RAJA, Spack)
- New products that enable exploration of emerging HPC requirements (e.g., SICM, zfp, UnifyCR)

<table>
<thead>
<tr>
<th>Example Products</th>
<th>Engagement</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPI – Backbone of HPC apps</td>
<td>Explore/develop MPICH and OpenMPI new features &amp; standards.</td>
</tr>
<tr>
<td>OpenMP/OpenACC –On-node parallelism</td>
<td>Explore/develop new features and standards.</td>
</tr>
<tr>
<td>Performance Portability Libraries</td>
<td>Lightweight APIs for compile-time polymorphisms.</td>
</tr>
<tr>
<td>LLVM/Vendor compilers</td>
<td>Injecting HPC features, testing/feedback to vendors.</td>
</tr>
<tr>
<td>Perf Tools - PAPI, TAU, HPCToolkit</td>
<td>Explore/develop new features.</td>
</tr>
<tr>
<td>Math Libraries: BLAS, sparse solvers, etc.</td>
<td>Scalable algorithms and software, critical enabling technologies.</td>
</tr>
<tr>
<td>IO: HDF5, MPI-IO, ADIOS</td>
<td>Standard and next-gen IO, leveraging non-volatile storage.</td>
</tr>
<tr>
<td>Viz/Data Analysis</td>
<td>ParaView-related product development, node concurrency.</td>
</tr>
</tbody>
</table>
Software Development Toolkit Motivation

- The exascale software ecosystem will be comprised of a wide array of software, all of which are expected to be used by DOE applications.

- The software must be:
  - interoperable
  - sustainable
  - maintainable
  - adaptable
  - portable
  - scalable
  - deployed at DOE computing facilities

- Provides intermediate coordination points to better manage complexity

- Without these qualities:
  - Value will be diminished
  - Scientific productivity will suffer
ECP ST SDK community policies: Important team building, quality improvement, membership criteria.

SDK Community Policy Strategy
- Review and revise xSDK community policies and categorize
  - Generally applicable
  - In what context the policy is applicable
- Allow each SDK latitude in customizing appropriate community policies
- Establish baseline policies in FY19 Q2, continually refine

xSDK compatible package: Must satisfy mandatory xSDK policies:
M1. Support xSDK community GNU Autoconf or CMake options.
M2. Provide a comprehensive test suite.
M3. Employ user-provided MPI communicator.
M4. Give best effort at portability to key architectures.
M5. Provide a documented, reliable way to contact the development team.

xSDK member package: An xSDK-compatible package, that uses or can be used by another package in the xSDK, and the connecting interface is regularly tested for regressions.

Prior to defining and complying with these policies, a user could not correctly, much less easily, build hypre, PETSc, SuperLU and Trilinos in a single executable: a basic requirement for some ECP app multi-scale/multi-physics efforts.

Recommended policies: encouraged, not required:
R1. Have a public repository.
R2. Possible to run test suite under valgrind in order to test for memory corruption issues.
R3. Adopt and document consistent system for error conditions/exceptions.
R4. Free all system resources it has acquired as soon as they are no longer needed.
R5. Provide a mechanism to export ordered list of library dependencies.

https://xsdk.info/policies

Initially the xSDK team did not have sufficient common understanding to jointly define community policies.
ECP ST Technologies that may be particularly suited to industry interactions

**Programming Models & Runtimes**
- Leverage new features in MPICH, OpenMP libraries
- Use C++ compile-time polymorphism to generate node-specific code from common source code (e.g., Kokkos, RAJA)
- Experiment with alternative programming models (Legion, UPC++/GASNet)

**Development Tools**
- Tools for performance analysis:
  - PAPI, TAU, HPC Toolkit, Dyninst:
  - Widely used in HPC community
- Portable, open-source LLVM compiler ecosystem to support expected ECP architectures, including support for F18

**Math Libraries**
- Use hypre, PETSc, SuperLU, Trilinos, others: All widely used parallel solvers being adapted for massive on-node concurrency.
  - APIs are largely unchanged
  - Provides performance portability across platforms
- Try STRUMPACK
  - Suitable SuperLU replacement
  - Highly scalable (for a direct solver).
  - Turnkey solver (easy to install and use)

**Data and Visualization**
- New storage software and workflows associated with non-volatile memory
  - Fundamental I/O game-changer
  - Examples: Fast offload of checkpoints, all-flash storage system
- Data compression tools: Same impact as increasing memory and storage size and bandwidth.
  - In situ workflows: Increased opportunities to analyze and transform data as part of the workflow.

