Toward a Leadership Software Center (LSC)

Transforming Science R&D into World-class Leadership Software
Disclaimer

- The following description is notional
- We have shared it with stakeholders
- Goal: Be ready to execute a plan for post-ECP sustainability
• The US DOE Exascale Computing Project (ECP) initiated the Extreme-scale Scientific Software Stack (E4S)
• E4S development will continue under ECP for two more years
• A brief reminder of E4S and SDKs
Extreme-scale Scientific Software Stack (E4S)

- **E4S**: HPC software ecosystem – a curated software portfolio
- **A Spack-based** distribution of software tested for interoperability and portability to multiple architectures
- Available from **source, containers, cloud, binary caches**
- Leverages and enhances SDK interoperability thrust
- Not a commercial product – an open resource for all
- Growing functionality: Nov 2021: E4S 21.11 – 91 full release products

Community Policies
- Commitment to software quality

Curated collection
- The end of dependency hell

Turnkey stack
- A new user experience

DocPortal
- Single portal to all E4S product info

Quarterly releases
- Release 1.2 – November

Build caches
- 10X build time improvement

Post-ECP Strategy
- LSSw; ASCR Task Force

Portfolio testing
- Especially leadership platforms

https://e4s.io
E4S lead: Sameer Shende (U Oregon)

Also includes other products, e.g.,
AI: PyTorch, TensorFlow, Horovod
Co-Design: AMReX, Cabana, MFEM
E4S delivers products needed now and into the future

Key themes:
- Focus: GPU node architectures and advanced memory & storage technologies
- Create: New high-concurrency, latency tolerant algorithms
- Develop: New portable (Nvidia, Intel, AMD GPUs) software product
- Enable: Access and use via standard APIs

Software categories:
- **Next generation established products:** Widely used HPC products (e.g., MPICH, OpenMPI, PETSc)
- **Robust emerging products:** Address key new requirements (e.g., Kokkos, RAJA, Spack)
- **New products:** Enable exploration of emerging HPC requirements (e.g., SICM, zfp, UnifyCR)

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

Levels of Integration
- Build all SDKs
- Build complete stack
- Containerize binaries

Product
- E4S
  - Source: ECP E4S team; Non-ECP Products (all dependencies)
  - Delivery: spack install e4s; containers; CI Testing

- SDKs
  - Source: SDK teams; Non-ECP teams (policy compliant, spackified)
  - Delivery: Apps directly; spack install sdk; future: vendor/facility

- ST Products
  - Source: ECP L4 teams; Non-ECP Developers; Standards Groups
  - Delivery: Apps directly; spack; vendor stack; facility stack

Source and Delivery

ECP ST Open Product Integration Architecture

ECP ST Individual Products
## E4S and SDKs as Platforms are providing tremendous value

