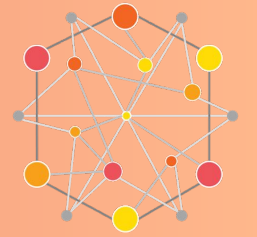
EXASCALE COMPUTING PROJECT

ExaWorks
https://exaworks.org

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

PEARC 2022



Lawrence Livermore National Laboratory · Argonne National Laboratory · Brookhaven National Laboratory · Oak Ridge National Laboratory · U.S. Department of Energy · Office of Science

Agenda

8:30 a.m. – 8:50 a.m.	Introduction and brief overviews of the tools, with Q&A	The team
8:50 a.m. – 9:00 a.m.	Logging into AWS / short break	
9:00 a.m. – 9:35 a.m.	RADICAL EnTk Exercises	Matteo Turilli
9:35 a.m. – 10:00 a.m.	Swift/T Exercises part 1	Justin Wozniak
10:00 a.m. – 10:30 a.m.	Coffee break	Ballroom B/Statler
10:30 a.m. – 10:45 a.m.	Swift/T Exercises part 2	Justin Wozniak
10:45 a.m. – 11:20 a.m.	Parsl Exercises	Kyle Chard
11:20 a.m. – 11:30 a.m.	Community outreach and wrap up	Rafael Ferreira da Silva

The Team

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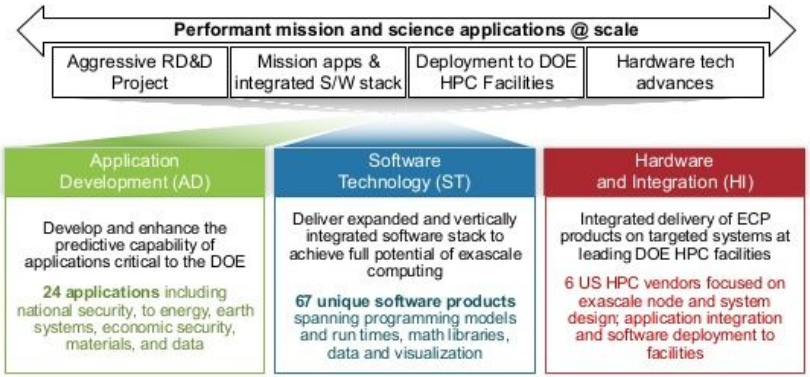
Exascale Computing Project (ECP)

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

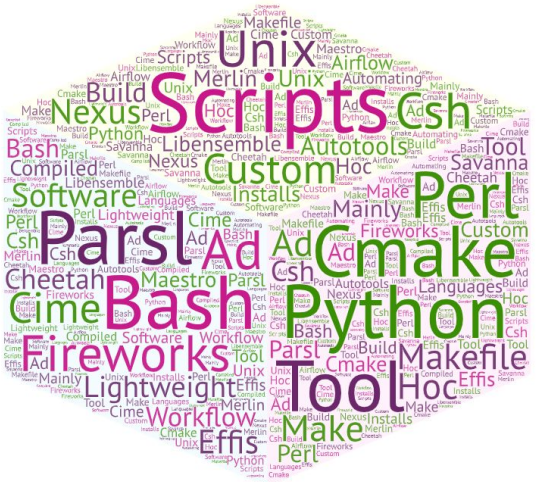
There is **duplication of effort** in these infrastructures

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



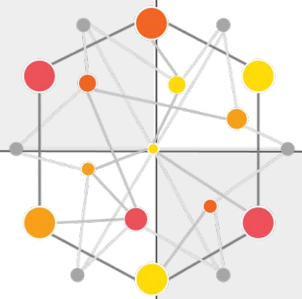
Our approach will ensure exascale readiness of a wide range of ECP workflows and improve their long-term sustainability

ECP Engagement

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

Facilities Engagement

Engage with DOE **compute facilities** to support deployment and use of workflows at scale; contribute requirements for next-generation systems

