Exascale Computing Project -- Software

Paul Messina, ECP Director
Stephen Lee, ECP Deputy Director

ASCAC Meeting, Arlington, VA

Crystal City Marriott
April 19, 2017
ECP scope and goals

- 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
- Develop a software stack that is both exascale-capable and usable on industrial & academic scale systems, in collaboration with vendors
- Partner with vendors to develop computer architectures that support exascale applications
- Train a next-generation workforce of computational scientists, engineers, and computer scientists

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

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Support national security

Develop a software stack that is both exascale-capable and usable on industrial & academic scale systems, in collaboration with vendors

Partner with vendors to develop computer architectures that support exascale applications

Train a next-generation workforce of computational scientists, engineers, and computer scientists
ECP has formulated a holistic approach that uses co-design and integration to achieve capable exascale systems.

**Application Development**
- Science and mission applications

**Software Technology**
- Scalable and productive software stack
  - Correctness
  - Visualization
  - Data Analysis
  - Co-Design
  - Programming models, development environment, and runtimes
  - Math libraries and Frameworks
  - Tools
  - System Software, resource management, and control
  - Memory and Burst buffer
  - Data management and file system
  - Node OS, runtimes

**Hardware Technology**
- Hardware technology elements

**Exascale Systems**
- Integrated exascale supercomputers

ECP’s work encompasses applications, system software, hardware technologies and architectures, and workforce development.
What is a capable exascale computing system?

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

• Delivers $50 \times$ the performance of today’s 20 PF systems, supporting applications that deliver high-fidelity solutions in less time and address problems of greater complexity

• Operates in a power envelope of 20–30 MW

• Is sufficiently resilient (perceived fault rate: ≤1/week)

• Includes a software stack that supports a broad spectrum of applications and workloads

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

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

Chief Technology Officer
Al Geist, ORNL

Exascale Computing Project
Paul Messina, Project Director, ANL
Stephen Lee, Deputy Project Director, LANL

Integration Manager
Julia White, ORNL

Communications Manager
Mike Bernhardt, ORNL

Project Management
Kathlyn Boudwin, Director, ORNL

Application Development
Doug Kothe, Director, ORNL
Bert Still, Deputy Director, LLNL

Software Technology
Rajeev Thakur, Director, ANL
Pat McCormick, Deputy Director, LANL

Hardware Technology
Jim Ang, Director, SNL
John Shalf, Deputy Director, LBNL

Exascale Systems
Terri Quinn, Director, LLNL
Susan Coghlan, Deputy Director, ANL
ECP Software Technology Overview

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

• Accomplished by extending current technologies to exascale where possible, performing R&D required to conceive of new approaches where necessary
  – Coordinate with vendor efforts; i.e., develop software other than what is typically done by vendors, develop common interfaces or services
  – Develop and deploy high-quality and robust software products
ST Level 3 WBS Leads

- **Programming Models and Runtimes**
  - 1.3.1
  - Rajeev Thakur, ANL

- **Tools**
  - 1.3.2
  - Jeff Vetter, ORNL

- **Mathematical and Scientific Libraries and Frameworks**
  - 1.3.3
  - Mike Heroux, SNL

- **Data Management and Workflows**
  - 1.3.4
  - Rob Ross, ANL

- **Data Analytics and Visualization**
  - 1.3.5
  - Jim Ahrens, LANL

- **System Software**
  - 1.3.6
  - Martin Schulz, LLNL

- **Resilience and Integrity**
  - 1.3.7
  - Al Geist, ORNL

- **Co-Design and Integration**
  - 1.3.8
  - Rob Neely, LLNL
# Vision and Goals for the ECP Software Stack

