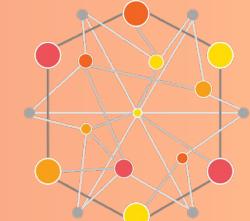


# An update on the ExaWorks Project

*Parsl & FuncX Fest '22*

*Daniel Laney*

LLNL-PRES-835634



# The Team



Dan Laney  
Lawrence Livermore National Laboratory



Aymen Alsaadi  
Brookhaven National Laboratory



Zeke Morton  
Lawrence Livermore National Laboratory



Kyle Chard  
Argonne National Laboratory



Ben Clifford  
Argonne National Laboratory



Mikhail Titov  
Brookhaven National Laboratory



Shantenu Jha  
Brookhaven National Laboratory



James Corbett  
Lawrence Livermore National Laboratory



Matteo Turilli  
Brookhaven National Laboratory



Rafael Ferreira da Silva  
Oak Ridge National Laboratory



Mihael Hategan  
Argonne National Laboratory



Andreas Wilke  
Argonne National Laboratory



Dong H. Ahn  
Lawrence Livermore National Laboratory



Ketan Maheshwari  
Oak Ridge National Laboratory



Justin M. Wozniak  
Argonne National Laboratory

## Previous Contributors



Stephen Herbein  
Lawrence Livermore National Laboratory



Yadu Babuji  
Argonne National Laboratory



Todd Munson  
Argonne National Laboratory

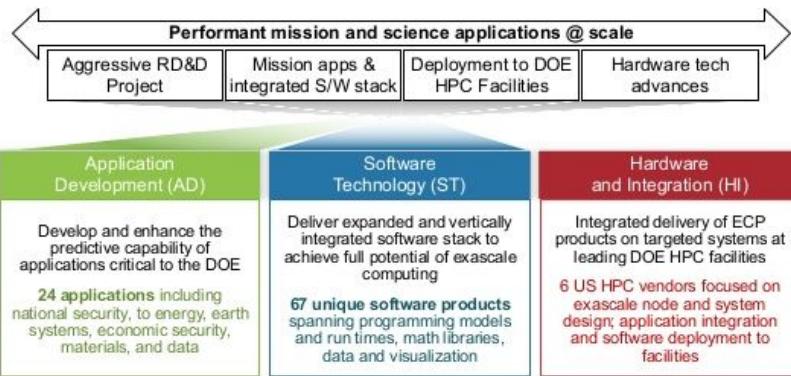


Andre Merzky  
Brookhaven National Laboratory

# 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

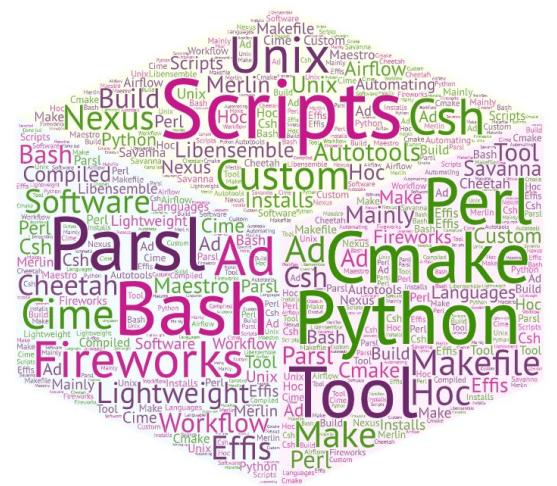
There is **duplication of effort** in these infrastructures

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

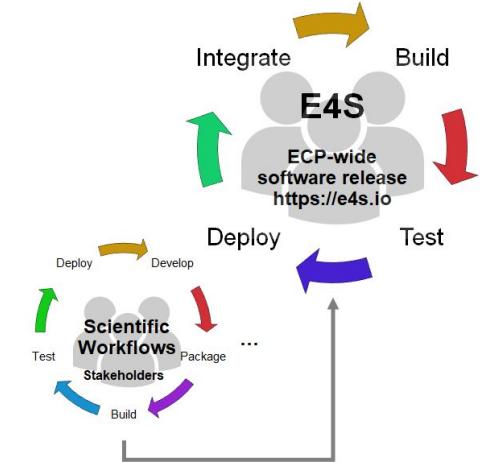
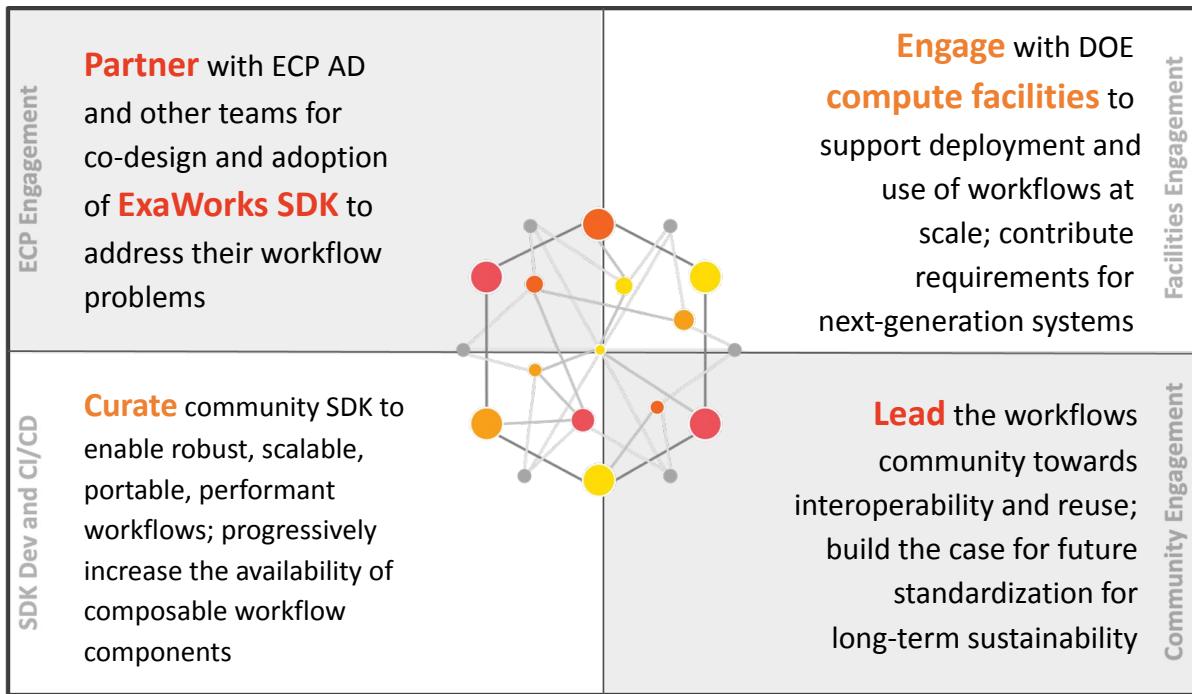
These tools do not always interface with facilities smoothly

