HEP-CCE Portable Applications and Workflows

Charles Leggett
for HEP-CCE

FAIROS-HEP Workshop on Workflows
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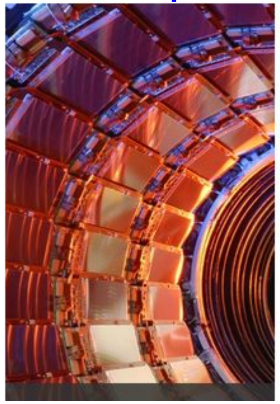
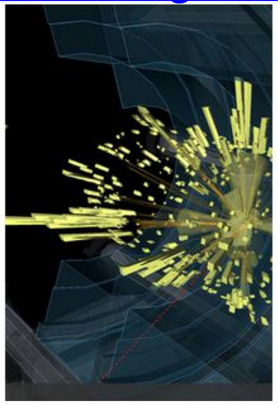
What is HEP-CCE?

Three-year (2020-2023) pilot project

- Explore intersectionality of modern GPU based HPCs and HEP experiment code bases
- Develop **practical** solutions to port hundreds of kernels to multiple GPU architectures
- Collaborate with HPC & networking communities on **data-intensive** use cases

1. PPS: Portable Parallelization Strategies
   - exploit massive concurrency
   - portability requirements
2. IOS: HEP I/O and HPC storage issues
   - new data models (memcpy-able, SOA,...)
   - fine-grained I/O, workflow instrumentation
3. EG: Optimizing event generators
4. CW: Complex workflows on HPCs

https://www.anl.gov/hep-cce


Four US labs, six experiments, ~12 FTE over ~35 collaborators.
PI: Salman Habib (ANL), Co-PI: Paolo Calafiura (LBNL)

Open collaboration https://indico.fnal.gov/category/1053/

Continuing Mission

- HEP experiments run mission-critical workflows on owned and pledged resources (such as **OSG** and **WLCG**), but also need to leverage **HPC** and **commercial cloud** facilities to deliver timely physics output.
- The (anticipated) increase of data volume exacerbates the need to use HPC resources at the DOE leadership class facilities (LCFs).
- In CCE Phase 1, **PPS** addresses **node-level** parallelization and portability issues of running HEP applications on LCFs, and we will continue to work with the experiments to address these issues and implement PPS solutions in production.
- In **Phase 2**, we will address the issues of running **complex workflows** on the LCFs, and develop a cross-cutting HEP **workflow portability** solutions to help HEP experiments build portable, high-throughput workflows across different computing facilities.

ASCR-Supported Tools

- DOE LCFs (NERSC, ALCF, and OLCF) are also developing tools to support experiment workflows. For example,
    - **Slate** at OLCF: container orchestration service for running user-managed persistent application services
    - **Spin** at NERSC: container-based platform to support user-defined services, workflows, databases and API endpoints.
    - The LCFs are also working on technologies to support cross-facility workflows. (Prelude to IRI, perhaps?)
- The US Exascale Computing Project (ECP) has generated a rich exascale-ready software ecosystem.
    - In particular, ExaWorks has developed a workflow SDK that can be adopted for HEP.

