INL/MIS-24-78521-Revision-1



# High Performance Computing User Group Meeting - June 12, 2024

June 2024

Stephanie J Parker, Ben Nickell, Shane T Grover, Bradlee Hope Rothwell, Matthew R Sgambati, Brandon S Biggs, Kit J Menlove, Scott M Serr, Trad Ryan Day, Kelly Anne Byrne, Jeremy Alexander Sharapov

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**June 2024**

**Idaho National Laboratory**
**Idaho Falls, Idaho 83415**

**http://www.inl.gov**

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**June 12, 2024**

Idaho National Laboratory

# High Performance Computing User Group Meeting

NSUF Nuclear Science User Facilities

# HPC User Group Meeting Agenda

- Bitterroot Updates and Release to Users
- SLURM
- Open OnDemand Upgrade
- Github Co-Pilot
- Grace-Grace architecture
- HPC Account Renewal System
- Storage Updates
- Sawtooth Updates
- Teton Updates
- Requesting RSICC Codes
- Trainings Supported by HPC


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# Bitterroot Status
# Hardware

- 384 Nodes
  - 336 nodes with 256 GB RAM
  - 48 nodes with 128 GB HBM
- 43,008 cores
- 200 Gb/s OmniPath network
- Dell C6620 4-in-2U Chassis as compute
- Dell R760 servers as logins and gateways
- Direct Liquid Cooled on-chip
- Will complement existing systems
- Release date of June 2024

Commodity Technology Systems-2 (CTS-2)

Deployed at LLNL & Sandia
Photo credit: Garry McLeod.



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# Bitterroot Status
# Images

- Imaging / Provisioning done with Warewulf4
  - Leverages Apptainer for image building
- Similar to Lemhi
  - Intel
  - OPA fabric
- Slurm
- Memory/Core (256/112 or 128/112)
  - Smaller in-memory image (HBM)
  - Larger image supporting X11 / Desktop

Commodity Technology Systems-2 (CTS-2)

Deployed at LLNL & Sandia
Photo credit: Garry McLeod.



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# Slurm for Bitterroot

- What is Slurm? (Simple Linux Utility for Resource Management)
  - A job schedule and resource management system similar to PBS
- Slurm is already in use on Hoodoo
- We plan to use Slurm on new clusters going forward
- Many PBS commands (like qstat) will continue to work

# Slurm for Bitterroot

- Submitting a batch job using Slurm

```
sbatch submission_script.slurm
```

- Simple way to start an interactive job

```
srun --nodes=1 --ntasks-per-node=112 --wckey=project_code --time=01:00:00
     --pty -I bash
```


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# Slurm for Bitterroot

PBS

```
#!/bin/bash
#PBS -N hello_world
#PBS -l select=1:ncpus=16
#PBS -l walltime=72:00:00
#PBS -j oe
#PBS -o $PBS_JOBNAME-$PBS_JOBID.log
#PBS -P project_code

cd $PBS_O_WORKDIR

module load mpich
mpiexec hello_world
```

Slurm

```
#!/bin/bash
#SBATCH --job-name "hello_world"
#SBATCH --nodes 1
#SBATCH --ntasks-per-node 16
#SBATCH --time 72:00:00
#SBATCH --output %x-%j.log
#SBATCH --wckey project_code

cd $SLURM_SUBMIT_DIR

module load mpich
mpiexec -n 16 hello_world
```