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



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

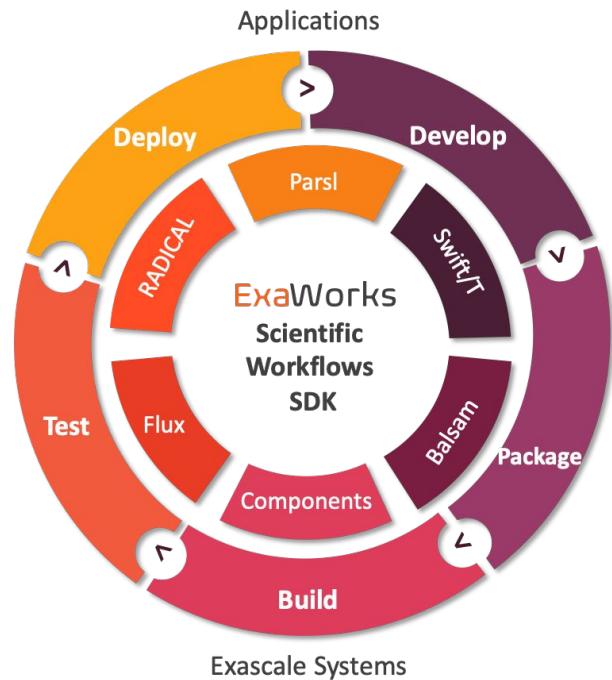
# ExaWorks is *not* funded to build another workflow system

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

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

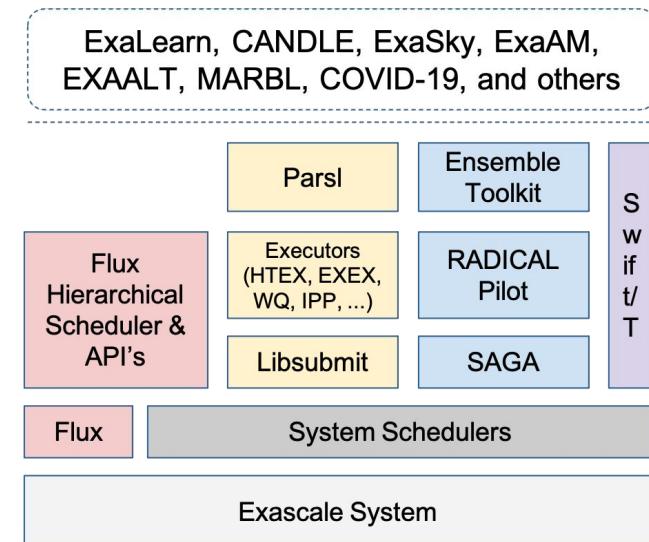
## Approach

- 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
- Work toward shared capabilities in the SDK



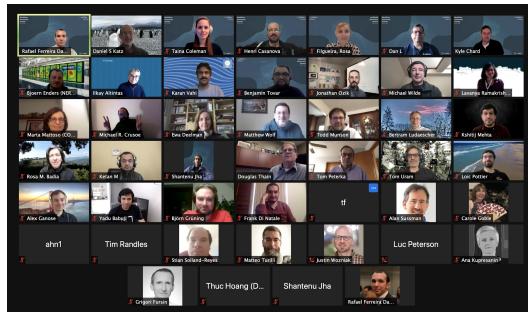
# ExaWorks SDK brings together five seed technologies currently impacting ECP applications

