INL/MIS-24-77636

17 April 2024

Idaho National Laboratory

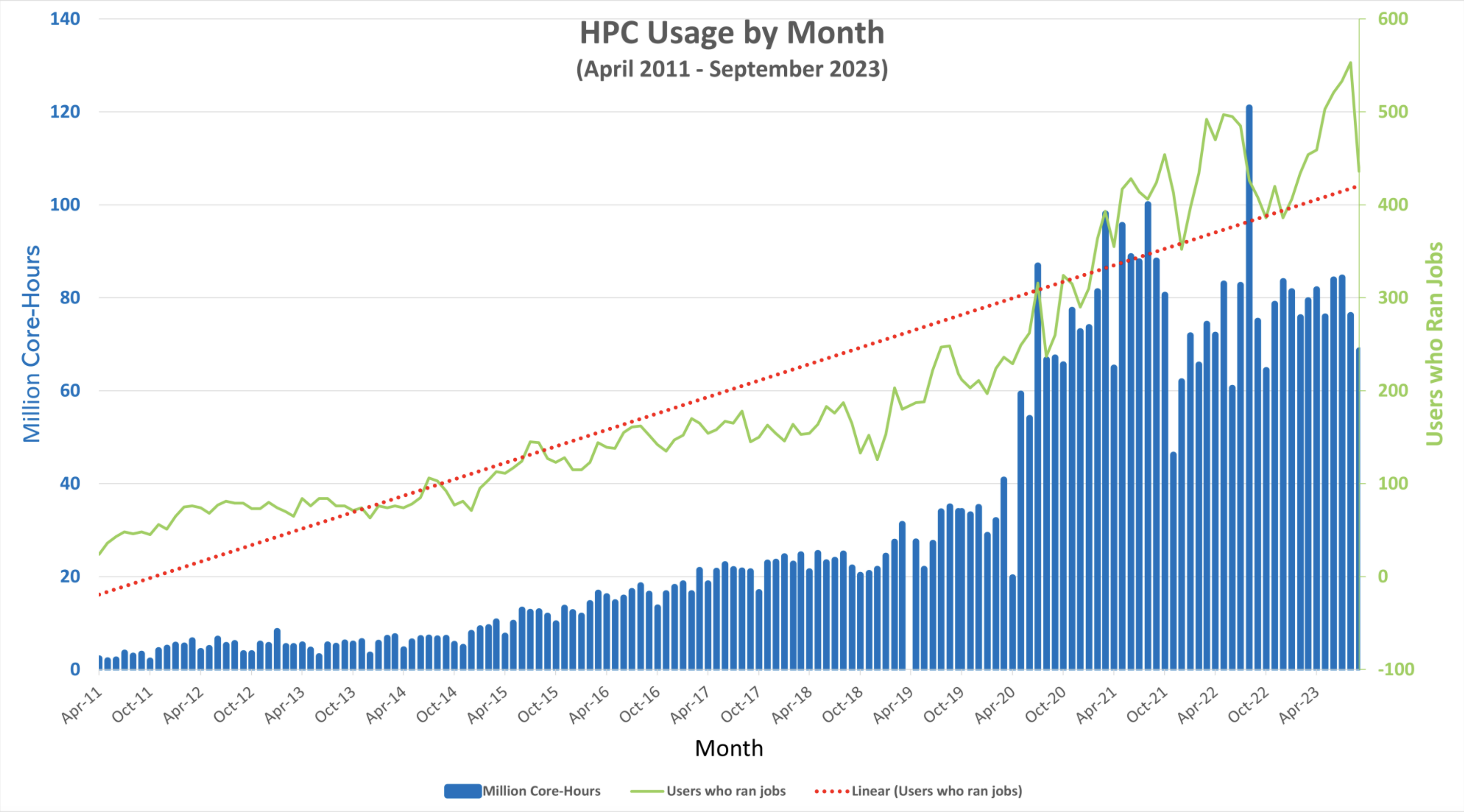
High Performance Computing Accomplishments

Nuclear Science User Facilities

HPC: Expanding computational research capabilities:

- Investing in scientific computing capacity
- Developing and validating innovative modeling tools
- Supporting data science gateways
- Supporting innovative software container strategies
- Expanding expertise in machine learning, artificial intelligence, advanced visualization, large-scale data processing and analytics