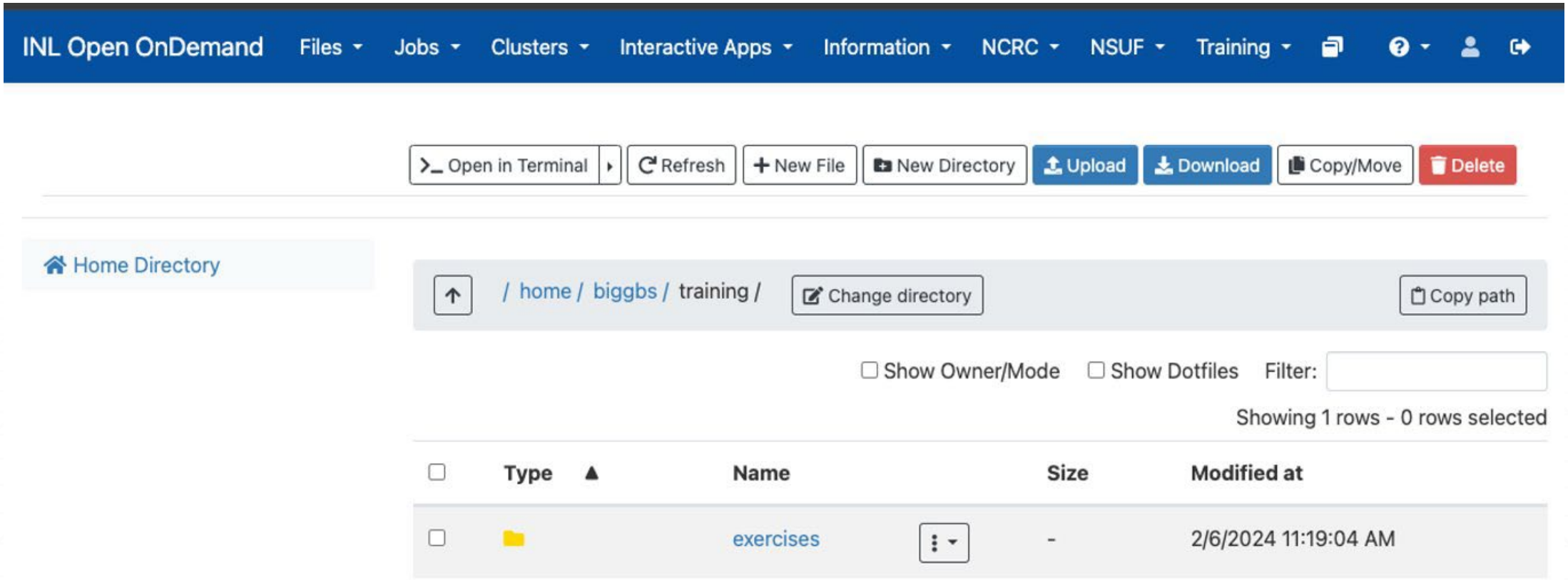
# Slurm for Bitterroot

- Some Slurm commands to be familiar with
  - squeue (shows listing of all currently queued jobs – similar to qstat)
  - scancel (cancels jobs, arrays or steps – similar to qdel)
  - sstat (status information on currently running jobs, including resource use)
  - sacct (tracks and reports job activity and resource usage)
- Stay tuned for upcoming training and documentation

# OnDemand Version Upgrade

- Upgrading from version 1.8 to 3.1
- New features
  - Support tickets
  - One click job submission
  - User profiles
  - Pinned applications
  - Updated files app
- Old functionality should remain

# New Files App





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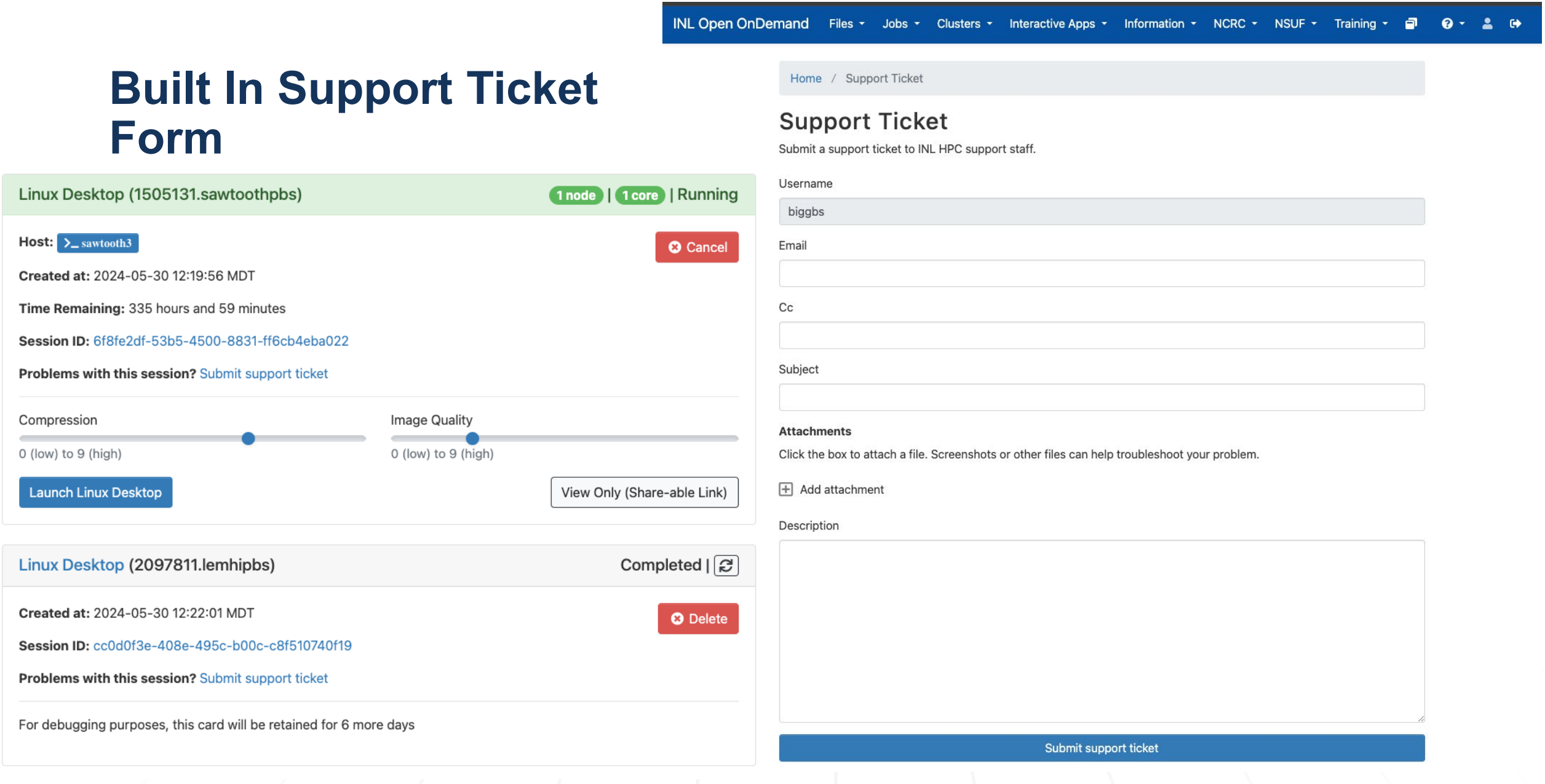
# Built In Support Ticket Form



