

# **Open OnDemand on Lawrencium**

**Sapana Soni**

# Outline

## **Part I : Using MyLRC portal**

Getting a user account on LRC

Getting access to project

Requesting project account and 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 kernels

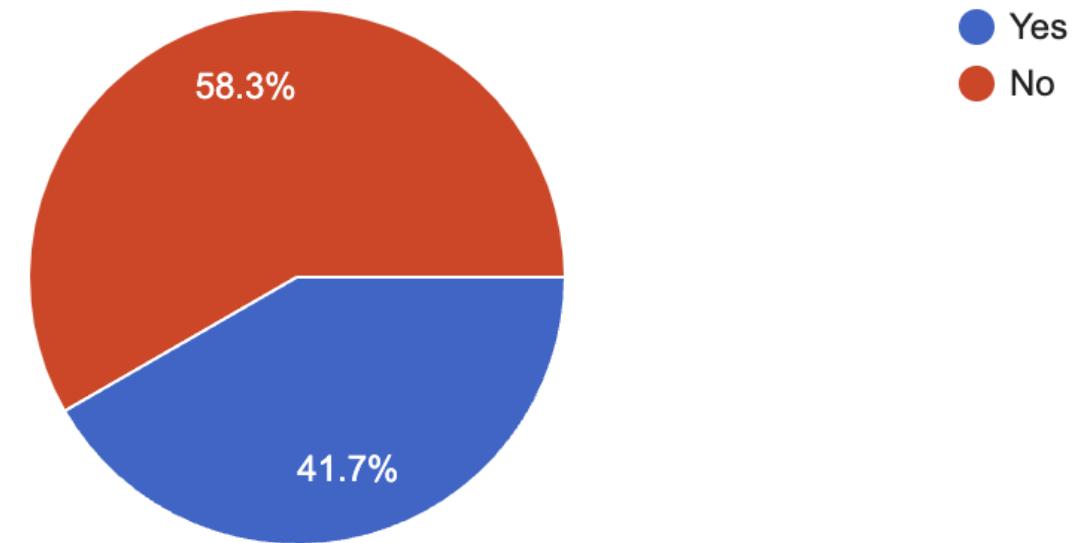
Job management and monitoring

# **Training style : mostly demonstration**

- If you have account on Lawrencium 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[<https://it.lbl.gov/resource/hpc/for-users/training-and-tutorials/>].
- How to use Lawrencium?
  - Documentation page [link](#)

# MyLRC User Portal: Getting and managing LRC accounts

- Getting a user account on LRC
- Getting access to project
- Requesting project account
  - Updating Project information
  - PCA Project renewal
  - Account deletion



MyLRC portal [login](#)

MyLRC [Documentation](#)

# Getting a user account on LRC

## Currentl Workflow:

1. Setup account on MyLRC [portal](#) as LBNL affiliate/UC bErkeley affiliate or as an External collaborator
2. Sign the User Access Agreement Form
3. Request to join existing project
4. PI approval
5. Lawrencium account creation by HPCS team
6. Users will 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**

 BERKELEY LAB  
Bringing Science Solutions to the World

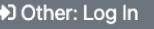
Home Center Summary Help 

## 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**

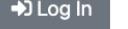
 BERKELEY LAB  
Bringing Science Solutions to the World

Home Center Summary Help 

## 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?](#)



A U.S. Department of Energy National Laboratory  
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](#)

Copyright © 2023 UC Regents. All rights reserved.

# 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. A dropdown menu is open, showing 'Google' as the selected option, followed by a list of other institutions: Lawrence Berkeley National Laboratory, 29 Mayis University, A\*STAR - Agency for Science, Technology and Research, A. T. Still University, AAF Virtual Home, aa.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, and Absalon University College. To the left of the dropdown is a section titled 'Select a' with a checkbox for 'Remember me'. At the bottom left is a note: 'By selecting "Log On", you agree to the [privacy policy](#)'.

The screenshot shows the same 'Consent to Attribute Release' page. The 'Google' option is now highlighted in blue at the top of the dropdown menu. The rest of the interface is identical to the first screenshot, including the 'CILogon' logo, search bar, list of institutions, and the 'Select a' section with the 'Remember me' checkbox and privacy policy note.

## Step 2: Sign the User Access Agreement Form

MyLRC - Laboratory Research Computing  
Access Management System



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 you can join a cluster project and gain access to the cluster.

| Task  | Status                      | Actions   |
|---|-----------------------------|---|
| 1. Sign the cluster user access agreement.  | <span>X Unsigned</span>     | <a href="#">Review and Sign</a> <span style="color: red;">Click here</span> |
| 2. Create or join a project. <span>?</span> | <span>X 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](#)

|   |   |
|---|---|
| <b>Software Use</b>                     | 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.  |
| <b>Altering Authorized Access</b>       | 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.   |
| <b>Data Modification or Destruction</b> | Users are prohibited from taking unauthorized actions to intentionally modify, delete, or reconstruct information or programs.  |
| <b>Malicious Software</b>               | 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.  |
| <b>Denial of Service Actions</b>        | Users may not deliberately interfere with other users accessing system resources.   |
| <b>Notification</b>                     | 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.   |
| <b>Account Usage</b>                    | Each user of this system must have a unique login. Users are not allowed to share their accounts with others.<br><br>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. |
| <b>Submit</b>                           | <span style="color: red;">→</span> <input type="checkbox"/> Acknowledge & Sign*<br><small>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.</small>  |
|   | <span style="color: red;">→</span> <a href="#">Submit</a>   |

## 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         | kewu    | dirac1         | DIRAC1     | Active | <a href="#">+ Join</a> |
| 2  | nano           | davidp  | nano           | NANO       | Active | <a href="#">+ Join</a> |
| 5  | catamount      | jbeaton | catamount      | CATAMOUNT  | Active | <a href="#">+ Join</a> |
| 6  | mhg            | mhg     | mhg            | MHG        | Active | <a href="#">+ Join</a> |
| 7  | ac_scsguest    | gmjung  | ac_scsguest    | LAWRENCIUM | Active | <a href="#">+ Join</a> |
| 8  | ac_nanotherapy | davidn  | ac_nanotherapy | LAWRENCIUM | Active | <a href="#">+ Join</a> |

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

PI will receive an email in following format.

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]{<https://mylrc.lbl.gov/project/7/review-join-requests/>}.

