

O2 Portal – Simplifying the Interaction and Experience of Using an HPC Environment

RC TRAINING | SUMMER 2023

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 Location: 1635 Tremont Street

 Office hours: Wednesdays 1:00-3:00 pm (Currently via Zoom - <https://rc.hms.harvard.edu/office-hours>)

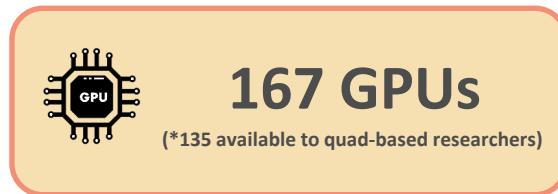
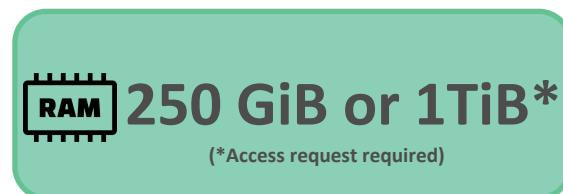


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What is O2?

- HMS Research Computing's newest High-Performance Compute cluster
- SLURM scheduler



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How to get an O2 account?

- Available to both, on-quad and off-quad researchers
 - off-quad - researchers from labs whose PIs **do not** have a primary or secondary faculty appointment in an [HMS Blavatnik Institute Basic or Social Science Department](#)
 - off-quad researchers are charged for O2 jobs and storage
- More information at [How to request or retain an O2 account](#)



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Important Note about O2 Storage

- O2 can only be used to store data of Harvard Security Level 3 and below.
- None of the standard filesystems are automatically encrypted, and **cannot** be used for HIPAA-protected or other secure data (Harvard's data security above level 3) unless those data have been de-identified.



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HMS Storage Offerings

- Options - <https://it.hms.harvard.edu/our-services/research-computing/services/storage>
- O2 Primary Storage
 - /home 100GiB
 - /n/data1, /n/data2, /n/groups
 - backups
- O2 Scratch
 - /n/scratch3
 - 10TiB; 30 day retention, no backups

	Active Compute (O2)	Scratch (O2)	Active Collaborations (research.files)	Standby	Cold
Description	Shared group or project folders connected to the High Performance Compute Cluster (O2).	Temporary storage (days to weeks) for data that can be easily regenerated (transient files). An automatic deletion process periodically removes files.	Shared group or project drives designed for active research data. Allows individuals to share documents and files within and outside of their department.	Shared group folders for infrequently accessed data; available for reference/retrieval.	Long-term storage of inactive research data; retained to meet data retention requirements.
Use Cases	Active research data that is frequently accessed, modified, or computed against. Next-gen sequencing analysis, molecular dynamics, mathematical	Pipeline that writes intermediate files that can be easily regenerated and do not require permanent retention. Temporary storage location	Storage location for data derived from tools, instruments, or desktops. Allows individuals to share documents and	An intermediary location; data associated with lab members who have recently departed or projects in the	Examples found in the Cold Storage Frequently Asked Questions ☰



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O2 Cluster Status

O2 Cluster Status

Created by Bergman, Andrew L., last modified about an hour ago

This page shows all service outages for the O2 cluster, including planned maintenance and unplanned events.

We also post updates on the [HMS RC Twitter page](#).

ONLINE

July 8: notes after the July OS/Slurm update

- Jupyter Notebooks users should start a new environment and remove any old runtime directories.
- "sbatch" no longer uses the "-x11" option in the new version of Slurm. Just remove it from your script and X forwarding should work by default.
 - "srun" commands still require "-x11" to enable X forwarding, though.
- If you have any custom built software, you may need to recompile or relink it on O2.