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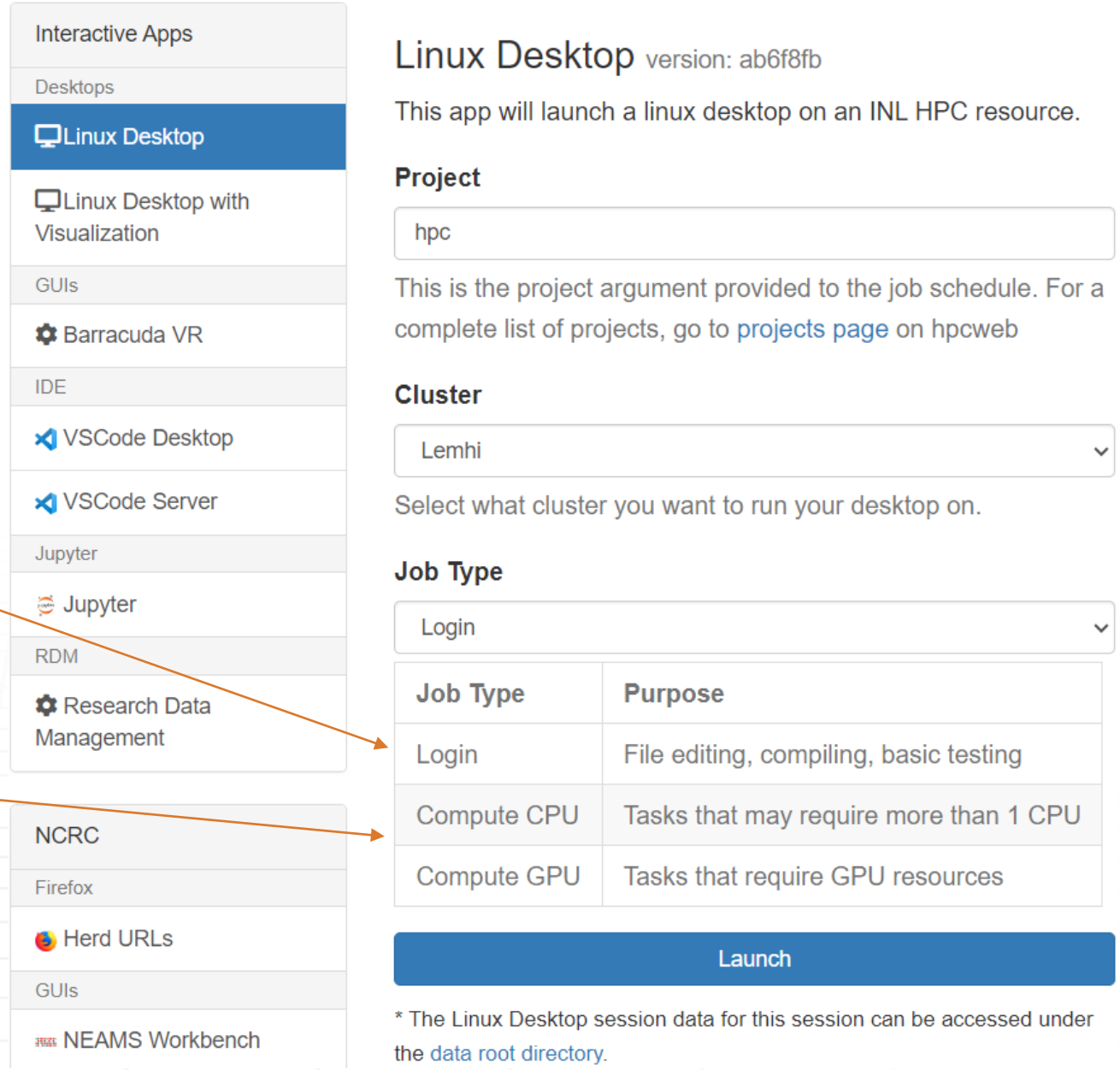
# Interactive Sessions Usage

- Please help us make good use of HPC resources!
- Feel free to leave a "Login"-type desktop session open for its duration.
- Please do not leave "Compute"-type sessions open and unused for significant periods of time.





