

# **Overview of Open OnDemand and MyLRC portal**

**Sapana Soni**

HPCS User Support Team

# Outline

## Part I : Using MyLRC portal

- Requesting a user account on Lawrencium super cluster
- Getting access to an existing project account
- Requesting a new project account and project management

## Part II : OOD Applications

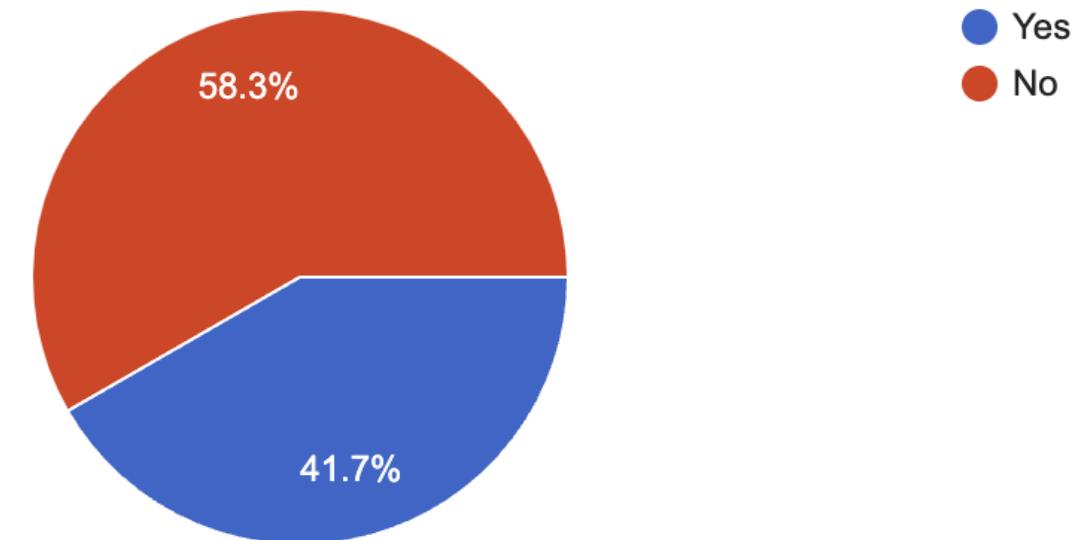
- Command-line shell access
- File management
- Interactive server and GUI applications, such Jupyter Notebook, Matlab and RStudio
- Full linux desktop streaming via web for GUI heavy jobs such as VMD, ParaView
- Customize Jupyter and Julia kernels
- Job management and monitoring

# **Training style : Mostly Demonstration**

- If you have an account on Lawrencium cluster then open OOD dashboard and try it yourself as we go.
- Don't have account on Lawrencium? Don't worry! You can watch for now and try it later using training material.
- Training material is available on GitHub([https://github.com/lbnl-science-it/OOD\\_training\\_Feb2023.git](https://github.com/lbnl-science-it/OOD_training_Feb2023.git))
- Recording for the training will be available [here](#).
- How to use Lawrencium?
  - Documentation page [link](#)

# MyLRC User Portal:

- Requesting a user account on Lawrencium super cluster
- Getting access to an existing project account
- Requesting a new project account and project management
  - Updating Project information
  - PCA Project renewal
  - Addition and removal/deletion of user accounts



MyLRC portal [login](#)

MyLRC [Documentation](#)

# **Requesting a user account on Lawrencium super cluster**

## **Current Workflow:**

1. Setup an account on MyLRC [portal](#). Portal uses CILogon for user authentication. Users can register using email address provided by LBNL or UC Berkeley or other institutions or google.
2. Sign the User Access Agreement Form on the welcome page
3. Request to join existing project
4. PI approval
5. Lawrencium account creation by HPCS team
6. Users will receive a confirmation email and PIN+OTP set up instructions.

**Step 1:** Use your LBNL email account to login. If you don't have LBNL email account then you can login using UC Berkeley email address or as an external collaborator.

**MyLRC - Laboratory Research Computing Access Management System**

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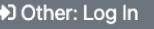
Home Center Summary Help 

## Welcome to MyLRC

MyLRC is a user portal for managing access to the clusters and other resources provided by the Laboratory Research Computing (LRC) program.

- Join projects and gain access to Lawrencium and other clusters.
- Create new projects and manage project users.
- Request or purchase computing allowances.
- View details of current and past jobs, and allowance usages.
- And more!

For more information, refer to our [documentation](#).

**MyLRC - Laboratory Research Computing Access Management System**

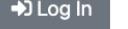
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## Log In: I am a...

 BERKELEY LAB

**Berkeley Lab User**  
I have a Berkeley Lab Identity.  


**UC Berkeley Collaborator**  
I do not have a Berkeley Lab Identity, but I do have a CalNet ID.  


**External Collaborator**  
I do not have a Berkeley Lab Identity, and I do not have a CalNet ID.  






# LBNL Credentials

CILogon

Consent to Attribute Release

Berkeley Lab, Laboratory Research Computing, MyLRC (Production) requests access to the following information. If you do not approve this request, do not proceed.

- Your CILogon user identifier
- Your name
- Your email address
- Your username and affiliation from your identity provider

**Selected Identity Provider**

Lawrence Berkeley National Laboratory  

Remember this selection 

**Log On**

By selecting "Log On", you agree to the [privacy policy](#).

 BERKELEY LAB

Log in with your Berkeley Lab Identity

Username  

Password  

**Log in**

A service named [CILogon](#) requested that you login.

[Lost or forgot password?](#)



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Managed by the University of California

[Questions & Comments](#)  
[Privacy & Security Notice](#)



# UC Berkeley Credentials

Logon

Consent to Attribute Release

Berkeley Lab | Laboratory Research Computing | MyLRC (Production) requests access to the following information. If you do not approve this request, do not proceed.

- Your CILogon user identifier
- Your name
- Your email address
- Your username and affiliation from your identity provider

**Selected Identity Provider**

University of California, Berkeley 

Remember this selection 

**Log On**

By selecting "Log On", you agree to the [privacy policy](#).

**Berkeley**  
UNIVERSITY OF CALIFORNIA

**CalNet Authentication Service**

CalNet ID:

Passphrase (Case Sensitive):

**SIGN IN** [HELP](#)

[FORGOT CALNET ID OR PASSPHRASE?](#)  
[MANAGE MY CALNET ACCOUNT](#)

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# External Collaborator :

Chose your institution from the drop down menu and enter your credentials for the account. If your institution is not listed then chose google to use a google account for login.

The screenshot shows a 'Consent to Attribute Release' page. At the top right is a 'CILogon' logo. Below it is a search bar with 'Type to search' placeholder text and a dropdown menu with 'Google' selected. The main content area displays a list of institutions:

- Lawrence Berkeley National Laboratory
- 29 Mayis University
- A\*STAR - Agency for Science, Technology and Research
- A. T. Still University
- AAF Virtual Home
- aai.lab.maeen.sa
- AAI@EduHr Single Sign-On Service
- Aalborg University
- Aalto University
- Aarhus School of Architecture
- Aarhus School of Marine and Technical Engineering
- Aarhus University
- AARNet
- Aba Teachers University
- Abertay University
- Aberystwyth University
- ABES - French Bibliographic Agency for Higher Education
- Abingdon and Witney College
- Absalon University College

Below the list is a 'Select a provider' button with a dropdown arrow, and a 'Remember me' checkbox. At the bottom is a 'Log On' button.

The screenshot shows a 'Consent to Attribute Release' page. At the top right is a 'CILogon' logo. Below it is a search bar with 'Type to search' placeholder text and a dropdown menu with 'Google' selected. The main content area displays a list of institutions, identical to the first screenshot.

At the top right of the main content area is a 'Select an Identity Provider' button with a dropdown arrow, and a 'Remember this selection' checkbox. At the bottom is a 'Log On' button.

## Step 2: Sign the User Access Agreement Form

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Home Center Summary Project Requests Jobs Help sapanasoni522@gmail.com

Successfully signed in as sapanasoni522@gmail.com.

Welcome

MyLRC is a new user portal available to all users of LRC clusters, starting on Oct. 4, 2022.

We'd love to hear your feedback. Please fill out this [Google Form](#) letting us know what you think.

If you would like to set up or update your access to a cluster, please complete the following steps.

First review and sign the cluster user agreement. Only then can you join a cluster project and gain access to the cluster.

Task	Status	Actions
1. Sign the cluster user access agreement.	<input checked="" type="checkbox"/> Unsigned	<input checked="" type="button"/> Review and Sign
2. Create or join a project. <small>?</small>	<input checked="" type="checkbox"/> 0 Project(s)	<input type="button"/> Create <input type="button"/> Join

Your LRC cluster account username: **No Cluster Account**

[My LRC Cluster Projects »](#)

ⓘ You are not part of any cluster projects at this time. Please click Join to join any of the existing projects. You can also click Create to request setup of a new project.

View all projects and managers

Software Use

All software used on LBNL computers must be appropriately acquired and used according to the appropriate licensing. Possession or use of illegally copied software is prohibited. Likewise, users shall not copy, store or transfer copyrighted software or data, except as permitted by the owner of the copyright.

Altering Authorized Access

Users are prohibited from changing or circumventing access controls to allow themselves or others to perform actions outside their authorized privileges or to circumvent security systems.

Data Modification or Destruction

Users are prohibited from taking unauthorized actions to intentionally modify, delete, or reconstruct information or programs.

Malicious Software

Users must not intentionally introduce or use malicious software such as computer viruses, Trojan horses, or worms. Users are responsible for taking reasonable steps to ensure the integrity and security of software they introduce to the system.

Denial of Service Actions

Users may not deliberately interfere with other users accessing system resources.

Notification

Users must notify LBNL immediately when they become aware that any of the accounts used to access LBNL have been compromised. LBNL reserves the right to temporarily disable accounts without prior notification in the event of a security compromise.

Account Usage

Each user of this system must have a unique login. Users are not allowed to share their accounts with others. IMPORTANT: The number one threat to this cluster is from a compromised endpoint (like your desktop computer) which allows your username/password to be stolen or your session to be hijacked. You are responsible for taking reasonable steps to ensure the security of any system you use to access LBNL systems.

Submit  Acknowledge & Sign\*

I have read the LBNL Policies and Procedures and understand my responsibilities in the use of LRC computing resources managed by the LBNL IT Division.

Submit

## Step 3: Request to join existing project

### Welcome

MyLRC is a new user portal available to all users of LRC clusters, starting on Oct. 4, 2022.

We'd love to hear your feedback. Please fill out this [Google Form](#) letting us know what you think.

If you would like to set up or update your access to a cluster, please complete the following steps.

First review and sign the cluster user agreement. Only then you can join a cluster project and gain access to the cluster.

Task	Status	Actions
1. Sign the cluster user access agreement.	<span style="color: green;">✓ Signed Dec. 12, 2022, 11:59 a.m.</span>	<a href="#">Review</a>
2. Create or join a project. <a href="#">?</a>	<span style="color: red;">✗ 0 Project(s)</span>	<a href="#">Create</a> <a href="#">Join</a>

Your LRC cluster account username: No Cluster Account

### My LRC Cluster Projects »

! You are not part of any cluster projects at this time. Please click Join to join any of the existing projects. You can also click Create to request setup of a new project.

[View all projects and managers](#)

### Join a Project

#### Requests Pending Manager Approval

Below is a list of join requests that await approval by project managers. **Please contact a project manager or PI if your request has not been reviewed in a reasonable time frame.**

Once a request is approved, a separate request for cluster access under the project will automatically be created, to be processed by cluster administrators. The statuses of those requests may be viewed on the [home page](#) or on the project's detail page.

! No requests await approval by project managers.

#### Make a New Request

If you are joining your first project and are not an LBL employee with a verified LBL email (@lbl.gov), you must select an eligible PI to become your host user when requesting to join a project.