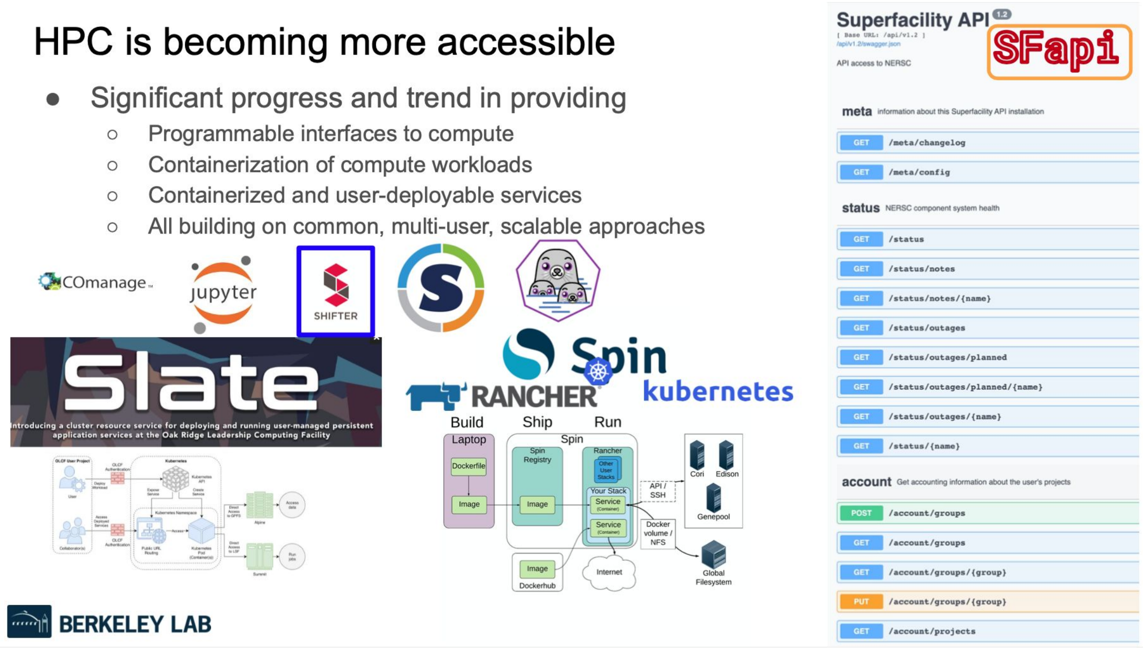
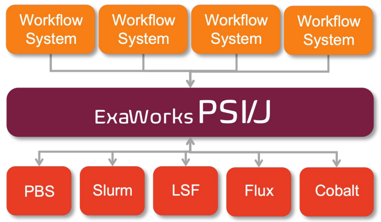


Figure 3: DOE LCFs are developing new tools to make HPC more accessible. Image taken from Wahid Bhimji (NERSC) presentation at Snowmass CompF4 topical workshop: https://indico.fnal.gov/event/53251/



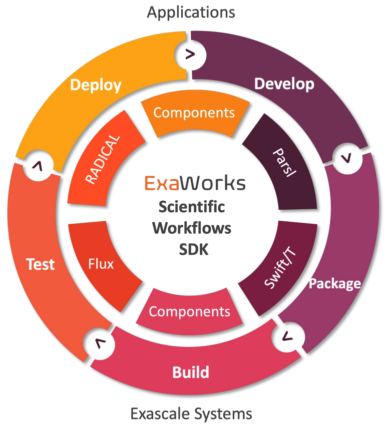
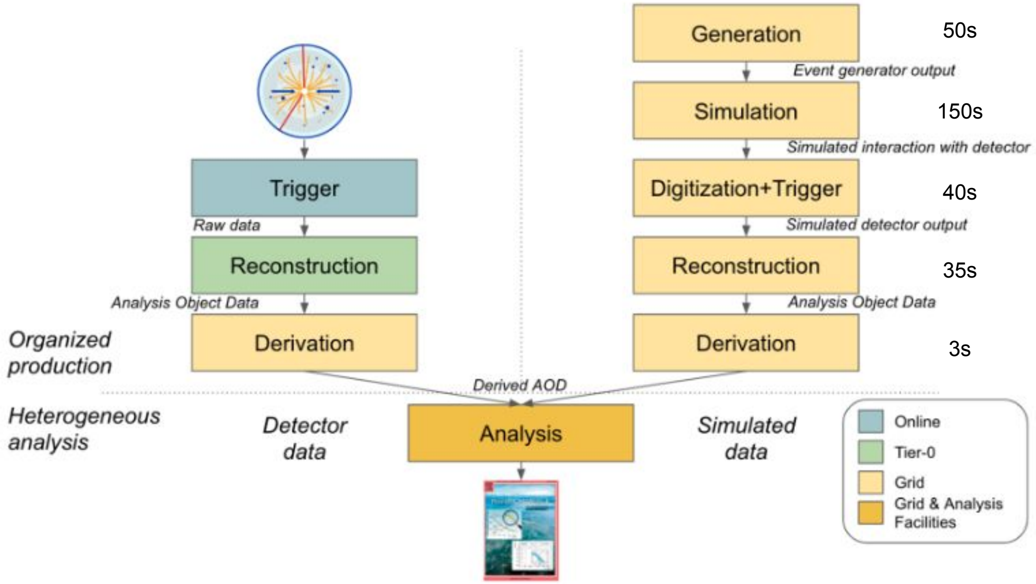