**Software Ecosystem**
- Advanced resource management:
  - Fast, scalable checkpoint/restart (leverage NVRAM).
  - Resource managers, e.g., Flux.
- SDKs and Spack are emerging as attractive combination for managing software components:
  - Involvement and input from industry can be beneficial both ways
Hardware and integration
Develop technology advances for exascale and deploy ECP products

Vendor R&D for exascale systems (PathForward)
Evaluation of hardware technology and performance
Software deployment and application integration at HPC facilities
Pre-exascale and exascale system utilization measurement and tracking
Community training and productivity

HI has primary ECP responsibility for the partnership with the Facilities and each HI project is collaborating with the Facilities.
## PathForward vendors, objectives, and R&D

<table>
<thead>
<tr>
<th>Company (HPC Vendor)</th>
<th>Objective</th>
<th>R&amp;D thrusts</th>
</tr>
</thead>
</table>
| AMD                  | Develop innovative technologies to enable our system integration partners to design and assemble a variety of world-class solutions for exascale computing | • Innovations in memory interfaces  
• CPU and GPU microarchitecture  
• Component integration  
• High-speed interconnects |
| Cray Inc.            | Improvements in sustained performance, power efficiency, scalability, and reliability | • Arm processor enhancements  
• Network enhancements  
• Memory architectures |
| Hewlett Packard Enterprise (HPE) | A system architecture and the integration technologies that can deliver an exascale system in a node-agnostic way | • System, node, and I/O design  
• Advance the Gen-Z interconnect  
• Optical interconnects |
| IBM                  | Optimize an exascale system for improved application performance and developer productivity while maximizing energy efficiency and reliability | • Architectural and system component innovations for a system combining processors, GPUs, high-performance networks, and high-performance storage |
| Intel Corp.          | Energy efficiency, fabric costs, memory and high-speed IO, performance, scalability and usability | • Energy efficiency  
• Reduced fabric costs and power  
• Scalable storage and memory arch.  
• Optimized communication characteristics |
| NVIDIA Corp.         | Accelerate efforts to develop highly efficient throughput computing technologies | • Energy-efficient GPU architectures  
• Resilience |
Application Matching to Facilities Plan and Status

**Strategy:** Match applications with existing facility readiness efforts

**Progress Assessment:** Progress towards technical execution plans measured quarterly; annual external assessment.

12 initial applications engaged by ALCF for Aurora. Other teams can follow best practices for Aurora readiness, and will be engaged as staffing allows.

An initial set of ~10 ECP applications will be identified to participate in CAAR-ECP in FY19. Applications may transition in and out of the program as progress is made.

5 ECP AD applications participating in NESAP for NERSC-9. Additional applications may participate with NERSC funding.

**Goal:** 22 performant exascale applications that run on Aurora and/or Frontier

Goal: Progress towards exascale readiness develops, and NESAP-ECP apps transition to LCF facilities.
Delivering a secure, easy-to-use Continuous Integration (CI) solution to support Software Product testing on DOE HPC environments

- Allows for the verification of development efforts through automated building & testing across sites to better identify errors and improve code efficiency
- Continuous Integration/Continuous Delivery pipelines enabled through a combination of the web application and project configuration files and are executed by a selected runners.

OnyxPoint + GitLab were chosen based upon a request for proposal with participation from the E6.
## Use cases being addressed and the solution being worked

### Use Cases

- Build, test, package, and deploy project code in a streamlined, repeatable workflow
- Develop CI pipelines that can directly leverage and submit jobs to HPC resources
- Target wider range of testing and deployment configurations by utilizing resources across facilities

### Solution

- Use GitLab for the entire DevOps lifecycle (plan, create, verify, release) coupled with runner components located across all sites
- Fund Facility staff to define the solution and to deploy and operate the service at their site
- Onyx Point developed runner improvements for DOE secure HPC data centers (identifying users uniquely and enabling submitting jobs directly to resource job management system)
- Centralized core repository managed by DOE Office of Scientific and Technical Information (OSTI) accessible by ECP and E6 users
- Shared runner strategy that offers security tied to user authentication while minimizing system administration overhead – A runner that serves all projects is called a shared Runner
Facilities and ECP Partnering is Key to ECI

- Mission is enduring
- ASCR has been delivering on its mission for decades

- Leverage ASCR capabilities
- Products delivered are accelerated apps, sw, and hw
- Shares in the deployment of exascale computing capabilities

- Mission ends with the project
- ECP is a few years old

- Leverage ECP capabilities
- Provides expertise, staff, and computer resources
- Acquires, deploys, and operates exascale computers
- Shares in the deployment of exascale computing capabilities
More detailed information about the applications will be available in the ECP Application Assessment Report

- Comprehensive assessment of ECP’s application projects and 7 co-design centers

- Primary document elements:
  - Completion requirements, including detailed description of exascale challenge problem and figure of merit (FOM) formula
  - FY18 milestone execution
  - DOE stakeholders
  - Software details, integration with ST projects

- Teams and AD leadership already acting on these findings

- Public version available May 2019
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