Hardware and Integration

Katie Antypas
Hardware and Integration Director

E4S Training
August 25, 2022
ECP’s Technical Focus Areas
Providing the necessary components to meet national goals

<table>
<thead>
<tr>
<th>Application Development (AD)</th>
<th>Software Technology (ST)</th>
<th>Hardware and Integration (HI)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Develop and enhance the predictive capability of applications critical to DOE</td>
<td>Deliver expanded and vertically integrated software stack to achieve full potential of exascale computing</td>
<td>Integrated delivery of ECP products on targeted systems at leading DOE HPC facilities</td>
</tr>
<tr>
<td>24 applications</td>
<td>71 unique software products spanning programming models and run times, math libraries, data and visualization</td>
<td>6 US HPC vendors focused on exascale node and system design; application integration and software deployment to Facilities</td>
</tr>
<tr>
<td>National security, energy, Earth systems, economic security, materials, data</td>
<td></td>
<td></td>
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<tr>
<td>6 Co-Design Centers</td>
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<td></td>
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<tr>
<td>Machine learning, graph analytics, mesh refinement, PDE discretization, particles, online data analytics</td>
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</table>
A capable exascale computing ecosystem made possible by “integrating” applications, software, and hardware innovations with training, outreach and allocation management with deep partnerships with DOE Facilities.

HI enables the “last mile.”
Deep Partnerships with Facilities to enable demonstration of AD challenge problems and deployment of software on Exascale Systems

- **PathForward (PF)**: Critical early vendor HW R&D for multiple exascale-capable system designs
- **Hardware Evaluation (HE)**: HW evaluations to influence system designs and to inform Facilities and ECP
- **Application Integration (AI)**: Facility support for ECP application development efforts to port and optimize for exascale or pre-exascale systems
- **Software Deployment (SD)**: Facility support for deploying ECP software at the Facilities and integrating with each Facility’s exascale software ecosystem
- **Facility Resource Utilization (FRU)**: Access to compute resources made available to ECP through the Facilities
- **Training and Productivity (T&P)**: Disseminated development knowledge, lessons learned, best practices to AD and ST teams in collaboration with AD, ST, and the Facilities
HI leadership team: Accomplished technical leaders with Facility experience

**Katie Antypas, HI Director (2.4)**
15 years experiencing supporting HPC users and deploying HPC systems (LBNL)

**Bronis de Supinski, PathForward (2.4.1)**
5 years as the CTO for the Livermore Computing facility (LLNL)

**Scott Pakin, HW Evaluation (2.4.2)**
17 years in performance analysis and SW development at the ACES Facility (LANL)

**Scott Parker, Application Integration at Facilities (2.4.3)**
13+ years experience working on performance optimization for scientific applications (ALCF)

**Ryan Adamson/Prout, Software Deployment at Facilities (2.4.4)**
12 years of systems and security administration, recently promoted to OLCF HPC Core Operations Group Lead (ORNL)

**Haritha Siddabathuni Som, Facility Resource Utilization (2.4.5)**
14 years in field and manager of the ALCF User Experience Team (ANL)

**Ashley Barker, Training and Productivity (2.4.6)**
8 years as a group leader of user assistance and outreach at the OLCF (ORNL)

**Susan Coghlan, HI Deputy Director (2.4)**
30 years experience acquiring, deploying, managing extreme scale systems at DOE Facilities (Argonne)

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What’s on deck for the next year?

**Software Deployment**
- Complete deployment and testing of ST products installed for initial and secondary deployment on Frontier and Aurora
- Improve E4S support model is accelerating build times

**Facility Resource Utilization**
- Successfully allocate and manage time on exascale system
- Tracking progress of AD and ST times
- Demonstration of KPP runs

**Application Integration**
- AD and ST teams continue to make productive use of early hardware including reporting bugs and issues that leads to the hardening and stabilization of systems
- Continue improving performance and functionality of AD/ST software

**Training and Productivity**
- Continue high quality trainings and hackathon
- Launch of broader engagement initiative

**Hardware Evaluation**
- Completes impactful report that influences next generation of systems and architectures
Software Deployment Highlights

• Recall the big decision that happened over a year ago. Software Deployment decided to leverage E4S software stack and packaging to simplify the testing, deployment and delivery of ST products at the facilities.

