

# Tutorial: Developing Robust and Scalable Next Generation Workflows Applications and Systems

ISC-HPC 2022









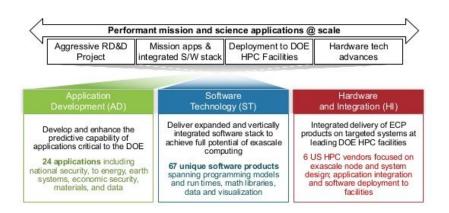




# Exascale Computing Project (ECP)

Seven-year, \$1.8B project that aims to accelerate R&D, acquisition, and deployment of exascale computing capability to DOE

Six core national laboratories are focused on software, applications, hardware, system engineering and testbed platforms

















# Scientific computing workflows underlie a significant number of projects in the Exascale Computing Project (ECP) portfolio

Many teams are creating infrastructures to:

- Couple multiple applications
- Manage jobs, sometimes dynamically
- Orchestrate compute/analysis and manage data

There is duplication of effort in these infrastructures

These customized workflows incur **significant costs** to port, maintain and scale

These tools do not always interface with facilities smoothly

The costs could be minimized by creating a reliable, scalable, portable software development kit (SDK) for workflows

#### ExaWorks Survey in 2020:

responses from 15/31 ECP application teams highlight the ad hoc workflows landscape













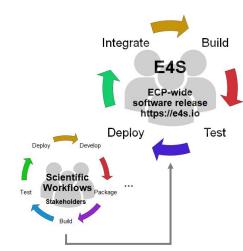


# Our approach will ensure exascale readiness of a wide range of ECP workflows and improve their long-term sustainability

Partner with ECP AD and other teams for co-design and adoption of ExaWorks SDK to address their workflow problems

Curate community SDK to enable robust, scalable, portable, performant workflows; progressively increase the availability of composable workflow components compute facilities to support deployment and use of workflows at scale; contribute requirements for next-generation systems

Lead the workflows
community towards
interoperability and reuse;
build the case for future
standardization for
long-term sustainability



The ExaWorks SDK is packaged, deployed, and tested using E4S and ECP Cl infrastructure













# ExaWorks is *not* funded to build another workflow system

We are funded to provide a production-grade Software Development Kit (SDK) for exascale workflows

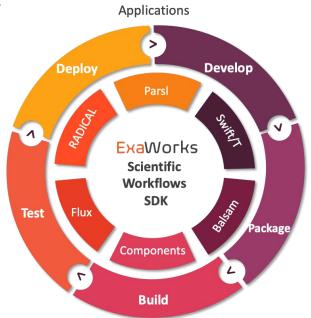
SDK democratizes access to hardened, scalable, and interoperable workflow management technologies and components

Implemented via community-based approach at progressively integrated levels

- Level 0: Technologies are packaged together
- Level 1: Component interfaces or pairwise integrations
- Level 2: Community developed and supported APIs

#### Approach

- Community policies for software quality (based on E4S)
- Open community-based design and implementation process
- Ensure scalability of components on Exascale Systems
- Standard packaging and testing



**Exascale Systems** 













## PSI/J: Portable Submission Interface for Jobs

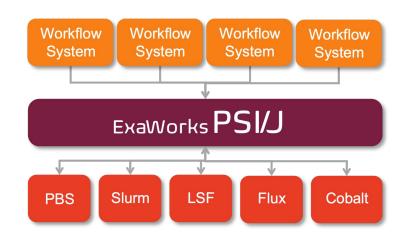
A set of **interfaces** that allow the specification and management of "jobs"

Support for Slurm, LSF, Cobalt, Flux, PBS

Open document to define a language-independent specification

Community specification

http://exaworks.org/job-api-spec/specification.html







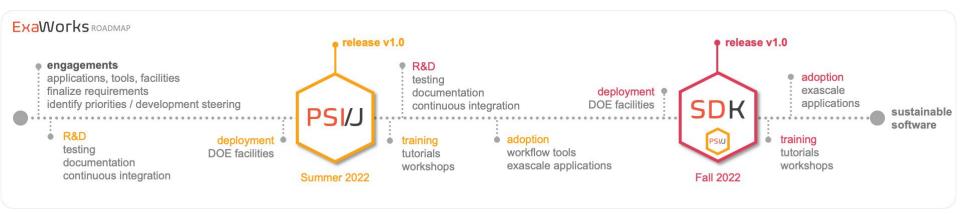








# ExaWorks RoadMap



## Exascale Workflows|Community













### Learn more...

### https://exaworks.org

- Join our Slack Channel
- Read the documentation

#### **Tutorial Sessions**

- ISC-HPC (May 2022)
- PEARC (July 2022)

### Engagements

 Get in touch to discuss how ExaWorks components can benefit your project

