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PAW Parallel Session Summary

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HEP-CCE All-Hands Meeting
July 22-24, 2024

Two most significant accomplishments of Year 1 so far



- Started the mini-app packaging with Spack (p2r) and containerization (FCS), including improving the functionalities of FCS and implementing CI/CD workflows
- Made considerable progress in understanding, reproducing and then porting two representative workflows to new facilities
 - DUNE 2x2 ND LAr Sim workflow to Polaris
 - ATLAS workflow on Perlmutter for integrating Globus Compute with Harvester

See Monday presentation.

Current focus areas of PAW

- Turning Phase 1 PPS testbeds into turnkey mini-apps that can be easily deployed on many different facilities and architectures
- Understanding complex HEP workflows from various stakeholders, porting them to new facilities, and adding new features and value

Plans for Year 2

- Finish the packaging of p2r and FCS;
 - Include WCT and patatrack in the next mini-app development
 - If traccc is complete and stable, would be good to add that too
- Work out how to run ATLAS workflows with Globus Compute on Perlmutter, and then try to port to a different system (Polaris, for example)
 - Rucio / Globus integration and testing at production scale (effort from LZ)
- Finish the DUNE workflow porting, testing and benchmarking on Polaris
 - then replicate on Frontier
- Cookbook based on PPS finding

These all match our stakeholders' priorities (HPC is important to them, but executing complex workflows on HPC is hard)

Collaboration With Other CCE Groups



SOP?

- Metadata is important/ maybe this is an area we can work with SOP on
 - start with a survey on what/how metadata are being captured across HEP experiments
 - Good metadata will help with workflow portability and reproducibility.

SML?

- We may want to use some ML workflows as our use cases/testbeds
- Conversely, maybe we can learn from the SML group what they have found on scaling up ML workflows

IRI/HPDF

We can provide input to IRI/HPDF based on our experience with the workflows

IRI could help standardize access to different compute facilities

- software environments, authentication/authorization, automation tools, etc.

CCE should play the role of HEP advocate to HPC facilities, and help IRI consider HEP's needs; our experience and the workflow portability layers can contribute to IRI's software considerations.

- Workflow “mini-apps” for benchmarking and testing of IRI infrastructure

IRI/HPDF Task Force should have both CCE stakeholders and CCE members involved

- HEP-CCE understands the commonalities of HEP compute challenges.

Maybe HEP-CCE can learn from the experience on the NSF HPC systems (more HEP-friendly)

- Outbound connectivity
- Willingness to support HEP
- cvmfs availability

AI/ML

- Could use LLMs to write a cookbook-style AI assistant for parallelization
- Or do automatic code optimization/parallelization
- Generate documentation with LLMs
- Or can we develop a HEP-specific LLM?
- Need to have a robust unit testing/CI/CD framework for verification and validation
- No in-house expertise in CCE, but can find some at our labs or larger groups
- Validation / Verification - ML model can point you to which variables you need to look at after code has been modified

FASST



- Contribute experience deploying and running complex workflows on a variety of facilities
- HEP-aware AI assistant for HPC software