- <https://harvardmed.atlassian.net/l/cp/zLMdWTYs>

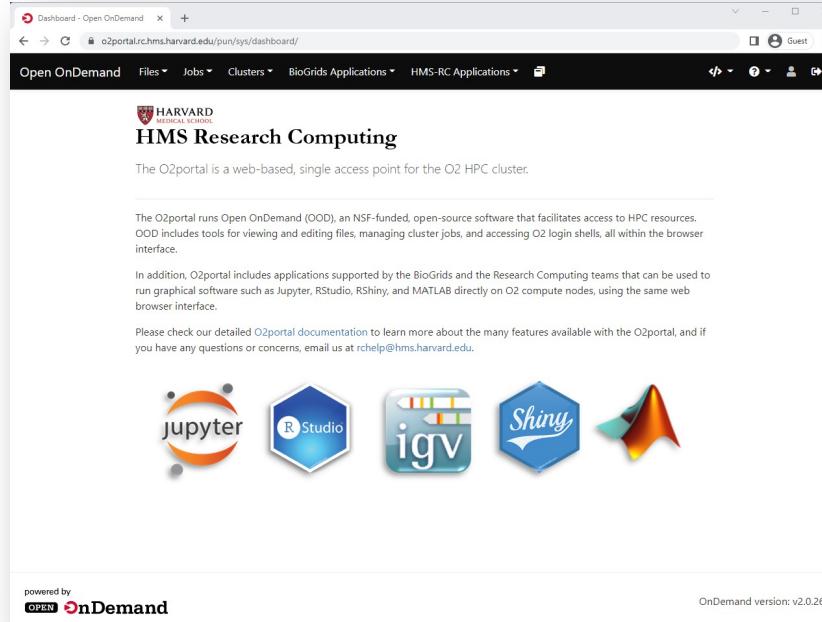


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O2 portal – O2 web-based access point

- Powered by Open OnDemand



A screenshot of a web browser displaying the O2 portal dashboard. The title bar shows 'Dashboard - Open OnDemand'. The main content area is titled 'HMS Research Computing' and includes the Harvard Medical School logo. It describes the O2portal as a web-based single access point for the O2 HPC cluster, powered by Open OnDemand. It lists various supported applications: Jupyter, R Studio, igv, Shiny, and MATLAB. At the bottom, it says 'powered by OPEN OnDemand' and 'OnDemand version: v2.0.26'.

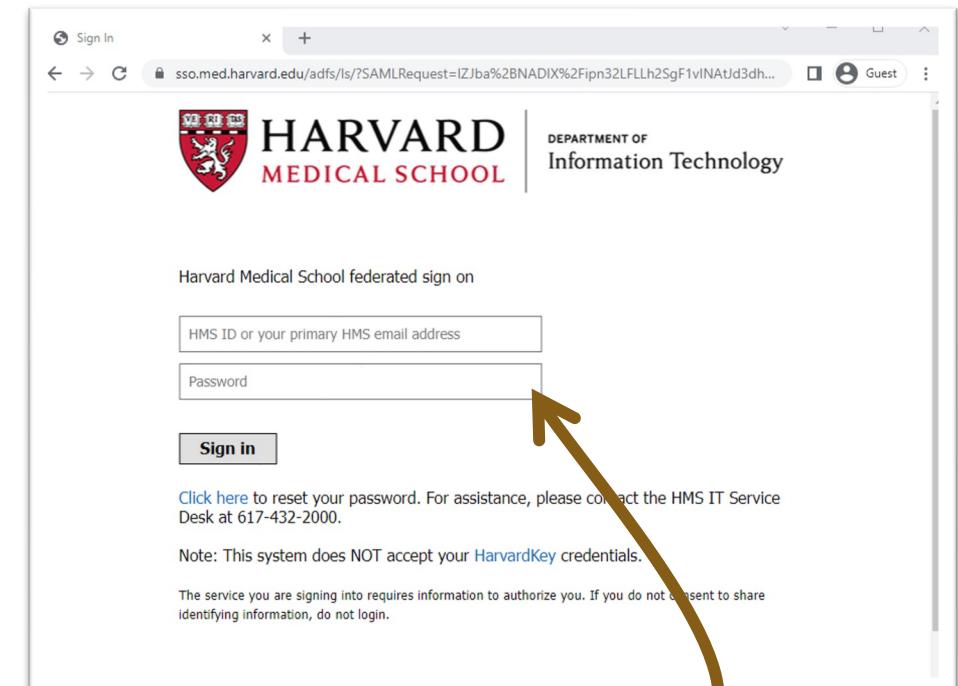


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Requirements to Access the O2 Portal