▼ Search +

Projects: 248

ID	Name	PIs	Title	Cluster	Status	Join
1	dirac1	pi1	dirac1	DIRAC1	Active	<span style="color: blue;">+ Join</span>
2	nano	pi2	nano	NANO	Active	<span style="color: blue;">+ Join</span>
5	catamount	pi3	catamount	CATAMOUNT	Active	<span style="color: blue;">+ Join</span>

## **Step 4:** Approval from Principal Investigator

PI will receive an email in the following format with link to the page.

Dear managers of ac\_scsguest,

User Sapana Soni (ssoni@lbl.gov) has requested to join your project, ac\_scsguest via the MyLRC User Portal.

Please approve/deny this request here.

Thank you,  
MyLRC User Portal team  
<https://mylrc.lbl.gov>  
Email:hpcshelp@lbl.gov

## **Step 5:** Account creation

HPCS team creates a user account on Lawrencium Super cluster. Users can check status of their account on MyLRC portal.

## **Step 6: Confirmation and Additional Information**

Dear Sapana Soni,

As requested, your user account on the LRC supercluster now has access to the project ac\_scsguest.

Your LRC supercluster username is - spsoni

Instructions on how to access the LRC supercluster, hardware details, filesystems, job scheduler etc... are all available at this user guide:  
<https://it.lbl.gov/service/scienceit/high-performance-computing/lrc/>

If this is the first time you are accessing the LRC supercluster, start with the below Logging In page: <https://it.lbl.gov/resource/hpc/for-users/getting-started/>

Please review online documentation. For any additional help or support questions contact us at [hpcshelp@lbl.gov](mailto:hpcshelp@lbl.gov)

Thank you,

MyLRC User Portal team  
<https://mylrc.lbl.gov>  
Email : [hpcshelp@lbl.gov](mailto:hpcshelp@lbl.gov)

# Getting access to project:

Once you get a user account on MyLRC portal and on lawrencium cluster, you can request to join other projects. Current workflow involves steps 3-6 from [Getting a user account on LRC](#).

Welcome

MyLRC is a new user portal available to all users of LRC clusters, starting on Oct. 4, 2022. X

We'd love to hear your feedback. Please fill out this [Google Form](#) letting us know what you think.

If you would like to set up or update your access to a cluster, please complete the following steps.

First review and sign the cluster user agreement. Only then you can join a cluster project and gain access to the cluster.

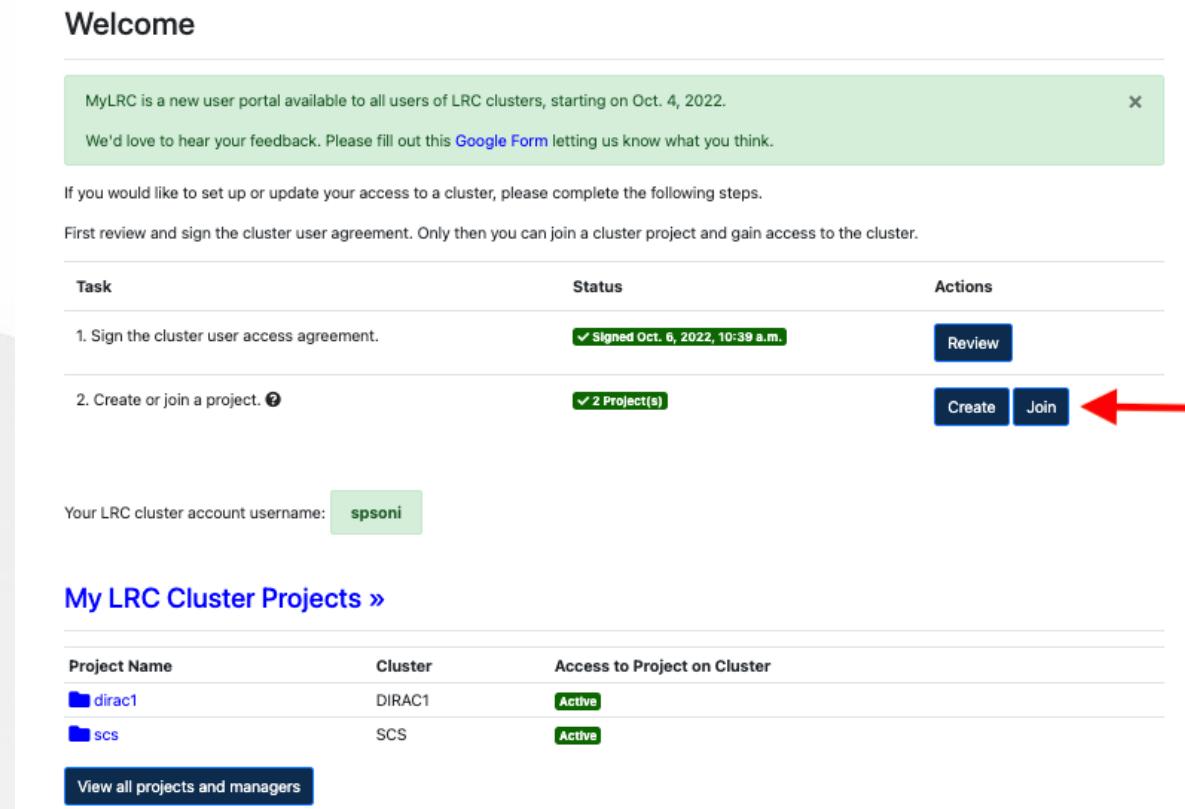
Task	Status	Actions
1. Sign the cluster user access agreement.	<span style="color: green;">✓ Signed Oct. 6, 2022, 10:39 a.m.</span>	<span style="background-color: #0070C0; color: white; padding: 2px 10px;">Review</span>
2. Create or join a project. <span style="color: red;">?</span>	<span style="color: green;">✓ 2 Project(s)</span>	<span style="background-color: #0070C0; color: white; padding: 2px 10px;">Create</span> <span style="background-color: #0070C0; color: white; padding: 2px 10px;">Join</span> <span style="color: red; font-size: 2em; margin-left: 10px;">←</span>

Your LRC cluster account username: spsoni

[My LRC Cluster Projects »](#)

Project Name	Cluster	Access to Project on Cluster
dirac1	DIRAC1	<span style="color: green;">Active</span>
scs	SCS	<span style="color: green;">Active</span>

View all projects and managers



# User account Features: Center Summary and Project

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Home Center Summary Project Requests Jobs Help

sponi@berkeley.edu

## LRC HPC Resources Scientific Impact

**Active Allocations and Users by Division or Department**

Division or Department	Active Allocation Count	User Count
Other	248	2384

Showing 1 to 1 of 1 entries  
Total Active Users: 1306  
Total Principal Investigators: 192

**Resources and Allocations Summary**

Allocations: 98.4%  
Active by Type: 100.0%

Resource Name (Type)	Active Allocation Count
LAWRENCIUM Compute (Cluster)	236
ALICE Compute (Cluster)	1
ALSACC Compute (Cluster)	1
CATAMOUNT Compute (Cluster)	1
DIRAC1 Compute (Cluster)	1
JBEI Compute (Cluster)	1
JGI Compute (Cluster)	1
JGICLOUD Compute (Cluster)	1
MHG Compute (Cluster)	1
NANO Compute (Cluster)	1

Showing 1 to 10 of 13 entries

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You have requested to join Project ac\_scsguest. The managers have been notified.

## Join a Project

Requests Pending Manager Approval

Below is a list of join requests that await approval by project managers. Please contact a project manager or PI if your request has not been reviewed in a reasonable time frame.

Once a request is approved, a separate request for cluster access under the project will automatically be created, to be processed by cluster administrators. The statuses of those requests may be viewed on the [home page](#) or on the project's detail page.

ID	Name	PIs	Title	Cluster
7	ac_scsguest	gmjung	ac_scsguest	LAWRENCIUM

**Make a New Request**

Search

Projects: 248

ID	Name	PIs	Title	Cluster	Status	Join
1	dirac1	kewu	dirac1	DIRAC1	Active	<a href="#">Join</a>

# User account Features: Requests and Jobs

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spsoni@berkeley.edu

The screenshot shows the 'Request Hub' section of the MyLRC interface. At the top, there are buttons for 'Collapse All -' and 'Expand All +'. Below them is a section titled 'Cluster Access Requests' with a blue link. The main focus is the 'Project Join Requests' section, which displays a table of pending requests. The table has columns for #, Username, User Email, Project, Date Requested, and Reason. One row is shown: # 1, spsoni@berkeley.edu, spsoni@berkeley.edu, ac\_scsguest, Feb. 05, 2023, Need to use LRC cluster. Below the table, it says 'Page 1 of 1' with 'Previous' and 'Next' buttons. A message 'No completed project join requests!' is displayed in a light blue box. Other sections like 'Project Removal Requests' and 'Project Renewal Requests' are also visible.

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spsoni@berkeley.edu

The screenshot shows the 'Job List' section of the MyLRC interface. At the top, there is a 'Filter' button. Below it is a form with fields for Status (dropdown), Slurm ID (text input), Project Name (dropdown), Partition (text input), Service Units (dropdown), Number of Service Units (dropdown), Submitted (dropdown), Started (dropdown), and Ended (dropdown). Below the form, a message 'No search results!' is displayed. The overall layout is clean with a white background and dark blue header.

# User account Features: Jobs

Home Center Summary Project Requests Jobs Admin Help spsoni

## Job List

Viewing only jobs belonging to you and belonging to projects in which you are a PI or manager. To view all jobs select "Show All Jobs" in the search form below and search, or click [here](#).

**Filter**

Status	Completed
Slurm ID	<input type="text"/>
Project Name	<input type="text"/>
Username	<input type="text"/>
Partition	<input type="text"/>
Service Units <span style="color: blue;">(1)</span>	<input type="text"/> Number of Service Units <input type="button" value=""/>
Submitted	<input type="text"/> MM/DD/YYYY
Started	<input type="text"/> MM/DD/YYYY
Ended	<input type="text"/> MM/DD/YYYY
<input type="checkbox"/> Show All Jobs	
<input type="button" value="Search"/> <input type="button" value="Reset"/>	
<a href="#"> Export Job List to CSV</a>	

Slurm ID <span style="color: blue;">(1)</span>	Username	Project	Job Status <span style="color: blue;">(1)</span>	Partition	Submit Date <span style="color: blue;">(1)</span>	Service Units <span style="color: blue;">(1)</span>
55640614	spsoni	scs	COMPLETED	es1	Feb. 02, 2023	8.02
55576553	spsoni	scs	COMPLETED	lr6	Jan. 31, 2023	0.01
55576498	spsoni	scs	COMPLETED	lr5	Jan. 31, 2023	1.64
55575037	spsoni	scs	COMPLETED	lr6	Jan. 31, 2023	0.43
55574967	spsoni	scs	COMPLETED	lr6	Jan. 31, 2023	0.71
55574932	spsoni	scs	COMPLETED	lr6	Jan. 31, 2023	0.16
55574901	spsoni	scs	COMPLETED	es1	Jan. 31, 2023	0.09
55574841	spsoni	scs	COMPLETED	es1	Jan. 31, 2023	0.03
55574834	spsoni	scs	COMPLETED	es1	Jan. 31, 2023	0.06
55574788	spsoni	scs	COMPLETED	lr6	Jan. 31, 2023	0.07
55574685	spsoni	scs	COMPLETED	lr5	Jan. 31, 2023	2.81
54500778	spsoni	scs	COMPLETED	lr6	Dec. 08, 2022	15.69
54500770	spsoni	scs	COMPLETED	lr6	Dec. 08, 2022	1.42
54500767	spsoni	scs	COMPLETED	lr6	Dec. 08, 2022	1.51
54500385	spsoni	scs	COMPLETED	lr6	Dec. 08, 2022	1.19
54489594	spsoni	scs	COMPLETED	lr6	Dec. 07, 2022	6.24
54488522	spsoni	scs	COMPLETED	lr6	Dec. 07, 2022	98.96
54488513	spsoni	scs	COMPLETED	lr6	Dec. 07, 2022	0.06
54477557	spsoni	scs	COMPLETED	o0d_inter	Dec. 06, 2022	0.00
54419270	spsoni	scs	COMPLETED	lr6	Dec. 02, 2022	0.11
54419227	spsoni	scs	COMPLETED	lr6	Dec. 02, 2022	0.06
54419214	spsoni	scs	COMPLETED	lr6	Dec. 02, 2022	0.22
54145360	spsoni	scs	COMPLETED	lr6	Nov. 17, 2022	0.04
54145353	spsoni	scs	COMPLETED	lr6	Nov. 17, 2022	0.07
54145352	spsoni	scs	COMPLETED	lr6	Nov. 17, 2022	0.07
54145277	spsoni	scs	COMPLETED	lr6	Nov. 17, 2022	0.04
54145275	spsoni	scs	COMPLETED	lr6	Nov. 17, 2022	0.02
54145166	spsoni	scs	COMPLETED	lr6	Nov. 17, 2022	0.11
54145161	spsoni	scs	COMPLETED	lr6	Nov. 17, 2022	0.11
54145156	spsoni	scs	COMPLETED	lr6	Nov. 17, 2022	0.09

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## Job Detail: 55640614

### Job Information

Slurm ID:	55640614
Username:	spsoni
Project:	scs
Job Status:	COMPLETED
Submit Date:	Feb. 2, 2023, 1:53 p.m.
Start Date:	Feb. 2, 2023, 1:53 p.m.
End Date:	Feb. 2, 2023, 3:54 p.m.
Partition:	es1
Nodes:	n0047.es1
Service Units <span style="color: blue;">(1)</span> :	8.02
Quality of Service:	es_normal
Number of CPUs:	4
Number of Required Nodes:	1
Number of Allocated Nodes:	1
Raw Time (seconds):	2.0055556
CPU Time (seconds):	8.022225

Science IT

# Requesting project account and management

LBNL affiliated PIs can request to create a project account on MyLRC portal. Manager role can be assigned to a project user for managing project account and project renewal (PCA account).