<table>
<thead>
<tr>
<th>Activity</th>
<th>SDKs</th>
<th>E4S</th>
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<tbody>
<tr>
<td><strong>Planning</strong></td>
<td>Transparent and collaborative requirements, analysis and design, delivery</td>
<td>Campaign-based portfolio planning coordinated with Facilities, vendors, community ecosystem, non-DOE partners</td>
</tr>
<tr>
<td><strong>Implementation</strong></td>
<td>Leverage shared knowledge, infrastructure, best practices</td>
<td>ID and assist product teams with cross-cutting issues</td>
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<tr>
<td><strong>Cultivating Community</strong></td>
<td>Within a specific technical domain: Portability layers, LLVM coordination, sparse solvers, etc.</td>
<td>Across delivery and deployment, with software teams, facilities’ staff</td>
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<tr>
<td><strong>Resolving issues, sharing solutions</strong></td>
<td>Performance bottlenecks and tricks, coordinated packaging and use of substrate, e.g., Desul for RAJA and Kokkos</td>
<td>Build system bugs and enhancements, protocols for triage, tracking &amp; resolution, leverage across &amp; beyond DOE</td>
</tr>
<tr>
<td><strong>Improving quality</strong></td>
<td>Shared practice improvement, domain-specific quality policies, reduced incidental differences and redundancies, per-commit CI testing</td>
<td>Portfolio-wide quality policies, documentation portal, portfolio testing on many platforms not available to developers</td>
</tr>
<tr>
<td><strong>Path-finding</strong></td>
<td>Exploration and development of leading-edge computational tools that provide capabilities and guidance for others</td>
<td>Exploration and development of leading-edge packaging and distribution tools and workflows that provide capabilities and guidance for others</td>
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<tr>
<td><strong>Training</strong></td>
<td>Collaborative content creation and curation, coordinated training events for domain users, deep, problem-focused solutions using multiple products</td>
<td>Portfolio installation and use, set up of build caches, turnkey and portable installations, container and cloud instances</td>
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<tr>
<td><strong>Developer experience</strong></td>
<td>Increased community interaction, increased overhead (some devs question value), improved R&amp;D exploration</td>
<td>Low-cost product visibility via doc portal, wide distribution via E4S as from-source/pre-installed/container environment</td>
</tr>
<tr>
<td><strong>User experience</strong></td>
<td>Improve multi-product use, better APIs through improved design, easier understanding of what to use when</td>
<td>Rapid access to latest stable feature sets, installation on almost any HPC system, leadership to laptop</td>
</tr>
<tr>
<td><strong>Scientific Software R&amp;D</strong></td>
<td>Shared knowledge of new algorithmic advances, licensing, build tools, and more</td>
<td>Programmatic cultivation of scientific software R&amp;D not possible at smaller scales</td>
</tr>
<tr>
<td><strong>Community development</strong></td>
<td>Attractive and collaborative community that attracts junior members to join</td>
<td>Programmatic cultivation of community through outreach and funded opportunities that expand the membership possibilities</td>
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Moving Forward

• To better ensure continued growth and sustainability beyond ECP, we are exploring ideas now to better orient E4S efforts toward the post-ECP era

• Engaging key US agencies and international institutions is essential to the longevity of E4S

• We propose a plan for
  • A DOE ASCR Leadership* Software Center (LSC)
  • A leadership and stewardship role in sustaining and growing E4S through LSC

*We intend leadership in our setting to mean emerging and leading-edge software for emerging and leading-edge scientific computing environments, including HPC, AI/ML for science, large-scale edge computing for science, quantum, and other scientific computing software products that complement industry efforts and facilitate scientific progress.
Mission

- Deliver a robust, reliable, high-quality and sustainable software stack that enables the rapid development of DOE scientific applications for the pursuit of scientific discovery in leading-edge computing environments
Vision

• Build the best leadership computing scientific software stack in the world
• that enables innovative computational and data science solutions
• to global challenges and breakthrough problems
• on leadership computing platforms
Values

We value software that

- addresses leading edge and emerging application needs,
- on leading edge and emerging computing platforms,
- and unambiguously adds value to the software ecosystem
- because of its usefulness, quality, sustainability & complementarity
Goals

1. Establish a sustainable organization to effectively & efficiently deliver DOE leadership scientific software
2. Deliver a portable, high-performance scientific computing development and execution software stack
3. Accelerate the augmentation of scientific solutions with integrated AI/ML and advanced workflows
4. Curate and deliver a software ecosystem for emerging edge workflows to support large-scale data
5. Prepare for software stack requirements to address emerging quantum computing technologies
6. Establish ecosystem partnerships with other DOE, agency, industry, academic and international institutions
7. Build a community and workforce around scientific software development
Requirements

1. **Single Org, distributed R&D teams:** Single LSC organization drawing from all DOE labs, universities, industry

2. **Sustained sponsor and affiliate support:** Clear commitment to attract the best and brightest

3. **Business model for interactions:** How to engage ecosystem partners: ASCR Research, SciDAC, Facilities, industry

4. **Domain leaders:** Thought leaders in each supported technical domain

5. **Strategic platform and problem information access:** Information on computing and scientific futures

6. **Distributed collaboration environment:** Information platforms, tools, processes and support staff
• ECP makes a compelling case for coordinated development and delivery of DOE software products
  • **Planning**: Portfolio of inter-related capabilities in collaboration with application teams, facilities, vendors, open-source communities
  • **Execution**: Development and dissemination of best practices; use of shared platforms (e.g., Atlassian tools), testing infrastructure, effective and efficient processes
  • **Tracking**: Coordinated and transparent progress tracking, adaptation to evolving requirements
  • **Assessment**: Regular assessment and reporting of progress to stakeholders and community

