Exascale Computing Project: Status and Next Steps

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Chair, ECP Laboratory Operations Task Force (LOTF)

DOE Office of Science Advanced Scientific Computing Advisory Committee (ASCAC)
April 17, 2018
ECP is a critical component of the broader ECI strategy

Computational and data science solutions for the Nation

• Broader ECI elements are essential for success
  – Deploying exascale systems quickly enough to impact schedule-sensitive mission problems
  – Maintaining and advancing the “HPC ecosystem” after ECP
  – Developing U.S. industry and academia partnerships to ensure the benefits of advanced computing have broad and enduring impacts

• ECP Vision (where ECP is headed)
  – *Accelerating innovation with exascale simulation and data science solutions that enhance US economic competitiveness, improve our quality of life, and strengthen our national security.*

• ECP Mission (purpose; reason for existence)
  – *Deliver* 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
  – *Leverage* US HPC vendor R&D activities and products into DOE HPC exascale systems.

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**ECP enables the continued US global strategic advantage in science and technology which is the foundation of future revolutions in technology development, energy security, scientific discovery, and national security.**
ECP History: from the Start of Project to Present

FY16
ECI: 10-year initiative
ECP CD-0 based on 10 years

2015
ECP
Apps
SW
Vendor R&D
Exascale Systems
NRE
Testbeds

2025

Q1-2 FY17
Acceleration & Data convergence
7 year ECP, novel arch 2021 system

2016
ECP
Apps
SW
Vendor R&D
Exascale Systems
NRE
Testbeds

2022

Present (since Q3 FY17)
Change in priorities reflected in DOE FY18 budget request:
- Push Argonne’s planned 2018 Intel system to 2021 and increase to exaflop
- Bring ORNL exascale system in to 2021 to help ensure mission success
- Move ECP ES scope to SC leadership facilities and NNSA HPC facilities via ECI

System Acquisition Target
ANL exascale system (2021) – A21
ORNL exascale system (2021-22) - Frontier
LLNL exascale system (2023) – El Capitan

Facilities
Exascale Systems, NRE, Testbeds

Emphasis on ECP/Facilities Integration
ECP Areas of Technical Focus

**Application Development**
The Application Development effort develops and enhances the predictive capability of applications critical to the DOE, including the science, energy, and national security mission space. The scope of the AD focus area includes:
- targeted development of requirements-based models, algorithms, and methods,
- integration of appropriate software and hardware via co-design methodologies,
- systematic improvement of exascale system readiness and utilization, and
- demonstration and assessment of effective software integration.

**Software Technology**
Software Technology spans low-level operational software to high-level applications software development environments, including the software infrastructure to support large data management and data science for the DOE SC and NNSA computational science and national security activities at exascale. Projects will have:
- line of sight to application’s efforts
- inclusion of a Software Development Kit to enhance the drive for collaboration, and
- delivery of specific software products across this focus area.

**Hardware and Integration**
This focus area is centered on the integrated delivery of specific outcomes (ECP Key Performance Parameters, or KPPs) and products (e.g., science as enabled by applications, software, and hardware innovations) on targeted systems at leading DOE computing facilities. Areas include:
- PathForward
- Hardware Evaluation
- Application Integration at Facilities
- Software Deployment at Facilities
- Facility Resource Utilization
- Training and Productivity
DOE Program and core laboratory agreements provide effective oversight, advisory bodies provide effective advice

**GOVERNANCE**

**ECP Board of Directors (BOD):**
- Laboratory directors of 6 core national labs
- ECP Project Director reports to the BOD

**Laboratory Operations Task Force (LOTF):**
- ALDs from each of the 6 core laboratories
- Meets with ECP project director and deputy weekly to discuss staffing, operational, and management issues

**Governance model has proven to be effective:**
- BOD provides oversight and advice to ECP Director, and high-level interface with stakeholders
- LOTF provides engaged and effective leadership, ensuring core partner labs work together and cooperatively
- DOE/NNSA provide clear programmatic guidance across office boundaries

**ADVICE**

- **Industry Council** provides communication and information exchange between ECP and industries reliant on computer and computational science
- **Science Council** will examine ECP scientific output and ECP plans from a science and engineering quality perspective
- Both bodies will examine ECP results, processes, and activities and provide respected and useful experience-based advice to ECP management
ECP Integrated Project Team (IPT)