<table>
<thead>
<tr>
<th>Deliver and Anticipate</th>
<th>Provide foundational software and infrastructure to applications and facilities necessary for project success in 2021-23, while also pushing to innovate beyond that horizon</th>
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<tbody>
<tr>
<td>Collaborate</td>
<td>Encourage and incentivize use of common infrastructure and APIs within the software stack</td>
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<tr>
<td>Integrate</td>
<td>Work with vendors to provide a balanced offering between lab/univ developed (open source), vendor-offered (proprietary), and jointly developed solutions</td>
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<td>Quality</td>
<td>Deploy production-quality software that is easy to build, well tested, documented, and supported</td>
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<td>Prioritize</td>
<td>Focus on a software stack that addresses the unique requirements of exascale – including extreme scalability, unique requirements of exascale hardware, and performance-critical components</td>
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<td>Completeness</td>
<td>Perform regular gap analysis and incorporate risk mitigation (including “competing” approaches) in high-risk and broadly impacting areas</td>
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ECP Requires Strong Integration to Achieve Capable Exascale

• To achieve a coherent software stack, we must integrate across all the focus areas
  – Understand and respond to the requirements from the apps but also help them understand challenges they may not yet be aware of
  – Understand and respond to the impact of hardware technologies and platform characteristics
  – Work with the facilities and vendors towards a successful stable deployment of our software technologies
  – Understand and respond to dependencies within the stack, avoiding duplication and scope creep
  – This is a comprehensive team effort — not a set of individual projects!
Requirements for Software Technology

Derived from

• Analysis of the software needs of exascale applications

• Inventory of software environments at major DOE HPC facilities (ALCF, OLCF, NERSC, LLNL, LANL, SNL)
  – For current systems and the next acquisition in 2–3 years (CORAL, APEX)

• Expected software environment for an exascale system

• Requirements beyond the software environment provided by vendors of HPC systems

• What is needed to meet ECP’s Key Performance Parameters (KPPs)
Example: An Exascale Subsurface Simulator of Coupled Flow, Transport, Reactions and Mechanics*

**Exascale Challenge Problem**

- Safe and efficient use of the subsurface for geologic CO$_2$ sequestration, petroleum extraction, geothermal energy and nuclear waste isolation
- Predict reservoir-scale behavior as affected by the long-term integrity of hundreds of thousands of deep wells that penetrate the subsurface for resource utilization
- Resolve pore-scale (0.1-10 µm) physical and geochemical heterogeneities in wellbores and fractures to predict evolution of these features when subjected to geomechanical and geochemical stressors
- Integrate multi-scale (µm to km), multi-physics in a reservoir simulator: non-isothermal multiphase fluid flow and reactive transport, chemical and mechanical effects on formation properties, induced seismicity and reservoir performance
- Century-long simulation of a field of wellbores and their interaction in the reservoir

**Applications & S/W Technologies**

**Applications**
- Chombo-Crunch, GEOS

**Software Technologies Cited**
- C++, Fortran, LLVM/Clang
- MPI, OpenMP, CUDA
- Raja, CHAI
- Chombo AMR, PETSc
- ADIOS, HDF5, Silo, ASCTK
- VisIt

**Development Plan**

**Y1:** Evolve GEOS and Chombo-Crunch; Coupling framework v1.0; Large scale (100 m) mechanics test (GEOS); Fine scale (1 cm) reactive transport test (Chombo-Crunch)

**Y2:** GEOS+Chombo-Crunch coupling for single phase; Coupling framework w/ physics; Multiphase flow for Darcy & pore scale; GEOS large strain deformation conveyed to Chombo-Crunch surfaces; Chombo-Crunch precip/dissolution conveyed to GEOS surfaces

**Y3:** Full demo of fracture asperity evolution-coupled flow, chemistry, and mechanics

**Y4:** Full demo of km-scale wellbore problem with reactive flow and geomechanical deformation, from pore scale to resolve the geomechanical and geochemical modifications to the thin interface between cement and subsurface materials in the wellbore and to asperities in fractures and fracture networks

**Risks and Challenges**

- Porting to exascale results in suboptimal usage across platforms
- No file abstraction API that can meet coupling requirements
- Batch scripting interface incapable of expressing simulation workflow semantics
- Scalable AMG solver in PETSc
- Physics coupling stability issues
- Fully overlapping coupling approach results inefficient.