- 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

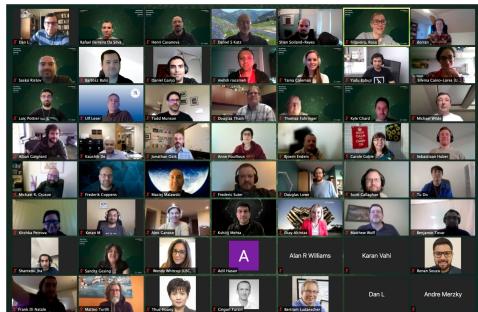


# We are engaging Workflow Communities and Computing Facilities

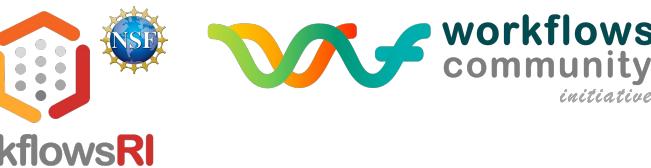
- **Workflows Community Summit: Researchers**
  - Brought together workflows leaders to develop a vision for community activities
  - <https://doi.org/10.5281/zenodo.4606958>
- **Workflows Community Summit: Developers**
  - Explored technical approaches for realizing the community vision
  - <https://doi.org/10.5281/zenodo.4915801>
- **Workflows Community Summit: Facilities**
  - Small group of facility representatives discussing facilities perspectives, challenges, and opportunities
- Invited Paper summarizing community roadmap: <https://arxiv.org/abs/2110.02168>



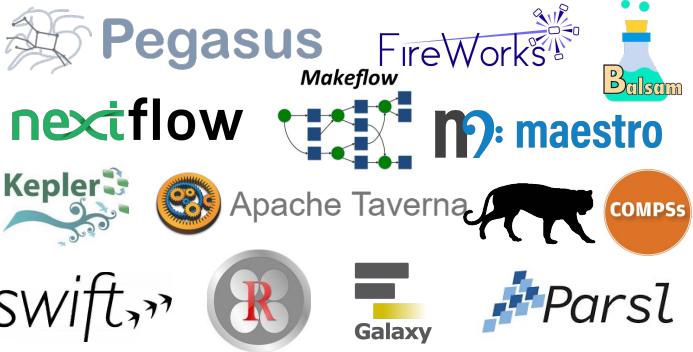
First Workflows Community Summit:  
45 participants, 27+ workflow systems



Second Workflows Community Summit:  
75 participants



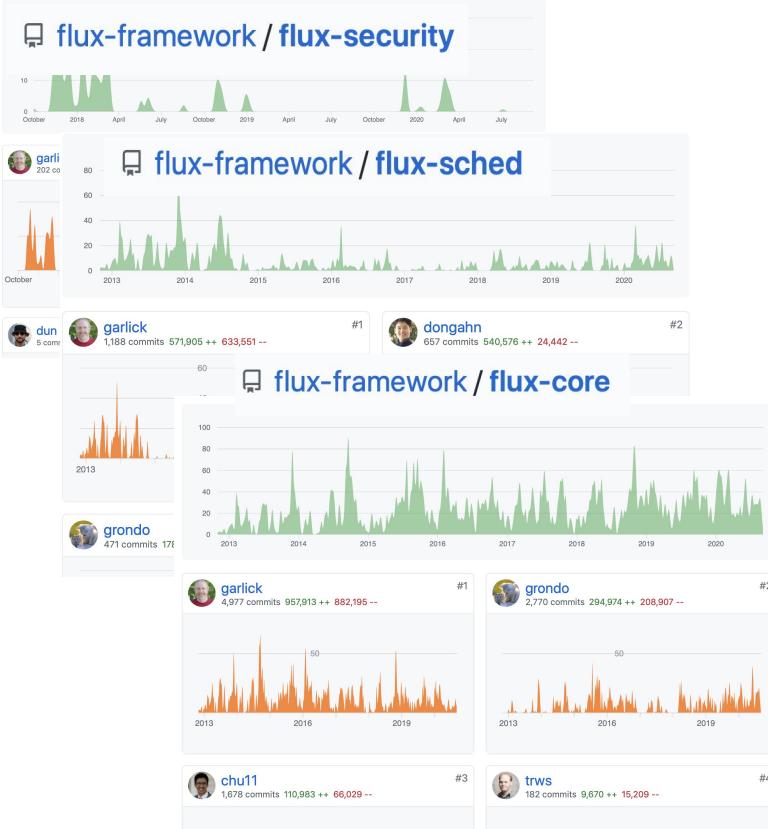
workflowsRI



Third Workflows Community Summit:  
9 participants, 8 facilities/centers (ALCF, OLCF, NERSC, LC, BNL, PSC, NREL, NCSA)



# A portable, flexible next gen job scheduler for emerging workflows



- Open-source project in active development at flux-framework GitHub organization with ~15 team members
- Single-user and multi-user (a.k.a. system instance) modes
  - Single-user mode has been used in production for ~3 years
  - Multi-user mode is having its debut on LLNL's Linux clusters
- Plan of record for **LLNL's El Capitan exascale** system
- Designed with heterogeneous systems and advanced workflows in mind
- Rich Python and C/C++ API's

# Parsl: a parallel programming library for Python

Apps define opportunities for **parallelism**

Python apps call Python functions

Bash apps call external applications

Apps return “futures”: a proxy for a result that might not yet be available

Apps run concurrently respecting dataflow dependencies. Natural parallel programming!

Parsl scripts are independent of where they run. Write once run anywhere!