- **IPT Members**: DOE program managers, Federal Project Director (FPD) and FPD Deputy, members from the ORNL site office, Oak Ridge Integrated Support Center (OR-ISC), Project Director (PD) and PD Deputy, CTO, focus area directors and deputies, and project office staff (when needed)

- **Mission**: Provide strategic planning, coordination, and communication for the ECP to ensure that the project’s objectives are achieved on schedule, within budget, and consistent with quality standards and DOE guidance
ECP’s Independent Project Review: Key Recommendations
From Jan 9-11, 2018 review

• Revise the ST gap analysis document regularly, at least annually.

• Revise initial ST Level 4 milestones by third quarter FY 2018 to remove vagueness and improve relevance.

• ECP and facilities need to work on an ongoing basis to achieve earliest possible access to test-beds, timelines, and information on chip/system architecture features.

• Add a HI and facilities breakout session to future independent project reviews including members of all the facilities in use by ECP.

• Expedite NDAs for the projects so AD and ST understand the hardware challenges and implications they will be facing early on.

• Refine and finalize the KPPs (including Figures of Merit and impact metrics) as soon as possible prior to CD-2.
ECP Funding thru FY18 and Plans for FY19

The FY18 budget was approved by Congress in March. The President’s Budget Request (PBR) for FY19 is public.

<table>
<thead>
<tr>
<th></th>
<th>FY-16 actual</th>
<th>FY-17 actual</th>
<th>FY-18 actual</th>
<th>FY-19 PBR</th>
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</thead>
<tbody>
<tr>
<td><strong>Total ECP Funding</strong></td>
<td>221</td>
<td>249</td>
<td>334</td>
<td>300</td>
</tr>
<tr>
<td>ASCR contribution</td>
<td>157</td>
<td>164</td>
<td>205</td>
<td>232</td>
</tr>
<tr>
<td>ASC contribution</td>
<td>64</td>
<td>85</td>
<td>129</td>
<td>68</td>
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**FY-18 looks good** with a slight increase over ASCR’s planned $197M and ASC contributing the planned amounts to AD and ST plus $54M rather than the planned $40M to PathForward.

**FY-19 contains challenges, most notable is a potential large drop in ASC support.**

The PBR specifies that ASC contribute $30M to AD, $35M to ST, and $0 to HI. The drop significantly affects PathForward and also reduces ST ATDM projects.
Execution is ECP’s highest FY18 priority

• **Execution of our plan** of record – FY18 budget enables the vigorous execution of our plan
  – The ECP plan of record includes additional scope and funding for some applications (seed and non-seed)

• **Complete detailed joint engagement and execution plans** with HPC Facilities
  – e.g., alignment of PathForward projects with NRE contracts once placed

• **Evaluate additional strategic scope** to enhance ECP’s long-term impact
  – Possible addition of data science scope (e.g., cyber) to the electrical grid application
  – Possible addition of a data science/artificial intelligence co-design center

• **Advancing project management toward CD-2**
  – Complete implementation of project dashboards for efficient project status and management
  – Complete clear plan to achieve CD-2 (in FY19) – Next IPR late fall, 2018

In addition to execution, our focus is on rapid evaluation, decision, and pushing out increased funding for added scope
### ECP Application Development (AD)

<table>
<thead>
<tr>
<th>Chemistry and Materials Applications</th>
<th>Describes underlying properties of matter needed to optimize and control the design of new materials and energy technologies</th>
</tr>
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<tbody>
<tr>
<td>Energy Applications</td>
<td>Model and simulation of existing and future technologies for the efficient and responsible production of energy to meet the growing needs of the U.S.</td>
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<tr>
<td>Earth and Space Science Applications</td>
<td>Spans fundamental scientific questions from the origin of the universe and chemical elements to planetary processes and interactions affecting life and longevity</td>
</tr>
<tr>
<td>Data Analytics and Optimization Applications</td>
<td>Applications partially based on modern data analysis and machine learning techniques rather than strictly on approximate solutions to equations that state fundamental physical principles or reduced semi-empirical models</td>
</tr>
<tr>
<td>National Security Applications</td>
<td>Stewardship of the US nuclear stockpile and assessment of future threats; related physics and engineering modeling and scientific inquiries consistent with that mission space</td>
</tr>
<tr>
<td>Co-Design</td>
<td>Focused on crosscutting algorithmic methods that capture the most common patterns of computation and communication in ECP applications</td>
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</tbody>
</table>
1. Deliver improved and impactful science & engineering (*performance*)
   - New or enhanced predictability on a problem of national importance (the “challenge problem”) measured in part by the application’s rate of executing useful work (W/t) on the CP