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*PI: Carl Steefel (LBNL)
Example: **NWChemEx: Tackling Chemical, Materials and Biomolecular Challenges in the Exascale Era**

**Exascale Challenge Problem**
- Aid & accelerate advanced biofuel development by exploring new feedstock for efficient production of biomass for fuels and new catalysts for efficient conversion of biomass derived intermediates into biofuels and bioproducts
- Molecular understanding of how proton transfer controls protein-assisted transport of ions across biomass cellular membranes; often seen as a stress responses in biomass, would lead to more stress-resistant crops thru genetic modifications
- Molecular-level prediction of the chemical processes driving the specific, selective, low-temperature catalytic conversion (e.g., Zeolites such as H-ZSM-5) of biomass-derived alcohols into fuels and chemicals in constrained environments

**Applications & S/W Technologies**

**Applications**
- NWChemEx (evolved from redesigned NWChem)

**Software Technologies Cited**
- Fortran, C, C++
- Global arrays, TiledArrays, ParSEC, TASCEL
- VisIt, Swift
- TAO, Libint
- Git, svn, JIRA, Travis CI
- Co-Design: CODAR, CE-PSI, GraphEx

**Risks and Challenges**
- Unknown performance of parallel tools
- Insufficient performance or scalability or large local memory requirements of critical algorithms
- Unavailable tools for hierarchical memory, I/O, and resource management at exascale
- Unknown exascale architectures
- Unknown types of correlation effect for systems with large number of electrons
- Framework cannot support effective development

**Development Plan**

**Y1:** Framework with tensor DSL, RTS, APIs, execution state tracking; Operator-level NK-based CCSD with flexible data distributions & symmetry/sparisity exploitation

**Y2:** Automated compute of CC energies & 1-/2-body CCSD density matrices; HT & DFT compute of >1K atom systems via multi-threading

**Y3:** Couple embedding with HF & DFT for multilevel memory hierarchies; QMD using HF & DFT for 10K atoms; Scalable R12/F12 for 500 atoms with CCSD energies and gradients using task-based scheduling

**Y4:** Optimized data distribution & multithreaded implementations for most time-intensive routines in HF, DFT, and CC.
Software Technologies
Aggregate of technologies cited in all candidate ECP Applications

• Programming Models and Runtimes
  – Fortran, C++/C++17, Python, C, Javascript, C#, R, Ruby
  – MPI, OpenMP, OpenACC, CUDA, Global Arrays, TiledArrays, Argobots, HPX, OpenCL, Charm++
  – UPC/UPC++, Co-Array FORTRAN, CHAPEL, Julia, GDDI, DASK-Parallel, PYBIND11
  – PGAS, GASNetEX, Kokkos, Raja, Legion/Regent, OpenShmem, Thrust
  – PARSEC, Panda, Sycl, Perilla, Globus Online, ZeroMQ, ParSEC, TASCEL, Boost

• Tools (debuggers, profilers, software development, compilers)
  – LLVM/Clang, HPCToolkit, PAPI, ROSE, Oxbow (performance analysis), JIRA (software development tool), Travis (testing),
  – ASPEN (machine modeling), CMake, git, TAU, Caliper, , GitLab, CDash (testing), Flux, Spack, Docker, Shifter, ESGF, Gerrit
  – GDB, Valgrind, GitHub, Jenkins (testing), DDT (debugger)

• Mathematical Libraries, Scientific Libraries, Frameworks
  – BLAS/PBLAS, MOAB, Trilios, PETSc, BoxLib, LAPACK/ScaLAPACK, Hypre, Chombo, SAMRAI, Metis/ParMETIS, SLEPc
  – SuperLU, Repast HPC (agent-based model toolkit), APOSMM (optimization solver), HPGMG (multigrid), FFTW, Dakota, Zero-RK
  – cuDNN, DAAL, P3DFFT, QUDA (QCD on GPUs), QPhiX (QCD on Phi), ArPack (Arnoldi), ADLB, DMEM, MKL, Sundials, Muelu
  – DPLASMA, MAGMA, PEBBL, pbdR, FMM, DASHMM, Chaco (partitioning), libint (gaussian integrals)
  – Smith-Waterman, NumPy, libcchem
Software Technologies
Cited in Candidate ECP Applications