NSUF HPC Trajectory

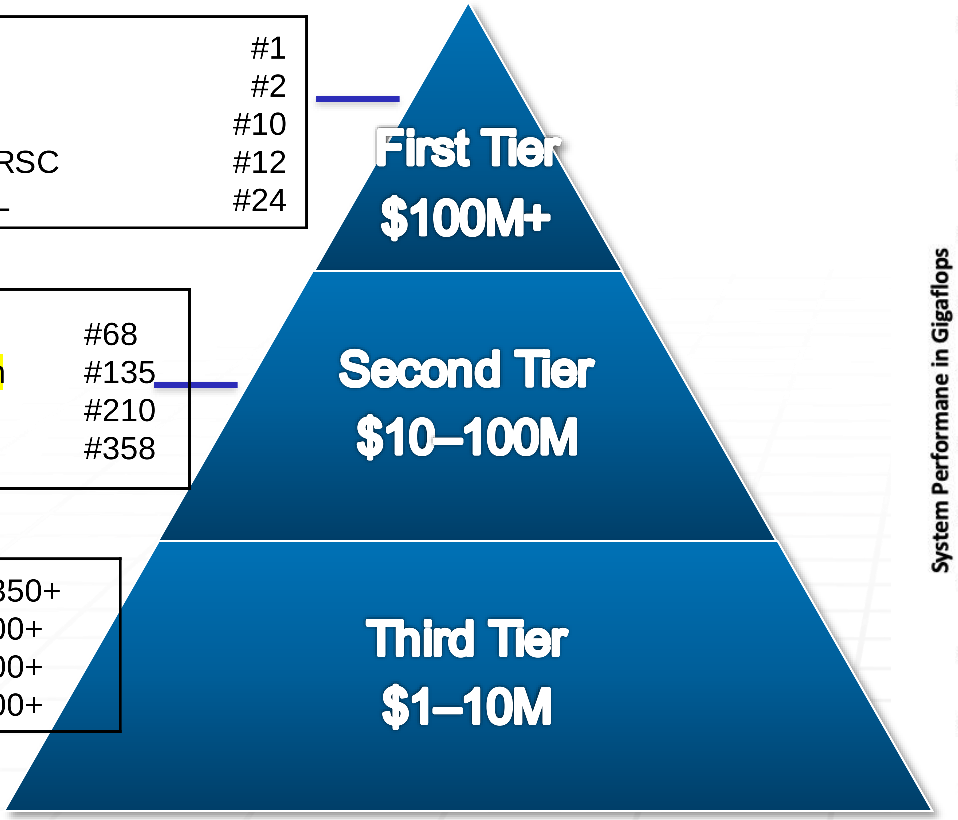


DOE Ecosystem – HPC Trends – INL positioning

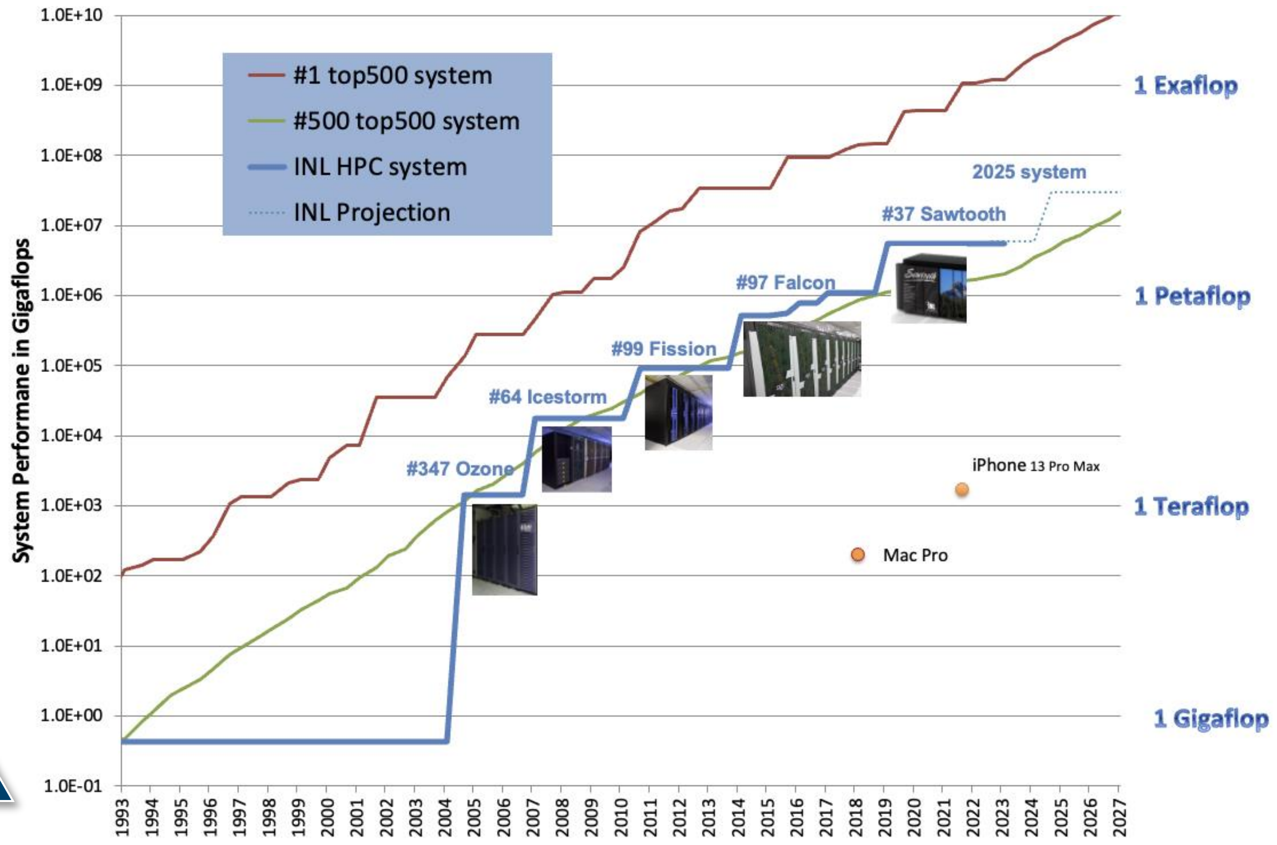
ORNL	#1
ANL	#2
LLNL	#10
LBNL/NERSC	#12
LANL/SNL	#24