Welcome

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Task	Status	Actions
1. Sign the cluster user access agreement.	Signed Oct. 6, 2022, 10:39 a.m.	<a href="#">Review</a>
2. Create or join a project. <a href="#">?</a>	✓ 2 Project(s)	<a href="#">Create</a> <a href="#">Join</a>

Your LRC cluster account username: **spsoni**

[My LRC Cluster Projects »](#)

Project Name	Cluster	Access to Project on Cluster
dirac1	DIRAC1	Active
scs	SCS	Active

[View all projects and managers](#)

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## Create a Project

Request to create a new project (Slurm account) on one of the clusters below. You may also request to [join](#) an existing project.

Lawrencium

## Project Accounts

- Three types of project accounts can be requested.
  1. **Primary Investigator (PI) Computing Allowance (PCA) account:** free 300K service units (SUs) per year (pc\_xxx)
  2. **Condo account:** PIs buy in compute nodes to be added to the general pool, in exchange for their own priority access and share the Lawrencium infrastructure (lr\_xxx)
  3. **Recharge account:** pay as you go with minimal recharge rate ~ \$0.01/SU (ac\_xxx)
- Check out more details here. [Project Accounts](#)
- PIs can grant PCA/condo/recharge project access to researchers/students and external collaborators.

# Chose a type of project account...

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## New Lawrencium Project

Eligible users may request to create a new project on the Lawrencium cluster, or pool their allowances with those of existing projects. The following allowances are available:

- PI Computing Allowance (PCA) **POOL**
- Condo Allocation
- Recharge Allocation (Pay for Used Time)

This form is intended for Principal Investigators (PIs) or users acting on behalf of PIs. The user who fills it out will become a manager on the project: the user will receive access to the project on the cluster, will have permissions to manage the project and its users, and cannot opt out of email notifications (unless at least one other user becomes a manager). If this does not sound like your role on the project, please ask the appropriate user to fill it out.

If you are filling out the form on behalf of another PI, that PI will be notified by email that a request is being made by you.

**MOU** The PI will be contacted to provide a signed Memorandum of Understanding as part of the approval process.  
**POOL** The allowance is eligible for pooling of service units.

Continue Back

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## Lawrencium: Computing Allowance

Select a computing allowance.

Computing Allowance\*

PI Computing Allowance (Computing Allowance)

PI Computing Allowance (Computing Allowance)  
Condo Allocation (Computing Allowance)  
Recharge Allocation (Computing Allowance)

Step 1 of 6

Example: For PCA account there will be allocation period...

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### Lawrencium: Computing Allowance

Select a computing allowance.

Computing Allowance\*

PI Computing Allowance (Computing Allowance)

Next Step

Step 1 of 6

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### Lawrencium: Allocation Period

Allowance: PI Computing Allowance

Select the time period during which the project's allocation will be valid. The listed number of service units will be usable between the start date and end date for the selected period.

A request for a time period that has not begun yet may be approved before its start date, but will not be fully processed (i.e., service units will not be usable) until then. Any service units not used by its end date will be forfeited.

Allocation Period\*

Allowance Year 2022 - 2023 (2022-10-01 - 2023-09-30) (200000.00 SUs)

First Step Previous Step Next Step

Step 2 of 8

Chose PI from the dropdown list and enter project details..

MyLRC - Laboratory Research Computing  
Access Management System

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Home Center Summary Project Requests Jobs Admin Help

spsoni

## Lawrencium: Principal Investigator

Allowance: PI Computing Allowance » Allocation Period: Allowance Year 2022 - 2023

Select an existing user to be a Principal Investigator of the project. You may search for the user in the selection field. If the desired user is not listed, you may skip this step and specify information for a new PI in the next step.

Note: Only LBL employees, users with an "@lbl.gov" email, can be selected as a PI.

Note: Each PI may only have one PI Computing Allowance at a time, so any that have pending requests or active allocations are not selectable.

Principal Investigator

- Aaron Fafarman (atf37@drexel.edu)
- Aaron Szasz (aszasz@berkeley.edu)
- Aaron Szasz (aszasz@lbl.gov)
- Aashish Sharma (asharma@lbl.gov)
- Aatif Jiwani (aatifjiwani@lbl.gov)
- Abdullah Cihan (acihan@lbl.gov)
- Abdullah Maruf (amaruf@lbl.gov)
- Abdulrahman Aldeessary (abdulrahman@berkeley.edu)

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spsoni

## Lawrencium: New Project Details

Allowance: PI Computing Allowance » Allocation Period: Allowance Year 2022 - 2023 » Existing PI: Gary Jung (gmjung@lbl.gov) » Not Pooling

You are creating a new project. Please provide the following details:

Name\*

Title\*

Description\*

First Step Previous Step Next Step

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Home Center Summary Project Requests Jobs Admin Help

spsoni

## Lawrencium: New Project Details

Allowance: PI Computing Allowance >> Allocation Period: Allowance Year 2022 - 2023 >> Existing PI: Gary Jung (gmjung@lbl.gov) >> Not Pooling

You are creating a new project. Please provide the following details:

Name\*

A unique name for the project, which must contain only lowercase letters and numbers. This will be used to set up the project's SLURM scheduler account.

Title\*

A unique, human-readable title for the project.

Description\*

A few sentences describing your project.

First Step Previous Step Next Step

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Home Center Summary Project Requests Jobs Admin Help

spsoni

## Lawrencium: Billing ID

Allowance: PI Computing Allowance >> Allocation Period: Allowance Year 2022 - 2023 >> Existing PI: Gary Jung (gmjung@lbl.gov) >> Not Pooling

Please provide an LBL Project ID, which may be used for billing:

Project ID\*

Example: 123456-789

First Step Previous Step Next Step

Step 6 of 7

Project creation request will be placed when survey is filled and submitted. Current status of the project will be available in Requests section.

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Access Management System

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Home Center Summary Project Requests Jobs Admin Help

spsoni

## Lawrencium: Survey

Allowance: PI Computing Allowance » Allocation Period: Allowance Year 2022 - 2023 » Existing PI: Gary Jung (gmjung@lbl.gov) » Not Pooling  
» Requested Project:

Please respond to the following questions to provide us with more information about your project and computational needs.

Scope and intent of research needing computation\*

Computational aspects of the research\*

Existing computing resources (outside of Lawrencium) currently being used by this project. If you use cloud computing resources, we would be interested in hearing about it.

Which of the following best describes your need for this system:

- Meets intermittent or small need for compute cycles
- Provides a resource since my group/area cannot purchase its own
- Provides additional compute cycles beyond what is provided on my own cluster
- Provides ability to run larger-scale jobs than those I can't run on my own cluster
- Provides an onramp to prepare for running on large systems or applying for grants and supercomputing center allocations
- Provides additional compute cycles

How many processor cores does your application use? (min, max, typical runs)

How many processor cores does your application use? (min, max, typical runs)

How much memory per core does your typical job require?

What is the run time of your typical job?

Estimate how many processor-core-hrs your research will need over the year.

LRC has a number of large memory nodes, each with hundreds of GB. Do you have a need to use these nodes? If so, what is your expected use of these nodes?

Describe your applications I/O requirements

Lawrencium provides a shared Lustre parallel filesystem for jobs needing access to high performance storage.

Interconnect performance

Select one...

Does your application require low latency communication between nodes?

Network connection from Lawrencium to the Internet

Do you need to transfer large amounts of data to and/or from the cluster? If yes, what is the max you might transfer in a day? What would be typical for a month? Do you have need for file sharing of large datasets?

What is the source of the software you use (or would use)?

Specify your software applications. If you have need for commercial software, please indicate that here.

Does your application require access to an outside web server or database? If yes, please explain.

First Step Previous Step Submit

Step 7 of 7

PI receives an email upon processing the project creation request.

Example email:

Dear LRC HPC Resources user,

Your request to create project pc\_test has been processed, and the project has been set up on the cluster.

You may manage your project at [https://mylrc.lbl.gov/project/<project\\_number>/](https://mylrc.lbl.gov/project/<project_number>)

If you have any questions, contact us at [hpcshelp@lbl.gov](mailto:hpcshelp@lbl.gov).

Thank you,

MyLRC User Portal team

<https://mylrc.lbl.gov>

Email : [hpcshelp@lbl.gov](mailto:hpcshelp@lbl.gov)

For other type of project creation chose the project type and follow the steps.

# Project Management : Applicable to project PIs and managers only

Navigate to project page by choosing a project listed under MyLRC Cluster Projects.

## Welcome

MyLRC is a new user portal available to all users of LRC clusters, starting on Oct. 4, 2022. X

We'd love to hear your feedback. Please fill out this [Google Form](#) letting us know what you think.

If you would like to set up or update your access to a cluster, please complete the following steps.

First review and sign the cluster user agreement. Only then you can join a cluster project and gain access to the cluster.

Task	Status	Actions
1. Sign the cluster user access agreement.	<span style="color: green;">✓ Signed Oct. 6, 2022, 10:39 a.m.</span>	<a href="#">Review</a>
2. Create or join a project. <span style="color: blue;">?</span>	<span style="color: green;">✓ 2 Project(s)</span>	<a href="#">Create</a> <a href="#">Join</a>

Your LRC cluster account username: spsoni

[My LRC Cluster Projects »](#)

Project Name	Cluster	Access to Project on Cluster
dirac1	DIRAC1	Active
scs	SCS	Active

[View all projects and managers](#)

## scs

[Manage Project](#) [Update Project Information](#) [Archive Project](#)

[Add Users](#) [Review Join Requests 0](#)

[Project Information](#)

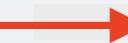
**Principal Investigators:**  
Gary Jung (gmjung)

**Title:** scs  
**Description:** This is a HPCS group, we manage Lawrencium cluster and departmental clusters. We also provide services such as software installation, HPC consultation and training.

**Cluster:** SCS  
**Project Status:** Active  
**Created:** Oct. 03, 2022  
**Requests to Join:** User requests to join the project must be approved by a PI.

**Project Information:** Project information can be modified using Update Project Information button.  
**Note:** PID change is not possible on the portal. PI/manager will have to open a ticket by sending an email to [hpcshelp@lbl.gov](mailto:hpcshelp@lbl.gov) with project name and new PID.