• Data Management and Workflows
  – Swift, MPI-IO, HDF, ADIOS, XTC (extended tag container), Decaf, PDACS, GridPro (meshing), Fireworks, NEDB, BlitzDB, CouchDB
  – Bellerophon, Sidre, Silo, ZFP, ASCTK, SCR, Sierra, DHARMA, DTK, PIO, Akuna, GridOPTICS software system (GOSS), DisPy, Luigi
  – CityGML, SIGMA (meshing), OpenStudio, Landscan USA
  – IMG/KBase, SRA, Globus, Python-PANDAS

• Data Analytics and Visualization
  – VisIt, VTK, Paraview, netCDF, CESIUM, Pymatgen, MacMolPlt, Yt
  – CombBLAS, Elviz, GAGE, MetaQuast

• System Software
Libraries used at NERSC
(similar data from other facilities)

Library Usage on Edison
(Mar 01, 2014 - Aug. 31, 2014)

Number of links

Libraries

- mpich
- darshan
- libsci
- hdf5
- fftw
- shmem
- petsc
- mpi
- openmpi
- metis
- dmapp
- netcdf
- upc
- superlu
- hdf5-para
- parmetis
- superlu_dist
- gsl
- HYPRE
- mumps
- scotch
- tpsl
- python
- rca
Conceptual ECP Software Stack

- Correctness
  - Programming Models, Development Environment, and Runtimes
- Visualization
  - Math Libraries/Frameworks
- Data Analysis
  - Tools
- Applications
  - Memory and Burst buffer
- Co-Design
  - Data Management, I/O and File System
- System Software, Resource Management, Threading, Scheduling, Monitoring, and Control
- Node OS, Low-Level Runtimes

Hardware interface
Current Set of ST Projects Mapped to Software Stack

Correctness
- VTK-m, ALPINE, Cinema

Visualization
- ALPINE, Cinema

Data Analysis

Applications
- 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
- Math Libraries/Frameworks
  - ScaLAPACK, DPLASMA, MAGMA, PETSc/TAO, Trilinos, xSDK, PEEKS, SuperLU, STRUMPACK, SUNDIALS, DTK, TASMANIAN, AMP, FleCSI, KokkosKernels, Agile Comp., DataProp, MFEM
- Memory and Burst buffer
  - Chkpt/Restart (VeloC, UNIFYCR), API and library for complex memory hierarchy (SICM)

Co-Design

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

Resources
- Node OS, low-level runtimes
  - Argo Global OS enhancements, SNL OS project
- System Software, Resource Management
  - Threading, Scheduling, Monitoring, and Control
  - Argo Global OS, Qthreads, Flux, Spindle, BEE, Spack, Sonar
- 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

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

Check point/Restart (VeloC, UNIFYCR), FSEFI, Fault Modeling

Resilience
Kokkos: On-Node Performance Portable Abstraction Layer

Description and Scope

Project Description:
• Enable application performance portability across next generation platforms (NGPs) on likely paths to exascale; especially DOE’s advanced technology systems (ATS)
• Sustain application developer productivity with effective programming model, support, and training that evolves with NGP architectures and sophistication of application algorithms

ECP Scope
• ASC/ATDM funded programming model R&D and ASC application support
• ECP-ST funded DOE-Lab-wide training and application support

Maturity Level and Accessibility

Maturity Indicators and Metrics
• Production since March 2015, support and R&D is ongoing
• Development of first prototyping began in 2010