• The ECP ST Portfolio approach promises improved effectiveness and efficiency of DOE software efforts vs independent software teams working alone

• The E4S/SDK open software architecture provides a framework for successful software development and delivery

• ECP has fostered a holistic approach to scientific software workforce development

• **A Leadership Software Center (LSC) provides a compelling approach as an enabler to coordinate the development and delivery of DOE software products after the end of ECP**
ECP Experience: Software sustainability requires a new kind of organization

**Leadership Software Center (LSC):** Will enable the sustainability of ECP contributions, and development and delivery of future capabilities, including new domains like AI/ML, Edge and Quantum

**Tailored Agile:** The LSC will use tailored project management practices, processes, tools, and a distributed multi-institutional organization to enable effective and efficient delivery of ASCR software investments.

**New Ecosystem Entity:** The LSC will establish an essential and new ecosystem entity to complement Facilities, ASCR Research, vendors, industry and other entities.

**Workforce Development:** Establishing the LSC assures the creation of a scientific software workforce for sustainable leadership scientific software development and delivery.
Key Elements of the LSC Structure

LSC Project Leadership
- Project Director/Deputy (2 FTE): Leads overall project, coordinates with DOE, Tech area leads, other stakeholders
- Project Controls & Admin (2 FTE): Manages budgets, funds, costs. Supports communication, processes & tools
- Overall responsibility for coordination and delivery of E4S (3 FTE)
- Conduit to vendor, facility stacks, open community platforms, standards (2 FTE)
- IDEAS/BSSw team (3 FTE)
- Training/Outreach (content curation, fellows) coordinated with Facilities (2 FTE)

Technical area SDKs
- Initial areas: Programming models & runtimes, development tools, math libs, data, viz, SW packaging & delivery
- Upcoming: ML/AI, Edge, Quantum
- Technical area SDK lead: Provides technical planning and oversight for the area as an aggregate
- One lead and deputy for each SDK collection of capabilities (1 FTE total per area)
- SDK leaders chosen for domain expertise and for broad institutional representation

Product development teams
- PI plus team (1 – 3 FTE per team).
- Team members include:
  - Domain expert developers
  - Project coordinator (shared across multiple product teams) to manage processes & deliverables
  - Career software professionals, research software engineers (RSEs)
Leadership Software Center Cadence
Ongoing + Campaigns

LSC Core

Initiate

Refine

Sustain

Leadership Software Campaigns

LSC-1 (2024-26)
- Next phase core SW*
- Establish AI/ML SDK
- Scope Edge SDK
- Contingency

LSC-2 (2027-2029)
- Next phase core SW
- Next phase AI/ML
- Establish Edge SDK
- Scope Quantum SDK
- Contingency

LSC-3 (2030-32)
- Next phase core SW
- Next phase AI/ML
- Next phase Edge
- Establish Quantum SDK
- Contingency

*Next phase core SW: Scope necessary to address emerging needs in programming models, runtimes, tools, math libs, data, visualization, workflows and other established software technologies. Often this scope will be new features in existing LSC products, such as AI linear algebra features being added, or support for the latest AI devices, or both, to our existing Math Libs SDK.
LSC Execution Approach

Plan, Execute, Track, Assess Lifecycle

- All activities governed by phased development process
- Executed as “campaigns”: LSC-1, LSC-2, ...
- Tailored agile approach
- Hierarchical approach:
  - Multi-year baseline as campaign
  - Refine annually
  - Add fidelity per milestone at “last responsible moment”

Change Management Process:

- Changes from campaign base plan managed by a process
- Any changes to cost, scope and schedule
- Explicit review process determined by degree of change
- Change control process assures lightweight transparency
- Objective: Always do most important work at any time
DOE software products have four primary integration targets:

- **Vendors**: Specific HPC enhancements, integrated into system vendor stacks
- **Community SW**: C++, Fortran, LLVM
- **Facilities**: Tuned open-source SW for key platforms
- **Direct to apps**: Application teams download and build

**Note**: Some products are available via 2 – 3 of the above targets

**LSC goals:**

- **Establish and ensure quality standards** for LSC product development and delivery
- Assure that funded projects **develop and deliver** to one or more integration targets
- **Track and assess** integration status of new capabilities
Building new infrastructure and business models toward a sustainable software ecosystem