• Software Deployment team deploys appropriate E4S packages at facility (selected packages depend on vendor offerings and architecture)

• E4S packages are deployed on Perlmutter, Cori, Spock and currently being built for Crusher

• Note: building software on first of a kind, large scale system is not turn key and is challenging when system software is frequently changing
  – Recent PCR approved to provide more support for building E4S

Ryan Adamson (OLCF)
ECP Software Stream: Incubation to Installation

External Contributors on GitHub

Facilities

Software Integration at Facilities
- Integration of Vendor Stack
- Local builds and testing
- System tuned configurations
- Local filesystem installation
- Local module scheme

Spack development branch
- Very Fresh: 400-600 changes/month
- Latest features and package versions
- CI for latest E4S and SDK versions

Spack release branches
- Stable Spack
- Stable package versions
- Bugfixes backported

E4S release branches
- Facility testing
- Curated public build caches
- Level 2 user support

ECP ST Product Teams
- Direct AD collaboration
- Incubation and Hardening
- Packaging into Spack Ecosystem
- Level 3 support for E4S

ECP AD Teams Consume Software From
- Direct source builds from ST teams
- Spack develop branch
- Spack releases
- E4S curated releases
- Facility Installed and Supported SW Stack

Incubate

Harden

Deliver

Deploy

Install
ECP Software Stream: Incubation to Installation

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Incubate

Currently 70% of ST products targeted for initial deployment are packaged and ported to Crusher

Ryan Adamson’s breakout goes into more details about packages deployed
## E4S Products Targeted For Deployment On Frontier (June 2022)

### Initially Targeted Products (23 / 24)

<table>
<thead>
<tr>
<th>Data &amp; Viz</th>
<th>Math Libraries</th>
<th>PMR</th>
<th>Tools</th>
</tr>
</thead>
<tbody>
<tr>
<td>ADIOS</td>
<td>BLAS: MAGMA</td>
<td>GASNet</td>
<td>AID: STAT</td>
</tr>
<tr>
<td>Darshan</td>
<td>Ginkgo</td>
<td>Kokkos</td>
<td>HPCToolkit</td>
</tr>
<tr>
<td>HDF5</td>
<td>hypre</td>
<td>Legion</td>
<td>PAPI</td>
</tr>
<tr>
<td>PnetCDF</td>
<td>Kokkoskernels</td>
<td>RAJA</td>
<td>TAU</td>
</tr>
<tr>
<td>UnifyFS</td>
<td>PETSc/TAO</td>
<td>UPC++</td>
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</tr>
<tr>
<td>VTK-m</td>
<td>ScaLAPACK: SLATE</td>
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<tr>
<td></td>
<td>STRUMPACK</td>
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<tr>
<td></td>
<td>SUNDIALS</td>
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<tr>
<td></td>
<td>SuperLU</td>
<td></td>
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<tr>
<td></td>
<td>Trilinos</td>
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- Core dependencies
- History of high usage
- Suggestions by ST