Accessibility
• github.com/kokkos/kokkos
• BSD 3 clause license

Current users
• numerous @ SNL, LANL, ORNL, U-Utah, ARL, NRL,

Collaborators

ASC and ECP Applications (AD, U, R)
• Sierra Mechanics
• Trilinos algorithms and enabling technologies
• EMPIRE/EMPRESS and SPARC
• Next-Generation Code (NGC) for multi-physics simulations
• Exascale Lattice Gauge Theory Opportunities and Requirements for Nuclear and High Energy Physics
• Molecular Dynamics at the Exascale: Spanning the Accuracy, Length and Time Scales for Critical Problems in Materials Science
• Exascale Predictive Wind Plant Flow Physics Modeling
• QMCPACK: A Framework for Predictive and Systematically Improvable Quantum-Mechanics Based Simulations of Materials
• Coupled Monte Carlo Neutronics and Fluid Flow Simulation of Small Modular Reactors
• Transforming Additive Manufacturing through Exascale Simulation (TrAMEx)
• Transforming Combustion Science and Technology with Exascale Simulations
• Cloud-Resolving Climate Modeling of the Earth’s Water Cycle

FY17 Development Plan
• Support application developers through training, consulting, and enhancements
• Develop initial capability enabling applications to manage and asynchronously utilize NGP node’s heterogeneous processing and memory resources
• Develop initial capability to support application algorithms using the on-node parallel pattern of a directed acyclic graph (DAG) of fine grain tasks
• Advocate for improvements to ISO/C++ and other standards for effective use of NGPs
**Extending HPCToolkit to Measure and Analyze Code Performance on Exascale Platforms**

### Description and Scope

**Project Description:**
Rice University’s HPCToolkit performance tools supports measurement, analysis, attribution, and presentation of parallel application performance.

**ECP Scope**
Extend HPCToolkit with improved capabilities for measurement and analysis of computation, data movement, communication, I/O, power, and energy consumption at extreme scale. Planned enhancements include improved support for lightweight measurement of massive node-level parallelism using hardware counters, measuring OS activity, recording measurement data efficiently, analyzing performance data in parallel, and integrating code-centric, time-centric, data-centric, and resource-centric views for analysis.

### Collaborators

**Potential or likely ties to other ECP Projects**
- Engage vendor and co-design efforts to design better instrumentation technologies for performance introspection on future platforms (HT/CD, D, E)
- Partner with developers of programming models and runtimes to add introspection interfaces that deliver insight into application performance (ST, D, E)
- Collaborate with NNSA and ST efforts developing instrumentation technologies for applications and runtimes, as well as measurement and analysis of data movement and network traffic (ST, U, E)
- Help ECP application teams use HPCToolkit to analyze code scalability and performance (AD, U, E)

**Synergistic projects**
- Exa-PAPI: The exascale performance and application programming interface
- ADTM projects: Caliper, Memtools, NetOpt, OMPT/OMPD

### Maturity Level and Accessibility

**Maturity Indicators and Metrics**
- Released in production
- 18 years in development

**Accessibility**
- [github.com/hpctoolkit](https://github.com/hpctoolkit), [github.com/dyninst](https://github.com/dyninst)
- BSD license

**Current users**
- Installed at ANL, LANL, LLNL, NERSC, ORNL, PNNL, SNL

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**First Year Development Plan**

- Curate releases of HPCToolkit in Q1 and Q4
- Finalize OMPT performance tools interface for OpenMP
- Leverage Linux `perf_events` interface to measure and attribute computation, data movement, OS activity, and blocked threads
- Parallelize program structure analysis to aid attribution of performance information
- Engage external collaborators and ECP application teams
**Project Description:**
The Exascale MPI project will design and develop enhancements to MPI that meet the critical needs of MPI applications. The project will focus on three primary capabilities: (1) improvements to the MPI implementation through MPICH; (2) improvements to the MPI standard; and (3) technology transfer to industry to ensure the availability of high-performance MPI implementations on DOE supercomputers.

**ECP Scope**
Exascale MPI will enable applications to effectively use the latest advances in MPI to scale to the largest supercomputers in the world. It will produce a high performance MPI implementation and affect changes to the MPI standard to meet application and architectural requirements.