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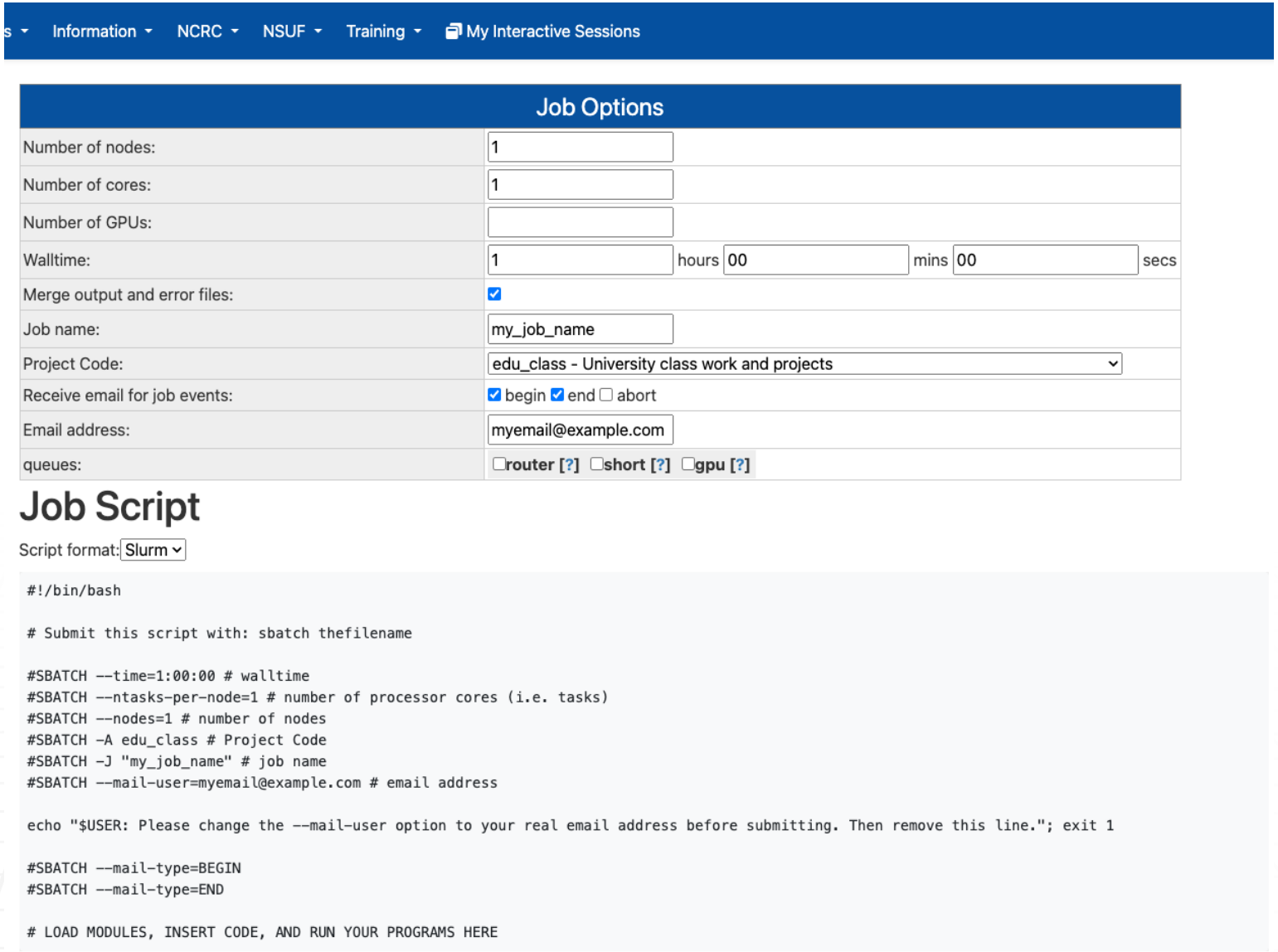
# Tool to Create Job Submission Scripts