2. As performance portable as possible and reasonable (*portability*)
   - No “boutique” one-off applications able to only execute on one (and likely ephemeral) system

3. Able to make effective use of a capable system (*readiness*)
   - *Effective* is app specific (weak, strong, ensembles, single-node performance)

4. Able to integrate latest relevant software technologies (*modern*)
   - Needed to demonstrate agility, flexibility, modern architecture; overall app portfolio must apply pressure to all key attributes of the system design characteristics

5. High priority (*strategic*)
   - Key stakeholders care about using application to make consequential decisions
**Selected FY18 AD Highlights**

**Release**

- CEED team released first software distribution (CEED 1.0), consisting of 12 integrated Spack packages for libCEED, mfem, nek5000, nekcem, laghos, nekbone, hpgmg, occa, magma, gslib, petsc and pumi, plus a new CEED “meta-package” (Milestone CEED-13).

**Algorithm or Physical Model Enhancement**

- WDMApp team completed coupling of GENE and XGC, first time a continuum core gyro-kinetic code (GENE) coupled to an edge gyro-kinetic code (XGC) based on the particle-in-cell (PIC) method, enabling a complete kinetic description of the entire plasma.

**Science Capability**

- E3SM-MMF successfully completed the milestone on GPU acceleration of ocean, and also completed the initial port of CRM to GPU.

**Performance**

- ExaSky ported the HACC code to Summit, and has already achieved excellent strong scaling and a 30-35X speedup over the CPU.
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
- Coordinate with and complement vendor efforts
- Develop and deploy high-quality and robust software products

56 WBS L4 subprojects executing RD&D
ECP SW Stack: Strategic Alignment & Synergies

Data & Visualization

Applications

Co-Design

Programming Models
Mathematical Libraries
Embedded Data & Visualization
Development Tools

Software Ecosystem & Delivery

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

ECP software projects
Each project to define (potentially ≥2) release vectors

More projects

SDKs
Reusable software libraries embedded in applications; cohesive/interdependent libraries released as sets modeled on xSDK

- Regular coordinated releases
- Hierarchical collection built on Spack
- Products may belong to >1 SDK based on dependences
- Establish community policies for library development
- Apply Continuous Integration and other robust testing practices

Fewer projects

OpenHPC
Potential exit strategy for binary distributions

- Target similar software to existing OpenHPC stack
- Develop super-scalable release targeting higher end systems

Direct2Facility
Platform-specific software in support of a specified 2021–2023 exascale system

- Software exclusively supporting a specific platform
- System software, some tools and runtimes

SDK Leadership Team: Decades of Software Experience
- Jim Willenbring – SDK Coordinator and Release Manager
- Sameer Shende – Programming Models & Runtimes
- Bart Miller – Development Tools
- Lois McInnes – Math Libraries
- Chuck Atkins - Data & Viz

94 – Number of Products ECP ST contributes to
(46, 23) – Number of Spack-ready products (Done, In progress)
Q2FY18 ECP ST Highlights

ECP ST Q2 Progress: 3 Examples

- Threaded execution of data compression: 16x time improvement.
  - Compression and threaded execution are essential.
- New OpenMP Runtime: 70% time overhead reduction.
  - Addresses the ‘+’ of MPI+X, essential for Exascale.
- New Checkpoint/Restart: 3s offload (purple), scale independent.
  - Rapid CPR is the ECP resilience strategy

Data Compression Speedups

- Speedup
  - 32 cores: 14~16
  - 64 cores: 15~17
- Breakdown performance
  - Speedup: up to about 40

Checkpoint/Restart Progress

- Preliminary experiments on Theta: Better scalability and performance for asynchronous vs synchronous mode

MPI+OpenMP Overhead Progress

- H: # of threads for horizontal parallelism
- V: # of threads for vertical parallelism
- Evaluated on a 16-core machine
- 2 x Intel Xeon CPU E5-2670
- Demonstration for vendor adoption