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

## Step 5 and 6: Account creation and confirmation

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 - viraat

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. You can follow 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> | <a href="#">Review</a>  |
| 2. Create or join a project. <span style="color: red;">?</span> | <span style="color: green;">✓ 2 Project(s)</span>                    | <a href="#">Create</a> <a href="#" style="color: red; border: 2px solid red; padding: 2px;">Join</a> <span style="color: red; font-size: 2em; position: absolute; left: -10px; top: 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

MyLRC - Laboratory Research Computing  
Access Management System

BERKELEY LAB  
Bringing Science Solutions to the World

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

MyLRC - Laboratory Research Computing  
Access Management System

BERKELEY LAB  
Bringing Science Solutions to the World

Home Center Summary Project Requests Jobs Help

sponi@berkeley.edu

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: Request and Jobs

MyLRC - Laboratory Research Computing  
Access Management System

BERKELEY LAB  
Bringing Science Solutions to the World

Home Center Summary Project Requests Jobs Help

spsoni@berkeley.edu

## Request Hub

Below are all of your requests in MyLRC. Click on a request section to view your requests of that type.

Collapse All - Expand All +

Cluster Access Requests

Project Join Requests

### Pending Project Join Requests

| # | Username            | User Email          | Project     | Date Requested | Reason                  |
|---|---------------------|---------------------|-------------|----------------|-------------------------|
| 1 | spsoni@berkeley.edu | spsoni@berkeley.edu | ac_scsguest | Feb. 05, 2023  | Need to use LRC cluster |

Page 1 of 1

Previous Next

No completed project join requests!

Project Removal Requests

Project Renewal Requests

New Project Requests

MyLRC - Laboratory Research Computing  
Access Management System

BERKELEY LAB  
Bringing Science Solutions to the World

Home Center Summary Project Requests Jobs Help

spsoni@berkeley.edu

## Job List

Viewing your jobs and the jobs belonging to projects in which you are a PI or manager.

Filter

Status

-----

Slurm ID

-----

Project Name

-----

Partition

-----

Service Units

-----

Number of Service Units

Submitted

-----

MM/DD/YYYY

Started

-----

MM/DD/YYYY

Ended

-----

MM/DD/YYYY

Search

Reset

No search results!

# 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  |

MyLRC - Laboratory Research Computing Access Management System

BERKELEY LAB Bringing Science Solutions to the World

Home Center Summary Project Requests Jobs Admin Help spsoni

## 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. Manager role can be assigned to a project user for managing project account and project renewal (for PCA projects)

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.     | 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](#)

MyLRC - Laboratory Research Computing  
Access Management System

BERKELEY LAB  
Bringing Science Solutions to the World

Home Center Summary Project Requests Jobs Admin Help

spsoni

## 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

MyLRC - Laboratory Research Computing  
Access Management System

 BERKELEY LAB  
Bringing Science Solutions to the World

Home Center Summary Project Requests Jobs Admin Help

 spsoni ▾

## 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**

MyLRC - Laboratory Research Computing  
Access Management System

 BERKELEY LAB  
Bringing Science Solutions to the World

Home Center Summary Project Requests Jobs Admin Help

 spsoni ▾

## Lawrencium: Computing Allowance

Select a computing allowance.

Computing Allowance\*

PI Computing Allowance (Computing Allowance)

**Next Step**

Step 1 of 6

MyLRC - Laboratory Research Computing  
Access Management System

 BERKELEY LAB  
Bringing Science Solutions to the World

Home Center Summary Project Requests Jobs Admin Help

spsoni

## Lawrencium: Computing Allowance

Select a computing allowance.

Computing Allowance\*

PI Computing Allowance (Computing Allowance)

Condo Allocation (Computing Allowance)

Recharge Allocation (Computing Allowance)

Step 1 of 6

MyLRC - Laboratory Research Computing  
Access Management System

 BERKELEY LAB  
Bringing Science Solutions to the World

Home Center Summary Project Requests Jobs Admin Help

spsoni

## 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

MyLRC - Laboratory Research Computing  
Access Management System

 BERKELEY LAB  
Bringing Science Solutions to the World

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)

MyLRC - Laboratory Research Computing  
Access Management System

 BERKELEY LAB  
Bringing Science Solutions to the World

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](#)

MyLRC - Laboratory Research Computing  
Access Management System

 BERKELEY LAB  
Bringing Science Solutions to the World

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](#)

MyLRC - Laboratory Research Computing  
Access Management System

 BERKELEY LAB  
Bringing Science Solutions to the World

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](#)

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

MyLRC - Laboratory Research Computing Access Management System

BERKELEY LAB  
Bringing Science Solutions to the World

Home Center Summary Project Requests Jobs Admin Help

sponi ▾

## 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

MyLRC - Laboratory Research Computing Access Management System

BERKELEY LAB  
Bringing Science Solutions to the World

Home Center Summary Project Requests Jobs Admin Help

sponi ▾

## 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)

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://mybrc.brc.berkeley.edu/project/<project\\_number>/](https://mybrc.brc.berkeley.edu/project/<project_number>)

If you have any questions, contact us at {{ hpcshelp@lbl.gov }}.

Thank you,

MyLRC User Portal team

<https://mylrc.lbl.gov>

Email : hpcshelp@lbl.gov

# Project Management

## 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: green;">?</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.

## 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 5px;">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 5px;">Create</span> <span style="background-color: #0070C0; color: white; padding: 2px 5px;">Join</span> |

Your LRC cluster account username: spsoni

[My LRC Cluster Projects »](#)

| Project Name | Cluster | Access to Project on Cluster   |
|--------------|---------|--|
| dirac1       | DIRAC1  | <span style="background-color: #0070C0; color: white; padding: 2px 5px;">Active</span> |
| scs          | SCS     | <span style="background-color: #0070C0; color: white; padding: 2px 5px;">Active</span> |

View all projects and managers

Title\*

Description\*

Save Cancel

# Project Join Requests from users

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.