Leadership Software Center (LSC): Some business needs overlap with Leadership Computing Facilities, but not all

Preparing E4S products requires additional early-access resources: Frontier and Aurora early-access systems are essential, but E4S teams need more

E4S products require tiered support: Beyond tier-1 support at the facilities, users need issues addressed by staff funded to do the support in collaboration with product dev teams

Partnering with commercial software companies for E4S support enables cost and benefit sharing: Cost of E4S support is shared, opens possibility for industry use of E4S because they can pay for support
Frank – Designed for Libs & Tools Developers

- Prep system for ECP libs & tools
- Access to latest non-NDA HW/SW
- Shared file system – 1 copy of SW
- Port to many device types at once
- Porting support from E4S team
- CI testing workhorse (500K builds)
- Next: Bare metal, BIOS-changing support for low-level software work
Software Support Challenges

Support for DOE libraries & tools has been challenging in the past:

- Support funding is a tax on incoming R&D funds
- External user support ad hoc and cautious: Chicken vs pig in ham & eggs breakfast

Impact: Uptake is risky

- Support is contingent on
  - Continued R&D funding (DOE users)
  - Minimal incompatibility with DOE user needs (external users)
- App teams (even DOE) reluctant to adopt – concerned about long-term support
Strategy: Commercial partnerships

• Fund external commercial support org
• Provide tier-2 facilities user support
• Triage E4S bugs
• Work with product teams to fix issues

Commercial partner leverage

• Commercial E4S expertise means industry, agencies can purchase support
• Creates broader E4S user base
• Spreads support costs
• Enables industry and agencies to adopt leading edge software more easily
Working toward software sustainability: ASCR Task force, community events

Leadership Scientific Software (LSSw) Portal  https://lssw.io

The LSSw portal is dedicated to building community and understanding around the development and sustainable delivery of leadership scientific software

- LSSw Town Hall Meetings (ongoing)
  - 3rd Thursday each month, 3 – 4:30 pm Eastern US time
  - 100+ attendees at each meeting, sessions recorded
- Town Hall Topics
  - Meeting 1: Overview of the ECP Software Technology Focus Area
  - Meeting 2: Progress, impediments, priorities & gaps in LSSw panel
  - Meeting 3: Expanding the LSSw User Communities - Panel
  - Meeting 4: Expanding the LSSw Developer Communities - Panel
  - Meeting 5: Other HPC Software Ecosystems - Panel
- Portal: Slack, Whitepapers & References: TBA

Workshop on Research Software Science
Software is an increasingly important component in the pursuit of scientific discovery. Both its development and use are essential activities for many scientific teams. At the same time, very little scientific study has been conducted to understand, characterize, and improve the development and use of software for science.

- 126 whitepaper submissions (at same time as RFI!)
- Whitepapers at: https://www.orau.gov/SSSDU2021
- 150 registrants (max), 100 registered observers
- 150 – 170 active participants across three days
- Goal: Leverage new skills applied to scientific SW
ASCR RFI Response

- **ASCR RFI** – Broad call, Dec 13, 2021 deadline

- **10 prompt sets:**
  - 1 Software Dependencies and Requirements
  - 2 Security and Integrity of Software and Data
  - 3 Software Development Infrastructure Requirements
  - 4 Developing and Maintaining Community Software
  - 5 Building a Diverse Workforce and Inclusive Environment
  - 6 Technology Transfer and Building Software Communities
  - 7 The Scope of Software Stewardship
  - 8 Stewardship Management and Oversight
  - 9 Assessment for Success
  - 10 Additional Topics

- **37 community responses** – From brief and long

- **ECP Response:**
  - 48 pages, addressing all prompts
  - Foundation for 2021 IPR Response

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A Response to the “Stewardship of Software for Scientific and High-Performance Computing” Request for Information

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December 13, 2021
2021 IPR Recommendation Response

- Revision of RFI response plus:
- A proposed transition timeline and rationale document for the relevant timeline scenarios
- Public release of the dependency database, or some releasable subset
- Release date: March 1, 2022
Questions?
"Any opinions, findings, conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Networking and Information Technology Research and Development Program."

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