Drona Composer Demo

Marinus Pennings
July 20, 2024
What will we discuss?

- OOD Dashboard
- **Drona composer**
  - submitting workflows
  - creating new workflows
- Drona job listing
OOD Dashboard

One stop shop for researchers to manage their resources, interact with HPRC helpdesk

- Cluster info
- Batch queue information
- Group management
- Account management
- Quota management
- Help request management
Demo Dashboard

Quick demo of dashboard

- How to access
- Show features
- Create dummy request
Drona Composer

A graphical user interface to run (and create) any type of workflow (environment) on ACES (and other HPRC clusters), removing typical barriers HPC researchers commonly face.
Motivation

Provide a more intuitive way for researchers to run their workflow

- novice users shouldn’t need to adapt to HPC
  - Might not be familiar with Linux (command line)
  - Not familiar with Batch schedulers
  - Need to learn about cluster configurations
- Expert users
  - Rapid (fast) prototyping
  - No need to write custom scripts
  - Create advanced workflows
- Reduce work for Helpdesk
  - HPRC helpdesk does receive tickets regularly with questions regarding to submitting (and submitted) jobs
Drona Composer GUI

Select workflow

workflow specific options

Job Directory
/scratch/user/pennings/job_composer/testAbaqus

Environment
Abaqus

Upload files?
File

Abaqus version
ABAQUS/2023

Input file (.inp)
testAbaqus.inp

Run in parallel
YES

ncpus value
60

user subroutine (optional)
myumat.for

Memory
10 GB

Expected time needed to run
Days 2 Minutes

Preview
Demo Composer

- Create and submit Base env job
  - show the generated template
- Show R job
  - Vary the number of cores and parallel mode
- Show Matlab Job
  - Different User Interface
- Preview AI/ML
Creating Workflows

Users can “specify” their own custom workflows.

- schemas.json  Specification to declare the input elements (front end)
- map.json Specification to map input values to placeholders
- template.txt  job/workflow template with placeholders values
- driver.sh    shell script to submit/run the workflow (optional soon)
- utils.py python script containing functions used in map.json (optional)
Creating Workflows

Frontend elements

Mapping placeholders

Mapping from placeholder $\rightarrow$ StringExpression, where a StringExpression is a combination of the following:

- variable: $\$NAME$ (where NAME is an input name defined in schemas.json)
- function call: $!FUNCTION(<parameters>)$
- literal strings: anything that is not a variable or a function call

Example:

```
{  
  "batchopts": "$!retrieve_batch_opts($cores, $walltime, $memory, $extra_params)",
  "MODULE": "module load $version"
}
```
Demo Workflows

- Show specifications for Base env
  - schema.json, structure maps.json, template
- Show specifications for R env
  - different driver and warnings
- Show specification for Matlab
  - different driver
Drona Joblisting

A graphical user interface to manage jobs

- Any stage (pending, running, finished)
- Provide stage specific option
  - Request help for failed jobs
  - Wall time extension for running jobs (beta)
- Provide workflow specific information (soon)
# Drona Joblisting

Tabs for all the job states

- Date range finished jobs
- Links to job directory

<table>
<thead>
<tr>
<th>ID</th>
<th>Name</th>
<th>Location</th>
<th>SU</th>
<th>Actual Walltime</th>
<th>End</th>
<th>State</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>144710</td>
<td>sys/dashb+</td>
<td>matlab/output/22492132-6d7f-4c13-b5f9-09c36bf6c60</td>
<td>0</td>
<td>04:00:14</td>
<td>(100.10 %)</td>
<td>timeout</td>
<td>TIMOUT</td>
</tr>
<tr>
<td>144711</td>
<td>test_ID-1</td>
<td>u.mp108705/job_composer/testMatlab</td>
<td>0</td>
<td>00:00:19</td>
<td>(0.26 %)</td>
<td>completed</td>
<td>COMPLETED</td>
</tr>
<tr>
<td>144714</td>
<td>Job5</td>
<td>scratch/user/u.mp108705</td>
<td>0</td>
<td>00:00:17</td>
<td>(9.44 %)</td>
<td>cancelled+</td>
<td>CANCELLED</td>
</tr>
<tr>
<td>144715</td>
<td>Job6</td>
<td>scratch/user/u.mp108705</td>
<td>0</td>
<td>00:03:04</td>
<td>(102.22 %)</td>
<td>timeout</td>
<td>TIMOUT</td>
</tr>
</tbody>
</table>

- Request help for finished jobs

[Data table image]
Demo Drona Joblisting

- Show various tabs
  - finished, running, pending
- filter finished jobs on date
- Request help
# Texas A&M at PEARC24

<table>
<thead>
<tr>
<th>Talk/Event</th>
<th>Date/Time</th>
<th>Room</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tutorial: Hands-on exercises on the Intel Data Center GPU Max 1100 (PVC-GPU) for AI/ML and Molecular Dynamics Workflows on the ACES Testbed</td>
<td>Mon, July 22, 2024 9:00 AM-12:30 PM ET</td>
<td>Room 553B</td>
</tr>
<tr>
<td>Seventh Workshop on Strategies for Enhancing HPC Education and Training (SEHET24)</td>
<td>Mon, July 22, 2024 9:00 AM-12:30 PM ET</td>
<td>Room 557</td>
</tr>
<tr>
<td>Workshop: Providing cutting-edge computing testbeds to the science and engineering community</td>
<td>Mon, July 22, 2024 1:30 PM-5:00 PM ET</td>
<td>Room 554A</td>
</tr>
<tr>
<td>Workshop: Engaging Secondary Students in Computing: K12 Outreach</td>
<td>Mon, July 22, 2024 1:30 PM-5:00 PM ET</td>
<td>Room 553A</td>
</tr>
<tr>
<td>Cultivating Cyberinfrastructure Careers through Student Engagement at Texas A&amp;M University High Performance Research Computing</td>
<td>Tue, July 23, 2024 11:00 AM-11:25 AM ET</td>
<td>Junior Ballroom</td>
</tr>
<tr>
<td>Insight Gained from Migrating a Machine Learning Model to Intelligence Processing Units</td>
<td>Tue, July 23, 2024 11:00 AM-11:25 AM ET</td>
<td>Room 551 A&amp;B</td>
</tr>
<tr>
<td>BOF 4: What's in it for me? How can we truly democratize the research computing and data community?</td>
<td>Tue, July 23, 2024 1:30 PM-2:30 PM ET</td>
<td>Room 551 A&amp;B</td>
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<tr>
<td>Memory Bandwidth Performance across Accelerators</td>
<td>Tue, July 23, 2024 3:25 PM-3:50 PM ET</td>
<td>Ballroom B</td>
</tr>
<tr>
<td>Container Adoption in Campus High Performance Computing</td>
<td>Wed, July 24, 2024 11:00 AM-11:25 AM ET</td>
<td>Ballroom B</td>
</tr>
<tr>
<td>Engaging Secondary Students in Computing and Cybersecurity</td>
<td>Wed, July 24, 2024 3:15 PM-3:30 PM ET</td>
<td>Room 557</td>
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<td>Exploring the Viability of Composable Architectures to Overcome Memory Limitations in High Performance Computing Workflows</td>
<td>Wed, July 24, 2024 3:45 PM-4:00 PM ET</td>
<td>Room 553 A&amp;B</td>
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Thank you

- We gratefully acknowledge support from National Science Foundation awards #2112356 (ACES),
- Please visit our talks and BoFs at PEARC24