Parsl scales to 100,000s of tasks on the largest HPC systems

pip install parsl

```
@python_app  
def hello():  
    return 'Hello World!'  
  
print(hello().result())
```



Hello World!

```
@bash_app  
def echo_hello(stdout='echo-hello.stdout'):  
    return 'echo "Hello World!"'  
  
echo_hello().result()  
  
with open('echo-hello.stdout', 'r') as f:  
    print(f.read())
```



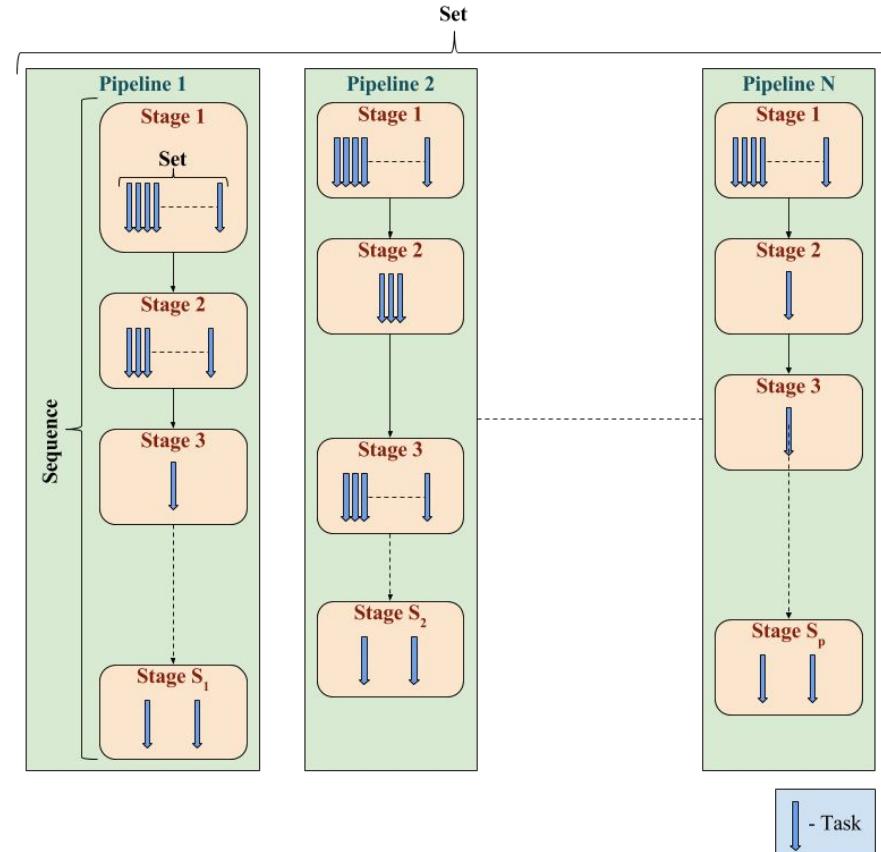
Hello World!

# RADICAL Cybertools: scalable Python abstractions for workflows

*RADICAL EnTk represents an ensemble application as a set of Pipelines.*

Two (pythonic) collections of objects:

- Set: contains objects that have no relative order with each other
- Sequence/List: contains objects that have a linear order, i.e. object ‘*i*’ depends on object ‘*i-1*’
- Pipelines can thus represent general DAG structures
- Pipelines can coordinate and communicate



# Swift/T: Enabling high-performance scripted workflows

Write site-independent scripts, translates to MPI

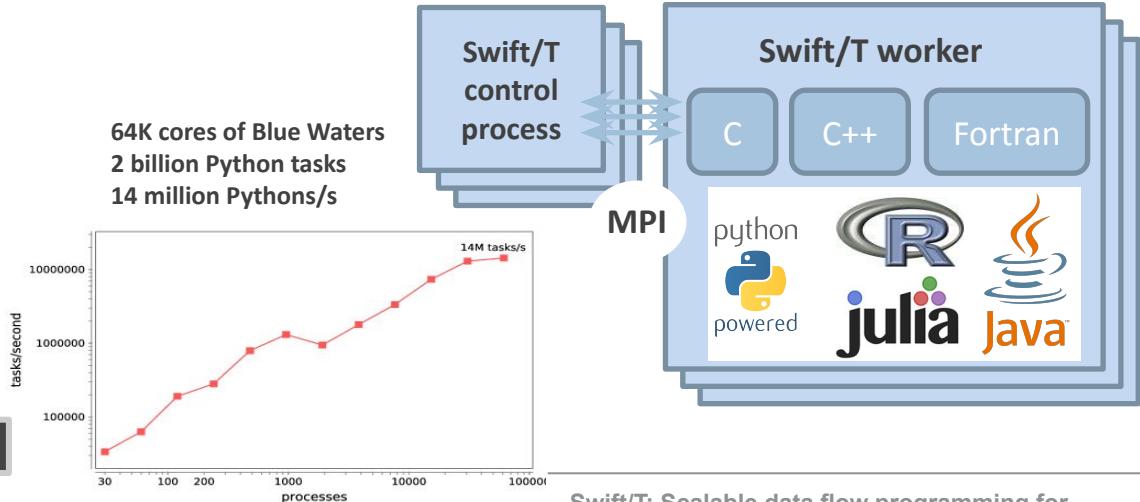
Automatic task parallelization and data movement

Invoke native code, script fragments  
in Python and R

Rapidly subdivide large  
partitions for MPI jobs  
in multiple ways (MPI 3.0)

```
$ spack install stc
```

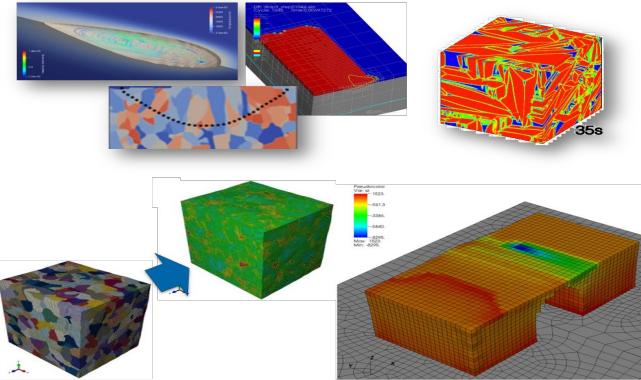
```
$ conda install -c lightsource2-tag swift-t
```



Swift/T: Scalable data flow programming for  
distributed-memory task-parallel applications  
Proc. CCGrid 2013.