SCS

Manage Project 

Add Users Review Join Requests 0

### Project Information

Principal Investigators:  
Gary Jung (gmjung)

Title: SCS  
Description: This is a HPCS group, we manage Lawrencium cluster and departmental clusters. We also provide services such as software installation, HPC consultation and training.

Cluster: SCS  
Project Status: Active  
Created: Oct. 03, 2022  
Requests to Join: User requests to join the project must be approved by a PI.

Title\*  
scs

Description\*  
This is a HPCS group, we manage Lawrencium cluster and departmental clusters. We also provide services such as software installation, HPC consultation and training.

Save Cancel

# Approving Project Join Request from users

SCS

Manage Project      [Update Project Information](#)      [Archive Project](#)

[Add Users](#)    [Review Join Requests 1](#) 

### Project Information

Principal Investigators:  
Gary Jung (gmjung)

Title: scs

Description: This is a HPCS group, we manage Lawrencium cluster and departmental clusters. We also provide services such as software installation, HPC consultation and training.

Cluster: SCS

Project Status: Active

Created: Oct. 03, 2022

Requests to Join: User requests to join the project must be approved by a PI. 

### Allocations 1

Show 10 entries      Search:

Resource Name	Information	Status	Start Date	End Date	More Details
SCS Compute	Service Units: 109166.37/100000000.00 (0.11 %)	Active	2000-01-01		

Showing 1 to 1 of 1 entries      Previous 1 Next

## Review requests to join project: scs

<input type="checkbox"/>	#	Username	First Name	Last Name	Email	Role	Need Host	Reason
<input type="checkbox"/>	1	spsoni@berkeley.edu	Sapana	Soni	spsoni@berkeley.edu	User	No	test join request for spsoni

[Approve Selected Users](#)    [Deny Selected Users](#)    [Back to Project](#)

**PCA Project Renewal:** PCA projects are renewed every Fiscal Year (1st October and- 30th September) and 300K SU are allocated in the beginning of the year. However, renewal can be requested through out the year. Prorated SU will be allocated to project. Condo(lr\_) and recharge accounts(ac\_) won't have this option since these project do not need renewal.

pc\_test

### Manage Project

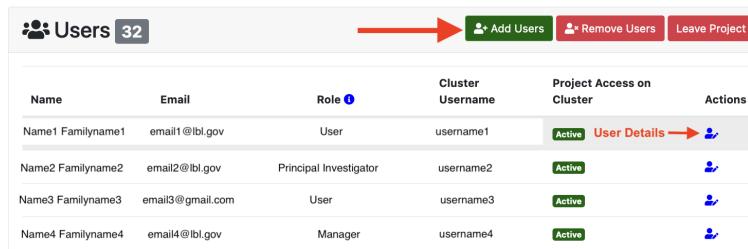
+ Add Users    + Review Join Requests 0    + Renew Allowance



### Project Information

Principal Investigators:

Existing Project users and their details.  
Managers or PIs can add user to project account.



Name	Email	Role	Cluster Username	Project Access on Cluster	Actions
Name1 Familyname1	email1@lbl.gov	User	username1	Active <a href="#">User Details</a> 	 
Name2 Familyname2	email2@lbl.gov	Principal Investigator	username2	Active	 
Name3 Familyname3	email3@gmail.com	User	username3	Active	 
Name4 Familyname4	email4@lbl.gov	Manager	username4	Active	 

### Add users to project: scs

Search String\*

Copy paste usernames separated by space or newline for multiple username search!

Search by\*

Exact Username Only  
 All Fields This option will be ignored if multiple usernames are entered in the search user text area.

 Search

### Project User Detail

Project: scs

**User Detail**

First Name:	Sapana
Last Name:	Soni
Email:	ssoni@lbl.gov
Role:	User
Enable Notifications:	<input type="checkbox"/>

**Cluster Access**

Cluster Username:	spsoni
Project Access on Cluster:	Active

# User Deletion

## 1. Remove users from project

User can request to leave the project or PI/manager can request removing users from the project on MyLRC portal. After removal from project user won't be able to submit jobs using that project account.

## 2. Remove from a project & delete user account

Project PI will be responsible to inform HPCS team about user's account deletion through ticketing system. User's account will be completely deleted from Lawrencium super cluster. A home and scratch directory will be removed. Account management charges of \$25 will be canceled from billing cycle. PI or user will be responsible for data backup.

**User's request to Leave Project**

Showing 1 to 1 of 1 entries

Name	Email	Role	Cluster Username	Project Access on Cluster
Aaron Culich	aculich@berkeley.edu	User	aculich	Action

**Leave Project**

**PI/manager request to remove a user from project.**

Remove users from project: scs

Below is a list of users with pending removal requests from project scs that must be reviewed and processed by admins.

No pending project removal requests!

Below is a list of users eligible to be removed from project scs. To initiate a removal request, click the "Remove" button next to the user to remove and click "Submit" in the confirmation window. Once a removal request is initiated, it must be reviewed and processed by admins.

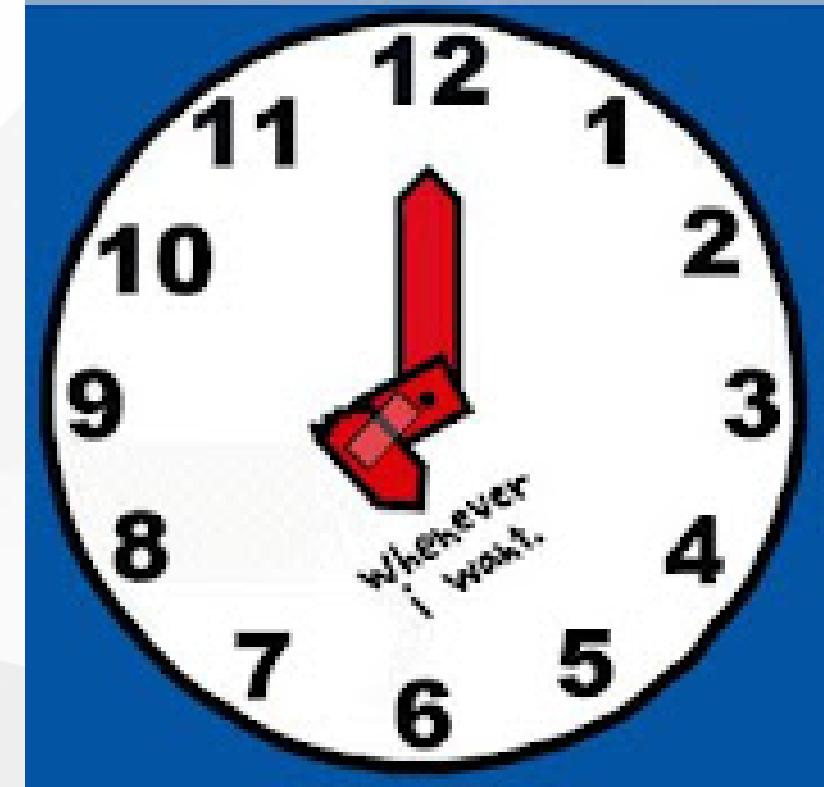
Select Users to Remove:

#	Username	First Name	Last Name	Email	Role	Status	Remove
	Username1	Name1	Family Name1	email1@lbl.gov	User	Active	<b>+ Remove</b>

# **Break Time!**

5 Minutes

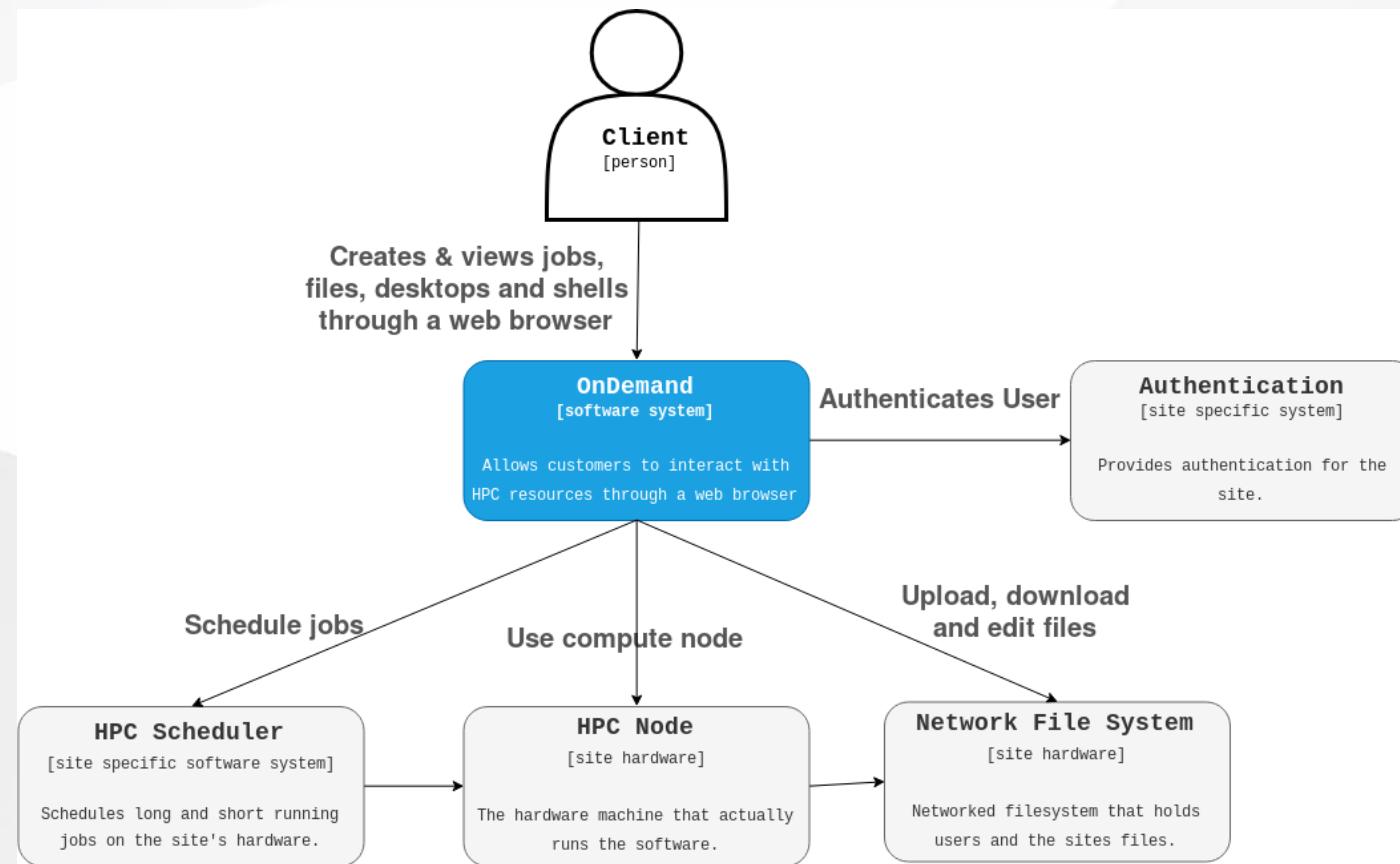
**WILL RETURN**



# Open OnDemand: Introduction

- What is Open OnDemand?
  - OpenOnDemand is a web platform that provides an easy access to the cluster's HPC resources and services.
  - Designed and developed by Ohio Supercomputer Center.
- Why OOD?
  - **New users:** intuitive and easy access to computing resources, removes barrier in using HPC resources for their research.
  - **Advanced users:** alternative and convenient way to traditional command line access

- How OOD works at system level?