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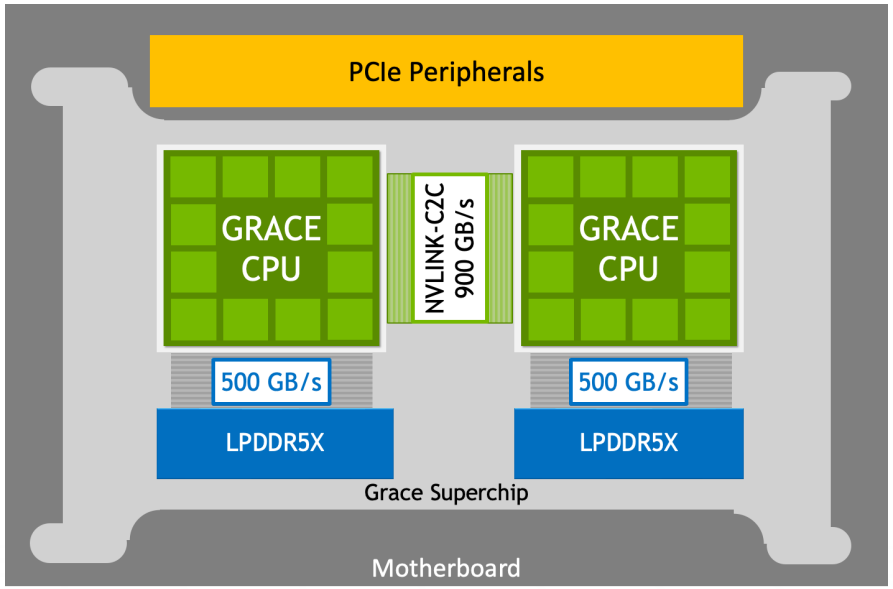
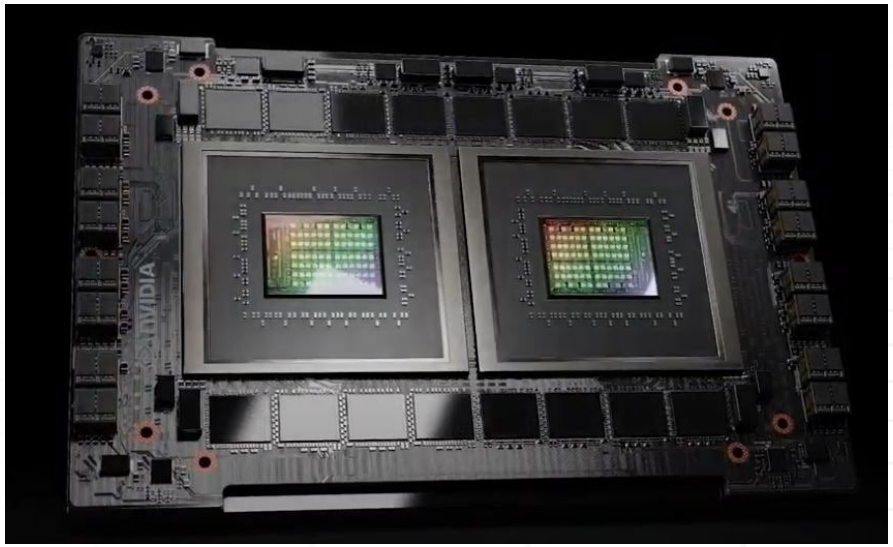
# Roadmap for Local GitHub CoPilot-like Tool

- Monitor feedback and resource utilization
- Support for Jetbrains IDEs
- Improved coding models

# Upcoming: Nvidia Grace-Grace

- The Grace-Grace superchip features dual Grace CPUs linked by a high-speed NVLink.
- Grace CPU
  - 480 GBs LPDDR5x memory with ECC
    - 1TB/s bandwidth
  - 144 Arm Neoverse V9 cores
- Total cores 288 and 960 GBs



What you need to know:

- We have acquired two grace-grace nodes, that will be available for testing in the near future. (Q4 2024)
- NOTE: Compilers greater impact performance
  - Upwards of 80% gains depending on the selected compiler

*product info pulled from Nvidia's publicly published information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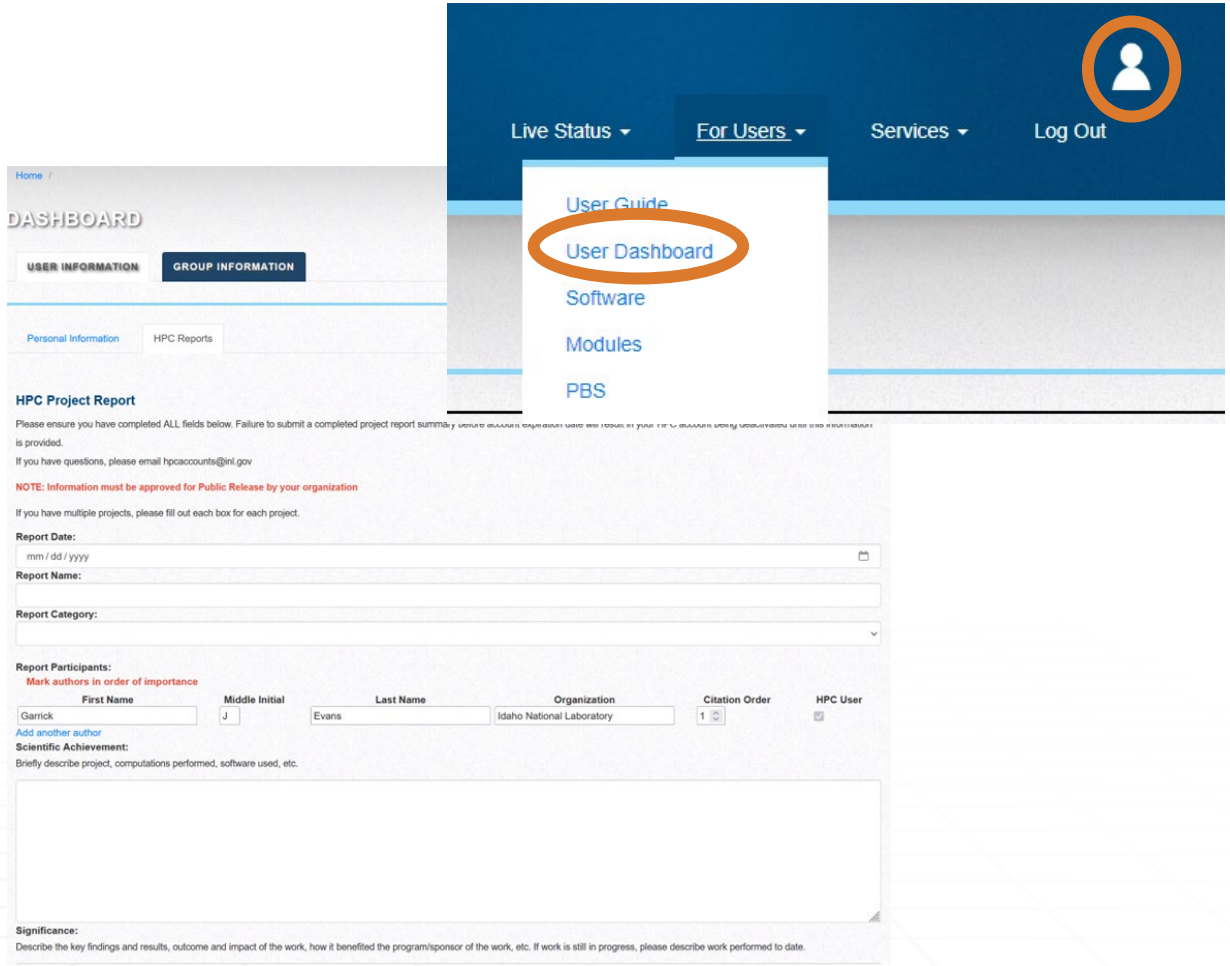
# HPC Account Renewal System

- New account renewal process for all external HPC users
  - INL employees can also fill out project report
- New authorship feature




## Steps to Renew

1. Receive an email saying that account is within 30 days of expiring
2. Go to the HPC Web Dashboard and fill out HPC Project Report
3. Report will be reviewed by a HPC Admin
4. Account will be extended for another year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# Isilon
# Home and Project space



- The Isilon is at **82%** full
  - At the current rate, the Isilon will be full by the end of the year
- The project space is taking **85%**
- Working on freeing up space
- New project space quotas
  - Newly created projects will have a 20TB quota
  - Previous projects will be given a 50TB quota
- Will work with project managers on projects over 50TB


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# IBM ESS
# Scratch

- Fast storage
- Scratch is available on all HPC systems
  - /scratch/<username>
- No quotas
- Files deleted after 90 Days

# Pure Flashblade Software stack

- New S200 Flashblade has been placed into production
- Faster hardware
- Five years support
- Easier upgrade paths


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# Sawtooth Update


- Renewed warranty on critical components for one year. (cooling, management, chassis, networking)
- Transition to INL support on compute nodes
  - Proactively filed cases on some potential failures
  - Currently only one of 2079 production compute nodes down
  - 4 tickets still open
- Anticipate additional component failures, primarily memory
  - Harder and more expensive to get DDR4 16GB RAM
  - Trying to procure and test more RAM
  - There are ~25,000 sticks of RAM in Sawtooth compute nodes
- Perhaps 1%-2% of nodes likely to fail and not be repaired in the next year
  - Repairs are time consuming
  - HPC staffing and personnel an issue
  - Time may be better spent making newer hardware available

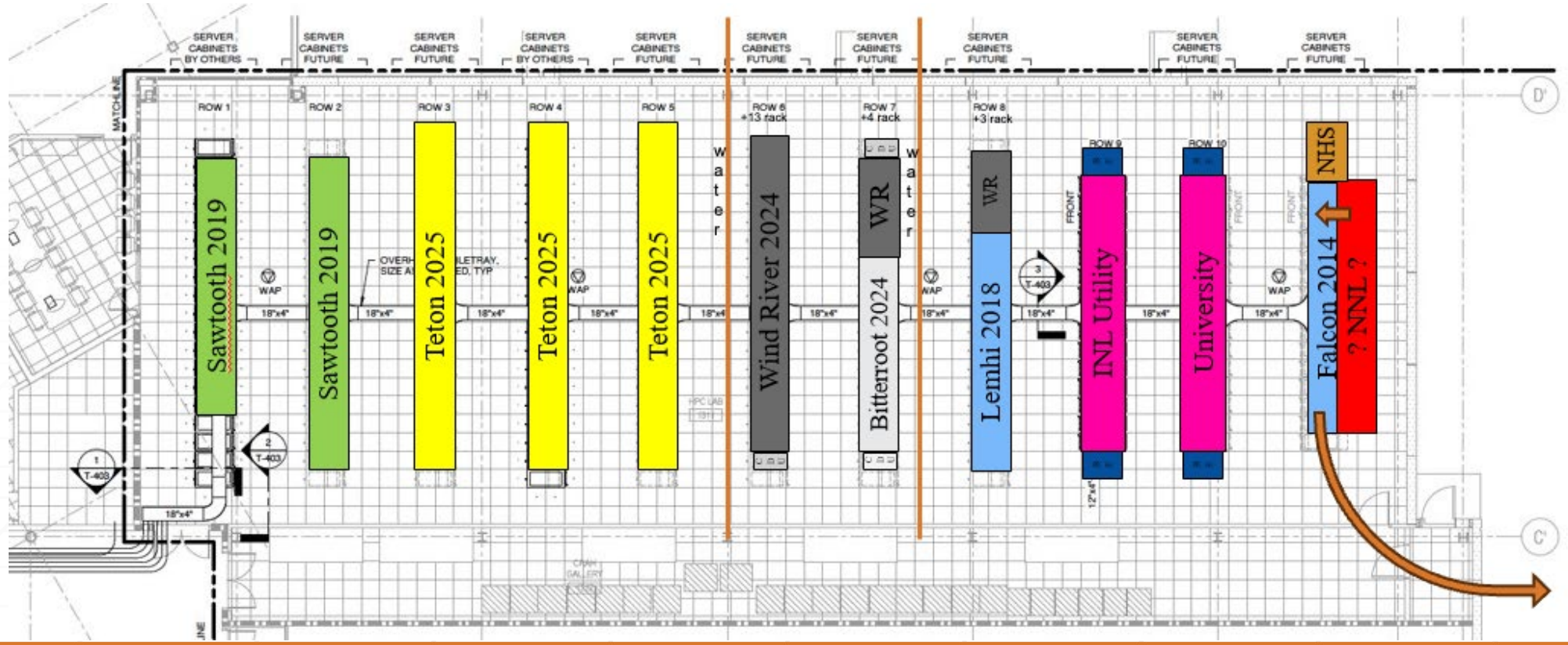
# Teton

Tetons from the Idaho side
Photo credit: Ben Nickell

- Next flagship INL HPC system
- Request for Proposals (RFP) is in progress
  - Hope to evaluate bids starting July 2024
- Targeting 400,000 cores at 2GB memory per core
- Fit within 3 rows in INL C3 data center
  - Power: 1.5 MW per row
- Target date: July 1, 2025
- INL HPC and purchasing worked for encourage competition among vendors to get the best possible system
  - Several vendors have indicated that they will be submitting a bid

# Wind River

- Possible INL purchased Dell CTS/2 - (6) Scalable Unit system – arriving late 2024
  - CTS/2 is ~200 nodes and 1.5 petaflops of computing power (per SU)
- Same hardware to Bitterroot, Intel Sapphire Rapids CPUs, w/o HBM nodes.
- 200GBps Cornelis Networks Omni-Path High Speed Interconnect
- 17.5 racks of compute nodes, direct to chip liquid cooling.





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# How to Gain Access to RSICC Codes on INL HPC Systems

- The Radiation Safety Information Computational Center (RSICC) at Oak Ridge National Laboratory is an information analysis center that collects, archives, evaluates, synthesizes and distributes information, data and codes that are used in various nuclear technology applications
- **Licensing:**
  - Register with RSICC and submit a request for code at: https://rsicc.ornl.gov/
  - Once a license is obtained from RSICC, go to the Request History link on RSICC's Customer Service homepage
  - Click on the "**Request History**" link and enter your RSICC Pass Number and Password
  - Once you verify the information is correct, an email will be sent to the address listed in your account
  - Forward this email to INL HPC at hpcsupport@inl.gov, indicating the package(s) to which you want access
  - INL HPC will review and grant access to requested code(s) on INL HPC systems
    - Affiliation on RSICC history must match affiliation for INL HPC account

**Example RSICC History Email:**

**From:** pdc@ornl.gov <pdc@ornl.gov>
**Date:** Wednesday, June 12, 2024
**To:** User's Email Address
**Subject:** RSICC User Software/Data History

Our records indicate the following software/data packages have been requested and received from RSICC. If this is incorrect, please contact RSICC at: (865)574-6176 or email pdc@ornl.gov.

Date Requested: 6/12/2024
Customer ID: xxxxx
Request Number: xxxxxx
Name: User's Full Name
Installation Name: USER'S AFFILIATION, UNITED STATES – This software is only valid for use while associated with this installation.
Software Package ID: C00834 MNYCP 07
Software Package Name: SCALE 6.2.4-EXE T

- **IMPORTANT:**
  - RSICC codes are only allowed to be accessed while located in United States. If plans to travel abroad, please contact INL HPC team at hpcsupport@inl.gov to remove access to codes while on travel.
  - RSICC code is only valid for use while associated with affiliation listed on RSICC history

