Drona Composer Demo

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High Performance
Research Computing
DIVISION OF RESEARCH

ACES
ACCELERATING COMPUTING
FOR EMERGING SCIENCES

What will we discuss?

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

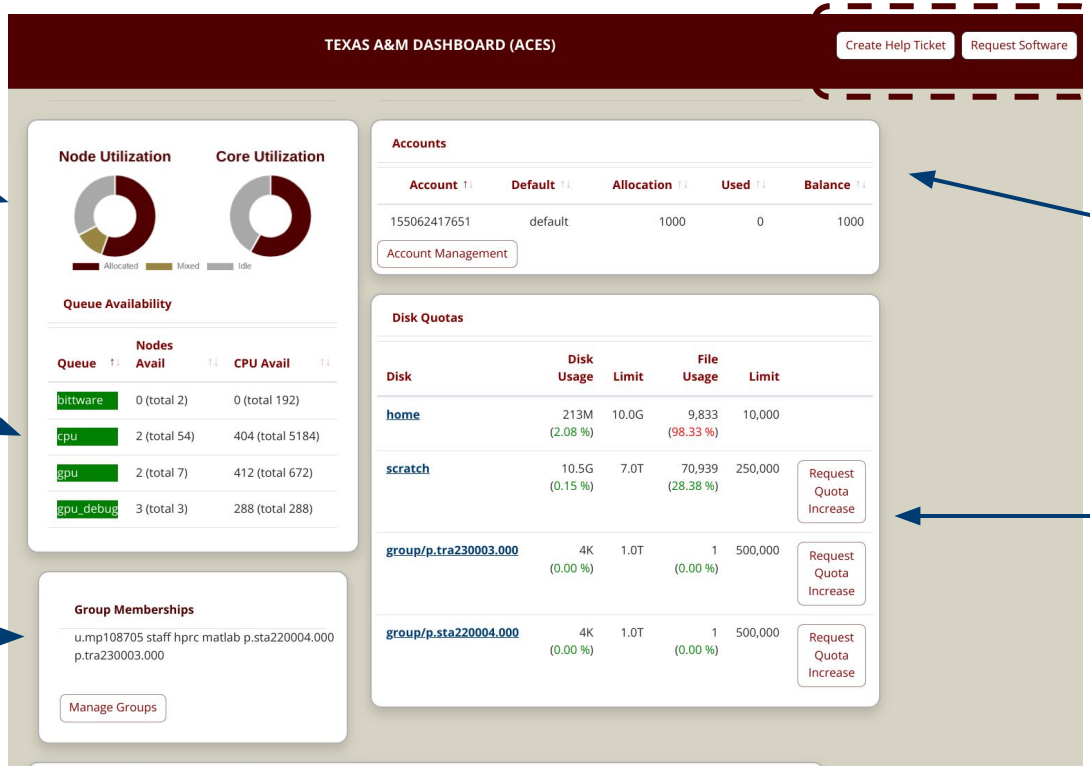
OOD Dashboard

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

Cluster info

Batch queue information

Group management



Help request management

Account management

Quota 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

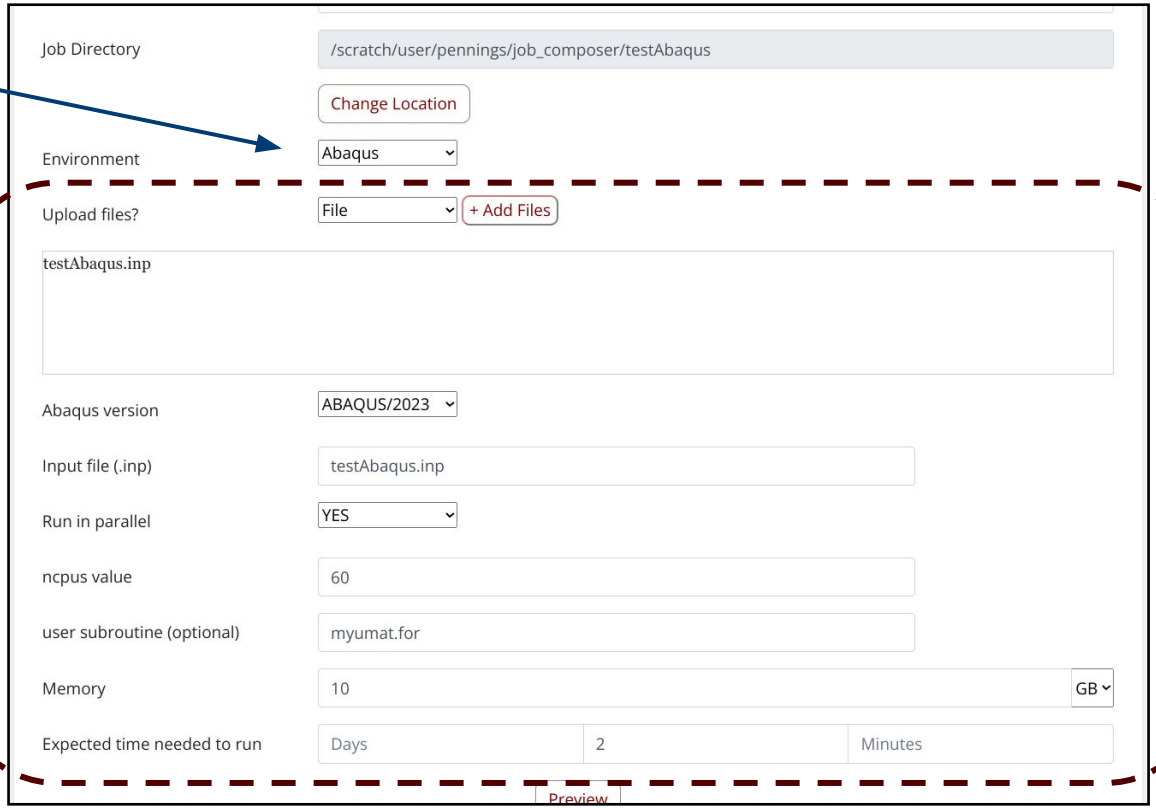
Provide a more intuitive way for researchers to run their workflow