# We are working closely with ECP Applications to impact deliverables

- **Approach:** Continuous engagement with ECP applications to address their workflow challenges and implement best practices, scalable, and performant workflows using the ExaWorks SDK.
- **ExaAM's** complex workflow simulates laser melt-pool additive manufacturing processes.
- **Colmena (ExaLearn):** open-source Python framework for ML-steering of simulation campaigns at scale.
- **CANDLE:** Relies on Swift/T for rapid development, scalability, and portability of DL-oriented cancer application suite on DOE systems
- **COVID:** National Virtual Biotechnology Lab used billions of core hours harnessed rapidly and effectively for heterogeneous workflows
- **Gordon Bell Prizes:** 3 of the 4 finalists used ExaWorks technologies



Gordon Bell submission	Description	ExaWorks Technologies Used
<b>WINNER: AI-Driven Multiscale Simulations Illuminate Mechanisms of SARS-CoV-2 Spike Dynamics</b>	Used DeepDriveMD built on <b>RADICAL-Cybertools</b> to steer ensembles of MD simulations using AI yielding <b>10x performance improvement</b> ; part of <b>CANDLE</b>	Entire <b>RADICAL</b> stack: <ul style="list-style-type: none"><li>▪ Ensemble-Toolkit</li><li>▪ RADICAL-Pilot</li><li>▪ SAGA</li></ul>
<b>Enabling Rapid COVID-19 Small Molecule Drug Design Through Scalable Deep Learning of Generative Models</b>	<b>Flux</b> is the scalable backbone of the Rapid COVID-19 Small Molecule Drug Design workflow whose scalable generative machine-learning task was featured in this paper; part of <b>CANDLE</b> and <b>ExaLearn</b>	The overall workflow is composed of <b>Flux</b> , the Maestro workflow manager, and a custom generative molecular design (GMD) workflow pipeline
<b>A Population Data-Driven Workflow for COVID-19 Modeling and Learning</b>	<b>Swift/T</b> managed a workflow containing the CityCOVID agent-based model and large numbers of small ML optimization tasks. The workflow consumed real-world infection data and produced data used by city and state governments	<b>Swift/T</b> managed the workflow

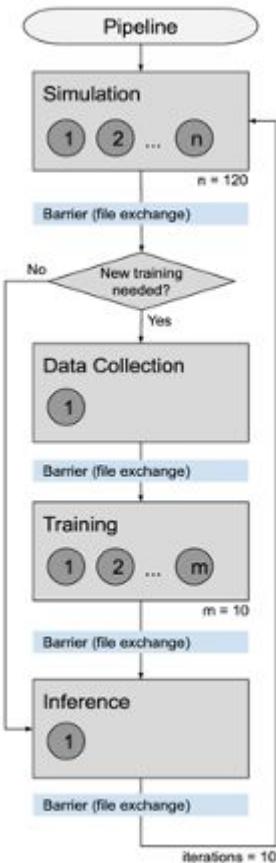
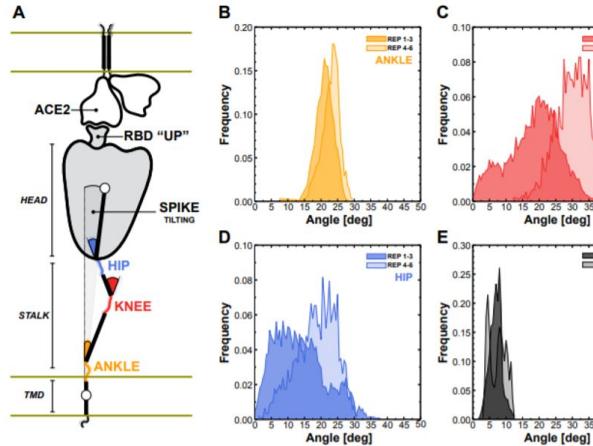
# ExaWorks technologies were leveraged in 3 of 4 finalists and the Winner of the SC21 Gordon Bell Covid-19 Competition

The Winner:

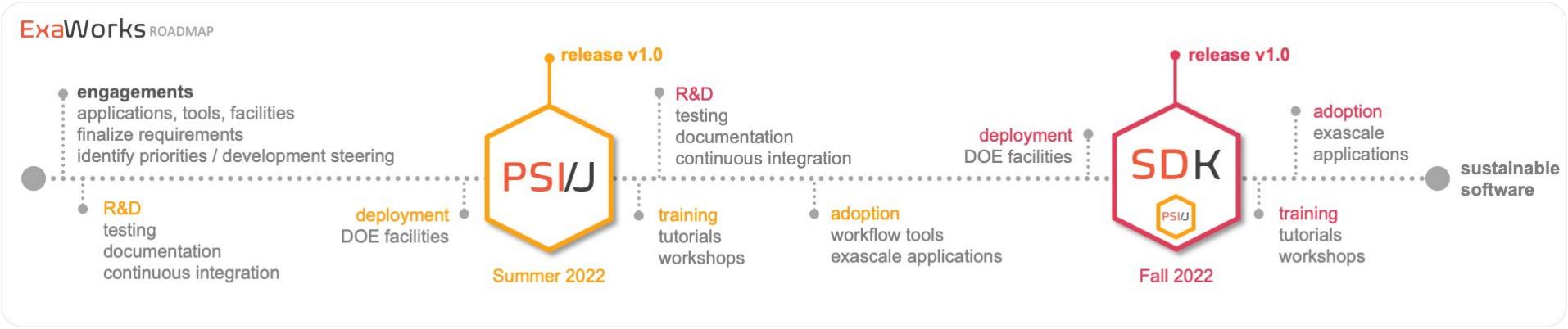
DeepDiveMD -- an extension of **RADICAL tools** -- workflow infrastructure adaptively couples ML + NAMD simulation workflow

