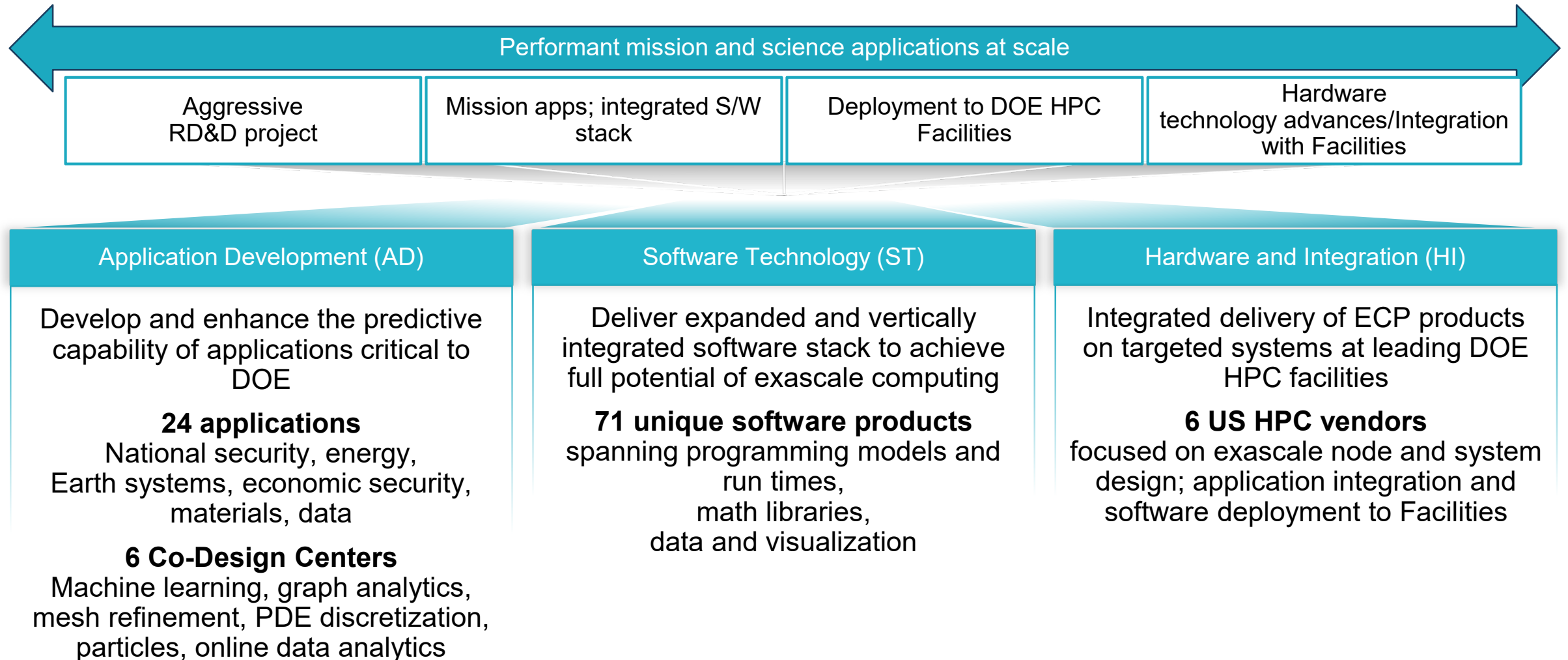# Hardware and Integration

Katie Antypas
Hardware and Integration Director

E4S Training
August 25, 2022

ECP's Technical Focus Areas
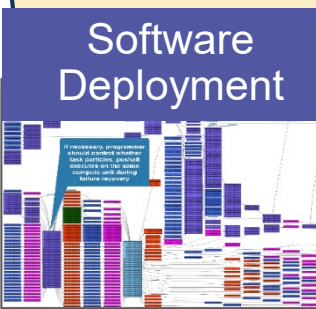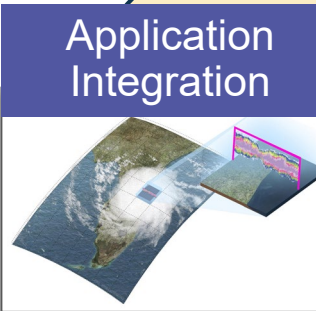Providing the necessary components to meet national goals

Performant mission and science applications at scale

| Aggressive RD&D project | Mission apps; integrated S/W stack | Deployment to DOE HPC Facilities | Hardware technology advances/Integration with Facilities |

Application Development (AD)

Develop and enhance the predictive capability of applications critical to DOE

24 applications
National security, energy, Earth systems, economic security, materials, data

6 Co-Design Centers
Machine learning, graph analytics, mesh refinement, PDE discretization, particles, online data analytics

Software Technology (ST)

Deliver expanded and vertically integrated software stack to achieve full potential of exascale computing

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

Hardware and Integration (HI)

Integrated delivery of ECP products on targeted systems at leading DOE HPC facilities

6 US HPC vendors
focused on exascale node and system design; application integration and software deployment to Facilities

ECP EXASCALE COMPUTING PROJECT

ECP **Hardware and Integration (HI)**

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."