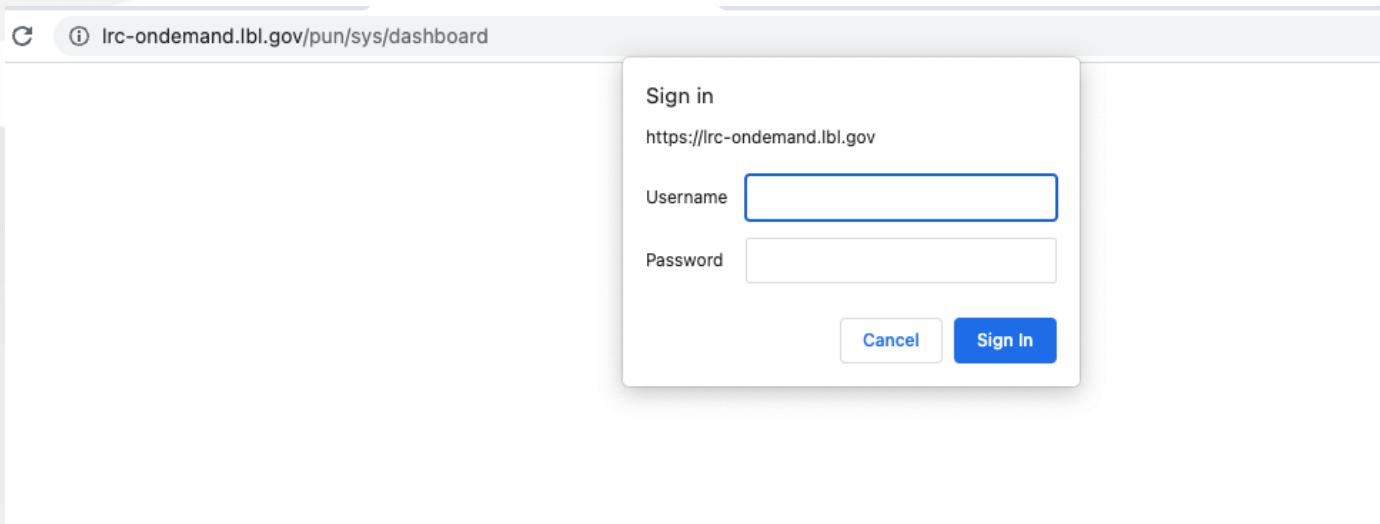


Users are able to use HPC services more efficiently through Open OnDemand.

# Accessing OOD on Lawrencium

1. Web link to connect : <https://lrc-on-demand.lbl.gov/>

**Note:** Use Chrome or Firefox to browse this page. Safari has known [authentication issues](#).



2. Use your LRC username and PIN+one-time password (OTP)
- same credentials you use to login Lawrencium cluster

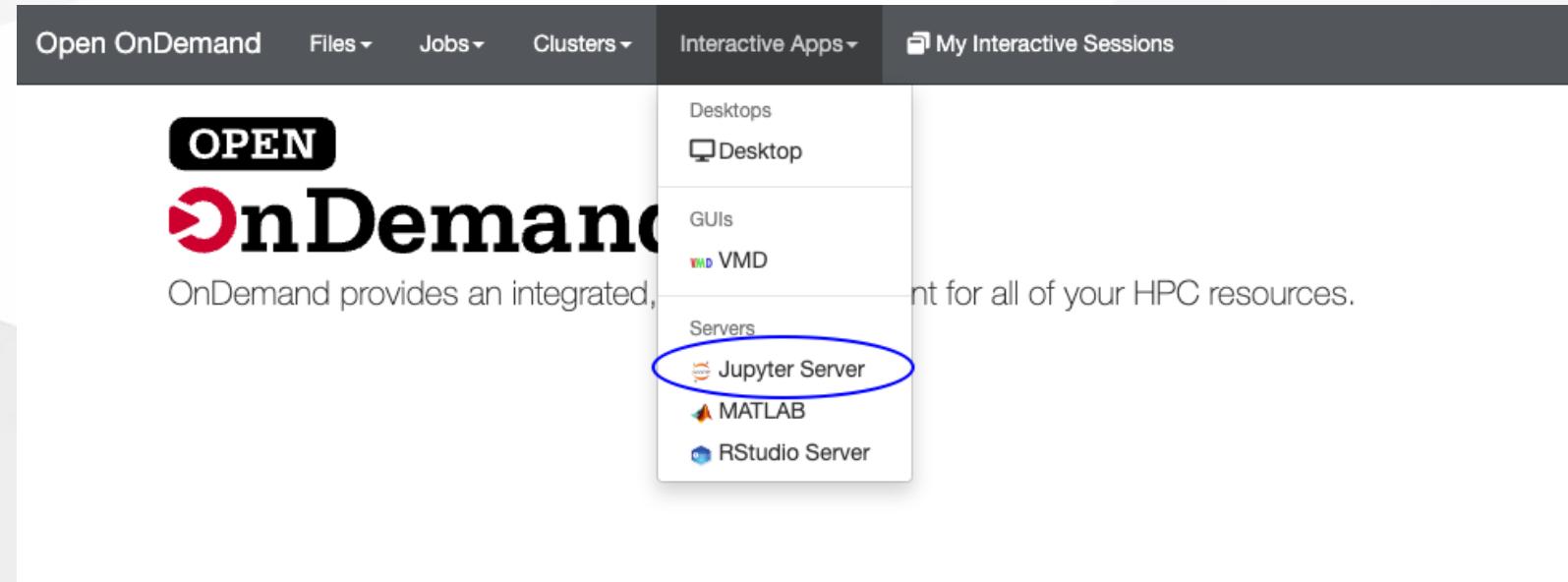
# OOD Dashboard on Lawrencium

On successful authentication you will see a OOD dashboard.

The screenshot shows the OnDemand (OOD) interface on the Lawrencium system. The top navigation bar includes links for Open OnDemand, Files, Jobs, Clusters, Interactive Apps, My Interactive Sessions, Help, and Log Out. The main content area features a large 'OPEN' button with a red arrow icon, followed by the 'OnDemand' logo. A descriptive text below the logo reads: "OnDemand provides an integrated, single access point for all of your HPC resources."

# Interactive Apps: Jupyter server

Click on **Interactive apps --> Jupyter Server** to open Jupyter notebook



# Interactive mode

Home / My Interactive Sessions / Jupyter Server

**Interactive Apps**

- Desktops
- Desktop
- GUIs
- VMD
- Servers
- Jupyter Server**
- MATLAB
- RStudio Server

**Jupyter Server** version: d96c37b

This app will launch a [Jupyter](#) server using [Python](#) on the [LBNL](#) Science-IT Laboratory Research Computing([LRC](#)) Infrastructure clusters.

**Type of use**

interactive\_mode, for exploration

Choose the mode of running your Jupyter Server

**Wall Clock Time**

1

How many hours do you want to run this Jupyter Server for ?

**Number of CPU cores per Node**

1

Please specify the number of CPU cores you want per node for this Jupyter Server

**Email address (optional)**

Enter your email address if you would like to receive an email when the session starts. Leave blank for no email.

**Launch**

\* The Jupyter Server session data for this session can be accessed under the [data root](#) directory.

# Compute mode

Interactive Apps

- Desktops
- Desktop
- GUIs
- VMs
- Servers
  - Jupyter Server
  - MATLAB
  - RStudio Server

**Jupyter Server** version: d96c37b

This app will launch a [Jupyter](#) server using [Python](#) on the [LBNL Science-IT](#) Laboratory Research Computing([LRC](#)) Infrastructure clusters.

Type of use

compute\_mode

Choose the mode of running your Jupyter Server

Wall Clock Time

1

How many hours do you want to run this Jupyter Server for ?

Name of the job

test

SLURM Partition

cf1

Choose the name of the SLURM Partition in which you want to launch this Jupyter Server

SLURM Project/Account Name

scs

For non Lawrencium partitions you can leave this blank.

SLURM QoS Name

cf\_debug

Most users can leave it black for default assignment, Lawrencium Condo users want to specify their condo QoS name

Number of Nodes

1

Please specify the number of nodes you want for this Jupyter Server

Email address (optional)

Enter your email address if you would like to receive an email when the session starts. Leave blank for no email.

Launch

\* The Jupyter Server session data for this session can be accessed under the [data root directory](#).

```
(base) [spsoni@n0003 ~]$ sacctmgr show association -p user=spsoni
Cluster|Account|User|Partition|Share|Priority|GrpJobs|GrpTRES|GrpSubmit|GrpWall|Grp
xTRES|MaxTRESPerNode|MaxSubmit|MaxWall|MaxTRESMins|QOS|Def QOS|GrpTRESRunMins|
perceus-00|dirac1|spsoni|ood_inter|1|||||||lr_interactive|||
perceus-00|dirac1|spsoni|dirac1|1|||||||normal|||
perceus-00|scs|spsoni|etna_shared|1|||||||normal|||
perceus-00|scs|spsoni|etna|1|||||||normal|||
perceus-00|scs|spsoni|etna_gpu|1|||||||normal|||
perceus-00|scs|spsoni|ood_inter|1|||||||lr_interactive|||
perceus-00|scs|spsoni|es1|1|||||||es_debug,es_lowprio,es_normal|||
perceus-00|scs|spsoni|cf1|1|||||||cf_debug,cf_lowprio,cf_normal|||
perceus-00|scs|spsoni|cm1|1|||||||cm1_debug,cm1_normal|||
perceus-00|scs|spsoni|lr_bigmem|1|||||||lr_debug,lr_normal|||
perceus-00|scs|spsoni|lr6|1|||||||lr6_lowprio,lr_debug,lr_normal|||
perceus-00|scs|spsoni|lr5|1|||||||lr_debug,lr_lowprio,lr_normal|||
perceus-00|scs|spsoni|lr4|1|||||||lr_debug,lr_lowprio,lr_normal|||
perceus-00|scs|spsoni|lr3|1|||||||lr_debug,lr_lowprio,lr_normal|||
```

Session was successfully created.

Home / My Interactive Sessions

Interactive Apps

- Desktops
- Desktop
- GUIs
- VMD
- Servers
- Jupyter Server
- MATLAB
- RStudio Server

**Jupyter Server (51665742)**

1 node | 64 cores | Starting

Created at: 2022-07-21 13:56:39 PDT

Time Remaining: 59 minutes

Session ID: 032d6e1a-efbc-406b-8ceb-4eab3c54dc95

Your session is currently starting... Please be patient as this process can take a few minutes.

Delete

Session was successfully created.

Home / My Interactive Sessions

Interactive Apps

- Desktops
- Desktop
- GUIs
- VMD
- Servers
- Jupyter Server
- MATLAB
- RStudio Server

**Jupyter Server (51665742)**

1 node | 64 cores | Running

Host: >\_n0014.ct1

Created at: 2022-07-21 13:56:39 PDT

Time Remaining: 58 minutes

Session ID: 032d6e1a-efbc-406b-8ceb-4eab3c54dc95

Connect to Jupyter

Delete



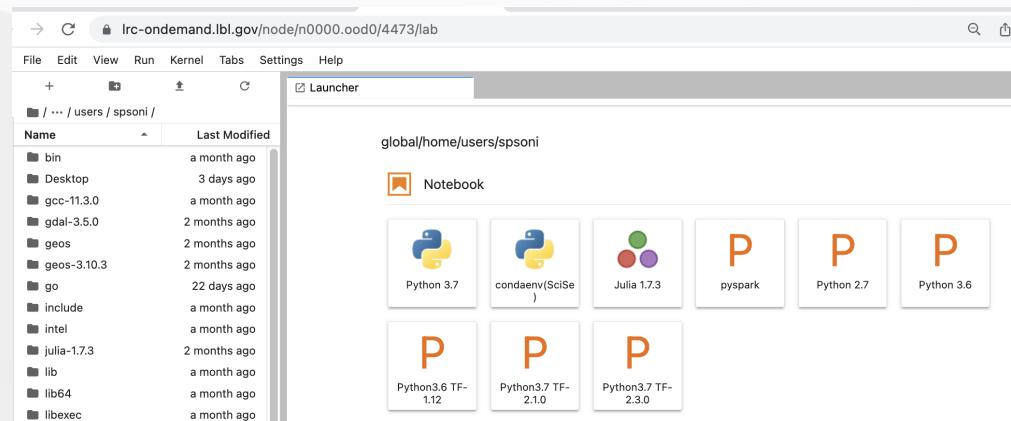
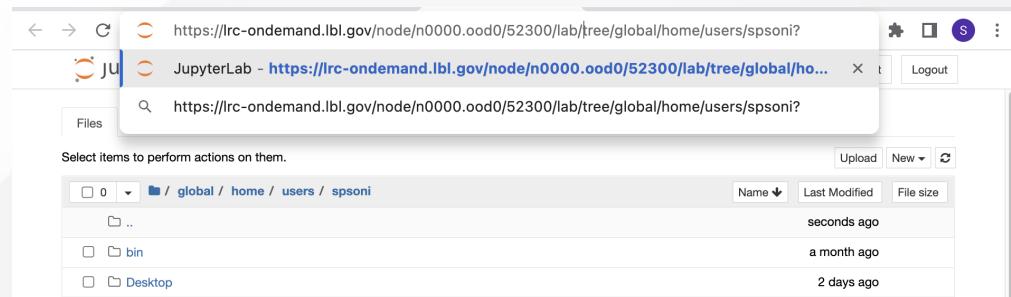
The screenshot shows a Jupyter Notebook cell. The code in the cell is:

```
In [3]: print("Hello World!")
```

The output of the cell is:

Hello World!