Effective speedup of 1 order of magnitude sampling efficiency: with DeepDriveMD observed 25% more conformations of the knee bending in only 12% of the time!

**RADICAL components of the ExaWorks tool set brought scalability, reliability, and agility to the project**



# ExaWorks RoadMap

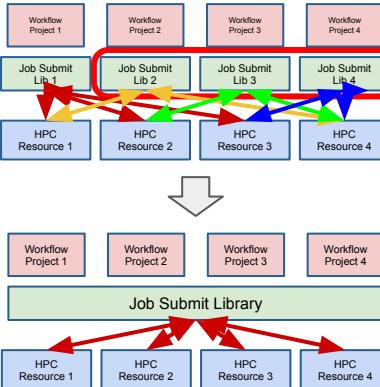


## Exascale Workflows|Community

# PSI/J was designed through an open community process

- Our survey, interviews, and co-design meetings highlighted need for portability layer for schedulers
- Community desired a light-weight user-space API
- Initial Python implementation is nearing version 1.0 release
  - Support for Slurm, LSF, Cobalt, Flux, RCT, SAGA
  - Working to add next set of schedulers (e.g., PBS)
  - Architected to allow seamless contributions from the community

## 1. Problem definition



## 2. Community specification

(<http://exworks.org/job-api-spec/specification.html>)

### Introduction

The purpose of this document is to provide an analysis of the design and implementation of a job management API capable for managing jobs that are on remote machines, as well as propose such an API. A job management API is a set of interfaces that allow the specification and management of the execution of application notebooks. The corresponding implementation of a job management API is a job management library, though its API is invoked by a client application.

Previously, this document is implemented in supercomputers by Local Resource Managers (LRMs), such as IBM's torque, SunGrid Engine, or Oracle's Grid Engine. Job management is understood as an abstraction layer on top of various LRMs.

A Note About Code Samples

There are various locations in this document where code is used to provide examples. Such code is not working code, but a Java/C++ inspired pseudo-code which almost surely will require modifications to be usable.

### Motivation and Design Goals

As designed, the number of clients is limited. These are concerned about availability and keeping the API and potential consumers simple, where clients must be made, such as deciding between local and remote implementations. Local simplicity is generally favored; however, an attempt is also made to distill and analyze the resulting complexities of a remote implementation in order to minimize the amount of work needed to be done with such an implementation.

Finally, the following sections describe the design in a significant amount of detail:

- A proposed API specification. A detailed description of the choice between synchronous and asynchronous APIs can be found here. In general, the synchronous API would not scale well in most languages. Additionally, if no need, the API provides a `wait()` method that allows client code to readily implement a synchronous wrapper around the API.
- Low-level API has been considered. The main reason for having such calls is to facilitate the use of more efficient mechanisms for transmitting job information to an underlying implementation. However, alternative methods exists that do not require a bulk call. Nonetheless, adding bulk calls to enable better performance in Layer 1-2, or even in Layer 0 if reasonably justified in the future, remains a possibility. For a technical discussion on the topic, please see Appendix C.

### Layers

There are at least three major ways in which a job management API can be used:

- Local: relevant API functions are invoked by programs running on the target resource (or a specific node on the target resource, such as a light-head node).
- Remote: the API functions are invoked by programs running on a different resource than the target resource; this requires some form of distributed architecture.

## 3. Open discussion

```
import jpsi

jex = jpsi.JobExecutor.get_instance('slurm')

def make_job():
    job = jpsi.Job()
    spec = jpsi.JobSpec()
    spec.executable = '/bin/sleep'
    spec.arguments = ['10']
    job.spec = spec
    return job

jobs = []
for i in range(N):
    job = make_job()
    jobs.append(job)
    jex.submit(job)

for i in range(N):
    jobs[i].wait()
```