Figure 4: ECP project ExaWorks is also developing tools to support complex workflows on HPC systems. https://exaworks.org/

HEP Experiment Workflows and HPC

- While HEP experiments can benefit greatly from the efficient use of the HPC systems, many challenges remain.
- HEP experiment workflows have unique characteristics and requirements that are not currently accommodated on the LCFs:
  - HEP workflows are highly **non-uniform:**
    - Different simulation and analysis steps have different potentials for HPC acceleration with varying computing resource requirements (some tasks take longer than others)



ATLAS/CMS Production Workflow

Figure from Megino, et al. "US ATLAS and US CMS HPC and Cloud Blueprint." *arXiv:2304.07376* (2023).

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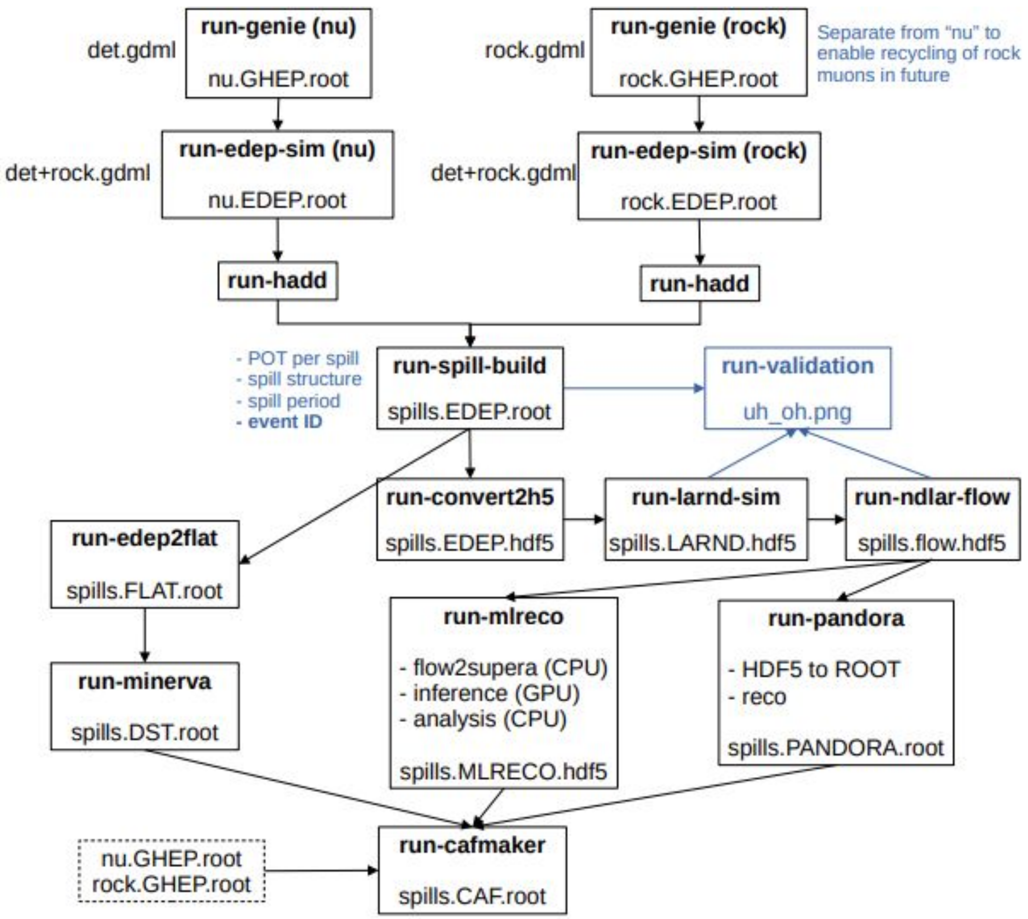
  - and increasingly **non-linear** and **heterogeneous**