**Maturity Level and Accessibility**

**Maturity Indicators and Metrics**
- MPICH is a production software that has been under continuous development for 23 years. MPICH derivatives are used on most supercomputers in the world as the primary MPI implementation.

**Accessibility**
- [http://www.mpich.org](http://www.mpich.org) (download and source links are available from there)
- BSD

**Current users**
- Practically all DOE applications and supercomputer centers use MPICH and derivatives. MPICH derivatives include Intel MPI, Cray MPI, IBM BG/Q MPI, Microsoft MPI, MVAPICH...

**Collaborators**

**Potential or likely ties to other ECP Projects**
- Most ECP applications employ MPI as part of their exascale strategy. We will collaborate with them to better understand the gaps in current implementations or the standard and will work closely with selected teams to develop solutions. Other potential collaborators:
  - SOLLVE: Scaling OpenMP with LLVM (ST, E)
  - Enhancing Qthreads (ST, E)
  - Argo: Operating System and Resource Management (ST, E)

**Synergistic projects**
- OpenMPI for Exascale

**First Year Development Plan**

- survey ECP apps teams to determine needs with respect to MPI implementation changes or standard changes;
- select key applications and mini-apps to guide and validate our work;
- prototype changes and work with applications to guide future changes;
- form teams with external participants to explore selected areas;
- integrate changes into releases and work with industry to incorporate first draft of changes for pre-exascale machines (such as CORAL)
Co-design in action: shared milestone examples

• OMPI-X ST project (Open MPI for exascale) will 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 Application Development teams to identify requirements about runtime coordination.
  – Interact with appropriate ECP Software Technology 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
Shared milestones examples

• SUNDIALS and the AMReX co-design center
  – Enable CVODE to be used from AMReX (Due 6/30/2017)
  – Description: AMReX will provide a build system and interface to CVODE within AMReX SUNDIALS will support AMReX in being able to link to CVODE from within the AMReX build system.

• Evaluation of VeloC (efficient checkpoint/restart) with the QCD application code

• Evaluation of VeloC (efficient checkpoint/restart) with the EXAALT application code (Molecular Dynamics at the Exascale application)
Next Steps for ST: Gap Analysis

- The results of a number of discussions (with vendors, facilities, applications) and responses to the ECP RFI to vendors are feeding into a gap analysis

- The gap analysis will specify what remaining pieces ECP needs to cover and what will be covered by vendors and other open source efforts

- Examples of known gaps:
  - Workflow infrastructure and tools
  - Software needed for applications in data analytics
  - Integration of ATDM ST efforts into overall architecture
  - Software co-design
  - Commonly used external software not covered in the current portfolio

- Will be reviewed by ECP leadership, senior lab leadership, and others
  - Update continuously based on feedback

- Contingent on available funding, we will issue an RFI/RFP later this year to close the gaps
Plan to involve additional Universities and Vendors

• The current set of Software Technology projects span 8 DOE national laboratories, 15 universities, and 2 independent software vendors.

• In FY17-18, budget permitting, we plan to issue additional solicitations for universities and vendors to cover gaps identified by the gap analysis.

• We plan to coordinate our activities with NSF to cover the broader university community through NSF.

• ECP has formed an Industry Council. This group will also serve as an interface for engaging independent software vendors and identifying industry users’ needs.

• Small businesses: DOE SBIR funding could support software of interest to ECP.
Update on ECP activities
Capable exascale system applications will deliver broad coverage of 6 strategic pillars