- O2 account
- Setup 2FA authentication



Authenticate with HMS ID



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Transfer Files



Submit Jobs



Monitor Jobs



Terminal



View/Edit Files



Applications



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View/Edit Files



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Transfer Files

Upload

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ BioGrids Applications ▾ HMS-RC Applications ▾ My Interactive Sessions ? Help ▾ Logged in as rc_training01 Log Out

Open in Terminal + New File + New Directory **Upload** Download Copy/Move Delete

Home Directory

Scratch

data1

data2

groups

no_backup2

Drop files here, [browse files](#) or
[browse folders](#)

Empty directories will be included in the upload only when a directory upload is initiated via drag and drop. This is because the File and Directory Entries API is available only on a drop event, not during an input change event.

Powered by Uppy

powered by
OPEN OnDemand

OnDemand version: v2.0.26



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Transfer Files

Download

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ BioGrids Applications ▾ HMS-RC Applications ▾ My Interactive Sessions ? Help ▾ Logged in as rc_training01 Log Out

Open in Terminal + New File New Directory Upload Download Copy/Move Delete

Home Directory

Scratch

data1

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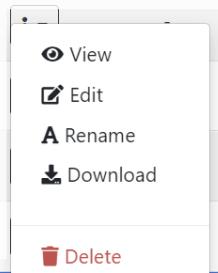
no_backup2

Up / home / rc_training01 / Change directory Copy path

Show Owner/Mode Show Dotfiles Filter:

Showing 5 of 16 rows - 1 rows selected

Type	Name	Size	Modified at
Folder	ondemand		8/8/2022 5:01:26 PM
Folder	programs		8/8/2022 4:00:36 PM
Folder	R		8/8/2022 5:09:16 PM
Folder	tissue_project		8/8/2022 3:59:27 PM
File	rstudio_launcher.sh	0 Bytes	8/8/2022 4:01:16 PM



powered by
OPEN OnDemand

OnDemand version: v2.0.26



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Transfer Files

Within O2

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ BioGrids Applications ▾ HMS-RC Applications ▾ My Interactive Sessions ? Help ▾ Logged in as rc_training01 Log Out

Open in Terminal + New File New Directory Upload Download Copy/Move Delete

Copy or move the files below from /home/rc_training01 to the current directory:

/ home / rc_training01 Change directory Copy path

Show Owner/Mode Show Dotfiles Filter: Showing 3 of 9 rows - 1 rows selected

Type	Name	Size	Modified at
programs	programs	-	8/8/2022 4:00:36 PM
tissue_project	tissue_project	-	8/8/2022 3:59:27 PM
rstudio_launcher.sh	rstudio_launcher.sh	0 Bytes	8/8/2022 4:01:16 PM

Home Directory Scratch data1 data2 groups no_backup2

Copy Move

powered by **OPEN** OnDemand OnDemand version: v2.0.26

- 1 Select file or directory
- 2 Click on “Copy/Move”
- 3 Move to target location
- 4 Click on Copy or Move



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Transfer Files

Within O2

c Open OnDemand Files ▾ Jobs ▾ Clusters ▾ BioGrids Applications ▾ HMS-RC Applications ▾ My Interactive Sessions ? Help ▾ Logged in as rc_training01 Log Out