## 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

## 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 year on 1st October and 300K SU are allocated for the Fiscal year. 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.

| Users 32          |                  |                        |                  |                           | <a href="#">Add Users</a> | <a href="#">Remove Users</a> | <a href="#">Leave Project</a> |
|-------------------|------------------|------------------------|------------------|---------------------------|---------------------------|------------------------------|-------------------------------|
| Name              | Email            | Role                   | Cluster Username | Project Access on Cluster | Actions                   |                              |                               |
| Name1 Familyname1 | email1@lbl.gov   | User                   | username1        | <a href="#">Active</a>    | <a href="#">Edit</a>      |                              |                               |
| Name2 Familyname2 | email2@lbl.gov   | Principal Investigator | username2        | <a href="#">Active</a>    | <a href="#">Edit</a>      |                              |                               |
| Name3 Familyname3 | email3@gmail.com | User                   | username3        | <a href="#">Active</a>    | <a href="#">Edit</a>      |                              |                               |
| Name4 Familyname4 | email4@lbl.gov   | Manager                | username4        | <a href="#">Active</a>    | <a href="#">Edit</a>      |                              |                               |

### Project User Detail

Project: scs

[User Detail](#)

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

[Update](#) [Back to Project](#)

[Cluster Access](#)

|                            |                        |
|----------------------------|------------------------|
| Cluster Username:          | spsoni                 |
| Project Access on Cluster: | <a href="#">Active</a> |

### Add users to project: scs

Search String\*

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

Search by\*

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

[Search](#)

## 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.

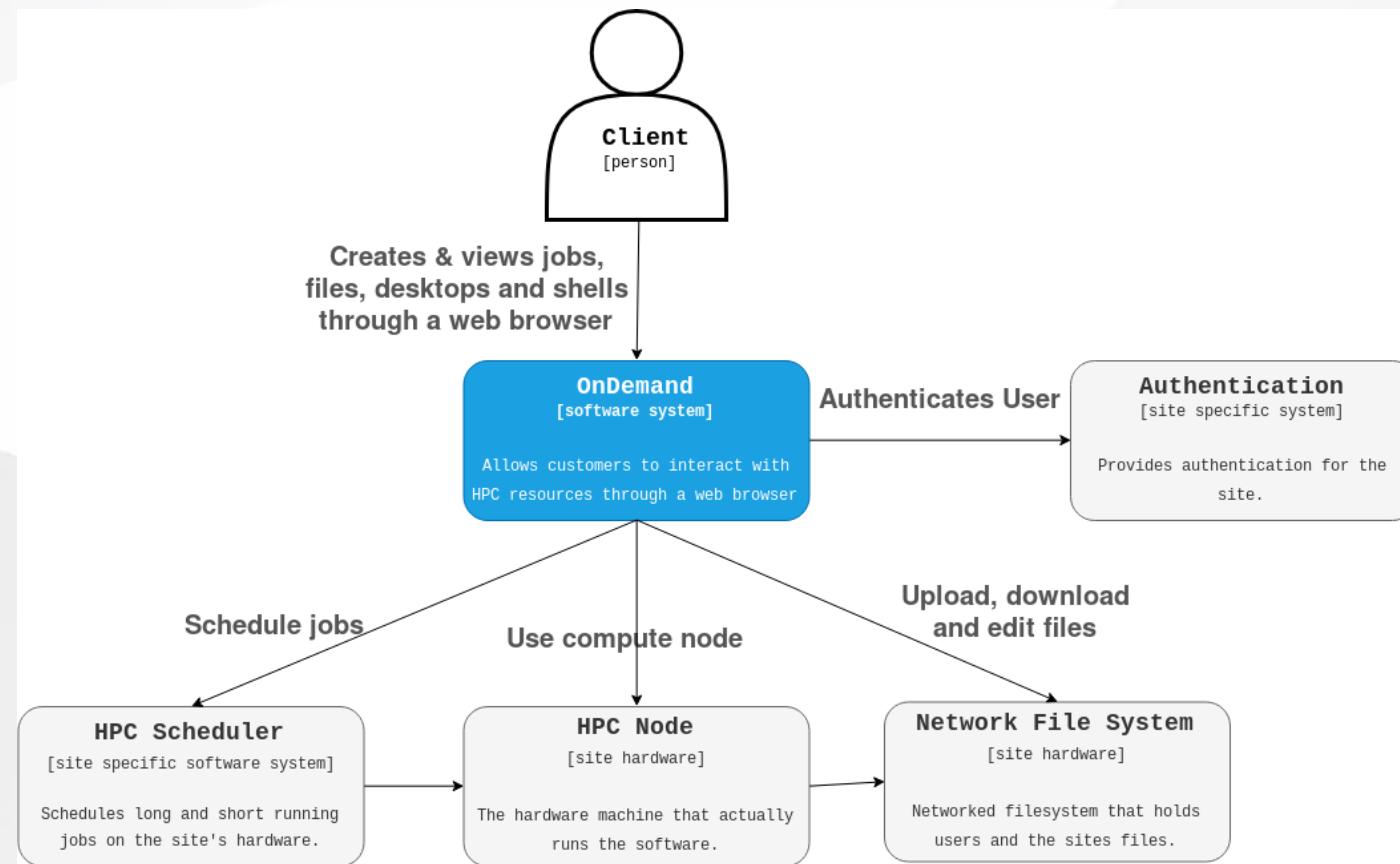
### 2. Remove from a project & delete user account

Project PI will be responsible to inform HPCS team to inform 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.

# 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?

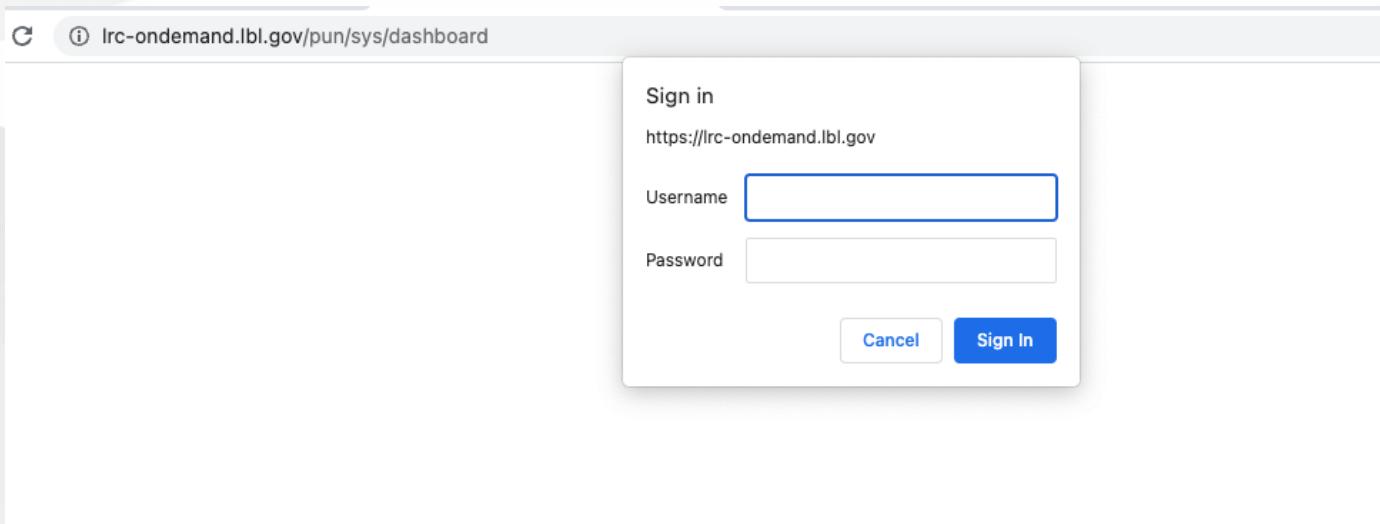


Users are able to use HPC services more efficiently through Open OnDemand.

