

HPC 101

Using the Open OnDemand Portal

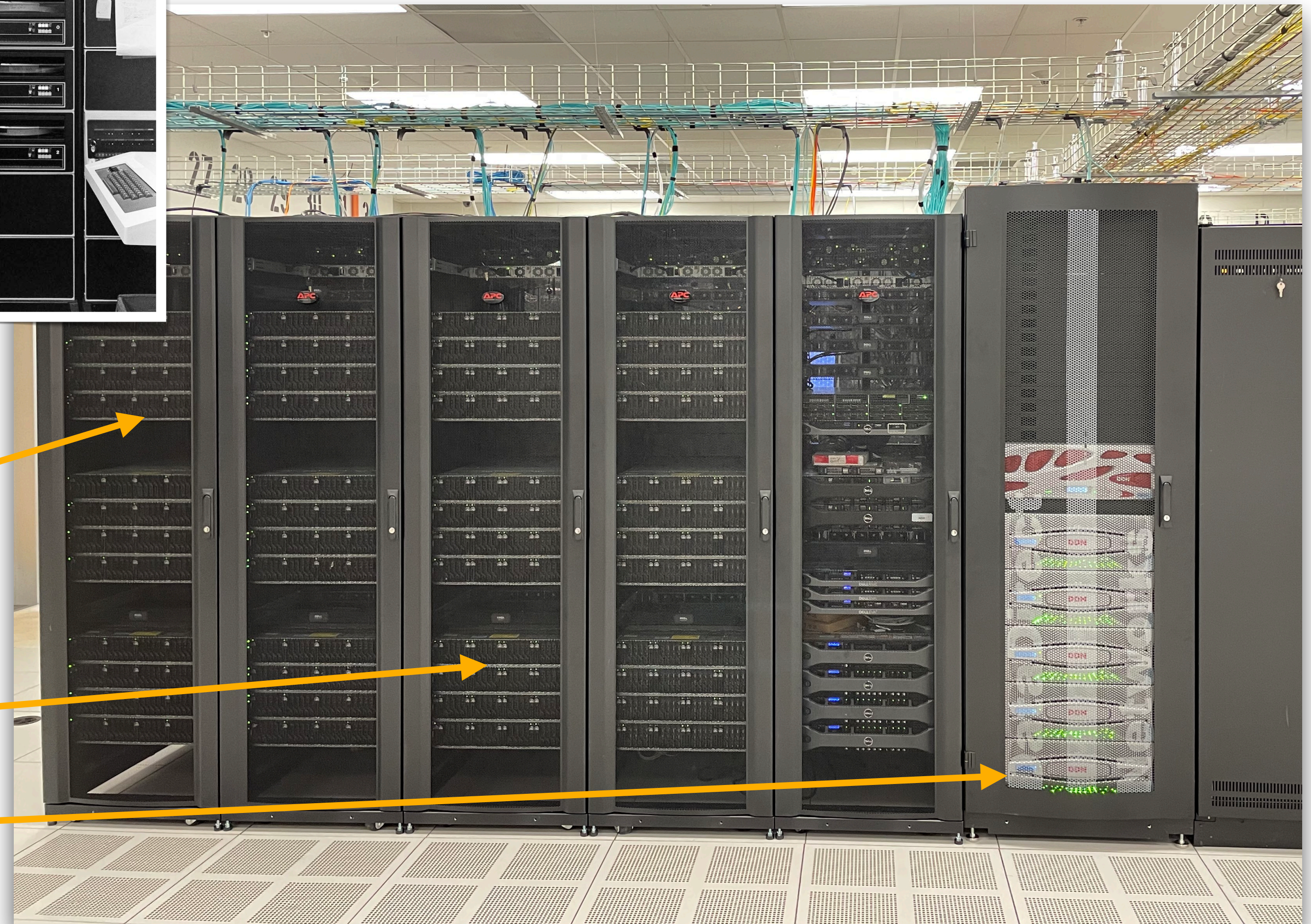
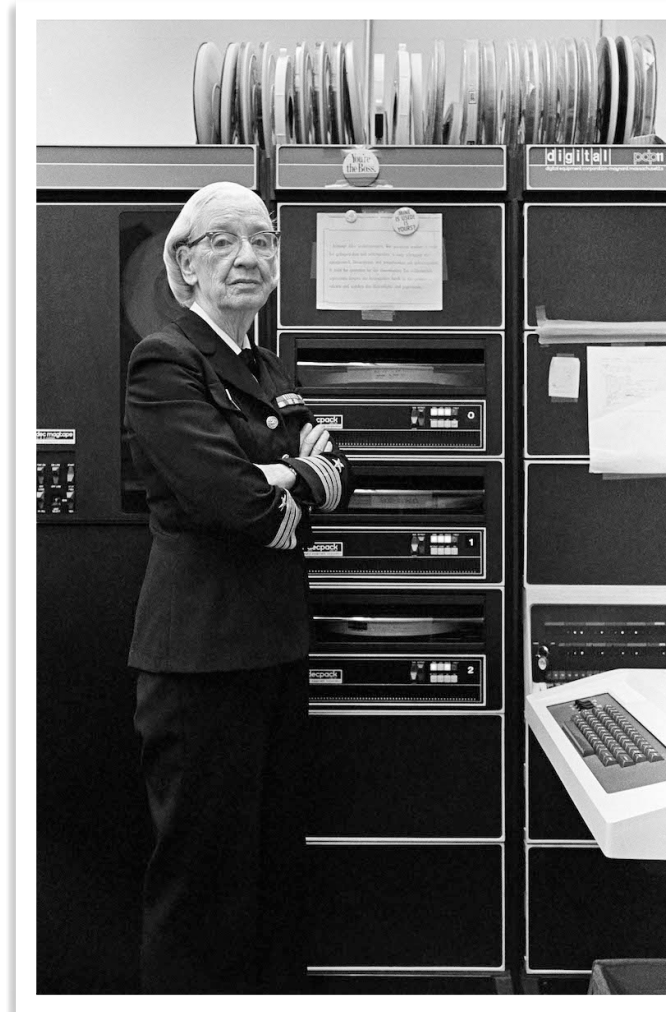
Joseph Utecht - May 17th 2021