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<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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<td>Stockpile stewardship</td>
<td>Turbine wind plant efficiency</td>
<td>Additive manufacturing of qualifiable metal parts</td>
<td>Cosmological probe of the standard model of particle physics</td>
<td>Accurate regional impact assessments in Earth system models</td>
<td>Accelerate and translate cancer research</td>
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<td>Design and commercialization of SMRs</td>
<td>Urban planning</td>
<td>Validate fundamental laws of nature</td>
<td>Stress-resistant crop analysis and catalytic conversion of biomass-derived alcohols</td>
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<td>Nuclear fission and fusion reactor materials design</td>
<td>Reliable and efficient planning of the power grid</td>
<td>Plasma wakefield accelerator design</td>
<td>Metagenomics for analysis of biogeochemical cycles, climate change, environmental remediation</td>
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<td>Subsurface use for carbon capture, petro extraction, waste disposal</td>
<td>Seismic hazard risk assessment</td>
<td>Light source-enabled analysis of protein and molecular structure and design</td>
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<td>High-efficiency, low-emission combustion engine and gas turbine design</td>
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<td>Find, predict, and control materials and properties</td>
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<td>Carbon capture and sequestration scaleup</td>
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<td>Predict and control stable ITER operational performance</td>
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<tr>
<td></td>
<td>Biofuel catalyst design</td>
<td></td>
<td>Demystify origin of chemical elements</td>
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Exascale Computing Project, www.exascaleproject.org
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)
  – **Motifs:** 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)
  – **Motifs:** 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
27 Application Development milestones delivered in Q2FY2017 so far; selected examples

• GAMESS (1.2.1.16)
  – Initiate the development of a GAMESS-QMCPACK interface in collaboration with the QMCPACK group
  – Complete and assess an initial threaded GAMESS RI-MP2 energy + gradient code, conduct benchmarks

• Urban (1.2.1.17)
  – Define data streams between the four proposed models, including what each model is capable of providing and what each model could leverage as input
  – Hold planning/strategy workshop with five-lab team and inviting ECP software teams to assist in evaluating existing coupling/data-exchange systems

• AMReX (1.2.5.3.03)
  – Performance characterization of current AMR application codes
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.
- 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-ECP – Advancing Software Productivity for Exascale Applications

Description and Scope

- **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

Collaborators

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 software productivity, quality, and sustainability

History and Accessibility

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)

- **WhatIs and HowTo docs**: concise characterizations & best practices
  - What is CSE Software Testing?
  - What is Version Control?
  - What is 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

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
IDEAS-ECP – Highlights of Recent Activities

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.1328697

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.

Productivity and Sustainability Improvement Planning (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.

Co-Lead PIs: M. Heroux (SNL) and L.C. McInnes (ANL); Partner sites: LBNL, LLNL, LANL, ORNL, Univ of Oregon

Exascale Computing Project, www.exascaleproject.org
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 doctoral students, postdocs, and scientists who are 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. Expect to select up to 70 participants.
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

<table>
<thead>
<tr>
<th></th>
<th>DSE (lab POCs)</th>
<th>Memory Technologies</th>
<th>Interconnect/System Simulators</th>
<th>Analytical Models</th>
<th>Node Simulators</th>
<th>Abstract Machine Models and Proxy Architectures</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>ANL</strong></td>
<td>Ray Bair</td>
<td></td>
<td>ROSS/CODES</td>
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<td>Gem5</td>
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<td><strong>LANL</strong></td>
<td>Jeff Kuehn</td>
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<td>CoNCEPTual</td>
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<tr>
<td><strong>LBNL</strong></td>
<td>David Donofrio</td>
<td></td>
<td>ExaSAT, Roofline Toolkit</td>
<td>Gem5, OpenSOC</td>
<td></td>
<td>Co-lead AMM v3</td>
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<td><strong>LLNL</strong></td>
<td>Robin Goldstone</td>
<td>LiME</td>
<td>ROSS/CODES</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>PALM</td>
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<tr>
<td><strong>SNL</strong></td>
<td>Rob Hoekstra</td>
<td>SST: VaultSimC, MemHierarchy</td>
<td>SST, Merlin, Ember, Firefly</td>
<td>SST: Miranda, Ariel, Gem5</td>
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<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