Hardware Innovations and Evaluation

Application Integration

Software Deployment

Training Outreach and Allocations

ANL Intel/Cray

EL CAPITAN **LLNL** Cray

FRONTIER **ORNL** Cray/AMD

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

ECP-Facilities Engagement Plan

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)

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

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)

Hardware and Integration
2.4
Antypas (LBNL)
Coghlan (ANL)

PathForward
2.4.1
de Supinski (LLNL)

- **PathForward Vendor 1**
  2.4.1.01
  Hughes (SNL)

- **PathForward Vendor 2**
  2.4.1.02
  Karlin (LLNL)

- **PathForward Vendor 3**
  2.4.1.03
  Goldstone (LLNL)

- **PathForward Vendor 4**
  2.4.1.04
  Atchley (ORNL)

- **PathForward Vendor 5**
  2.4.1.05
  Pakin (LANL)

- **PathForward Vendor 6**
  2.4.1.06
  Daley (LBNL)

Hardware Evaluation
2.4.2
Pakin (LANL)

- **Hardware Evaluation Working Groups**
  2.4.2.01
  Pakin (LANL)

Application Integration
2.4.3
Parker (ALCF)

- **Aurora Application Integration**
  2.4.3.01
  Knight (ANL)

- **Frontier Application Integration**
  2.4.3.02
  Nichols (ORNL)

- **Pre-exascale Application Integration**
  2.4.3.03
  Bard (LBNL)

- **HIP on Aurora**
  2.4.3.05
  Videau (ANL)

Software Deployment
2.4.4
Prout (ORNL)

- **Software Integration**
  2.4.4.01
  Siddiqui (LBNL)

- **Shasta System Software Testing**
  2.4.4.03
  Srinivasan (LBNL)

- **Continuous Integration Infrastructure**
  2.4.4.04
  Bryant (ORNL)

- **Slingshot and System Testing**
  2.4.4.05
  Srinivasan (LBNL)

Facility Resource Utilization
2.4.5
Siddabathuni Som (ANL)

- **Facility Resource Utilization**
  2.4.5.01
  Siddabathuni Som (ANL)

Training and Productivity
2.4.6
Barker (ORNL)

- **Training**
  2.4.6.01
  Marques (LBNL)

- **Productivity**
  2.4.6.02
  Curfman (ANL)

ECP EXASCALE COMPUTING PROJECT

What's on deck for the next year?