# 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.

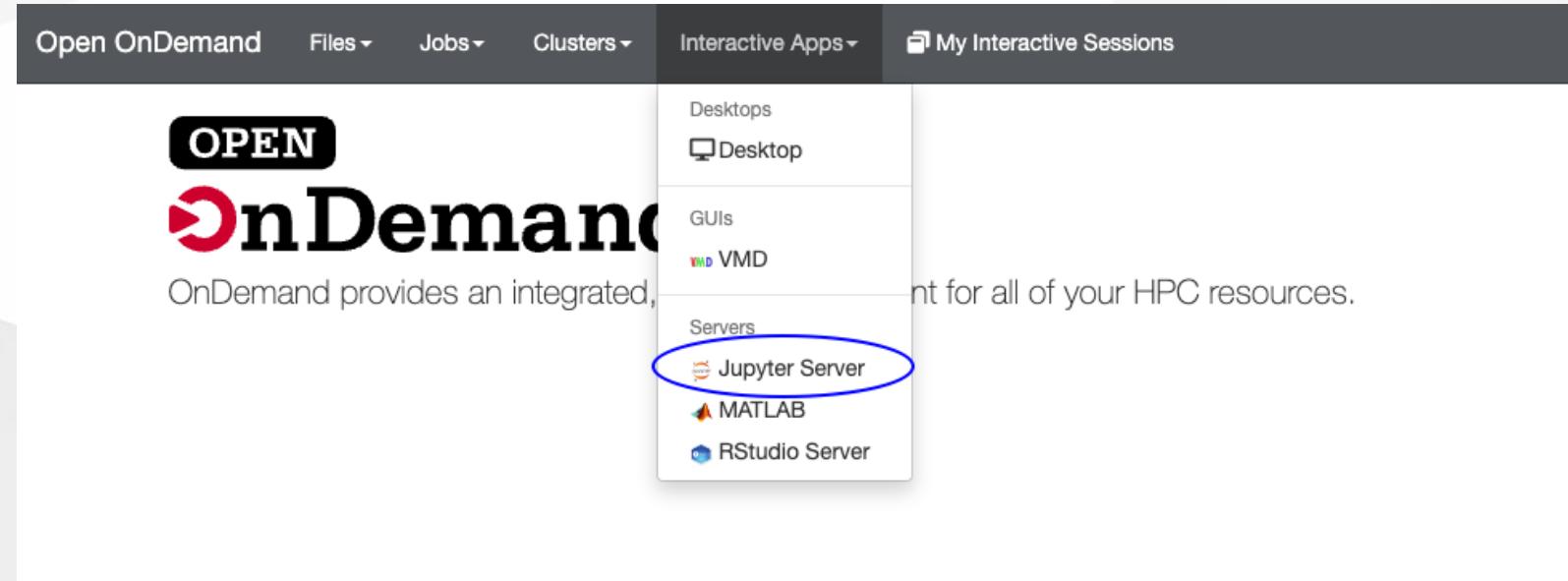
Open OnDemand    Files ▾    Jobs ▾    Clusters ▾    Interactive Apps ▾    My Interactive Sessions    Help ▾    Logged in as spsoni    Log Out

**OPEN**  
**OnDemand**

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

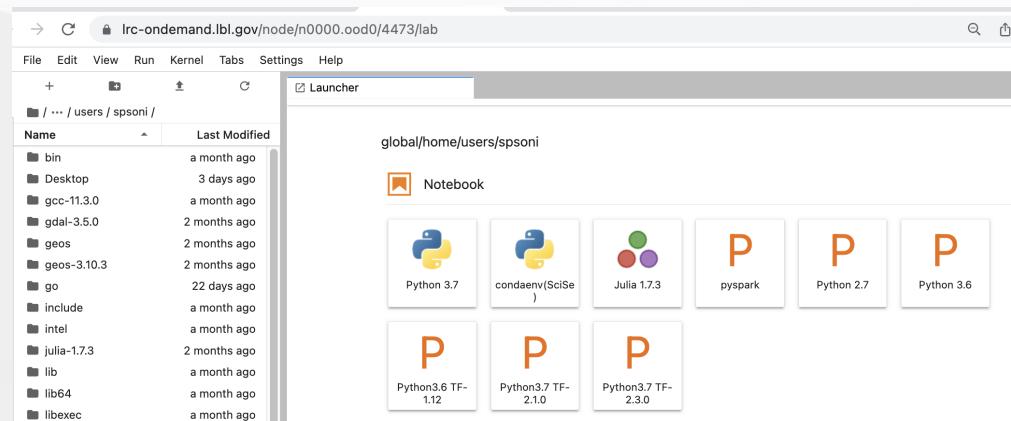
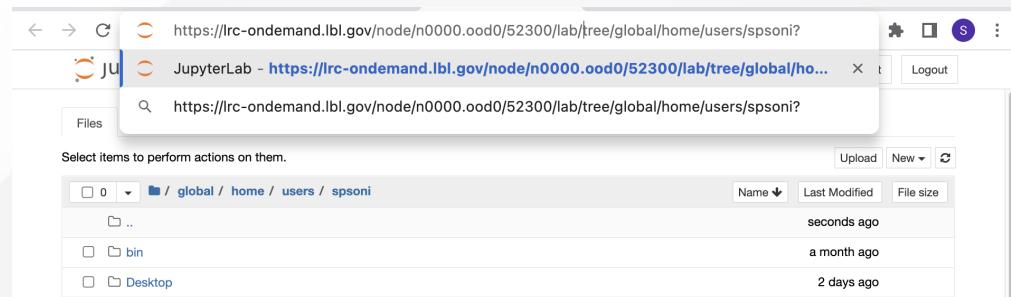
Connect to Jupyter

Delete



The screenshot shows a Jupyter Notebook cell titled 'Untitled1'. The cell contains the code 'In [3]: print("Hello World!")'. When run, the output 'Hello World!' is displayed below the code. The notebook interface includes a header with a logo, the title 'Untitled1', a 'Logout' button, and a menu bar with 'File', 'Edit', 'View', 'Insert', 'Cell', 'Kernel', 'Widgets', and 'Help'. A toolbar below the menu bar provides various editing and navigation tools. The kernel selected is 'Python 3.6'.