To load Jupyter lab simply add  
**lab/** before **tree/** in jupyter  
server url.



# **Customizing Jupyter Kernels : Python and Julia**

If you'd like to use a different language or version of python or different conda environment not indicated in the drop-down menu of jupyter notebook you'll need to create your own kernel.

## **Python:**

There are two ways to add python kernel to jupyter notebook.

1. Using conda environment
2. Manually creating a new kernel

[Click here for details.](#)

## Customizing python kernel using conda environment

```
# Creating a pykernel for 3.9.12 version of python and installing packages
module load python/3.9.12
# Create the environment in your home directory:
conda create --name=py39 python=3.9 ipykernel
source activate py39
python -m ipykernel install --user --name py39 --display-name="py39(Sci)"
conda install -c conda-forge scipy
```

Creating environment in scratch space: \$USER is your own username.

```
conda create -p /global/scratch/users/$USER/py39_scr python=3.9 ipykernel
source activate /global/scratch/users/$USER/py39_scr
python -m ipykernel install --name=py39_scr --prefix=/global/scratch/users/$USER/py39_scr --display-name="py39_scratch"
#create symlink to kernel in custom path
ln -s /global/scratch/users/spsoni/py39test_scr/share/jupyter/kernels/py39_scr /global/home/users/spsoni/.local/share/jupyter/kernels/py39_scr
```

You need to create a symlink in /global/home/users/\$USER/.local/share/jupyter/kernels/ directory so that kernel appears in the jupyter notebook.

## Julia:

Julia kernel can be added in Jupyter for writing a Julia code in Jupyter notebook. To add a Julia kernel to Jupyter we only need to add the IJulia package.

```
module load julia/1.0.3
julia --version
julia
using Pkg
Pkg.add("IJulia")
Pkg.build("IJulia")
```

To remove unwanted jupyter kernel use following commands.

```
module load python/3.9.12
jupyter kernelspec list
jupyter kernelspec uninstall julia-1.0
jupyter kernelspec uninstall py39
```

# Interactive Apps: RStudio

The screenshot shows the OnDemand interface. At the top, there is a navigation bar with links for Open OnDemand, Files, Jobs, Clusters, Interactive Apps (which is currently selected), and a search icon. Below the navigation bar, the main content area features a large "OPEN OnDemand" logo. To the right of the logo, a message reads "OnDemand provides an integrated, singl..." followed by "all of your HPC resources." A vertical sidebar on the right lists several interactive application options: Desktops, GUIs (with VMD listed), Servers (with Jupyter Server and MATLAB listed), and RStudio Server. The "RStudio Server" option is highlighted with a blue oval.

The screenshot shows the "My Interactive Sessions" page. A green banner at the top indicates "Session was successfully deleted." Below this, a table lists the session details for an "RStudio Server" session. The session ID is 51666842, it was created at 2022-07-21 15:59:49 PDT, and it has 1 node, 1 core, and is running. The session host is n0001.cml. The session has 57 minutes remaining. A "Connect to RStudio Server" button is visible. The sidebar on the left lists the same interactive application options as the previous screenshot.

# Compute and interactive mode

Home / My Interactive Sessions / RStudio Server

Interactive Apps
Desktops
<i>Desktop</i>
GUls
<i>VMD</i>
Servers
<i>Jupyter Server</i>
<i>MATLAB</i>
RStudio Server

## RStudio Server version: d96c37b

This app will launch a RStudio Server an IDE for R on the LBNL Science-IT Laboratory Research Computing(LRC) Infrastructure clusters.

### Type of use

interactive\_mode, for exploration

Choose the mode of running your Rstudio Server

### Wall Clock Time

1

How many hours do you want to run this Rstudio Server for ?

### Number of CPU cores per Node

1

Please specify the number of CPU cores you want per node for this Rstudio Server

### Email address (optional)

Enter your email address if you would like to receive an email when the session starts. Leave blank for no email.

Launch

\* The RStudio Server session data for this session can be accessed under the data root directory.

Home / My Interactive Sessions / RStudio Server

Interactive Apps
Desktops
<i>Desktop</i>
GUls
<i>VMD</i>
Servers
<i>Jupyter Server</i>
<i>MATLAB</i>
RStudio Server

## RStudio Server version: d96c37b

This app will launch a RStudio Server an IDE for R on the LBNL Science-IT Laboratory Research Computing(LRC) Infrastructure clusters.

### Type of use

compute\_mode

Choose the mode of running your Rstudio Server

### Wall Clock Time

1

How many hours do you want to run this Rstudio Server for ?

### Name of the job

test

### SLURM Partition

cf1

Choose the name of the SLURM Partition in which you want to launch this Rstudio Server

### SLURM Project/Account Name

scs

For non Lawrencium partitions you can leave this blank.

### SLURM QoS Name

cf\_normal

Most users can leave it black for default assignment, Lawrencium Condo users want to specify their condo QoS name

### Number of Nodes

1

Please specify the number of nodes you want for this Rstudio Server

### Email address (optional)

Enter your email address if you would like to receive an email when the session starts. Leave blank for no email.

Launch

\* The RStudio Server session data for this session can be accessed under the data root

# Interactive Apps: MATLAB

The screenshot shows the Open OnDemand web interface. At the top, there's a navigation bar with links for Desktop, Open OnDemand, Files, Jobs, Clusters, Interactive Apps, and a search icon. The 'Interactive Apps' dropdown is open, showing options like Desktops, GUIs (with VMD), Servers (with Jupyter Server, MATLAB circled in blue, and RStudio Server), and MATLAB. Below the menu, the text "OnDemand provides an integrated, singl..." is visible, followed by "all of your HPC resources."

The screenshot shows a MATLAB session details page. The top header says "Home / My Interactive Sessions". The main section is titled "MATLAB (51666979)" with status "1 node | 1 core | Running". It displays session metadata: Host (>\_n0000.ood0), Created at: 2022-07-21 16:24:34 PDT, Time Remaining: 59 minutes, and Session ID: 58dfcbce-9c5e-432d-b02d-87043985df5c. It also includes compression and image quality sliders, and a "Launch MATLAB" button. A "View Only (Shareable Link)" button is located at the bottom right.

# Interactive Apps: Desktop

The screenshot shows the Open OnDemand web interface. At the top, there is a navigation bar with links for 'Open OnDemand', 'Files', 'Jobs', 'Clusters', 'Interactive Apps', and 'My Interactive Sessions'. Below the navigation bar, the 'Interactive Apps' menu is open, displaying several options: 'Desktops' (selected), 'GUIs', 'VMD', 'Servers', 'Jupyter Server', 'MATLAB', and 'RStudio Server'. A blue oval highlights the 'Desktops' option. To the right of the menu, there is a brief description of OnDemand: 'OnDemand provides an integrated access point for all of your HPC resources.'

Home / My Interactive Sessions / Desktop

**Interactive Apps**

Desktops

**Desktop**

GUIs

VMD

Servers

Jupyter Server

MATLAB

RStudio Server

**Desktop** version: 31a024e

This app will launch an interactive desktop on the [LBNL Science-IT](#) Laboratory Research Computing([LRC](#)) Infrastructure clusters. You will be able to launch GUI applications directly on the desktop.

**Name of the Job**

OOD\_desktop\_test

**SLURM Partition**

cf1

The SLURM Partition in which you want to launch this Desktop session.

**SLURM Account/Project Name**

scs

The SLURM account (i.e., the value of the -A or --account flag used when submitting a SLURM job).

**SLURM QoS Name**

cf\_debug

The QoS you want run under.

**Number of Compute Nodes**

1

The number of nodes you want for your Desktop session.

**Wall Clock Time**

1

The maximum number of hours your Jupyter session will run for. To save PCA credits or free up resources for your condo group members, you should delete your session when you are done.

**Email Address (Optional)**

Enter your email address if you would like to receive an email when the session starts. Leave blank for no email.

**Launch**

\* The Desktop session data for this session can be accessed under the [data root](#) directory.

Session was successfully deleted.

Home / My Interactive Sessions

**Interactive Apps**

Desktops

**Desktop**

GUIs

VMD

Servers

Jupyter Server

MATLAB

RStudio Server

**Desktop (51668171)**

Host: [2001:4d8:1001:1::1](#)

Created at: 2022-07-21 18:17:33 PDT

Time Remaining: 59 minutes

Session ID: 645aabba-caa9-4f1b-a5c0-973421f951fb

Compression

0 (low) to 9 (high)

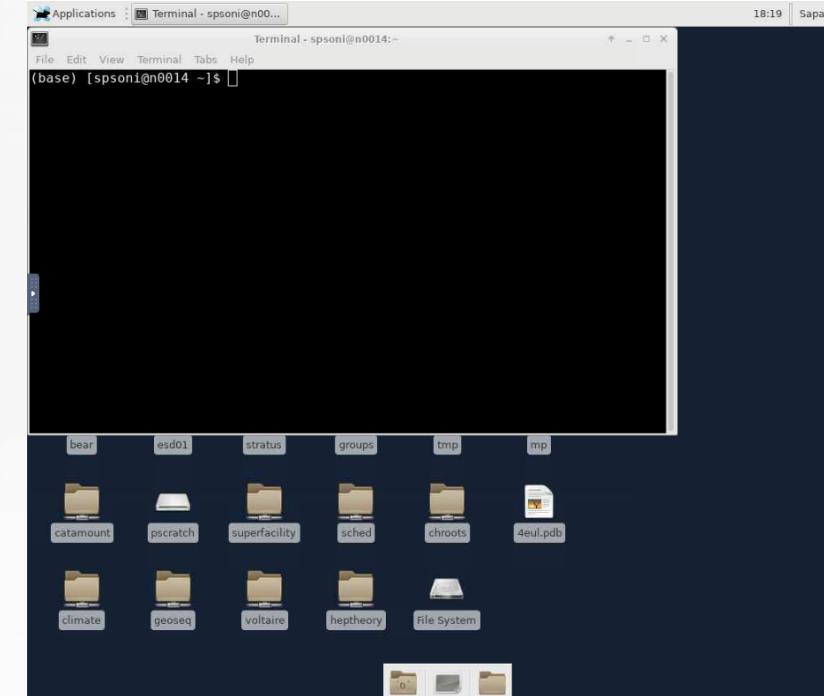
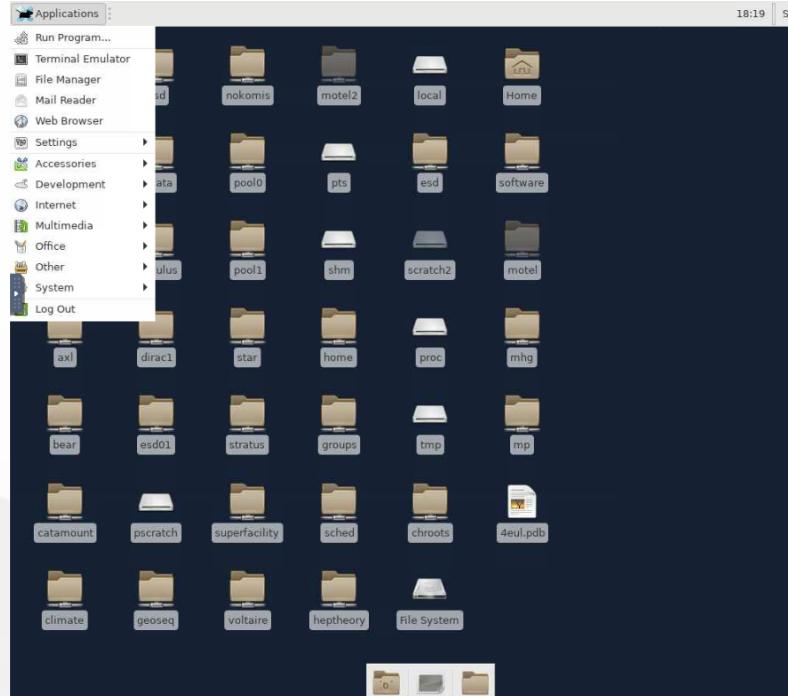
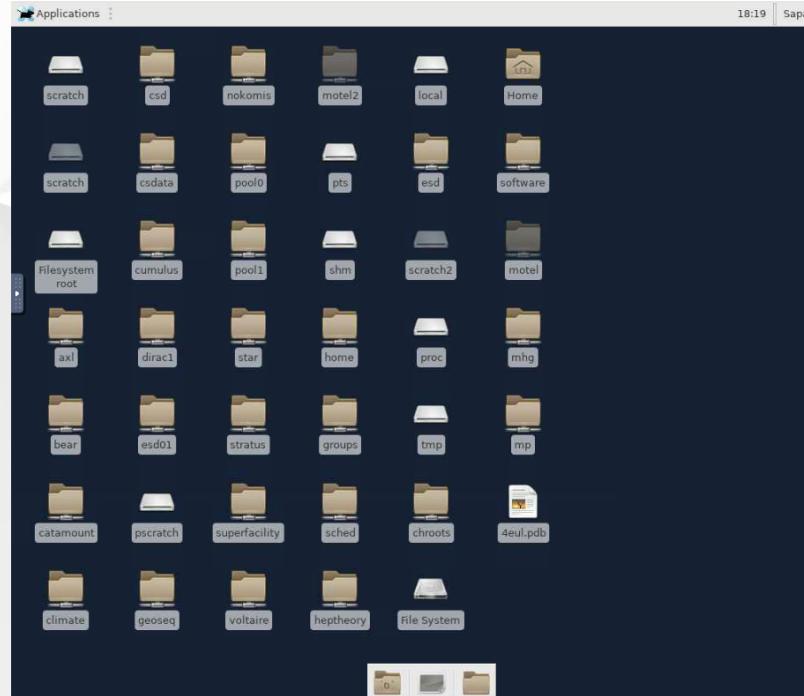
Image Quality