**New topics every other Monday at 11am
See hpc.uams.edu for schedule**

UAMS High Performance Computer

Grace

- 96 Xeon CPU Nodes
28 cores at 2.4 GHz and 128GB of memory
- 96 Xeon Phi CPU Nodes
64 cores at 1.30 GHz and 192GB or 384GB of memory
- 1.9 PB High speed storage
Connected via 100Gb/s Omni-Path interconnects



HPC Users

Rights and Responsibilities

- Grace's computing resources are freely available to UAMS researchers
- Grace is a shared resource
- Sensitive material should never be stored on the system
 - Grace is not a HIPAA or FERPA repository
- Storage on Grace is redundant and highly reliable but not backed up
- Grace is a self-service resource, you are mostly on your own
- Full Terms and Conditions are available on the wiki found at hpc.uams.edu

Open OnDemand Portal

Full featured web portal to the HPC

- Submit Jobs
- Transfer files
- Launch interactive sessions
- Monitor status
- Obtain shell access
- Accessible anywhere from the browser

The screenshot displays the Open OnDemand web portal interface. At the top, it shows the user's current location: "Grace Open OnDemand / Active Jobs". Below this, there are navigation buttons for "Your Jobs" and "All Clusters".

The main section is titled "Active Jobs" and includes a "Show 50 entries" dropdown and a "Filter:" input field. A table lists active jobs with columns for ID, Name, User, Account, Time Used, Queue, Status, Cluster, and Actions. One job is visible: ID 49299, Name sys/dashboard/sys/RStudio, User jutecht, Account any, Time Used 00:26:16, Queue any, Status Completed, and Cluster Grace.

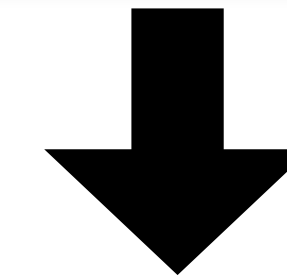
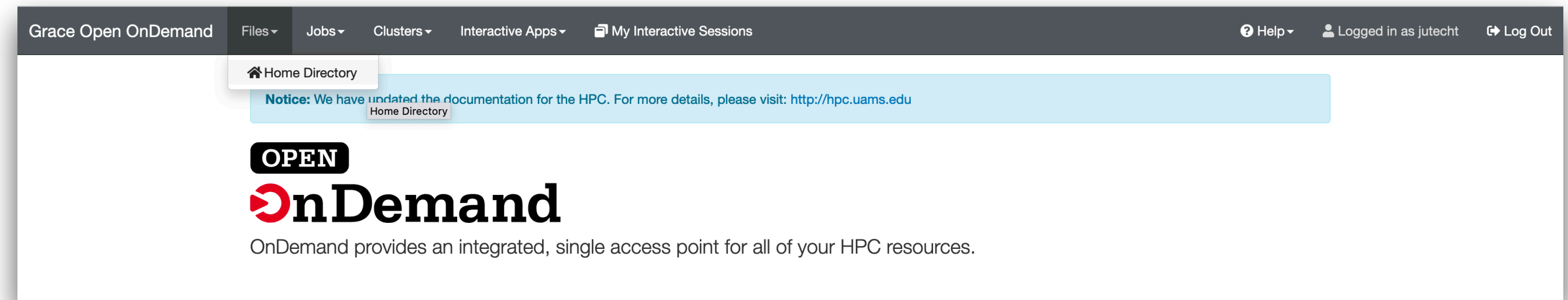
Below the job list, there are two panels. The left panel shows details for the selected job (ID 49299), including Cluster, Job Id, Job Name, User, Account, Partition, State, and Reason. The right panel shows a file manager view for the directory "/home/jutecht/moving_pictures/". It includes a sidebar with a file tree, a top navigation bar with "Go To...", "Open in Terminal", "New File", "New Dir", "Upload", "Show Dotfiles", and "Show Owner/Mode". The main area shows a table of files and directories with columns for name, size, and modified date. Files include "core-metrics-results", "emp-single-end-sequences", "aligned-rep-seqs.qza", "alpha-rarefaction.qzv", "ancom-Subject.qzv", "comp-gut-table-l6.qza", "comp-gut-table.qza", "demux.qza", "demux.qzv", "emp-single-end-sequences.qza", "gg-13-8-99-515-806-nb-classifier.qza", "gut-table-l6.qza", "gut-table.qza", "l6-ancom-Subject.qzv", "masked-aligned-rep-seqs.qza", "moving_pictures.script", "qiime", "rep-seqs.qza", "rep-seqs.qzv", and "rooted-tree.qza".