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/$USER/py39_scr --display-name="py39_scratch"
#create symlink to kernel in custom path
ln -s /global/scratch/users/$USER/py39 /global/home/users/$USER/.local/share/jupyter/kernels/py39
```

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:

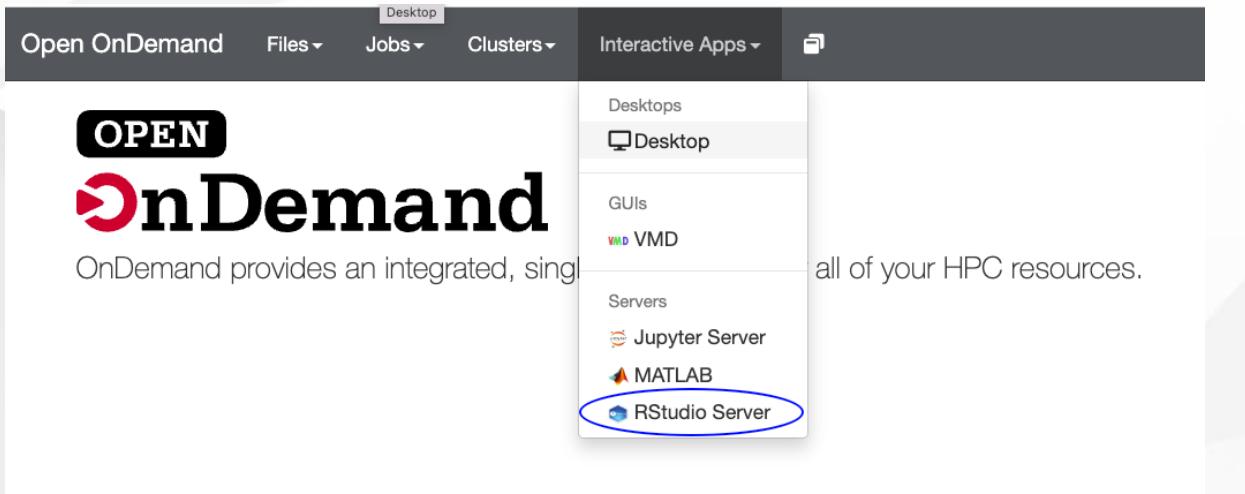
Julia kernel can be added in Jupyter for writing a Julia code in Jupyter notebook. To add a Julia kernel to Jupyter we only need to add the IJulia package.

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

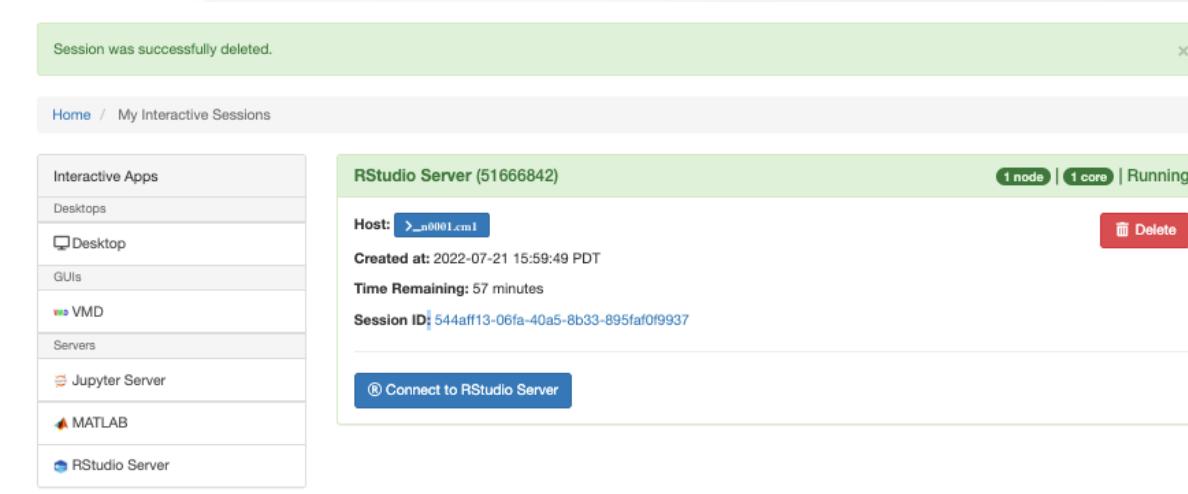
To remove unwanted jupyter kernel use following commands.

```
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's a navigation bar with 'Open OnDemand', 'Files', 'Jobs', 'Clusters', 'Interactive Apps', and a search icon. Below this, the main area features the 'OnDemand' logo and the text 'OnDemand provides an integrated, sing...'. To the right, there's a sidebar with a list of interactive applications: Desktops (selected), GUIs (VMD), Servers (Jupyter Server, MATLAB), and RStudio Server (circled in blue). The main content area displays the message 'all of your HPC resources.'



The screenshot shows the 'My Interactive Sessions' page. It displays a green success message 'Session was successfully deleted.' Above the list of sessions. The list includes: 'Interactive Apps' (Desktops, GUIs, VMD, Servers, MATLAB, RStudio Server), 'RStudio Server (51666842)' (Host: >\_n0001.cml, Created at: 2022-07-21 15:59:49 PDT, Time Remaining: 57 minutes, Session ID: 544aff13-06fa-40a5-8b33-895faf0f9937, Connect to RStudio Server button), and a 'Delete' button.

# 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 navigation bar includes Home, My Interactive Sessions, and a search icon. The main area displays the session information for "MATLAB (51666979)". It shows the host as >\_n0000.ood0, created at 2022-07-21 16:24:34 PDT, with 59 minutes remaining. The session ID is 58dfcbce-9c5e-432d-b02d-87043985df5c. There are compression and image quality sliders, and a "Launch MATLAB" button. A "View Only (Shareable Link)" button is also present.