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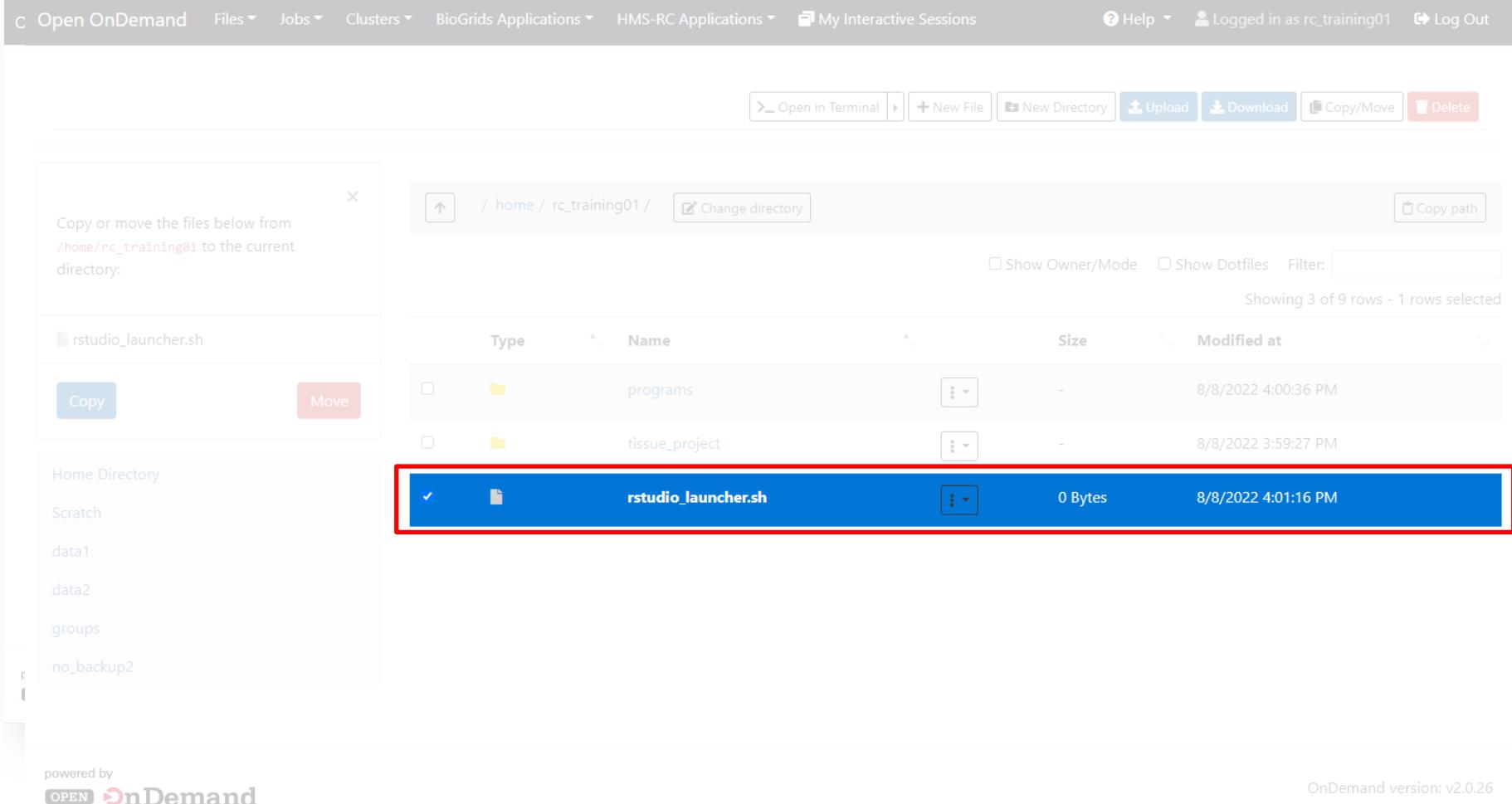
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Home Directory Scratch data1 data2 groups no_backup2

powered by **OPEN** OnDemand OnDemand version: v2.0.26



1 Select file or directory

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15



Transfer Files

Within O2

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ BioGrids Applications ▾ HMS-RC Applications ▾ My Interactive Sessions ? Help ▾ Logged in as rc_training01 Log Out