At the bottom, there is a section for "Interactive Apps" with a sidebar listing "Desktops" (Grace Desktop), "Jupyter Servers" (Jupyter Lab, Jupyter Notebook), and "R Servers" (RStudio Server). The main area shows a "Jupyter Lab (49306)" session that is "Running" on "1 node | 4 cores". It includes the host name "_kn1081.uams-hpc", creation time "2021-05-14 11:05:15 CDT", time remaining "59 minutes", and session ID "9c81c553-89a6-42a4-8db1-16500ed6adbe". A "Delete" button and a "Connect to Jupyter" button are also visible.

The footer of the page includes the text "powered by OPEN OnDemand" and "OnDemand version:".

File Management

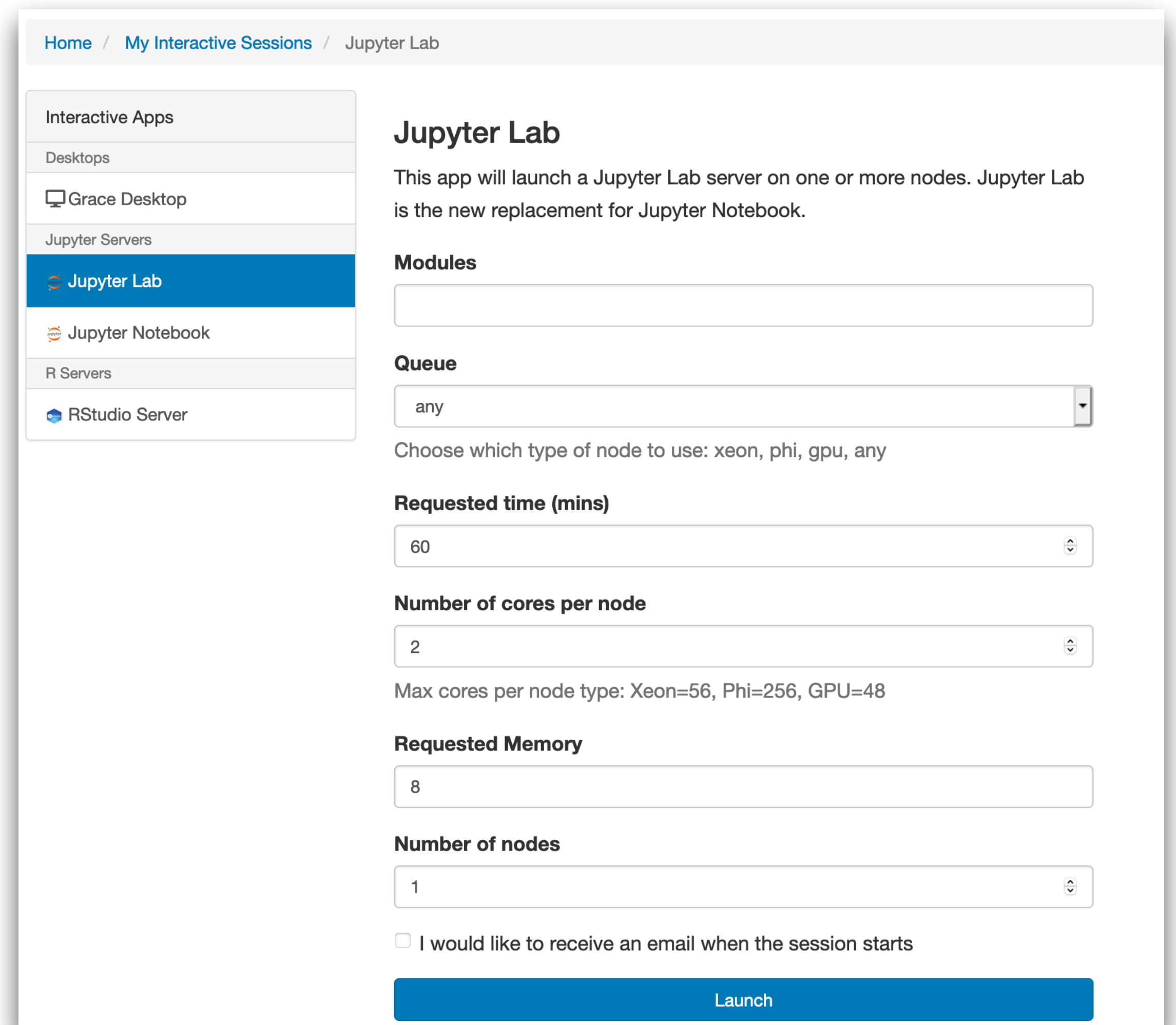
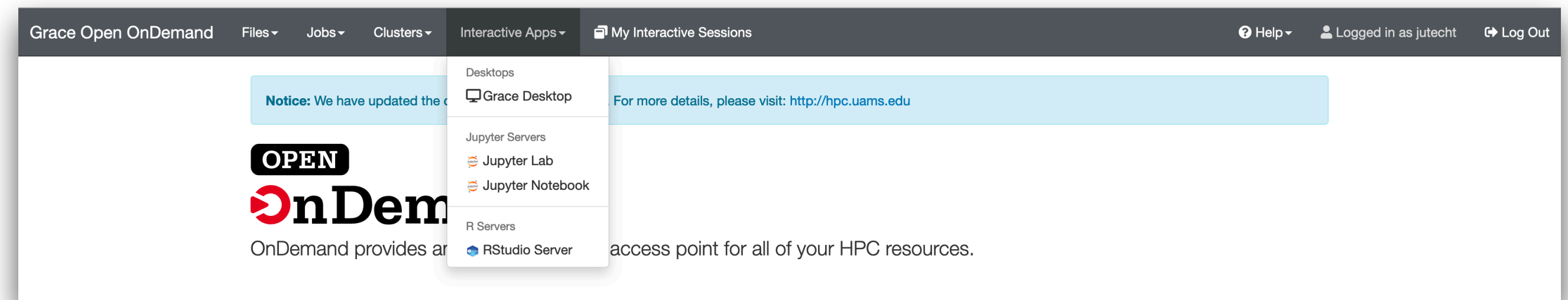
- File system is shared between login and compute nodes
- Your home directory should not be used to store large files for long time periods
- Relative vs absolute file paths
- ~/ is a shortcut to the base of your home directory