## 4. Community SDK component

Author	Label	Projects	Assignee	Sort
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✓ JobExecutor constructor missing	✓ API Compatibility Across Implementations	✓ get_instance	✓ 17	✓
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✓ 481 opened on Nov. 8, 2020 by andre-metrey	✓ 482 opened on Nov. 8, 2020 by andre-metrey	✓ 483 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 482 opened on Nov. 8, 2020 by andre-metrey	✓ 483 opened on Nov. 8, 2020 by andre-metrey	✓ 484 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 483 opened on Nov. 8, 2020 by andre-metrey	✓ 484 opened on Nov. 8, 2020 by andre-metrey	✓ 485 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 484 opened on Nov. 8, 2020 by andre-metrey	✓ 485 opened on Nov. 8, 2020 by andre-metrey	✓ 486 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 485 opened on Nov. 8, 2020 by andre-metrey	✓ 486 opened on Nov. 8, 2020 by andre-metrey	✓ 487 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 486 opened on Nov. 8, 2020 by andre-metrey	✓ 487 opened on Nov. 8, 2020 by andre-metrey	✓ 488 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 487 opened on Nov. 8, 2020 by andre-metrey	✓ 488 opened on Nov. 8, 2020 by andre-metrey	✓ 489 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 488 opened on Nov. 8, 2020 by andre-metrey	✓ 489 opened on Nov. 8, 2020 by andre-metrey	✓ 490 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 489 opened on Nov. 8, 2020 by andre-metrey	✓ 490 opened on Nov. 8, 2020 by andre-metrey	✓ 491 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 490 opened on Nov. 8, 2020 by andre-metrey	✓ 491 opened on Nov. 8, 2020 by andre-metrey	✓ 492 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 491 opened on Nov. 8, 2020 by andre-metrey	✓ 492 opened on Nov. 8, 2020 by andre-metrey	✓ 493 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 492 opened on Nov. 8, 2020 by andre-metrey	✓ 493 opened on Nov. 8, 2020 by andre-metrey	✓ 494 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 493 opened on Nov. 8, 2020 by andre-metrey	✓ 494 opened on Nov. 8, 2020 by andre-metrey	✓ 495 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
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✓ 498 opened on Nov. 8, 2020 by andre-metrey	✓ 499 opened on Nov. 8, 2020 by andre-metrey	✓ 500 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
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✓ 500 opened on Nov. 8, 2020 by andre-metrey	✓ 501 opened on Nov. 8, 2020 by andre-metrey	✓ 502 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 501 opened on Nov. 8, 2020 by andre-metrey	✓ 502 opened on Nov. 8, 2020 by andre-metrey	✓ 503 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 502 opened on Nov. 8, 2020 by andre-metrey	✓ 503 opened on Nov. 8, 2020 by andre-metrey	✓ 504 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 503 opened on Nov. 8, 2020 by andre-metrey	✓ 504 opened on Nov. 8, 2020 by andre-metrey	✓ 505 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 504 opened on Nov. 8, 2020 by andre-metrey	✓ 505 opened on Nov. 8, 2020 by andre-metrey	✓ 506 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 505 opened on Nov. 8, 2020 by andre-metrey	✓ 506 opened on Nov. 8, 2020 by andre-metrey	✓ 507 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 506 opened on Nov. 8, 2020 by andre-metrey	✓ 507 opened on Nov. 8, 2020 by andre-metrey	✓ 508 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 507 opened on Nov. 8, 2020 by andre-metrey	✓ 508 opened on Nov. 8, 2020 by andre-metrey	✓ 509 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
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✓ 509 opened on Nov. 8, 2020 by andre-metrey	✓ 510 opened on Nov. 8, 2020 by andre-metrey	✓ 511 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
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✓ 511 opened on Nov. 8, 2020 by andre-metrey	✓ 512 opened on Nov. 8, 2020 by andre-metrey	✓ 513 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 512 opened on Nov. 8, 2020 by andre-metrey	✓ 513 opened on Nov. 8, 2020 by andre-metrey	✓ 514 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 513 opened on Nov. 8, 2020 by andre-metrey	✓ 514 opened on Nov. 8, 2020 by andre-metrey	✓ 515 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 514 opened on Nov. 8, 2020 by andre-metrey	✓ 515 opened on Nov. 8, 2020 by andre-metrey	✓ 516 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 515 opened on Nov. 8, 2020 by andre-metrey	✓ 516 opened on Nov. 8, 2020 by andre-metrey	✓ 517 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 516 opened on Nov. 8, 2020 by andre-metrey	✓ 517 opened on Nov. 8, 2020 by andre-metrey	✓ 518 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 517 opened on Nov. 8, 2020 by andre-metrey	✓ 518 opened on Nov. 8, 2020 by andre-metrey	✓ 519 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
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✓ 519 opened on Nov. 8, 2020 by andre-metrey	✓ 520 opened on Nov. 8, 2020 by andre-metrey	✓ 521 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 520 opened on Nov. 8, 2020 by andre-metrey	✓ 521 opened on Nov. 8, 2020 by andre-metrey	✓ 522 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 521 opened on Nov. 8, 2020 by andre-metrey	✓ 522 opened on Nov. 8, 2020 by andre-metrey	✓ 523 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 522 opened on Nov. 8, 2020 by andre-metrey	✓ 523 opened on Nov. 8, 2020 by andre-metrey	✓ 524 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 523 opened on Nov. 8, 2020 by andre-metrey	✓ 524 opened on Nov. 8, 2020 by andre-metrey	✓ 525 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 524 opened on Nov. 8, 2020 by andre-metrey	✓ 525 opened on Nov. 8, 2020 by andre-metrey	✓ 526 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 525 opened on Nov. 8, 2020 by andre-metrey	✓ 526 opened on Nov. 8, 2020 by andre-metrey	✓ 527 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 526 opened on Nov. 8, 2020 by andre-metrey	✓ 527 opened on Nov. 8, 2020 by andre-metrey	✓ 528 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
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✓ 528 opened on Nov. 8, 2020 by andre-metrey	✓ 529 opened on Nov. 8, 2020 by andre-metrey	✓ 530 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 529 opened on Nov. 8, 2020 by andre-metrey	✓ 530 opened on Nov. 8, 2020 by andre-metrey	✓ 531 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 530 opened on Nov. 8, 2020 by andre-metrey	✓ 531 opened on Nov. 8, 2020 by andre-metrey	✓ 532 opened on Nov. 8, 2020 by andre-metrey	✓ 15	✓
✓ 531 opened on Nov. 8, 2020 by andre-metrey	✓ 532 opened on Nov. 8, 2020 by andre-metrey	✓ 533		