Software Available from all projects:

- SZ Compression: New release (1.4.13.0) can be downloaded from github (https://github.com/disheng222/SZ/releases/tag/v1.4.13.0).
- OpenMP: BOLT v1.0b1 and v1.0a1 (http://www.bolt-omp.org/downloads) and Argobots v1.0b1 and v1.0a1 (http://www.argobots.org/downloads)
- CPR: Veloc Backend software (xgitlab.cels.anl.gov/ecp-veloc)
Hardware Integration: Designed to Enable Integration of ECP’s products into HPC Environments at the Facilities

ECP will meet its objectives on Facility resources

**ECP products**
- Applications
- Software
- Early HW R&D

**Hardware and Integration**
- Facility resource utilization
- Developer training and productivity
- PathForward
- HW evaluation

**Facilities**
- Application integration at Facilities
- SW deployment at Facilities
- DOE SC and NNSA HPC Facilities
- US vendor system offerings
<table>
<thead>
<tr>
<th>HI project</th>
<th>FY18 Q1 and Q2 Accomplishments</th>
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<tbody>
<tr>
<td>Application Integration at Facilities</td>
<td>• Developed a plan jointly with the Facilities to prepare and deploy ECP applications on the Facilities’ pre-exascale and exascale systems&lt;br&gt;• Prepared paperwork to send funds to the Facilities for this project</td>
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<tr>
<td>Software Deployment at Facilities</td>
<td>• Developed a plan jointly with the Facilities to deploy ECP software on the Facilities’ pre-exascale and exascale systems&lt;br&gt;• Prepared paperwork to send funds to the Facilities for this project&lt;br&gt;• Collaborated with ST on awarding and managing a contract to develop a secure automated testing capability</td>
</tr>
<tr>
<td>Training and Productivity</td>
<td>• Developed and hosted multiple training and educational events&lt;br&gt;• Awarded the 2018 Better Scientific Software (BSSw) Fellows&lt;br&gt;• Made available on ECP’s public website recordings of training events and material</td>
</tr>
<tr>
<td>HI project</td>
<td>• FY18 Q1 and Q2 Accomplishments</td>
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<tr>
<td>Facility Resource Allocation</td>
<td>• Stood up the ECP Resource Allocation Council (RAS)</td>
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<td></td>
<td>• Allocated, managed, and reported on ECP’s initial computer allocations</td>
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<tr>
<td></td>
<td>• Drafted a user program for managing future computer allocations</td>
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<tr>
<td>PathForward</td>
<td>• 2nd review held March 2018 – all 6 contractors reported progress to be reviewed by a team of Lab/Gov’t experts</td>
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<td>• ~25% of milestones completed; another ~25% in progress</td>
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<td></td>
<td>• PF research efforts are expected to significantly enhance the CORAL2 bids</td>
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<tr>
<td>Hardware Evaluation</td>
<td>• Published first version of an Abstract Machine Model document to be used as a aid for understanding key architectural features without revealing proprietary information</td>
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<td>• Completed a memory performance study</td>
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HI has three main challenges: 1) time pressures 2) developing and maintaining strong partnerships, and 3) standing up HI two years into ECP

- Shortened timeline: less time for HW innovations, app and SW development, facilities preparation and acquisition
- Integration with 6 facilities: building strong collaborations, aligning priorities and schedules
- HI late start: reduced time to achieve objectives, budgetary constraints
- Integration with AD and ST: many projects, connecting them with the facilities, building collaboration between many stakeholders
Software Projects

- ADIOS
- ATDM
- LLVM
- Kokkos
- RAJA
- Legion
- Trilinos

SDKs

- SDK 1
- SDK 2
- SDK 3
- ... Software Development Kits (SDKs) (delivery specs and mechanism)

Communication and Release

- GitLab
- openHPC
- Workshops
- Conferences
- Publications
- ...