Open in Terminal + New File New Directory Upload Downloads Copy/Move Delete

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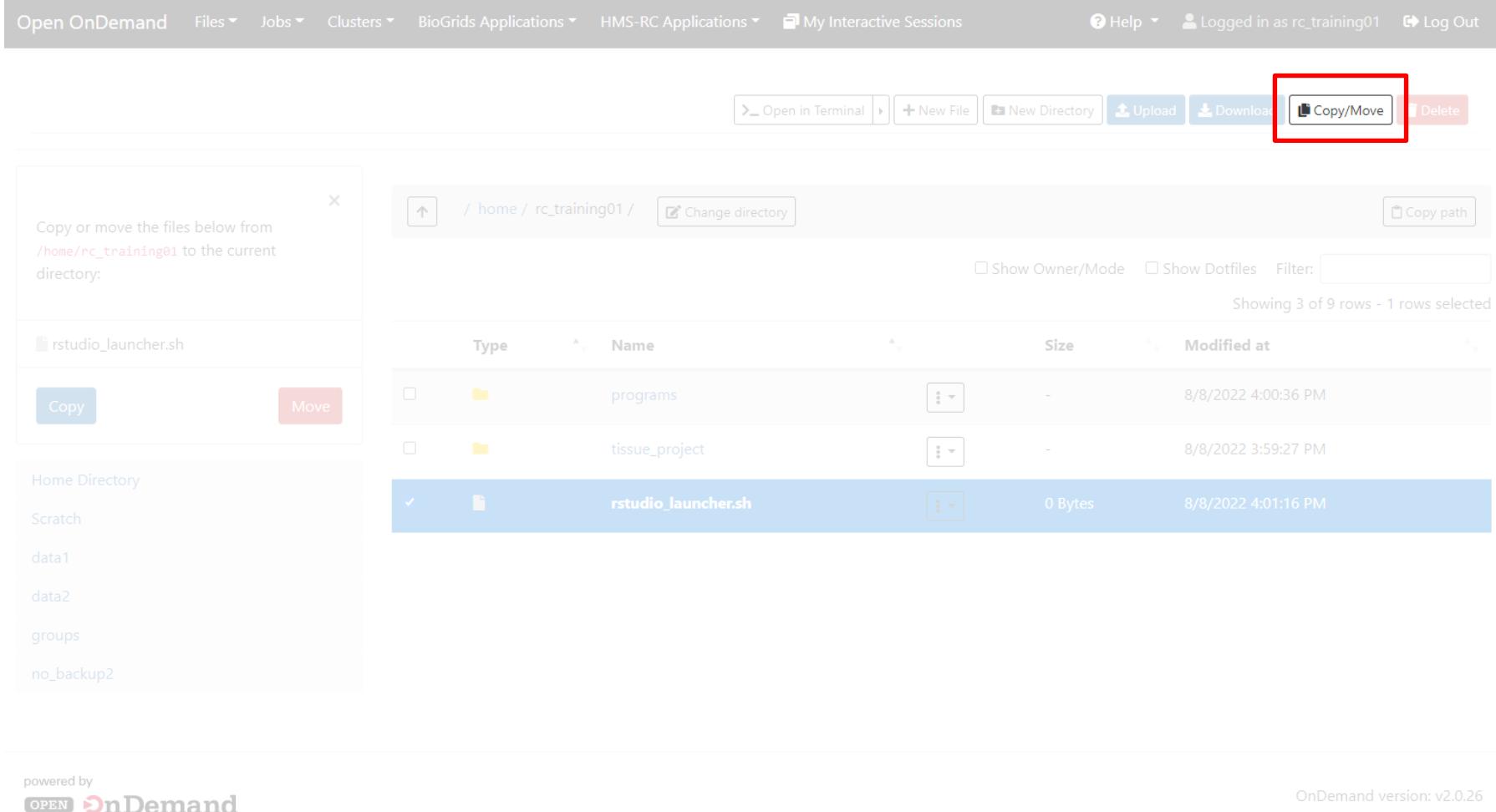
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Copy Move