# Interactive Apps: Desktop

The screenshot shows the OnDemand interface. At the top, there is a navigation bar with links for Open OnDemand, Files, Jobs, Clusters, Interactive Apps, and My Interactive Sessions. The 'Interactive Apps' menu is open, displaying options: Desktops (selected), GUIs (VMD), Servers (Jupyter Server, MATLAB, RStudio Server). A blue oval highlights the 'Desktops' link. Below the menu, there is a message: "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)

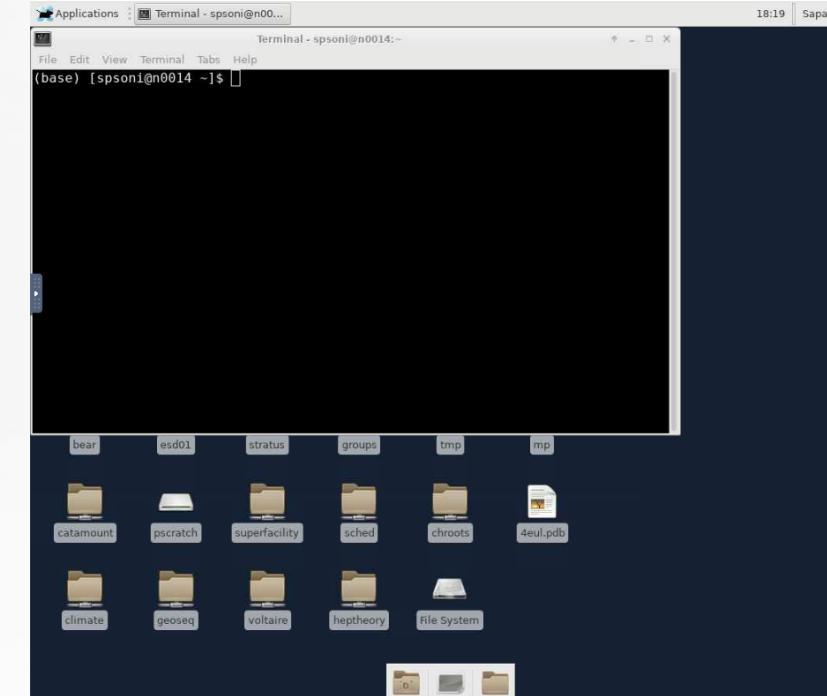
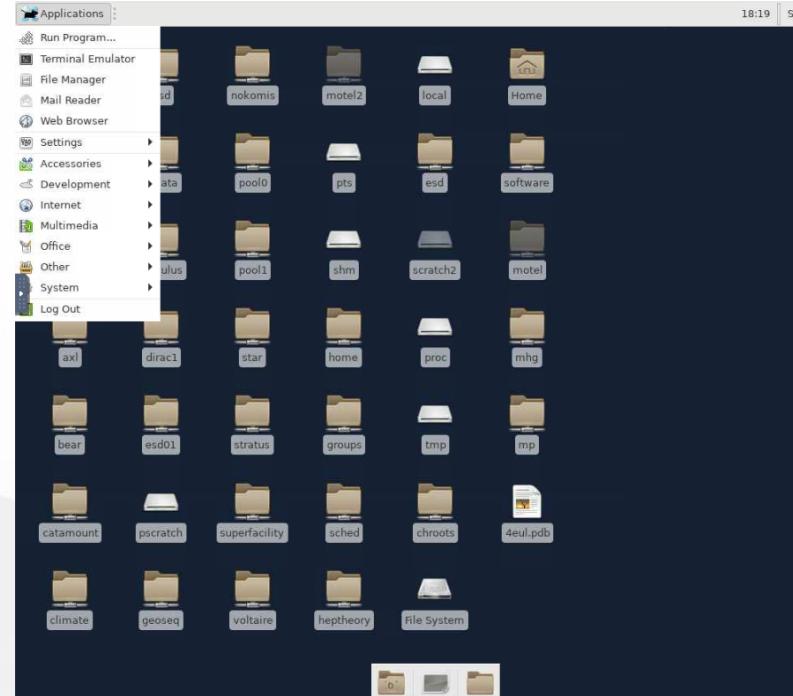
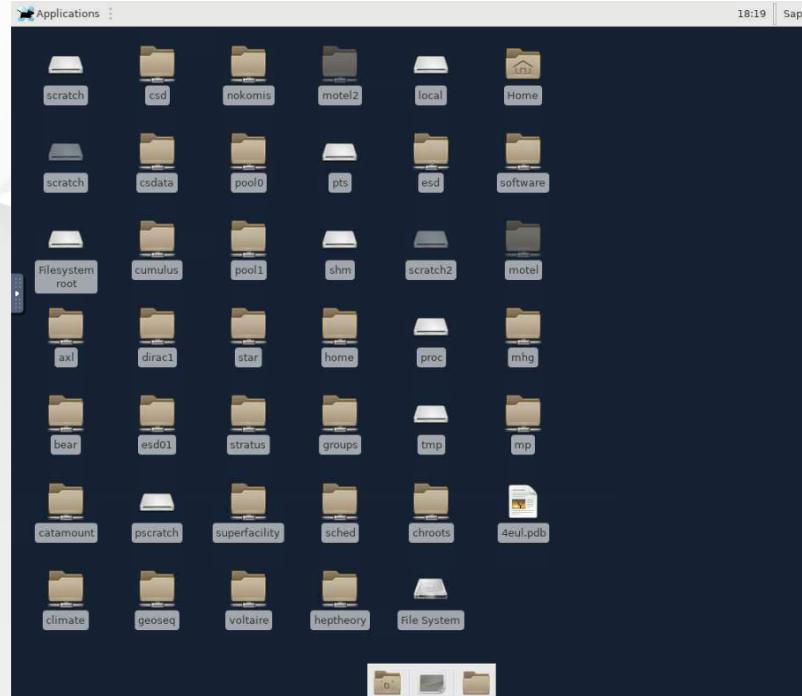
Image Quality

0 (low) to 9 (high)