Applications
Integration of ST products via SDK

APIs

S/W R&D

Continuous Integration

Release

Integration with vendor s/w

Deploy to Facilities

S/W deployment

Facilities

- A21
- Frontier
- El Capitan
- Pre-Exascale

The ECP Exascale Computing Ecosystem

HPC and Scientific Community
Dashboard Being Developed to Track Progress
Attributes currently being prototyped – ECP will evolve what we learn is most useful

• Applications
  – Mission (priority, uniqueness)
  – Exascale challenge problem status (on track, caution, trouble)
  – Figure of Merit (FOM) status (ratio of required challenge problem work rate / current work rate)
  – Node- and system-level performance and scalability (relative to baseline)
  – Readiness and portability (facility platforms supported & specs associated with successful execution)
  – Facility commitment (readiness, acceptance, early science)
  – Ecosystem Requirements (coverage of motifs & ST products)

• Software Technologies
  – Utilization: by applications, facilities, and overall users
  – Continuous integration results: regression tests, performance, integrity, scaling
  – Impact goal status (on track, caution, trouble)

• Hardware and Integration
  – PathForward milestone deliverables (how many, mapping to exascale hardware challenges)
  – Status of application and software deployment at DOE HPC Facilities
  – EPC application and software HPC resource usage at DOE HPC Facilities
ECP Risks and Challenges

• Cost/funding issues
  – Accept (track funding issues; implement flexible contracts; design for agility)

• Exascale platform meeting requirements unavailable to ECP
  – Mitigate (impart 12 months of schedule contingency, re-baseline)

• Unclear messaging to stakeholders
  – Mitigate (develop common talking points and training)

• Standard programming models are insufficient for applications
  – Mitigate (formal constraints on s/w ecosystem delivered by vendors, regular assessments)

• PathForward funding does not align with costs
  – Mitigate (realign funding commitments to profiles, re-negotiate vendor milestones)

• Relationship between ECP and Facilities
  – Mitigate (facility engagement plans, track interactions and facility utilization)
ECP Status: Summary

• Great team, great plan, executing full bore
• Great stakeholder support and high priority to DOE
• Moving into a product development stage with more quantitative metrics
• Actively managing our highest risks
• Putting facility engagement plans into action
• Still have work to do: tracking progress (dashboard), maintaining agility for highest ROI on RD&D, adjusting plan to ever-changing budget and cost profiles
Thank you!
ECP Governance: DOE Program & Lab Agreements

• MOU between DOE/SC and NNSA/DP to define roles & responsibilities of Programs responsible for ECI & ECP

• MOA between six national labs (“core partners”) responsible for leading and managing ECP: ANL, LANL, LBNL, LLNL, ORNL, SNL

• ECP Board of Directors serves an advisory, oversight, line-management role for ECP
  – Advise Project Director (PD) on strategic direction and performance goals; evaluate PD performance on an annual or as-needed basis; support ECP SLT in managing interfaces with key stakeholders
  – Comprised of the laboratory directors from each core partner laboratory and 2-3 external members
  – Operations: establish a standing Laboratory Operations Task Force (LOTF) comprised of one delegate from each core partner laboratory with management responsibility at their laboratory for the resources needed for ECP to be successful
    • Rick Stevens (ANL); John Sarrao (LANL); Kathy Yelick (LBNL)
    • Mike McCoy (LLNL); Jeff Nichols (ORNL); Scott Collis (SNL)
  – LOTF currently meets weekly with the PD to discuss staffing, operational and management issues

Governance model has proven to be effective. LOTF provides engaged and effective leadership to ECP and in keeping ECP core partner labs working together consistently and cooperatively.
ECP Advisory Bodies: Industry and Science Councils

• Industry Council (meetings Mar & Oct 2017, teleconference Jun 2017)
  – Provides two-way communication and information exchange between ECP and private sector software and hardware companies and broader engagement with the computational science and HPC user community from an industry perspective
  – Member companies represent computer and computing technology, design and engineering, consumers of scientific computing resources as part of their business activities, and ISVs
  – Current activity: provide ECP with industry exascale challenge problem drivers and requirements
  – Future activities: participate in red team reviews, provide feedback on milestone reports and accomplishments, provide feedback on project office’s approach to incorporating agile with formal PM

• Science Council (not yet chartered)
  – SC will be asked to examine and provide technical feedback and advice to ECP leadership on the plan for and quality of the science, engineering, and technology achievements and milestone deliverables
  – SC will be composed of leading computer scientists, computational scientists, and applied mathematicians (e.g., NAS, NAE members)

ECP will benefit in FY18 and beyond from increased external SC/IC advice on its plans and milestone deliverables