0 (low) to 9 (high)

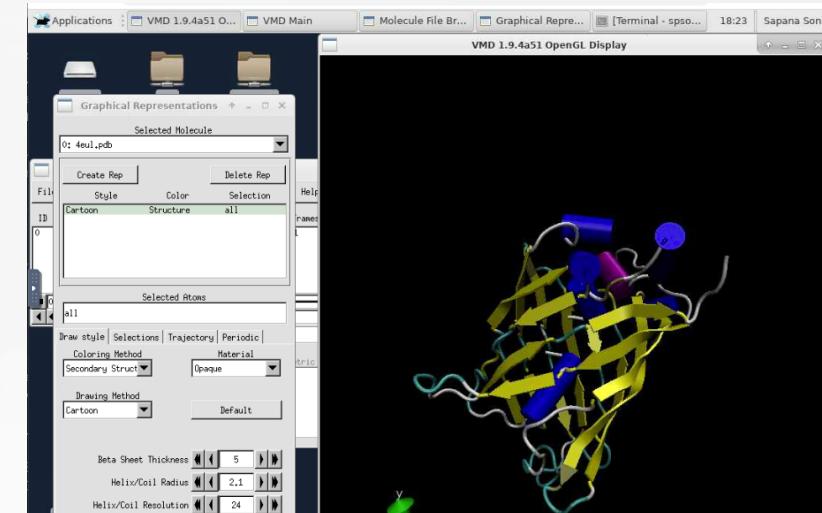
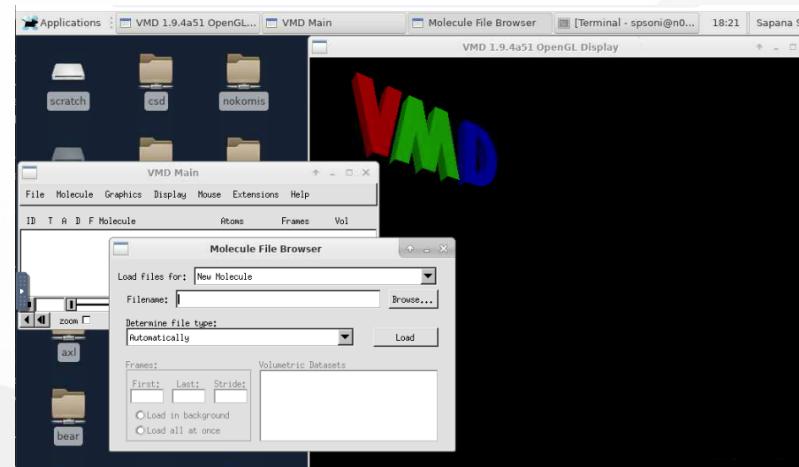
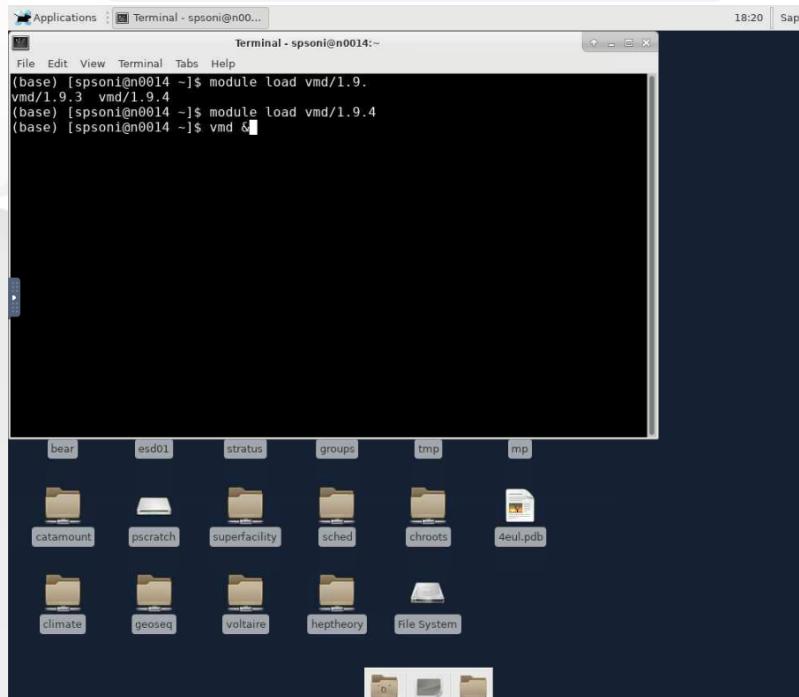
**Launch Desktop**