DUNE Near Detector 2x2 Simulation Workflow

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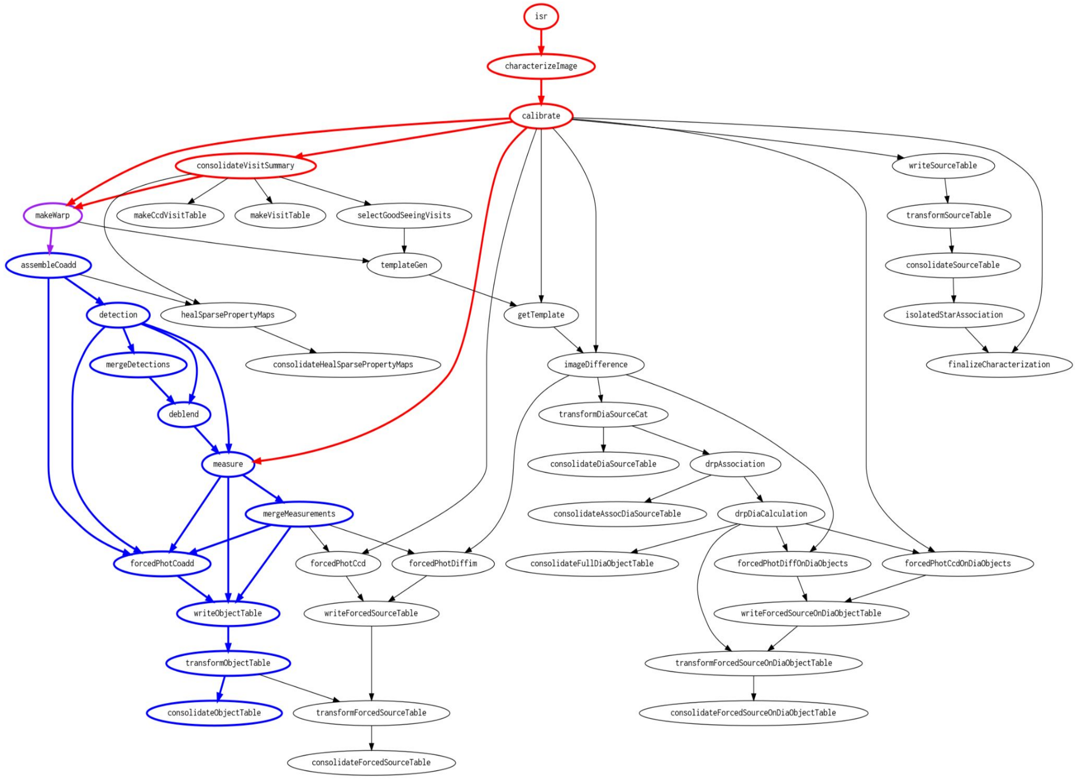

Rubin LSST Image Processing Pipeline

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  - Need for **real-time** or **on-demand** access to resources
  - Large data volumes make data delivery, cataloging, and storage challenging
  - Many HEP computational tasks are still CPU-based, with spare use of GPUs, while HPC systems are increasingly GPU-based.