# ExaWorks is working towards a production quality continuous integration and deployment infrastructure for workflow tools

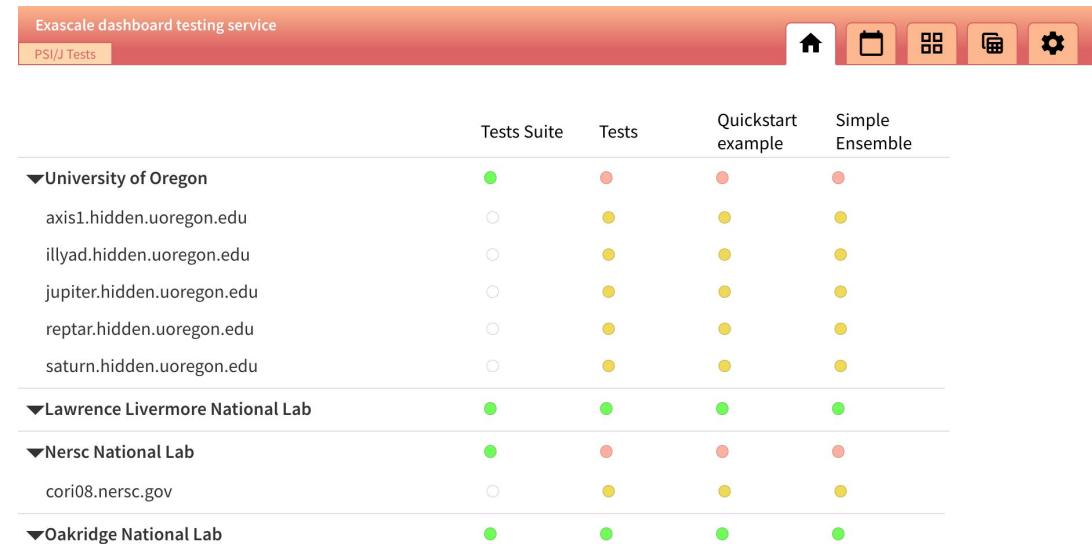
We have developed a GitLab CI infrastructure

We have set up CI at LLNL, ORNL, and ANL for the SDK components

We are testing PSI/J on an ECP testing cluster

We have developed a testing server to collect results of tests and enable dashboards and reporting from multiple sites

We are creating **Status Dashboard** to view what tests have been run on which systems



# PSI/J: Portable Submission Interface for Jobs

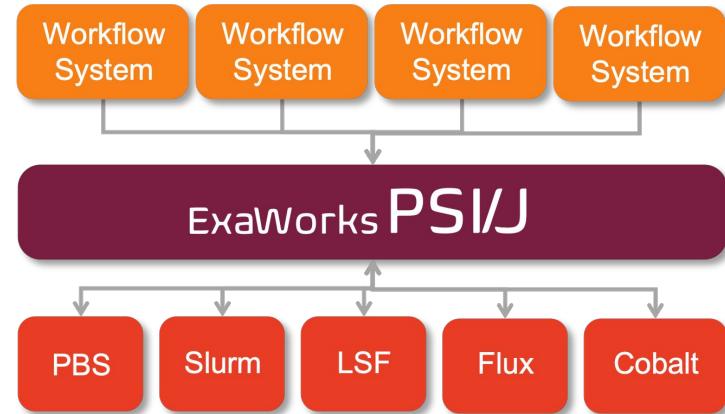
A set of **interfaces** that allow the specification and management of “jobs”

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>



# PSI/J Python binding provides an intuitive Python-futures based API for job management

- PSI/J Python binding
  - Python library with asynchronous interface for interacting with job schedulers
  - Support for Slurm, LSF, Cobalt, Flux, RCT, SAGA
  - Working to add next set of schedulers (e.g., PBS)
  - Architected to allow seamless contributions from the community
- Eventually the PSI/J specification will cover more advanced job-management functionality, such as job submission on remote clusters (“layer 1”).
  - All effort so far has been on “Layer 0”, in which PSI/J talks only to the local resource manager.
- We have integrated PSI/J into both RADICAL CyberTools and Parsl

```
import jpsi

jex = jpsi.JobExecutor.get_instance('slurm')

def make_job():
    job = jpsi.Job()
    spec = jpsi.JobSpec()
    spec.executable = '/bin/sleep'
    spec.arguments = ['10']
    job.spec = spec
    return job

jobs = []
for i in range(N):
    job = make_job()
    jobs.append(job)
    jex.submit(job)

for i in range(N):
    jobs[i].wait()
```

# 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

The ExaWorks website features three main sections:

- SDK:** Describes the ExaWorks Scientific Workflows SDK, which provides access to hardened and tested workflows technologies. It includes a circular diagram illustrating the workflow cycle from Applications to Exascale Systems.
- PSI/J:** Describes the ExaWorks PSI/J, a portable submission interface for jobs. It shows a diagram of a portability layer across different HPC workload managers.
- Workflows for Exascale:** A research paper presented at the 2021 IEEE Workshop on Workflows in Support of Large-Scale Science (WORKS), November 2021. It includes a thumbnail of the paper cover.

# Thank you!

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC