

jsub (Open OnDemand)

Submitting a New Job

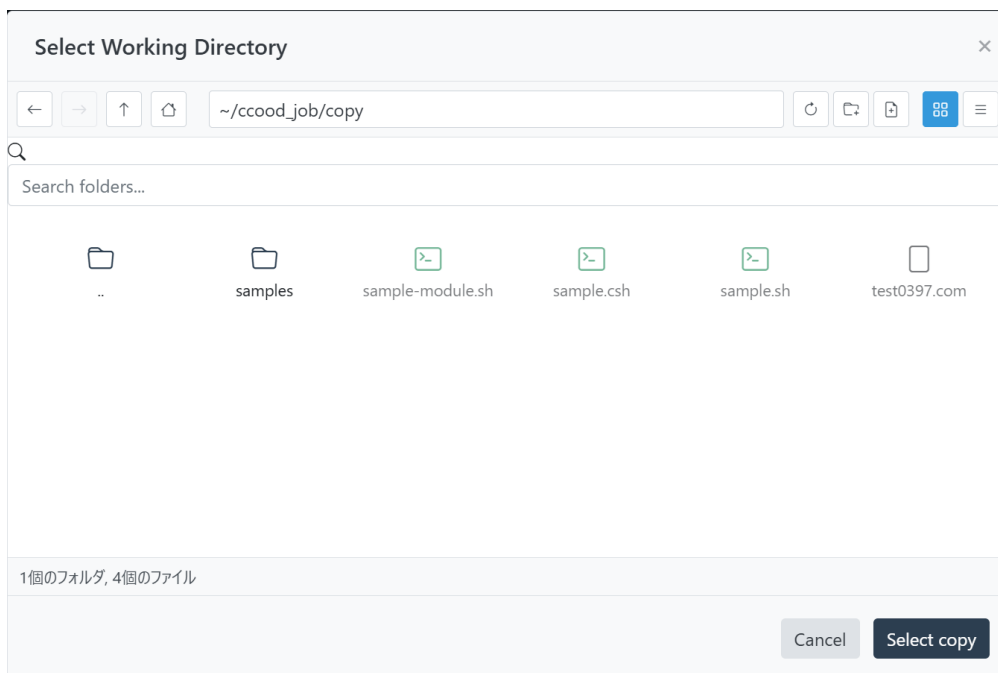
Submitting a new job involves the following three steps:


1. Data Preparation: Set the working directory and prepare input files
2. Script & Resource Settings: Select or edit the execution script and configure computational resources
3. Submission Confirmation: Review your settings and submit the job

Use the tabs at the top of the screen to switch between steps.

Data Preparation

Setting Working Directory



- Enter the path directly in the "Working Directory" field, or click the "Browse" button to select a directory
- To create a new directory, click the  button, enter a name, and click "Create".

Checking Disk Resources

The "Disk Resources" panel displays available disk capacity and usage.
Click "Refresh" to get the latest information.

Reviewing File List

The "File List" tab shows files and folders in the working directory.
Click the "Update List" button to refresh the contents.

File Upload

Drag & Drop Upload

Drag and drop files here or click to select (max 500MB)

The "File Upload" tab allows you to upload files from your local computer to the server.

1. Drag and drop files into the dashed area, or click to select files
2. Once upload is complete, files are automatically added to the file list

File Copy

The "File Copy" tab allows you to copy files from other locations on the server.

Destination:

~

Browse

Specify the path where selected files/folders will be copied

☒ Copy folder contents recursively

☐ Overwrite existing files

Execute Copy

Refresh

Home

Up

Current Location: /apl

Shortcuts

Home

Applications

Files

Filter...

abcluster

ABINIT-MP

aiida

alphafold

amber

aocc

aocl

apptainer

autoconf

autodock

autodock-gpu

autodock-vina

bio

boost

censo

1. Navigate to the source directory by clicking the left panel or double-clicking folders
2. Select the files or folders you want to copy
3. Enter the destination path in "Destination" or select using the "Browse" button
4. Select options as needed, such as recursive copy or overwrite.
5. Click the "Execute Copy" button

Script & Resource Settings

Selecting/Editing Execution Scripts

Script Content

Execution Script

Path to the script file to execute

```
#!/bin/sh
#PBS -l select=1:ncpus=18:mpiprocs=1:ompthreads=18
#PBS -l walltime=00:30:00

if [ ! -z "${PBS_O_WORKDIR}" ]; then
    cd "${PBS_O_WORKDIR}"
    WORK=/lwork/users/${USER}/${PBS_JOBID}/gaussian
else
    WORK=/gwork/users/${USER}/tmp.$$
fi

if [ ! -d ${WORK} ]; then
    mkdir ${WORK}
```

1. Enter the path directly in the "Execution Script" field, or click the "Browse" button to select a script file
2. To create a new script, click the "New" button

? Using the Script Editor

1. Click the "Edit in Editor" button to open the script editor
2. Make changes to the script and click "Save" to apply them
3. Click the "Refresh" button to reload the script content

Configuring Computational Resources

You can configure script resource settings in the right form:

- Job Type: Choose from Standard Computation, GPU Computation, or Large Memory
- Node Count: Number of nodes to use
- CPU Cores: Number of CPU cores to use (or select from "Core Preset" buttons)
- GPU Count: For GPU computation, number of GPUs to use
- Wall Time: Set the job's maximum runtime (HH:MM:SS format)
- MPI Processes: Number of MPI parallel processes
- OpenMP Threads: Number of OpenMP parallel threads

? Additional Options

Expanding the "Options" panel allows the following settings:

- Merge Standard Output and Error: Combine standard output and error into a single file
- No Rerun: Prevent automatic rerun of jobs in case of system failure

? Script Integration

- Load Settings from Script: Automatically load settings from PBS directives in the script
- Apply Settings to Script: Apply current settings to the script

Submission Confirmation and Execution

Options

? Setting Job Name

Enter a job identifier in the "Job Name" field.

If left blank, the script name will be used.

? Email Notification Settings

1. Check "Use Email Notifications"
2. Enter the notification email address (default is the address registered with RCCS)
3. Select notification timing (on start, on completion, on abnormal termination)

Reviewing Settings

The "Submission Confirmation" tab displays all settings configured so far.

Items to review:

- Data and work environment (working directory, execution script, job name)
- Resource settings (job type, node count, CPU cores, GPU count, execution time, etc.)
- Notification settings (output merge, email notifications)

Job Submission

1. Review the settings
2. If all settings are correct, click "Submit Job"
3. Upon successful submission, a confirmation message is displayed and a job ID is issued
4. You' ll be automatically redirected to the "Job List" screen, where your submitted job will appear.