Home Directory
Scratch
data1
data2
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no_backup2

powered by **OPEN** OnDemand OnDemand version: v2.0.26



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Transfer Files

Within O2

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Copy Move

Home Directory Scratch data1 data2 groups no_backup2

powered by **OPEN** OnDemand OnDemand version: v2.0.26

1 Select file or directory

2 Click on “Copy/Move”

3 Move to target location

4 Click on Copy or Move



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Transfer Files

Within O2

The screenshot shows the OnDemand interface with the 'Transfer Files' tab selected. The top navigation bar includes links for Open OnDemand, Files, Jobs, Clusters, BioGrids Applications, HMS-RC Applications, My Interactive Sessions, Help, Log In, and Log Out. Below the navigation is a toolbar with buttons for Open in Terminal, New File, New Directory, Upload, Download, Copy/Move, and Delete. The main area displays a file list in a table format. The table has columns for Type, Name, Size, and Modified at. It shows three rows: 'programs' (directory), 'tissue_project' (directory), and 'rstudio_launcher.sh' (file). The 'rstudio_launcher.sh' row is highlighted with a blue background. To the left of the table is a sidebar with a message about moving files from /home/rc_training01 to the current directory, and a list of home directory contents: Home Directory, Scratch, data1, data2, groups, and no_backup2. A red box highlights the 'Copy' and 'Move' buttons for the 'rstudio_launcher.sh' file.

Copy or move the files below from `/home/rc_training01` to the current directory:

<code>rstudio_launcher.sh</code>	<button>Copy</button>	<button>Move</button>
----------------------------------	-----------------------	-----------------------

Home Directory

Scratch

data1

data2

groups

no_backup2

Powered by OnDemand

OnDemand version: v2.0.26

- 1 Select file or directory
- 2 Click on “Copy/Move”
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Transfer Files



Submit Jobs



Monitor Jobs

Terminal



View/Edit Files



Applications



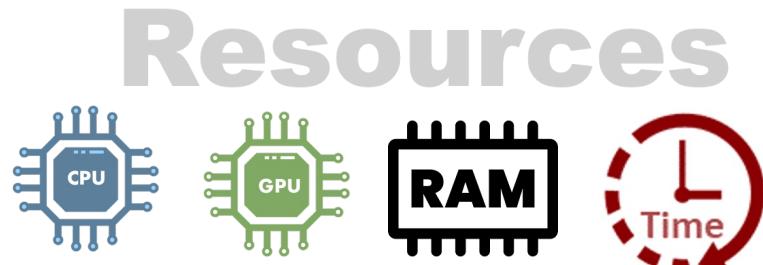
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Submit Jobs

A job is a **resource** request sent to O2 via the O2 Portal containing one or more **tasks**.



Launch Application



Data Analysis



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Transfer Files



Submit Jobs



Monitor Jobs

Terminal



View/Edit Files



Applications



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Monitor Jobs

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ BioGrids Applications ▾ HMS-RC Applications ▾ **My Interactive Sessions** ? Help ▾ Logged in as rc_training01 Log Out

RStudio Environment (59163745)

Queued

Deleted

RStudio Environment (14087611)

1 node | 1 core | Running

Deleted

Job Status

Host: compute-e-16-230.o2.rc.hms.harvard.edu

Created at: 2022-08-08 17:03:32 EDT

Time Requested: 1 hour

Ses:

Ple

req

Time Remaining: 58 minutes

Session ID: d262e7ff-eee2-4bb9-97e3-89c6ce0e4959

Progress & Error log: [output.log](#)