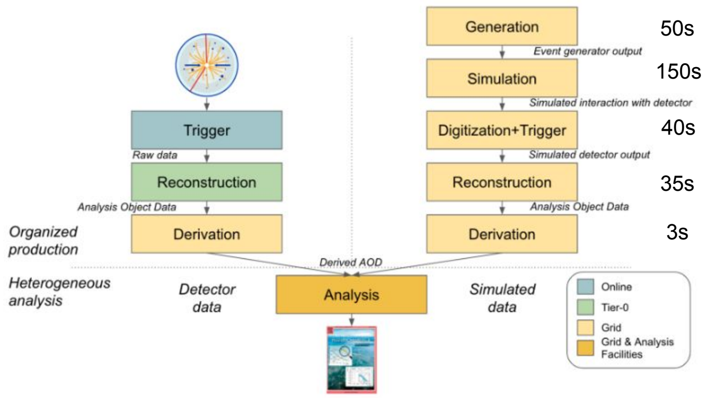
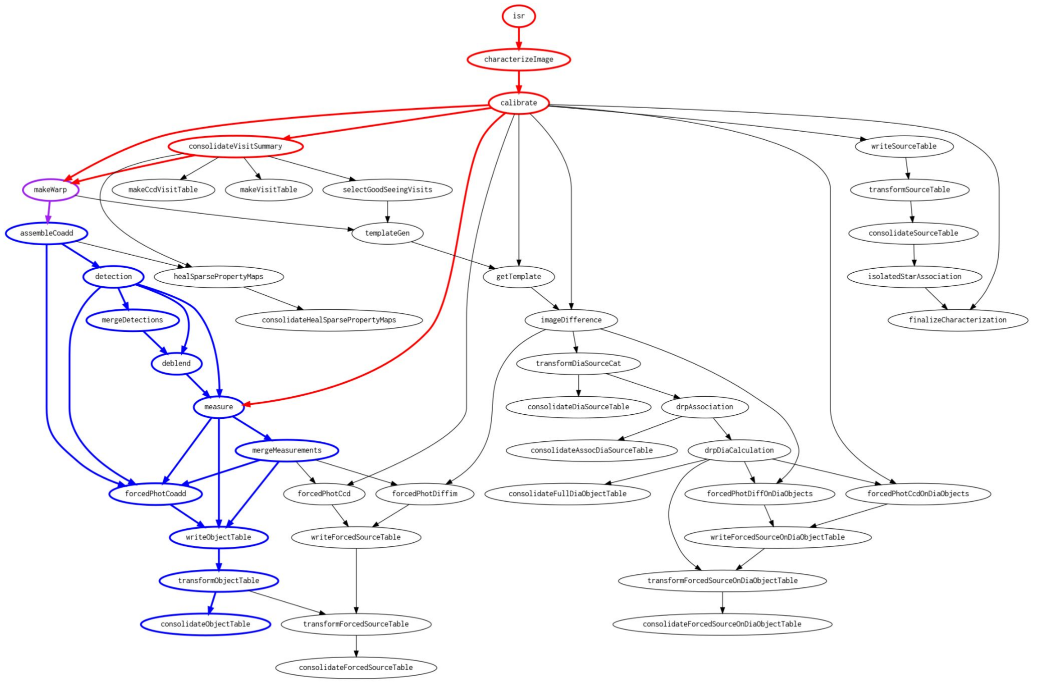


Figure 1: Workflow overview in the ATLAS and CMS experiments.

Figure from Megino, et al. "US ATLAS and US CMS HPC and Cloud Blueprint." *arXiv:2304.07376* (2023).



Rubin LSST Image Processing Pipeline

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Challenges of HEP Workflows on HPC Systems - I

- **Resource Access Challenge**
  - HPC centers have decentralized identity management, unlike WLCG
  - HEP compute resource needs may be non-linear, sometimes requiring **burst or real-time access** for specific science needs, for example,
    - transient alerts from the Rubin Observatory
    - candidate supernova neutrino flashes detected in DUNE (data intensive, time critical)
  - "Small" experiments may have to rely on HPCs for real-time monitoring of detector performance or calibration quality, such as the LZ experiment
- **Data Challenge**
  - HEP experiments deal with Peta to ExaBytes of data. Data on HPC will be transient in nature.
    - Good data cataloging and delivery mechanism is needed.
  - Some experiments will have extremely **high data rates for relatively short periods** of time, such as during supernova neutrino burst events for DUNE.
  - Getting the data in and out of the HPC centers efficiently requires commonly supported high-throughput services.