name	size	modified date
..	dir	
core-metrics-results	dir	05/03/2019
emp-single-end-sequences	dir	05/03/2019
aligned-rep-seqs.qza	57.17kb	05/03/2019
alpha-rarefaction.qzv	421.45kb	05/03/2019
ancom-Subject.qzv	390.31kb	05/03/2019
comp-gut-table-l6.qza	63.91kb	05/03/2019
comp-gut-table.qza	35.84kb	05/03/2019
demux.qza	19.64mb	05/03/2019
demux.qzv	291.15kb	05/03/2019
emp-single-end-sequences.qza	27.75mb	05/03/2019
gg-13-8-99-515-806-nb-classifier.qza	27.06mb	01/30/2019
gut-table-l6.qza	58.97kb	05/03/2019
gut-table.qza	30.68kb	05/03/2019
l6-ancom-Subject.qzv	412.73kb	05/03/2019
masked-aligned-rep-seqs.qza	59.27kb	05/03/2019
moving_pictures.script	4.82kb	05/03/2019
qiime	2.57gb	05/03/2019
rep-seqs.qza	47.03kb	05/03/2019
rep-seqs.qzv	273.78kb	05/03/2019
rooted-tree.qza	60.99kb	05/03/2019

Interactive Sessions

- Use familiar tools in a powerful environment
- See results in real time
- Compute nodes have no internet access
- Modules and packages needed must be managed ahead of time
 - Conda environments are the recommended approach



Exercise

Basic Workflow

- Log in to portal.hpc.uams.edu
- Transfer file from your computer to the HPC
- Launch an interactive session Jupyter/RStudio
- Read the file you uploaded in Python/R from your interactive session
- Create a figure or file from Python/R
- Close your interactive session
- Download the file you created back to your computer

Thank you

Next Training - May 31st 11am

Slurm Basics - Submitting jobs on the HPC

Sign ups at hpc.uams.edu

Please send suggestions for
future topics of interest to
jrutecht@uams.edu