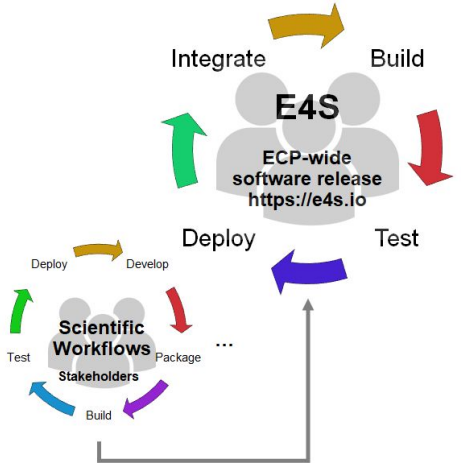


SDK Dev and CI/CD

Curate community SDK to enable robust, scalable, portable, performant workflows; progressively increase the availability of composable workflow components

Community Engagement

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 CI 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

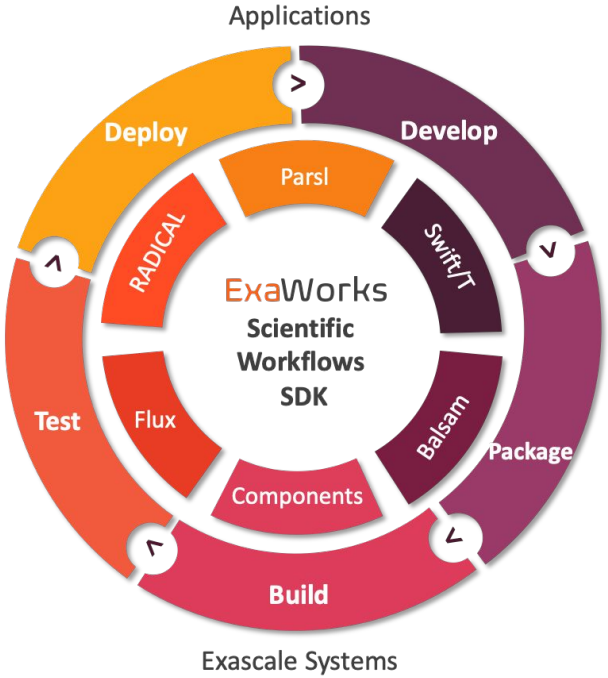
SDK democratizes access to hardened, scalable, and interoperable workflow management technologies and components

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

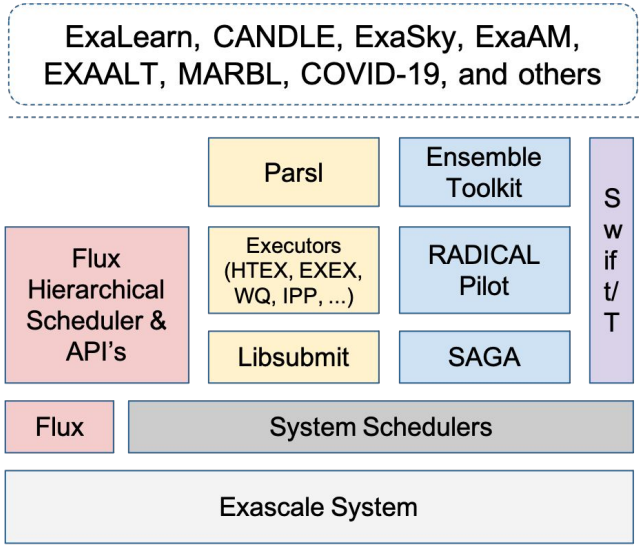
Approach

- 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



ExaWorks SDK brings together five seed technologies currently impacting ECP applications

- Scientific workflows SDK includes four seed technologies
  - **Flux** – hierarchical resource and job management software
  - **Parsl** – flexible and scalable parallel programming library for Python
  - **RADICAL** – component-based workflow middleware
  - **Swift/T** – high performance dataflow computing



PSI/J: Portable Submission Interface for Jobs

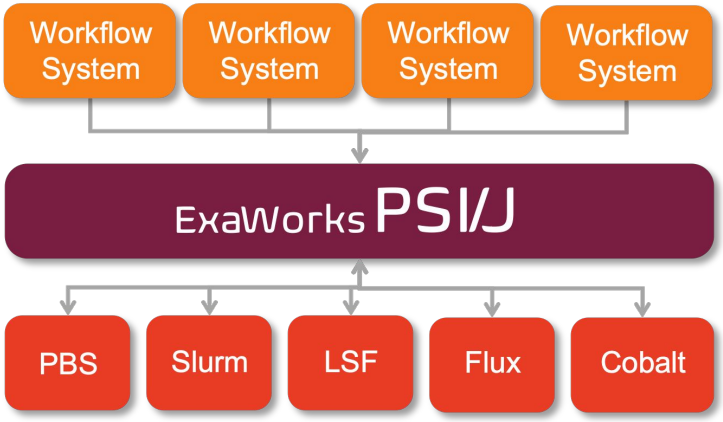
A set of interfaces that allow the specification and management of “jobs”