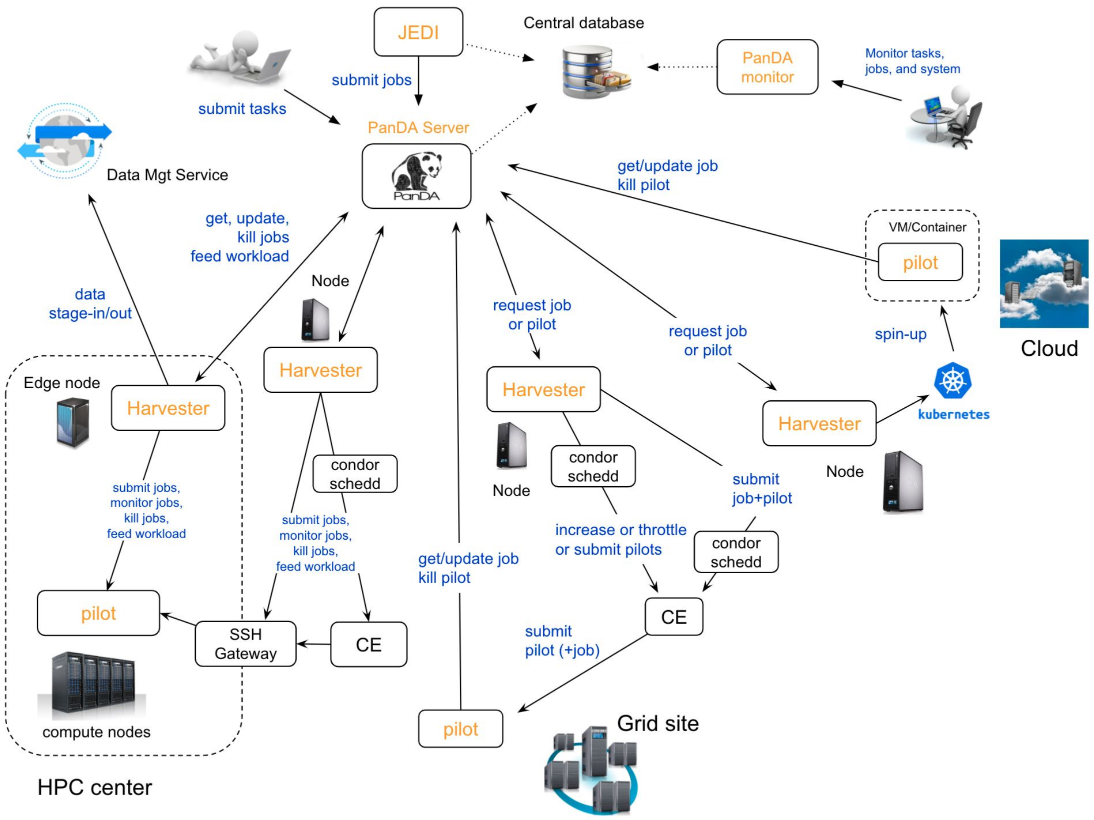
Challenges of HEP Workflows on HPC Systems - II

- **Software Environment Challenge**
  - HEP software support for HPC architectures varies
    - Different CPUs and GPUs (AMD, Intel and NVIDIA)
    - Partially addressed by **CCE Phase 1**
  - HPC center software environments differ
    - Different OS, compilers, batch systems (PBS, Slurm, …)
    - Even the supported container technologies may be different
  - Integration of HEP software frameworks with HPC services is non-trivial
    - cvmfs, eos
    - Each experiment has tended to develop its own middleware tools

- **Performance, Reliability and Reproducibility Considerations**
  - With the diversity of architectures and software environments, how to guarantee reproducibility of the results becomes a challenge.
    - Need to have careful data cataloging and documentation
  - Heterogeneous and hybrid tasks in a HEP workflow may perform best on different hardware architectures (some work better on CPUs while others on GPUs)
    - Need to maximize performance with careful allocation and mapping of resources
  - Can we resume critical workflows elsewhere if the current system fails?
    - Need to look into resubmission/restart mechanism

Leveraging Current Workflow Technologies

- Both the **HEP** and **ASCR** communities have recognized these challenges and started developing tools and services to address them.
- **ATLAS** has developed a distributed workflow system that can interact with HPC, Cloud and Grid.
  - HEP-developed tools such as **Harvester, PanDA** may be leveraged for other workflows.
- **CMS** has successfully integrated their workflows with user-facility-type HPC centers through the **HEPCloud** portal.
  - Running on LCFs remains challenging
- **DUNE** offline computing CDR explicitly targets HPCs
  - Current plan to use a combination of **JobSub, GlideinWMS,** and **HEPCloud** for both Grid and HPC sites



ATLAS distributed workflow management system

HEP-CCE Phase 2 Plan

- In HEP-CCE Phase 2, our goal is to provide the experiments with both a validated, ready-to-use portability solution and a suite of portability tools that can be integrated into their production systems.
  - To reconcile different services and tools provided by HEP and ASCR.
  - To reduce the operation and maintenance overhead of deploying HEP workflows on HPC systems