Facility Resource Utilization

- Successfully allocate and manage time on exascale system

- Tracking progress of AD and ST times

- Demonstration of KPP runs

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

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

ECP EXASCALE COMPUTING PROJECT
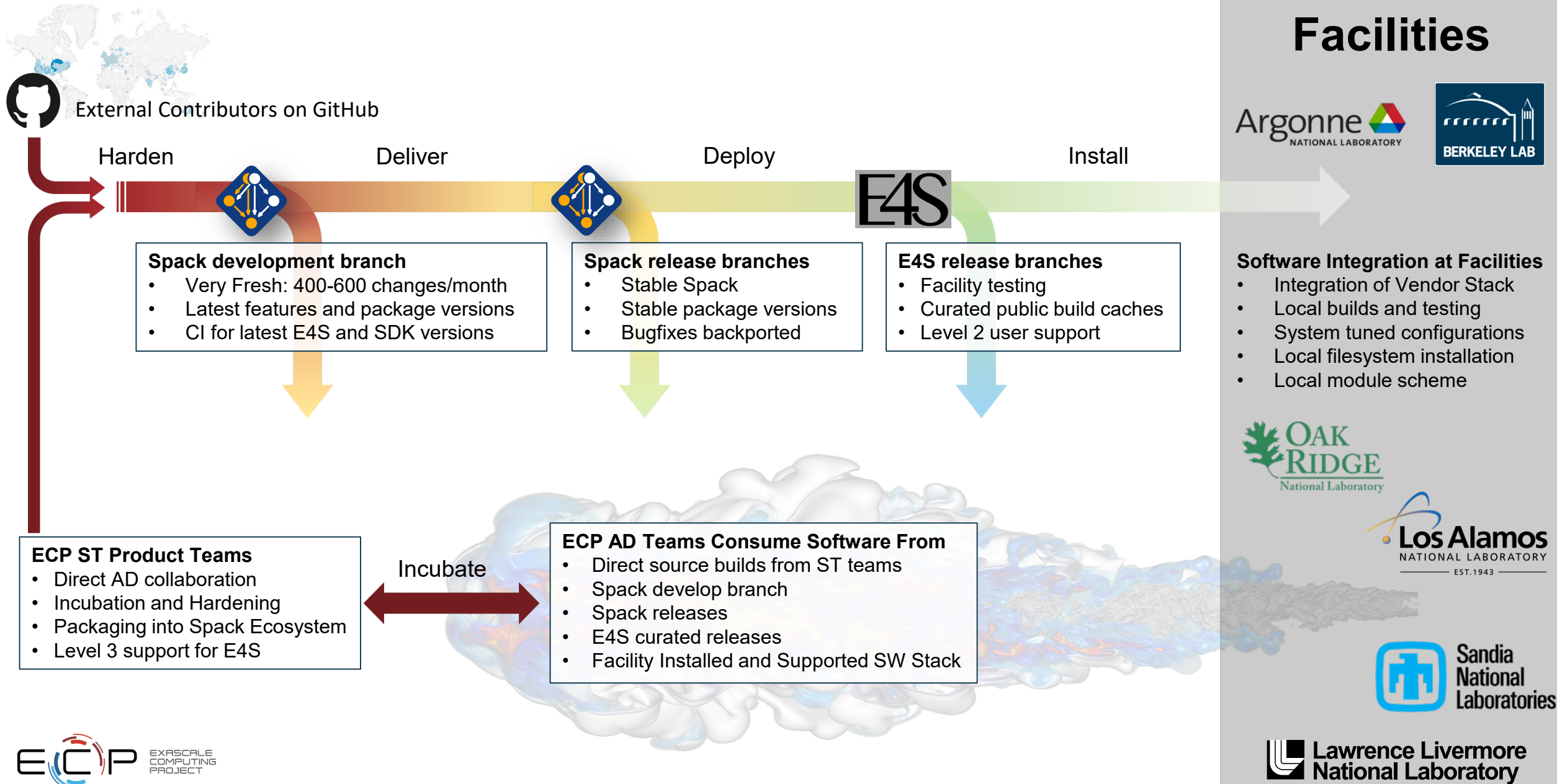
Software Deployment Highlights
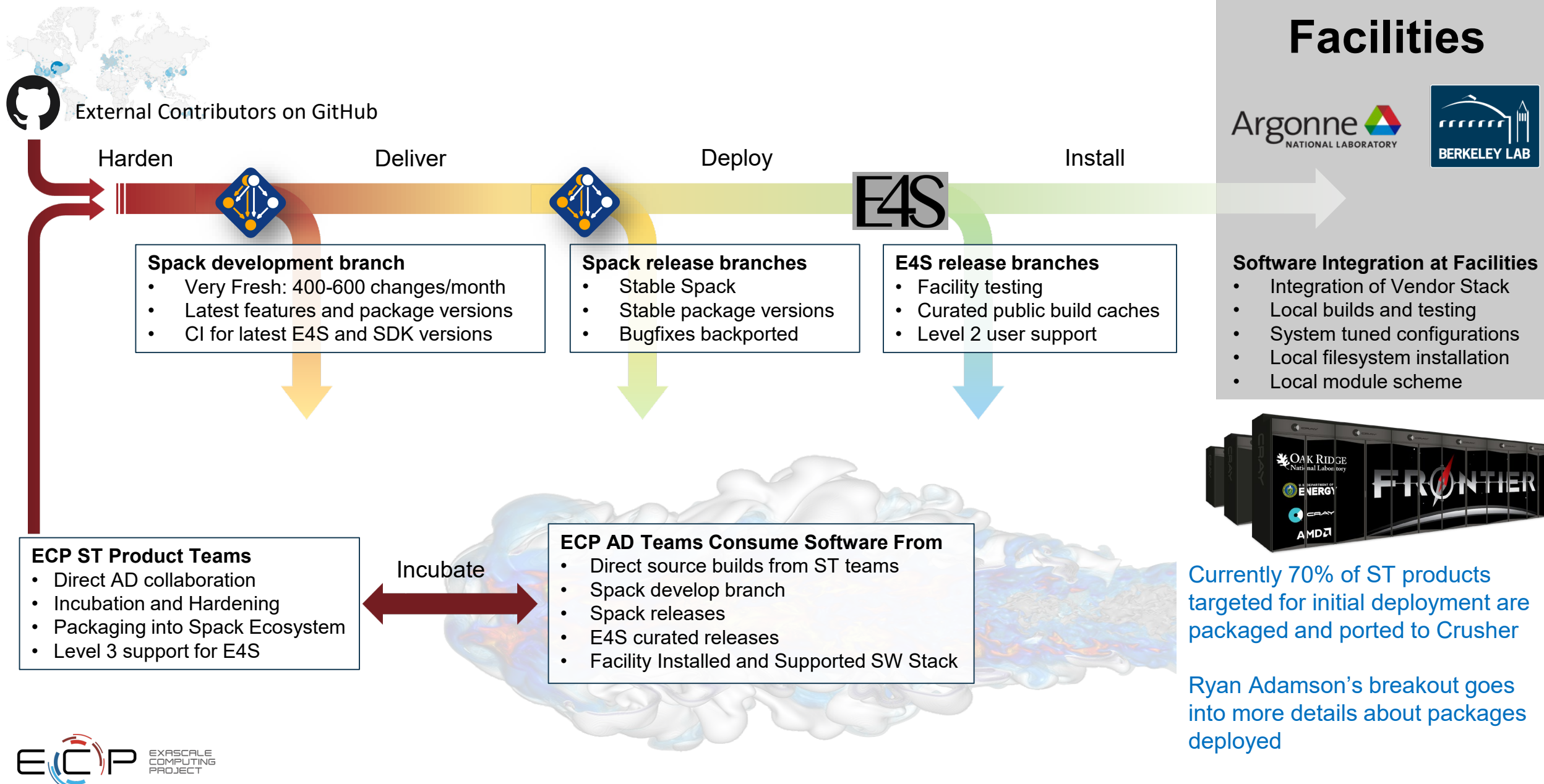
Ryan Adamson (OLCF)