Support for Slurm, LSF, Cobalt, Flux, PBS

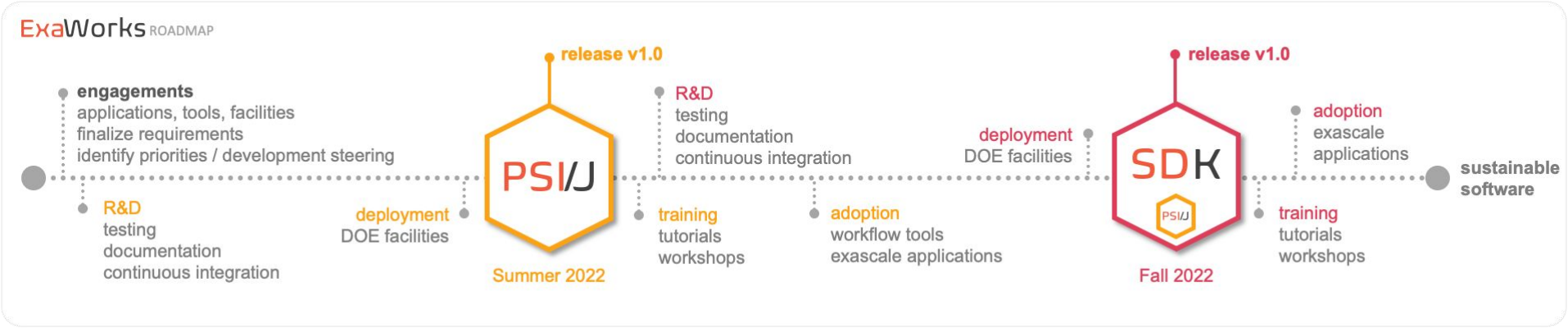
Open document to define a language-independent specification

Community specification

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



ExaWorks RoadMap



Exascale Workflows|Community

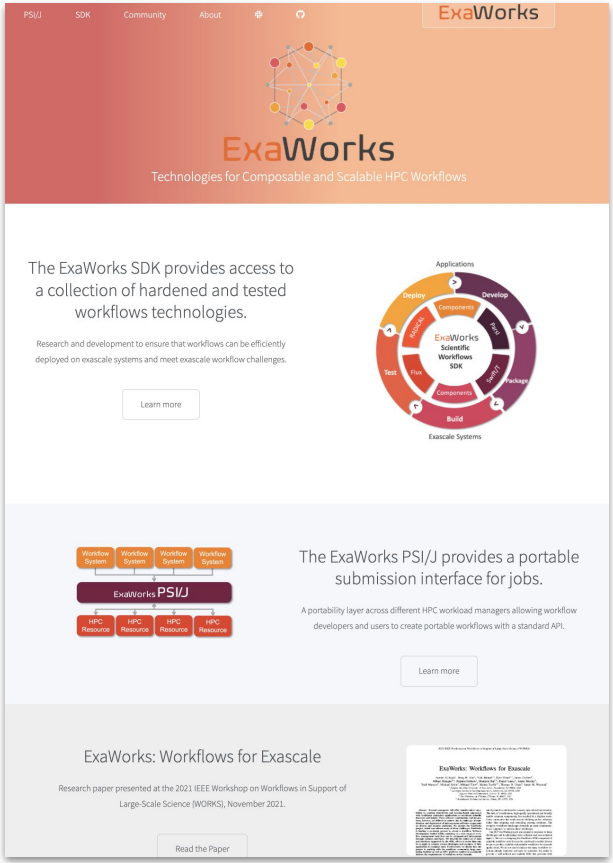
Learn more…

https://exaworks.org

- Join our Slack Channel
- Read the documentation

Engagements

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



ExaWorks

https://exaworks.org

https://tinyurl.com/exaworks

Thank you!

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