- Building on the experience of **PPS** and **CW** groups in HEP-CCE Phase I, we will have two main tasks in Phase 2:
  - **Task 1:** apply lessons learned in PPS to help HEP experiments develop portability solutions in their applications
  - **Task 2:** develop portable, experiment-agnostic, workflow overlays to interface existing HEP workflows with HPC centers

Task 1: Applying Lessons Learned to HEP Experiments

- The goal of this task is two-fold:
  - capitalize on the Phase 1 PPS findings to help experiments develop portable solutions on more components of their workflows for HPC,
  - help HPC centers understand and consider HEP requirements for future software and hardware
- Phase 2 activities include:
  - Work with experiments to develop tailored application portability recommendations depending on the experiment size, codebase, data, and timescale.
  - Turn Phase 1 PPS test beds into representative HEP mini-apps to share with ASCR facilities to help define requirements and KPPs for facility infrastructure.
  - Develop experiment-independent algorithmic examples/benchmarks that could be used for training and form the basis of a portable parallelization “cookbook.”
  - Some of the benchmarks can be contributed to community standard benchmarks such as SPEChpc, HEPScore, etc. to ensure HEP requirements are well supported by future HPC software and hardware

Task 2: Develop Workflow Portability Solutions

- The overarching goal of this task is to enable diverse HEP experiment workflows to run efficiently on LCFs and other HPC centers with little overhead.

- This will be done through the development of a portability overlay that would include a set of tools and services to seamlessly integrate HEP workflows with HPC, such as
  - Software delivery and container management
  - Scalable, distributed execution engines
  - Application services including Function as a Service (FaaS) microservices like funcX
  - Accelerator/Inference as a Service (AaaS) microservices like NVIDIA Triton, DLHub, etc.
  - Identity management (following rules of engagement as set by the facilities)
  - Computing and storage resource brokering with a focus on resource availability and overall throughput.
  - Edge services, including pilot management (Harvester, HEPCloud), remote logging and reporting, and database access
  - Data cataloging, delivery, and access, leveraging XRootD, Globus, Rucio

Year 1 Plan

Task 1 - Application Portability:

- Develop a **cookbook** for portability layers based on Phase 1 findings
- Outreach to experiments for portable solution implementation (**workshops/hackathons**, followed by regular office hours)
  - Understand the experiments' timescales for portable accelerator uses
- Create **mini-apps** based on two of the Phase I PPS testbeds that can be executed at NERSC, OLCF and ALCF, preferably with the same software environment (FCS, p2r)
- Use mini-apps to extract **figures of merit** for ASCR facilities and LCFs to use as baselines

Task 2 - Workflow Portability:

- Complete **survey** of existing HEP experiment workflow technologies on HPC; also look into workflow technologies used by **other experiment facilities such as light sources**.
  - Find commonalities between experiment workflow systems
- Explore the needs of HEP in terms of **ML workflows/pipelines and microservices** (synergistic with the distributed ML activity)
- Investigate common layers and interfaces (batch scheduler, policies, pilots, …) to facilitate portability and interoperability across ASCR facilities in collaboration with **IRI testbeds**
- Create **2 representative HEP experiment workflows** to run two different HPC systems. Candidates include: LSST/DESC, LZ, DUNE, LHC Experiments (ATLAS/CMS).
  - have tentatively selected **DUNE 2x2 Sim** (Fireworks + MongoDB on SPIN), and **ATLAS** Simulation (PanDA + Harvester -> FuncX + GlobusCompute) workflows
  - would also like to look at Light Sources

Big Questions

Why has each experiment developed its own workflow tools?

- do they really have different requirements, or is it just historical and the fundamental desire of physicists to reinvent the wheel?

Can we find common workflow tools that will support all the HEP experiments (LHC and others)?

- are the tools sufficiently extensible?
- is it possible to get the experiments to adopt them, or is there too much inertial?
- are there any lessons to be learned from Light Sources or BioMed?

How can we integrate seamlessly with all the facilities?

- Europe, USA, Asia, etc
- Grid, Cloud, HPC, HTC

Thoughts About A Few Necessary Components

Integrated data movement and data provenance tracking

- rucio, xrootd, gridftp, spade, globus ...

Authentication and Identity Management

- individual and federated

Real time monitoring and logging

- job/stage resubmission on error detection

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