- 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



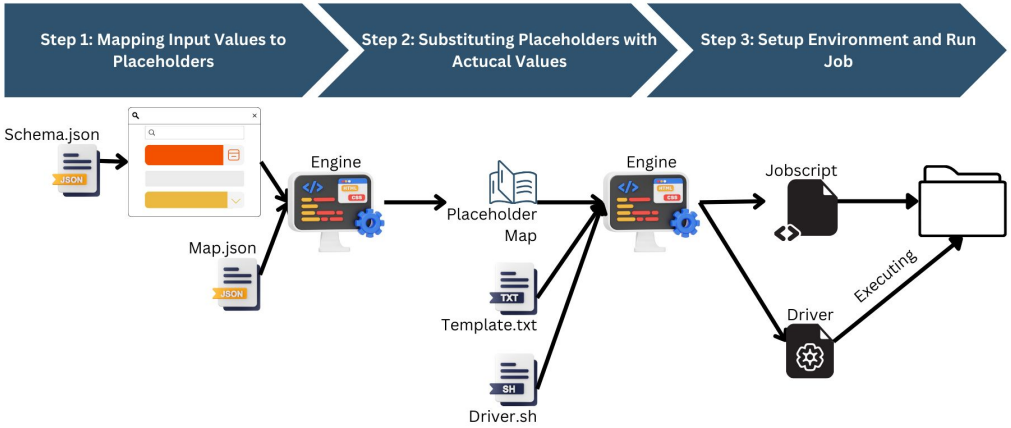
Demo Composer

- 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

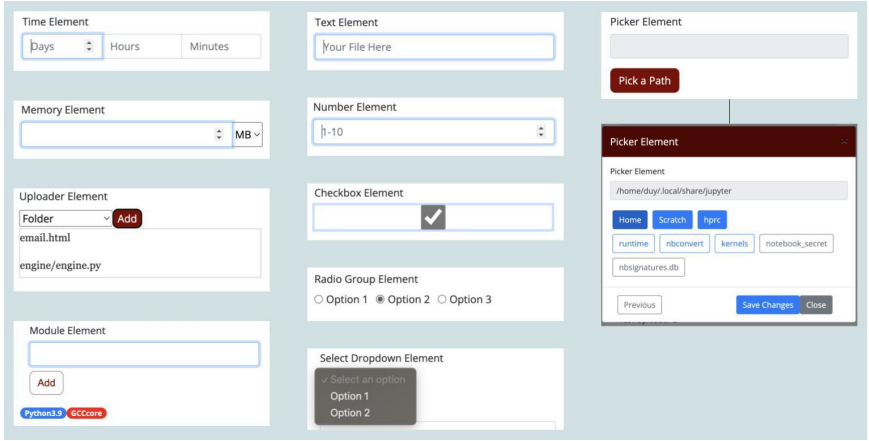
Users can “specify” their own custom workflows.

- 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 ← StringExpression, where a StringExpression is a combination of the follopwing:

- 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)