Connect to RStudio Server

```
graph LR; JS[Job Status] --> Q[Queued]; JS --> R[Running]
```



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Monitor Jobs

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ BioGrids Applications ▾ HMS-RC Applications ▾ **My Interactive Sessions** Help ▾ Logged in as rc_training01 Log Out

RStudio Environment (14087611) **1 node | 1 core | Running**

Host: compute-e-16-230.o2.rc.hms.harvard.edu [Delete](#)

Created at: 2023-08-01 16:05:01 EDT

Time Remaining: 58 minutes

Session ID: [d262e7ff-eee2-4bb9-97e3-89c6ce0e4959](#)

Progress & Error log: [output.log](#)

[Connect to RStudio Server](#)

Important!
(Stop the job)



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Monitor Jobs

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ BioGrids Applications ▾ HMS-RC Applications ▾ **My Interactive Sessions** Help ▾ Logged in as rc_training01 Log Out

RStudio Environment (14087611) **1 node | 1 core | Running**

Host: compute-e-16-230.o2.rc.hms.harvard.edu [Delete](#)

Created at: 2023-08-01 16:05:01 EDT

Time Remaining: 58 minutes

Session ID: [d262e7ff-eee2-4bb9-97e3-89c6ce0e4959](#)

Progress & Error log: [output.log](#) **Link to log file** ←

[Connect to RStudio Server](#)



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Monitor Jobs

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ BioGrids Applications ▾ HMS-RC Applications ▾ **My Interactive Sessions** ? Help ▾ Logged in as rc_training01 Log Out

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Time Remaining: 58 minutes

Session ID: [d262e7ff-eee2-4bb9-97e3-89c6ce0e4959](#)

Progress & Error log: [output.log](#)

[Connect to RStudio Server](#)

Open Application



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Transfer Files



Submit Jobs



Monitor Jobs

Terminal



View/Edit Files



Applications



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Terminal

The O2portal is a web-based, single access point for the O2 HPC cluster.

The O2portal runs Open OnDemand (OOD), an NSF-funded, open-source software that facilitates access to the O2 HPC cluster.

Host: transfer.rc.hms.harvard.edu
running kernel 3.10.0 born on 2020-08-11

Host: o2.hms.harvard.edu
running kernel 3.10.0 born on 2021-09-27

News (Jan 3 2022)

Contact HMS Research Computing:

E-mail rchelp@hms.harvard.edu
Web it.hms.harvard.edu/rc
Twitter @hms_rc

[rc_training01@transfer06 ~]\$

[rc_training01@login02 ~]\$



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Transfer Files



Submit Jobs



Monitor Jobs



Terminal



View/Edit Files



Applications



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View/Edit Files

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ BioGrids Applications ▾ HMS-RC Applications ▾ My Interactive Sessions ? Help ▾ Logged in as rc_training01 Log Out

Open in Terminal + New File New Directory Upload Download Copy/Move Delete

Home Directory

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/ home / rc_training01 / Change directory Copy path

Show Owner/Mode Show Dotfiles Filter: Showing 3 of 9 rows - 0 rows selected

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View Edit Rename Download Delete

powered by **OPEN** OnDemand OnDemand version: v2.0.26



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Transfer Files



Submit Jobs



Monitor Jobs

Terminal



View/Edit Files



Applications



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Applications

- Two sets of scientific software applications provided by BioGrids and HMS Research Computing

BioGrids Applications

GUIs
IGV
IDE
Jupyter
RStudio

HMS-RC Applications

GUIs
Desktop Mate
Graphical User Interface (GUI)
MATLAB
Relion
IDE
VSCode
Jupyter
MATLAB-proxy-app
RStudio Environment
Shiny (Internal)



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Applications

1. Select Application



2. Specify Resources



3. Launch Application

Launch



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Survey

- Short (3-min or less)
- Suggest new content!
- Share your feedback!!



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