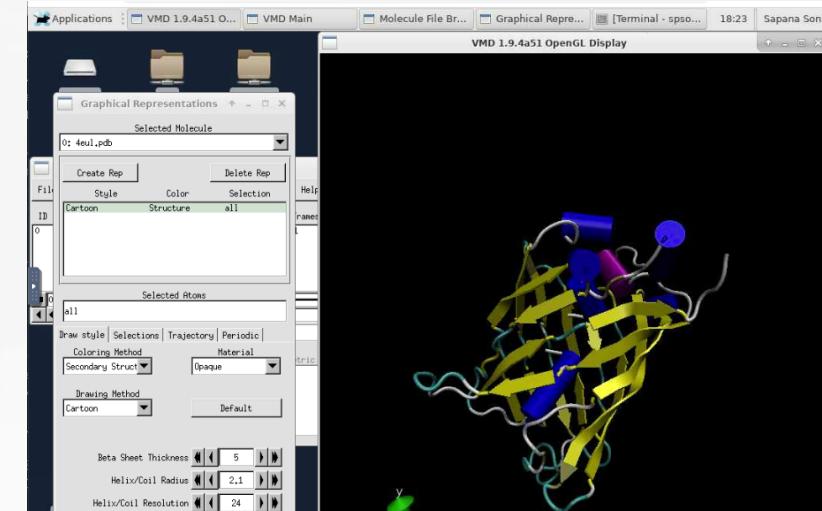
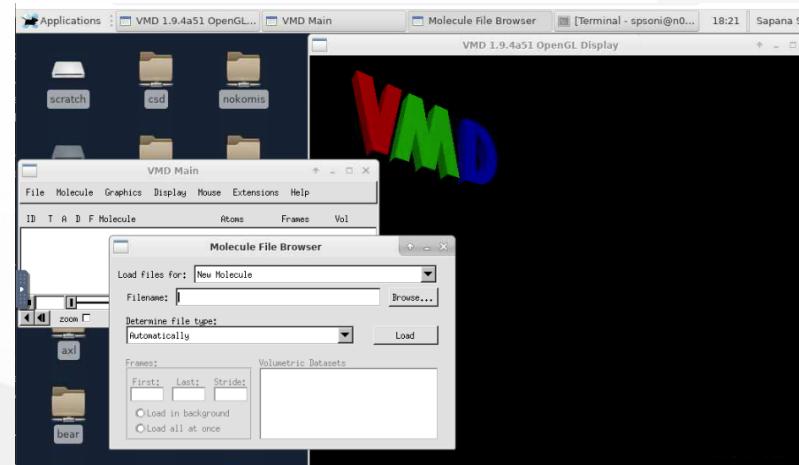
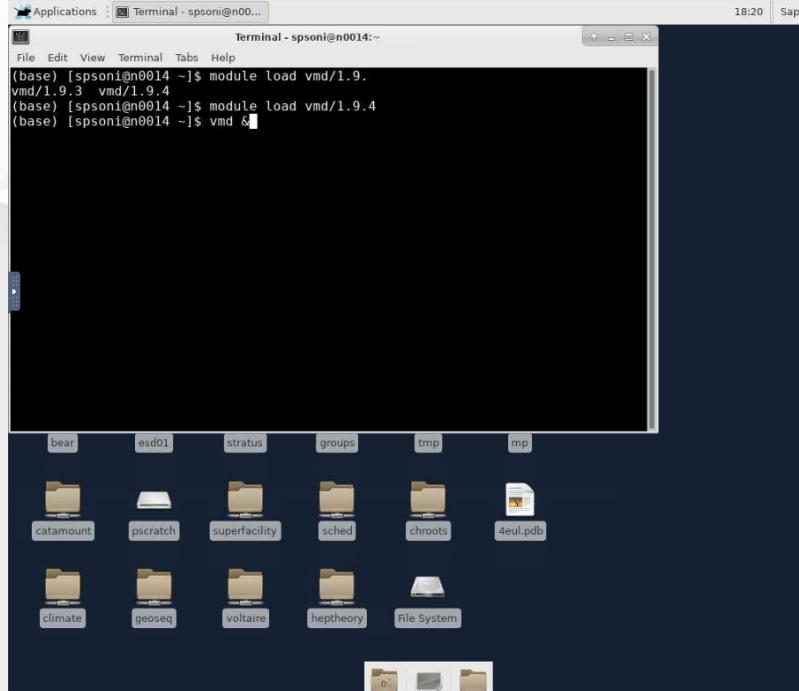
**Launch Desktop**