= Ported and Packaged in E4S

### Secondarily Targeted Products (27 / 27)

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<th>Math Libraries</th>
<th>PMR</th>
<th>Tools</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALPINE: Ascent</td>
<td>DTK</td>
<td>AML</td>
<td>AID: Archer</td>
</tr>
<tr>
<td>SZ</td>
<td>FleCSI</td>
<td>Chai</td>
<td>AID: FLiT</td>
</tr>
<tr>
<td>VeloC</td>
<td>MFEM</td>
<td>SICM: Metall</td>
<td>AID: ReMPI</td>
</tr>
<tr>
<td>zfp</td>
<td>ArborX</td>
<td>MPI: Qthreads</td>
<td>Caliper</td>
</tr>
<tr>
<td></td>
<td>FFT: heFFTe</td>
<td>PaRSEC</td>
<td>OpenMP: Bolt</td>
</tr>
<tr>
<td></td>
<td>SWIG</td>
<td>Umap</td>
<td>Papyrus</td>
</tr>
<tr>
<td></td>
<td>Tasmanian</td>
<td>Umpire</td>
<td>Dyninst</td>
</tr>
<tr>
<td></td>
<td>ForTrilinos</td>
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= Ported and Packaged in E4S

- Other additional ST Products that are not provided by vendor and that integrate easily into Frontier stack
ECP and the ASCR Facilities have agreed to a Level 2 support Plan

- Facility staff have the ability to engage E4S L2 support regarding build, installation, testing, and issue support for E4S products and the E4S portfolio.

- Facilities and E4S L2 support will use the E4S issue tracker on GitHub as a single point of collaboration. ([https://github.com/E4S-Project/e4s/issues](https://github.com/E4S-Project/e4s/issues))

- The engagement model between E4S L2 support and the Facilities should provide flexibility for facilities to best determine how to integrate their own existing ticket-triage and user-troubleshooting processes into the E4S issue tracker.

- The facilities and E4S L2 support will collaboratively create a new-issue template for creating new E4S issues including the ability to identify issues as facility-submitted.

- E4S L2 support will address facility-submitted E4S issues by E4S L2 support staff within 3 business days. (In this context address means resolve or communicate a path or plan to resolution.)

- The facilities have ability to reasonably raise prioritization of facility-impacting issues above other issues tracked by E4S L2 support.

- E4S issue tracker should be updated by E4S product teams as progress is being made on an issue so facility staff can be updated in a timely manner.

- E4S L2 support will provide regular reporting of E4S support metrics to facility staff including the number of resolved issues, number of open issues, time-to-acknowledge, and time-to-resolution metrics within the reporting time period. Discussion and description of particularly troublesome, difficult or high priority issues.
E4S / Facility Software Support Model

The Kokkos parallel reduce operation in the facility-provided E4S installation is not using the A100 GPU, while the Kokkos parallel for operation is.

Facility User

User creates ticket in Facility System (Facility Ticket #20081)

Facility Staff Evaluates Facility Ticket #20081

Facility Staff works Facility Ticket #20081 until resolution

No

Yes

Does ticket require external E4S support?

Yes

Facility Staff creates ticket in E4S Issue Tracker: https://github.com/E4S-Project/E4S-Issues (E4S Issue #72)

Facility Staff updates E4S Issue #72

E4S Level 2 Support Acknowledges and Evaluates E4S Issue #72

E4S Level 2 Support Contacts E4S Product Team and updates E4S Issue #72 Regularly

No

Contact will be through the preferred issue tracker of the E4S product as documented within E4S

E4S Support Staff

E4S Level 2 Support Fixes Issue

No

E4S Product Team solves issue and provides a fix

All relevant parties work to diagnose and fix the issue

E4S Issue #72 is used as central information sharing hub for all parties

Yes

Is collaborative debugging required?

No

E4S Product Developer

E4S Level 2 Support Patches issue

Any temporary workarounds are provided to appropriate parties as a stopgap and merged back into Spack/Develop or the software package where possible

Facility Support Staff

Facility Staff updates and closes Facility Ticket #20081

Stop

Relevant user-provided information should be included within E4S Issue #72 where appropriate

If appropriate, link to HPC User GitHub account to E4S Issue #72

Sensitive information should not be put into E4S Issues since they are publicly viewable

There will be positive acknowledgement of issues created by Facility Support Staff within 3 business days

E4S Issues will be updated regularly by E4S Level 2 Support and Facility Support Staff will update Facility tickets periodically

Facility Staff Links to E4S Issue #72 from within Facility Ticket #20081