- 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

ECP Software Stream: Incubation to Installation

Facilities

External Contributors on GitHub

Harden   Deliver   Deploy   Install

E4S

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

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

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

Incubate

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

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Argonne NATIONAL LABORATORY   BERKELEY LAB

Harden   Deliver   Deploy   Install

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OAK RIDGE National Laboratory   ENERGY   CRAY   AMD   FRONTIER

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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

ECP EXASCALE COMPUTING PROJECT

E4S Products Targeted For Deployment On Frontier (June 2022)

Initially Targeted Products (23 / 24)

Data & Viz
- ☑ ADIOS
- ☑ Darshan
- ☑ HDF5
- ☑ PnetCDF
- ☑ UnifyFS
- ☑ VTK-m

PMR
- ☑ GASNet
- ☑ Kokkos
- ☑ Legion
- ☑ RAJA
- ☑ UPC++

Math Libraries
- ☑ BLAS: MAGMA
- ☑ Ginkgo
- ☑ hypre
- ☑ Kokkoskernels
- ☑ PETSc/TAO
- ☑ ScaLAPACK: SLATE
- ☑ STRUMPACK
- ☑ SUNDIALS
- ☑ SuperLU
- ☑ Trilinos

Tools
- AID: STAT
- HPCToolkit
- ☑ PAPI
- ☑ TAU

- Core dependencies
- History of high usage
- Suggestions by ST

Secondarily Targeted Products (27 / 27)

Data & Viz
- ☑ ALPINE: Ascent
- ☑ SZ
- ☑ VeloC
- ☑ zfp

Software Ecosystem
- ☑ Flux

Math Libraries
- ☑ DTK
- ☑ FleCSI
- ☑ MFEM
- ☑ ArborX
- ☑ FFT: heFFTe
- ☑ SWIG
- ☑ Tasmanian
- ☑ ForTrilinos

PMR
- ☑ AML
- ☑ Chai
- ☑ SICM: Metall
- ☑ MPI: Qthreads
- ☑ PaRSEC
- ☑ Umap
- ☑ Umpire

Tools
- ☑ AID: Archer
- ☑ AID: FLiT
- ☑ AID: ReMPI
- ☑ Caliper
- ☑ OpenMP: Bolt
- ☑ Papyrus
- ☑ Dyninst

- Other additional ST Products that are not provided by vendor and that integrate easily into Frontier stack

ECP EXASCALE COMPUTING PROJECT

☑ = Ported and Packaged in E4S

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)

- 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