# INL Nuclear Codes Available for License via the NCRC

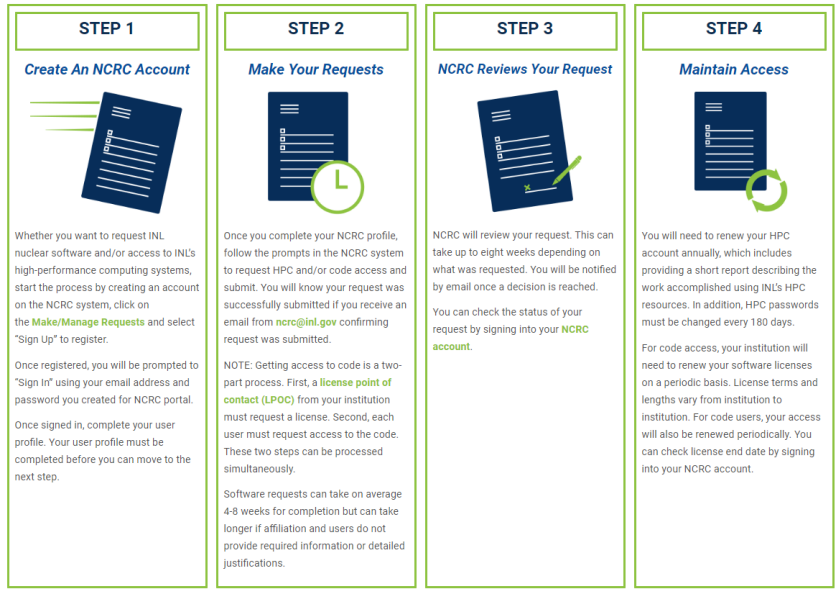
## Available for License

- BISON
- BLUECRAB
- DIREWOLF
- GRIFFIN
- GRIZZLY
- MARMOT
- RELAP5-3D
- RELAP-7
- SOCKEYE
- PRONGHORN

## Other Available Codes (Non-INL Licensed)

- SAM

- The Nuclear Computational Resource Center (NCRC) distributes several Nuclear Energy Advanced Modeling and Simulation (NEAMS)-developed applications.
  - 10 INL-licensed software tools require a license by INL to be used by researchers
  - 1 non-INL licensed software tool (SAM) requires a license by Argonne National Laboratory to be used by researchers
- To request access to INL Nuclear codes, go to NCRC portal: https://inl.gov/ncrc/



**STEP 1**

*Create An NCRC Account*

Whether you want to request INL nuclear software and/or access to INL's high-performance computing systems, start the process by creating an account on the NCRC system, click on the **Make/Manage Requests** and select "Sign Up" to register.

Once registered, you will be prompted to "Sign In" using your email address and password you created for NCRC portal.

Once signed in, complete your user profile. Your user profile must be completed before you can move to the next step.

**STEP 2**

*Make Your Requests*

Once you complete your NCRC profile, follow the prompts in the NCRC system to request HPC and/or code access and submit. You will know your request was successfully submitted if you receive an email from **ncrc@inl.gov** confirming request was submitted.

NOTE: Getting access to code is a two-part process. First, a **license point of contact (LPOC)** from your institution must request a license. Second, each user must request access to the code. These two steps can be processed simultaneously.

Software requests can take on average 4-8 weeks for completion but can take longer if affiliation and users do not provide required information or detailed justifications.

**STEP 3**

*NCRC Reviews Your Request*

NCRC will review your request. This can take up to eight weeks depending on what was requested. You will be notified by email once a decision is reached.

You can check the status of your request by signing into your **NCRC account**.

**STEP 4**

*Maintain Access*

You will need to renew your HPC account annually, which includes providing a short report describing the work accomplished using INL's HPC resources. In addition, HPC passwords must be changed every 180 days.

For code access, your institution will need to renew your software licenses on a periodic basis. License terms and lengths vary from institution to institution. For code users, your access will also be renewed periodically. You can check license end date by signing into your NCRC account.

# Trainings Supported by INL HPC

- Availability and access to training on Nuclear Energy Advanced Modeling and Simulation (NEAMS) code is instrumental to continued adoption and refinement of capabilities
- INL HPC staff, in collaboration with NCRC staff, have supported **16** external training sessions and workshops between December 2022 – June 2024 that required HPC access to provide hands on exercises using NEAMS codes for attendees.
  - HPC staff created a HPC account for each attendee, setup the OnDemand app, and scheduled a reservation to meet the requirements for each training
  - HPC staff were made available throughout the training sessions to assist with HPC-related questions from meeting organizers and attendees
- Training opportunities, such as these, promote the development of national computational science expertise

| Date: | Training Supported by INL HPC: |
|---|---|
| December 2022 | Bison Training |
| 27-28 June 2023 | Bison Training |
| 18 July 2023 | Rolls Royce Workshop |
| 16-17 August 2023 | Bison Training for X-energy |
| 23-27 October 2023 | 2023 IAEA Lise Meitner Programme 2 (LMP2) |
| 7-8 November 2023 | Bison Training for BWXT |
| 4-8 December 2023 | International RELAP5-3D User Group Meeting (IRUG) |
| 11 December 2023 | Griffin Training - NRC |
| 18 December 2023 | SAM Training - NRC |
| 16-19 January 2024 | Bison Fuels Performance Training @MIT January |
| 18 January 2024 | SAM Training - NRC |
| 6-7 February 2024 | Canadian Nuclear Laboratories (CNL) Bison Training |
| 21 April 2024 | ART/NEAMS M&S Pebble Bed Reactors |
| 21 April 2024 | ART/NEAMS M&S Molten Salt Reactors |
| 6-8 May 2024 | NRC Griffin/Pronghorn Training GC-PBR |
| 16 June 2024 | NEAMS Griffin Neutronics Fast Reactor Modeling and Simulation |

# Next HPC User Group Meeting

- Wednesday, September 11, 2024
- HPC team will send out dial-in information closer to meeting date

# Questions

- Please type your questions into chat