**View Only (Share-able Link)**

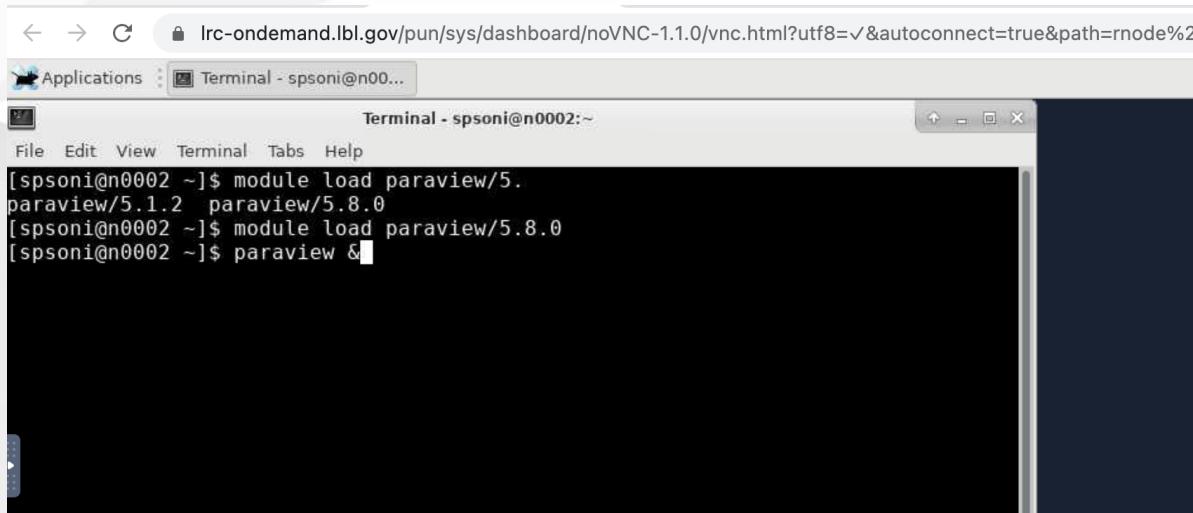
# Desktop



# Using Desktop to launch VMD

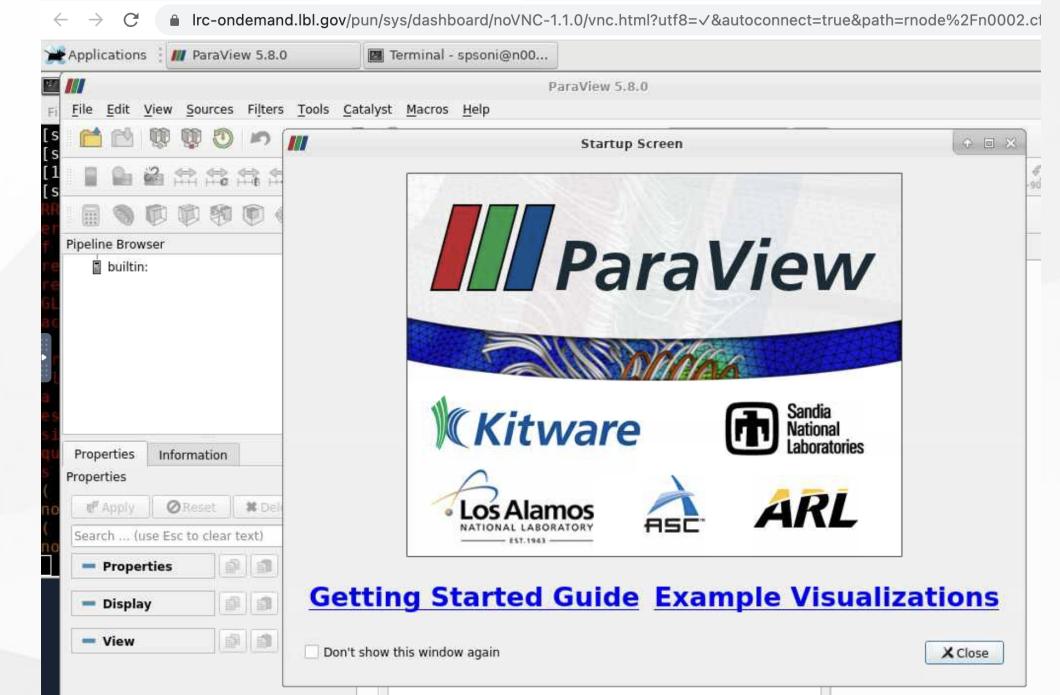


# Using Desktop to launch ParaView



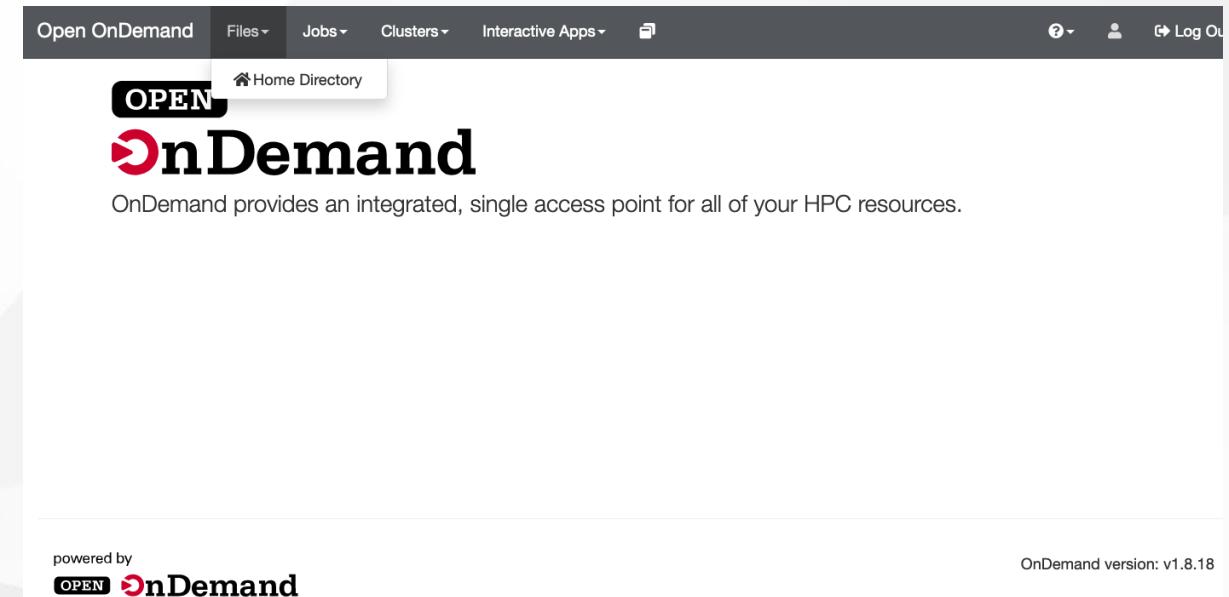
A screenshot of a terminal window titled "Terminal - spsoni@n002:~". The window shows the following command history:

```
[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 modified dates range from 05/17/2022 to 07/24/2022. The list includes: .., Desktop, OCEAN, R, bin, gcc-11.3.0, gdal-3.5.0, geos, geos-3.10.3, go, include, intel, julia-1.7.3, lib, lib64, libexec, libssh, libssh2, libssh2-0.9, myproject, and 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, there is a banner with the text "OPEN OnDemand". The main content area displays the message "OnDemand provides an integrated, single access point for all of your HPC resources." At the bottom left, it says "powered by OPEN OnDemand", and at the bottom right, it indicates "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 regarding computer system usage under contract with the U.S. Department of Energy. It states that the system may be monitored for security purposes and that unauthorized access is prohibited, subject to criminal and civil penalties under Federal Laws. It also mentions Public Laws 83-703 and 99-474. The notice concludes with a list of emergency contact information: 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>). Below this, there is a section about weekly office hours on Wednesdays starting July 24, 2019, and a request for virtual consultations at <https://sites.google.com/a/lbl.gov/hpc/getting-help>. 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 search 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" heading. A message states: "OnDemand provides an integrated, single access point for all of your HPC resources." In the center, there is a "Active Jobs" section with a sub-menu for "Job Composer". At the bottom, 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 "Active Jobs" and it says "Showing 1 to 1 of 1 entries". There is one entry listed:

| 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 right, there are buttons for "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

★ Create Template

### 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

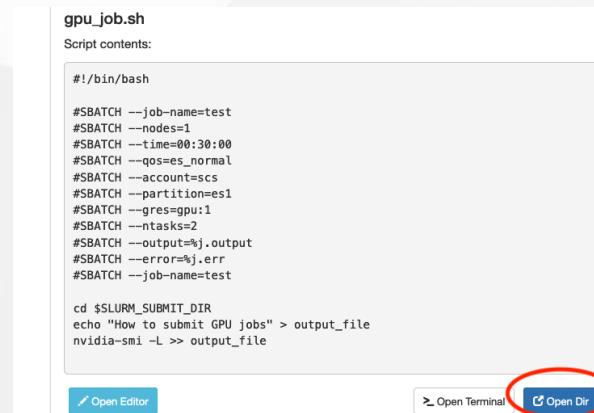
Open Terminal

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/*
```

# 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](#)