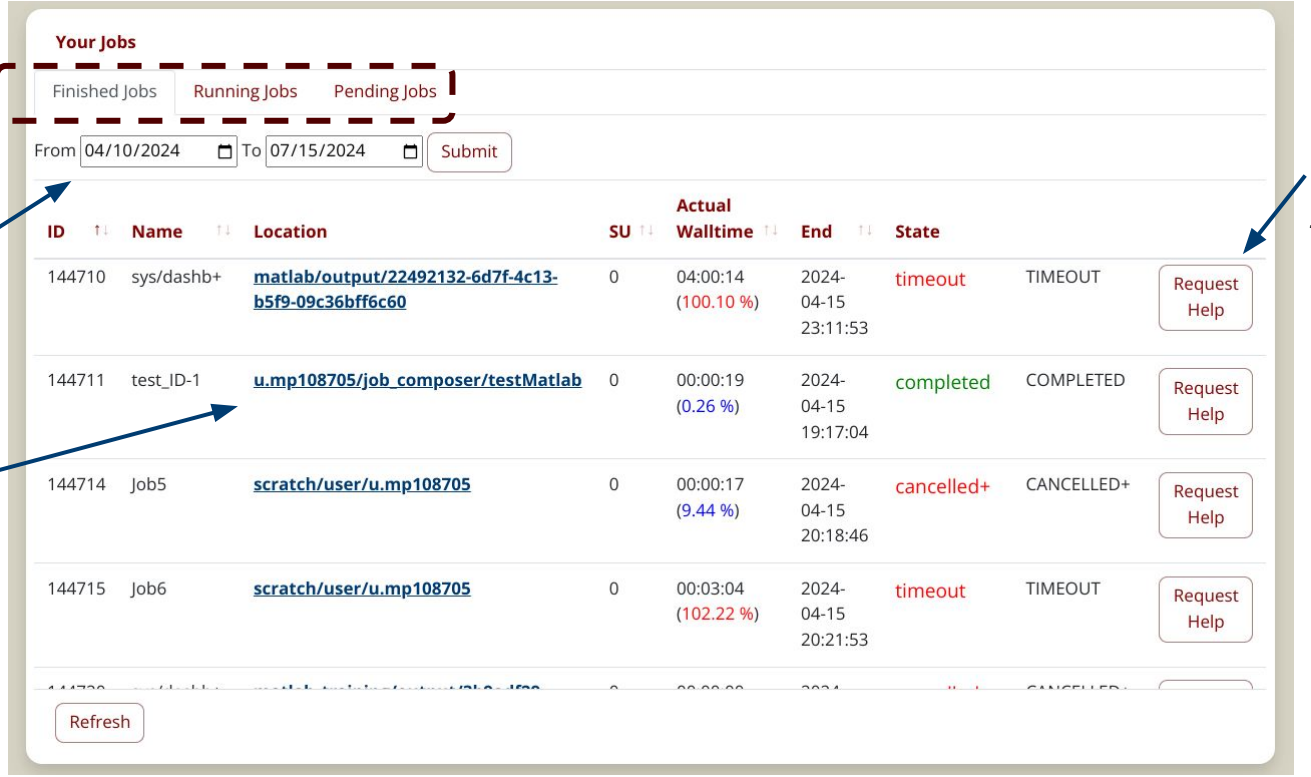
Drona Joblisting

Tabs for all the job states

date range finished jobs

links to job directory

request help for finished jobs



Demo Drona Joblisting

- Show various tabs
  - finished, running, pending
- filter finished jobs on date
- Request help

Texas A&M at PEARC24

Talk/Event	Date/Time	Room
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	Mon, July 22, 2024 9:00 AM-12:30 PM ET	Room 553B
Seventh Workshop on Strategies for Enhancing HPC Education and Training (SEHET24)	Mon, July 22, 2024 9:00 AM-12:30 PM ET	Room 557
Workshop: Providing cutting-edge computing testbeds to the science and engineering community	Mon, July 22, 2024 1:30 PM-5:00 PM ET	Room 554A
Workshop: Engaging Secondary Students in Computing: K12 Outreach	Mon, July 22, 2024 1:30 PM-5:00 PM ET	Room 553A
Cultivating Cyberinfrastructure Careers through Student Engagement at Texas A&M University High Performance Research Computing	Tue, July 23, 2024 11:00 AM-11:25 AM ET	Junior Ballroom
Insight Gained from Migrating a Machine Learning Model to Intelligence Processing Units	Tue, July 23, 2024 11:00 AM-11:25 AM ET	Room 551 A&B
BOF 4: What's in it for me? How can we truly democratize the research computing and data community?	Tue, July 23, 2024 1:30 PM-2:30 PM ET	Room 551 A&B

Texas A&M at PEARC24

Talk/Event	Date/Time	Room
BRICCs: Building Pathways to Research Cyberinfrastructure at Under Resourced Institutions	Tue, July 23, 2024 3:25 PM-3:50 PM ET	Junior Ballroom
Memory Bandwidth Performance across Accelerators	Tue, July 23, 2024 3:25 PM-3:50 PM ET	Ballroom B
Container Adoption in Campus High Performance Computing	Wed, July 24, 2024 11:00 AM-11:25 AM ET	Ballroom B
Engaging Secondary Students in Computing and Cybersecurity	Wed, July 24, 2024 3:15 PM-3:30 PM ET	Room 557
Exploring the Viability of Composable Architectures to Overcome Memory Limitations in High Performance Computing Workflows	Wed, July 24, 2024 3:45 PM-4:00 PM ET	Room 553 A&B
Performance of Molecular Dynamics Acceleration Strategies on Composable Cyberinfrastructure	Wed, July 24, 2024 4:15 PM-4:30 PM ET	Room 551 A&B
BOF 17: Fantastic ACCESS Cyberinfrastructure Resources and Where to Find Them	Wed, July 24, 2024 4:45 PM-5:45 PM ET	Room 553 A&B
BOF 18: Recipes to build successful cross-institutional collaborative computing	Wed, July 24, 2024 4:45 PM-5:45 PM ET	Junior Ballroom

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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