DOE Cross-facility Workflows Training

April 12, 2023
8:00 AM PST, 11:00 AM EST

Argonne NATIONAL LABORATORY Leadership Computing Facility

NERSC National Energy Research Scientific Computing Center

OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

Introduction

Agenda

8 - 8:10 a.m. (PST)	Welcome and introduction	Bill Arndt (NERSC)
8:10 - 9:10 a.m.	GNU Parallel tutorial + exercises	Ketan Maheshwari (OLCF) and Bill Arndt (NERSC)
9:10 - 9:15 a.m.	Break	
9:15 - 10:15 a.m.	Parsl tutorial + exercises	Bjoern Enders (NERSC) and Tyler Skluzacek (OLCF)
10:15 - 11:00 a.m.	Lunch	
11 a.m. -12 p.m.	FireWorks tutorial + exercises	Laurie Stephey (NERSC) and Sean Wilkinson (OLCF)
12 - 12:05 p.m.	Break	
12:05 - 1:05 p.m.	Balsam tutorial + exercises	Andrew Naylor (NERSC), Christine Simpson (ALCF), and Nick Tyler (NERSC)

Materials and Communications

- Github repository containing training materials:
  - https://github.com/CrossFacilityWorkflows/DOE-HPC-workflow-training
- Google document for questions and responses:
  - https://docs.google.com/document/d/1YXYvPKw8JaXQMxSed_m2dQZthbeKeAG9jAV_1Ej9BAE/edit
- Workflows.community Slack, channel #doe_workflow_training_2023
  - https://join.slack.com/t/workflowscommunity/shared_invite/zt-1t6n6r4zl-~8duS3haBCr6B6OP6iHXsQ
- Workflow Tool Decider
  - https://crossfacilityworkflows.github.io/workflow-tool-decider/
- Exit Survey:
  - https://forms.gle/CUnDt33CyxKp3fqZ6

System Reservations Available

- Perlmutter and Cori (NERSC) training reservation details:
  - `export SBATCH_ACCOUNT=ntrain7`
  - `export SBATCH_RESERVATION=doe_workflows_2023_cpu`
  - `#export SBATCH_RESERVATION=doe_workflows_2023_gpu`
  - `#export SBATCH_RESERVATION=doe_workflows_2023_cori`
- Polaris (ALCF) training reservation details:
  - Project: **WALSforAll**
  - Queue: **R476170**

Acknowledgement

- Haritha Siddabathuni Som, Beth Cerny, and Madelyn Blair - Administration Support
- Urjoshi Sinha and Daniel Fulton - Training Infrastructure Support
- Anubhav Jain - Fireworks Support
- Logan Ward, Kyle Chard, and Yadu Babuji - Parsl Support
- Murat Keceli, Chris Knight, and Neil Mehta - LAAMPS Support for Balsam Demo
- Yasaman Ghadar, Rafael Ferreira da Silva, and Helen He - Training Guidance