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<tr>
<th>Access to Office of Science Systems</th>
<th>Access to testbeds supported with ECP funds</th>
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<tr>
<td><strong>NERSC’s Cori II</strong></td>
<td><strong>ALCF’s Theta</strong></td>
</tr>
<tr>
<td>Cori II early access</td>
<td>ECP allocation is 37+M hours on Theta for 2017</td>
</tr>
<tr>
<td>• Shared access with other users</td>
<td>• Intel Xeon Phi cpus</td>
</tr>
<tr>
<td>• Intel Xeon Phi (KNL) nodes</td>
<td>• 3,624 nodes</td>
</tr>
<tr>
<td>• Through June 30, 2017</td>
<td>• 64 core processor per node</td>
</tr>
<tr>
<td><strong>OLCF’s Titan</strong></td>
<td><strong>OLCF’s Summitdev</strong></td>
</tr>
<tr>
<td>2016 ALCC Reserve Award to ECP</td>
<td>ECP allocation is the equivalent of 18 nodes on Summitdev</td>
</tr>
<tr>
<td>• 13M Titan-core hours</td>
<td>• Power 8+</td>
</tr>
<tr>
<td>• March 30 to June 30, 2017</td>
<td>• NVIDIA Pascal GPGPUs</td>
</tr>
<tr>
<td>• 10 AD, 6 ST, and 1 HT teams are getting access</td>
<td>• NVLINK1</td>
</tr>
</tbody>
</table>

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

• We have a website
  – www.ExascaleProject.org

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

• A newsletter *The ECP Update* has been launched
  – https://exascaleproject.org/newsletter/ecp-update-1/
  – will be published at a minimum on a monthly basis, but we will use this vehicle to send our more frequent updates as we have topics of interest to report on.
  – Mailed to website followers plus Confluence registrants.
ECP Industry Council Charter

• The Exascale Computing Project (ECP) Industry Council is an advisory body that serves the ECP director and leadership team by providing advice and feedback on project scope and requirements, technical approaches, progress, strategic directions and other issues.

• The ECP Industry Council provides two-way communication and information exchange between the ECP and the high performance computing (HPC) industrial user community as well as the commercial HPC software community.
Industry Council Organization

- ECP IC Chair – Michael McQuade, United Technologies
- ECP Director – Paul Messina, Argonne National Laboratory
- ECP IC Co-Executive Directors – Suzy Tichenor, Oak Ridge National Laboratory and David Martin, Argonne National Laboratory
- ECP IC Members – 18 senior executives, 15 from industry and 3 from ISVs
- Members are appointed by ECP Director for a two-year term
- Members represent their company as well as their industry sector
Industries Represented (Forbes Categories)

- Conglomerates
- Oil & Gas Operations
- Nuclear Power
- Heavy Equipment
- Air Currier
- Household Personal Care
- Pharmaceuticals
- Food, Drink and Tobacco
- Auto & Truck Manufacturers
- Household Appliance
- Diversified Chemicals
- Fusion Energy
- Media (Animation)
- Independent Software Vendors
Wall of Logos
First ECP Industry Council Meeting

- Held March 6-7, 2017 at Argonne National Laboratory
- Tour of the Advanced Photon Source
- Detailed Presentations from ECP Director and Focus Area Leads
- Presentation on International Exascale Competition
- Time for Feedback on Direction and Plans
- Outcome: Exascale is Critical to US, Desire to Provide Detailed Input on Industry Needs
For More Information

• Industry Council Web Site: https://exascaleproject.org/advisory-councils/


• Industry Council Co-Executive Directors:
  – David Martin <dem@alcf.anl.gov>
  – Suzy Tichenor <tichenorsp@ornl.gov>
THE ECP ECOSYSTEM

- 800 Researchers
- 26 Application Development Projects
- 66 Software Development Projects
- 5 Co-Design Centers

DOE LABORATORIES & AGENCY PARTNERS: 22
PRIVATE SECTOR PARTNERS: 9
UNIVERSITY RESEARCH PARTNERS: 39
INDUSTRY COUNCIL MEMBERS: 18
Thank you!

www.ExascaleProject.org