**View Only (Shareable Link)**

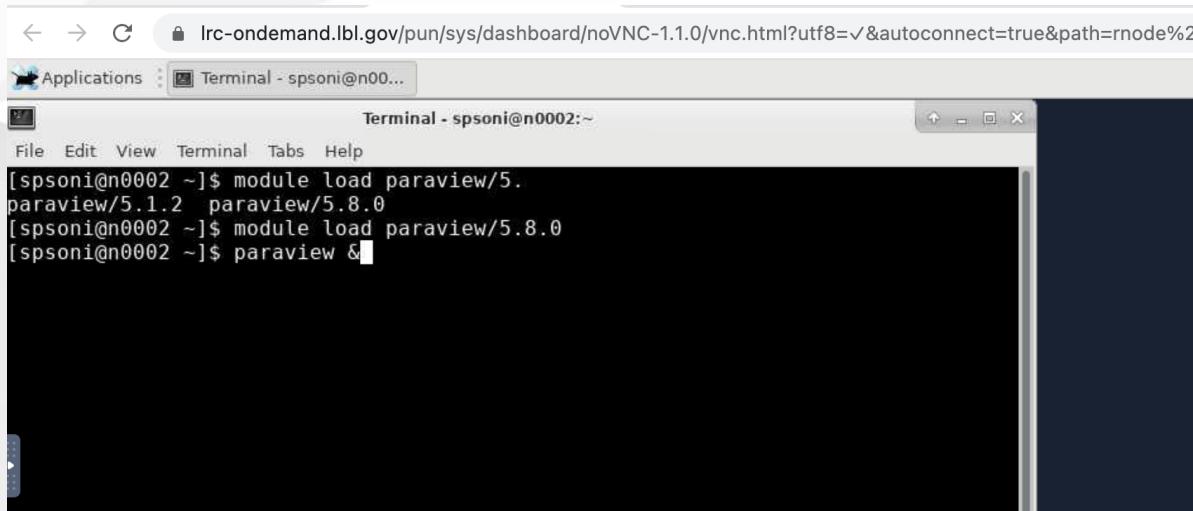
# Desktop



# Using Desktop to launch VMD

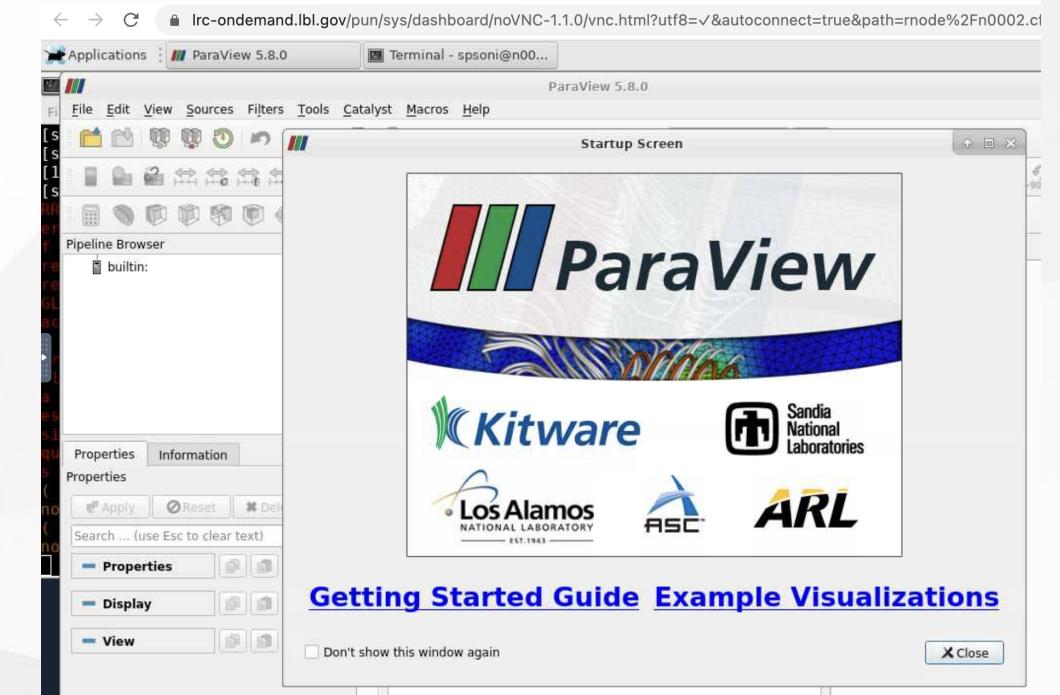


# Using Desktop to launch ParaView



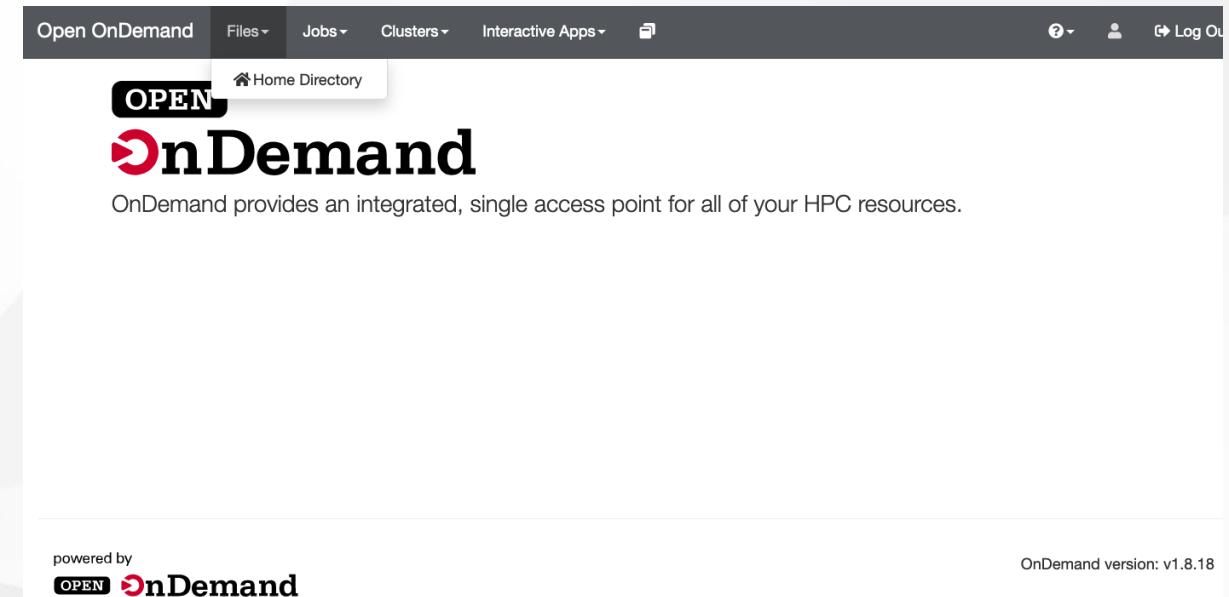
A screenshot of a terminal window titled "Terminal - spsoni@n002:~". The window shows the following command history:

```
[spsoni@n002 ~]$ module load paraview/5.  
paraview/5.1.2 paraview/5.8.0  
[spsoni@n002 ~]$ module load paraview/5.8.0  
[spsoni@n002 ~]$ paraview &
```



# Files: file management

- **Conventional approach: command line**
  - Linux file editors for editing files: vi, vim, nano, emacs
  - File transfer: scp, rsync
- **Globus for file transfer**
- **Open OnDemand: Files feature**
  - view and edit text files
  - create or rename or delete files
  - create or rename or delete directories
  - file/directory upload and download



# Files : Home directory

The screenshot shows a file manager interface with the following details:

- Toolbar:** Go To..., Open in Terminal, New File, New Dir, Upload, Show Dotfiles, Show Owner/Mode.
- Path:** /global/home/users/spsoni/
- Buttons:** View, Edit, A-Z Rename/Move, Download, Copy, Paste, (Un)Select All, Delete.
- Table Headers:** name, size, modified date.
- Table Data:** The table lists numerous directories, all of which are empty (size 0). The last modified date for most is 06/13/2022, except for Desktop, OCEAN, R, bin, and lib, which are from 06/09/2022 to 07/24/2022.

name	size	modified date
..	dir	07/24/2022
Desktop	dir	07/08/2022
OCEAN	dir	06/09/2022
R	dir	06/13/2022
bin	dir	06/14/2022
gcc-11.3.0	dir	06/09/2022
gdal-3.5.0	dir	06/09/2022
geos	dir	06/09/2022
geos-3.10.3	dir	06/09/2022
go	dir	07/05/2022
include	dir	06/29/2022
intel	dir	06/16/2022
julia-1.7.3	dir	05/17/2022
lib	dir	06/13/2022
lib64	dir	06/29/2022
libexec	dir	06/13/2022
libssh		
libssh2		
libssh2-0.9		
myproject		
ondemand		

# Clusters: LRC shell access

The screenshot shows the OnDemand web interface. At the top, there is a navigation bar with links for Open OnDemand, Files, Jobs, Clusters (which is the active tab), Interactive Apps, and a search icon. Below the navigation bar, the main content area has a header "OPEN OnDemand". The header includes a "LOG IN" button and a "Log Out" link. A sub-header "OnDemand provides an integrated, single access point for all of your HPC resources." is displayed. In the center, there is a large "OPEN OnDemand" logo with a red "O" and a black "n". Below the logo, there is a brief description of what OnDemand offers. At the bottom of the page, there is a footer with the text "powered by OPEN OnDemand" and "OnDemand version: v1.8.18".

The screenshot shows a terminal window with a black background and white text. It displays a security notice from Lawrence Berkeley National Laboratory. The notice states that the system is operated under a contract with the U.S. Department of Energy and is for authorized use only. It warns against unauthorized access for security purposes and outlines legal consequences under Federal Laws 83-703 and 99-474. It also mentions that LBNL may detain, access, and copy files from non-LBNL computers if misuse is suspected. Below the notice, there is a list of emergency contacts: LBNL Computer Protection Emergency phone number (486-7770), LBNL Security Webpage (<http://www.lbl.gov/security/>), and LBNL Backup Services (<https://commons.lbl.gov/display/itdivision/Backups>). Further down, it indicates weekly office hours on Wednesdays starting July 24, 2019. It also mentions virtual consultations at <https://sites.google.com/a/lbl.gov/hpc/getting-help> between 10:30am and noon on Wednesdays. The terminal window ends with a prompt "[spsoni@n000 ~]\$".

# Job submission and management

The screenshot shows the OnDemand web interface. At the top, there is a navigation bar with links for Open OnDemand, Files, Jobs, Clusters, Interactive Apps, and a user icon. Below the navigation bar is the main content area. On the left, there is a sidebar with a "OPEN OnDemand" logo and a "OnDemand" section containing the text: "OnDemand provides an integrated, single access point for all of your HPC resources." In the center, there is a "Active Jobs" section with a table showing one entry:

ID	Name	User	Account	Time Used	Queue	Status	Cluster	Actions
51694850	OOD_desktop_test	sponi	scs	00:00:09	cf1	Running	LRC	

At the bottom of the page, there is a footer with the text "powered by OPEN OnDemand" and "OnDemand version: v1.8.18".

The screenshot shows the "Active Jobs" list page. The title is "Open OnDemand / Active Jobs". There are two buttons at the top right: "Your Jobs" and "All Clusters". Below the title, there is a search bar with the placeholder "Filter: [ ]". The main content is a table titled "Active Jobs" with the following data:

ID	Name	User	Account	Time Used	Queue	Status	Cluster	Actions
51694850	OOD_desktop_test	sponi	scs	00:00:09	cf1	Running	LRC	

Below the table, it says "Showing 1 to 1 of 1 entries". At the bottom right, there are navigation buttons: "Previous", "1", and "Next".

# Job composer and template

Open OnDemand / Job Composer Jobs Templates ⚡ Help

## Jobs

+ New Job ▾

Edit Files Job Options Open Terminal Submit Stop Delete

Show 25 entries Search:

Created	Name	ID	Cluster	Status
July 24, 2022 5:24pm	GPU Slurm Job	51694976	LRC	Not Submitted
July 24, 2022 5:16pm	MPI Slurm Job	51694976	LRC	Completed
July 24, 2022 5:12pm	GPU Slurm Job	51694958	LRC	Completed

Showing 1 to 3 of 3 entries Previous 1 Next

Job Details

Job Name: GPU Slurm Job

Submit to: LRC

Account: Not specified

Script location: /global/home/users/spsoni/ondemand/data/sys/myjobs/projects/d

Open OnDemand / Job Composer Jobs Templates ⚡ Help

## Templates

To create a new job, select a template to copy, fill out the form to the right, and click "Create New Job".

+ New Template Copy Template

View Files Open Terminal Delete

Show 10 entries Search:

Name	Cluster	Source
GPU Slurm Job	Lrc	System Templates
MPI Slurm Job	Lrc	System Templates
Simple Sequential Slurm Job	Lrc	System Templates

Showing 1 to 3 of 3 entries Previous 1 Next

Create New "GPU Slurm Job"

A basic template for GPU job on a Slurm system

Job Name: GPU Slurm Job

Cluster: LRC

Script Name: gpu\_job.sh

Create New Job Reset

# Submission script

★ Create Template

ch:

Delete

Status: Not Submitted

Completed

Completed

Previous 1 Next

### Job Details

Job Name: **GPU Slurm Job**

Submit to: LRC

Account: Not specified

Script location: /global/home/users/spsoni/ondemand/data/sys/myjobs/projects/default/4

Script name: gpu\_job.sh

Folder Contents:

Folder Contents:

gpu\_job.sh

### Submit Script

gpu\_job.sh

Script contents:

```
#!/bin/bash

#SBATCH --job-name=test
#SBATCH --nodes=1
#SBATCH --time=00:30:00
#SBATCH --qos=es_normal
#SBATCH --account=scs
#SBATCH --partition=es1
#SBATCH --gres=gpu:1
#SBATCH --ntasks=2
#SBATCH --output=%j.output
#SBATCH --error=%j.err
#SBATCH --job-name=test

cd $SLURM_SUBMIT_DIR
echo "How to submit GPU jobs" > output_file
nvidia-smi -L >> output_file
```

Open Editor

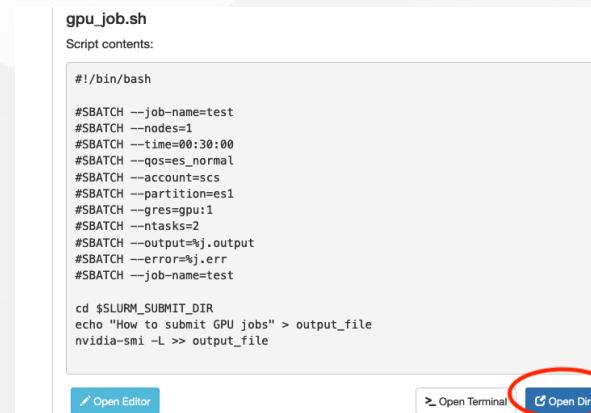
Open Terminal

Open Dir

# Jobs: submission directory

Job composer creates a working directory by default on the path  
/global/home/users/spsoni/ondemand/data/sys/myjobs/projects/default

- **Use default path:** Copy/upload all the files required for the jobs on this path before hitting Submit button.
  - click 'Open Dir' button at the bottom of the job script content.
  - using a file explorer upload or transfer files



**OR**

- **Set different working directory:** If you want to use files saved on different location and would like to run job in that directory, for example: scratch.
  - add following command line in your job script

```
cd /global/scratch/users/spsoni/my_working_dir
```

**Note:** Use path you aim to set for your working directory.

# Log out and clean up

- Log out of the portal
- Clean up
  - The portal stores temporary files for interactive apps on the path \$HOME//ondemand/data/sys/dashboard/batch\_connect/sys
  - It is a good practice to clean up this directory periodically.

```
rm -rf $HOME/ondemand/data/sys/dashboard/batch_connect/sys/*
```

The screenshot shows a user interface for managing interactive sessions. At the top, there are navigation links: Jobs, Clusters, Interactive Apps, My Interactive Sessions, Help, Logged in as sponi, and Log Out. A green success message box says "Session was successfully created." Below this, the "Interactive Apps" section lists Desktops, GUIs, VMD, Servers, Jupyter Server, MATLAB, and RStudio Server. Two sessions are listed: "Desktop (55835388)" and "RStudio Server (55835387)". Each session card includes details like Host, Created at, Time Remaining, Session ID, and configuration sliders for Compression and Image Quality. Red arrows point to the "Delete" buttons for both the Desktop and RStudio Server sessions.

# Getting help

- Virtual office hours:
  - Time: 10.30 am to noon every Wednesday
  - Online [request](#)
- Send us tickets at [hpcshelp@lbl.gov](mailto:hpcshelp@lbl.gov)
- More information about LBNL Supercluster and scientific computing services can be found [here](#).

Your feedback is important to us for improving HPC services and training.

Please fill out [training survey](#)