NREL	#68
INL Sawtooth	#135
NETL	#210
PNNL	#358

INL Bitterroot	~#350+
INL Lemhi	#500+
Bettis	#500+
Knolls	#500+



November 2023 Top500 Rankings



Continual updates are required: ~20–30PF for 2025 system

High Performance Computing Resources

- NSUF HPC systems support a wide range of users and programs as a shared-use resource for national laboratories, universities, and industry
- Bitterroot (2024)
  - 374 nodes, 41,888 cores
  - Powered on 16 April 2024
- Sawtooth (2020)
  - 6 Petaflops performance
  - 2,079 compute nodes, 99,972 compute cores
  - #37 on November 2019 TOP500 list
  - Open for users: 17 March 2020
- Lemhi (2018)
  - 1 Petaflop performance
  - 504 compute nodes, 20,160 compute cores
  - #427 on November 2018 TOP500 list
  - Open for users: 28 Feb 2019

A right-sized solution for DOE Nuclear Energy research and development

Bitterroot

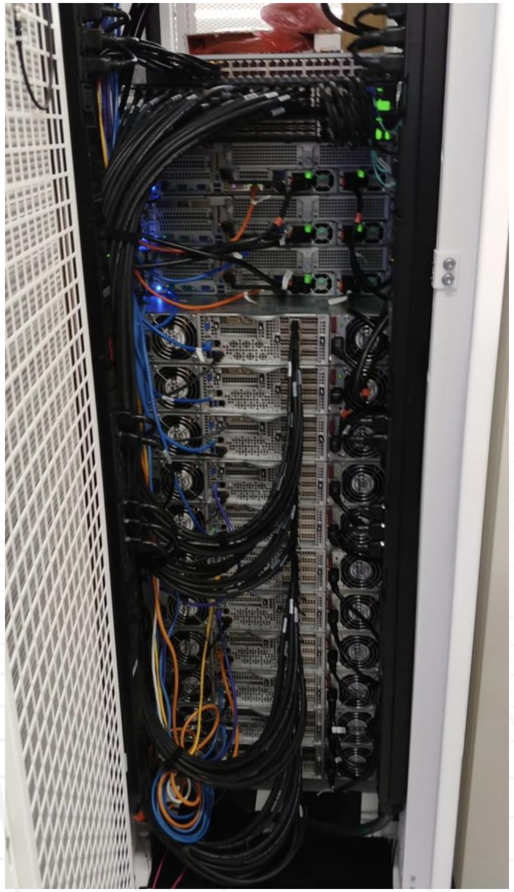
Sawtooth

Lemhi

Artificial Intelligence and Visualization Systems

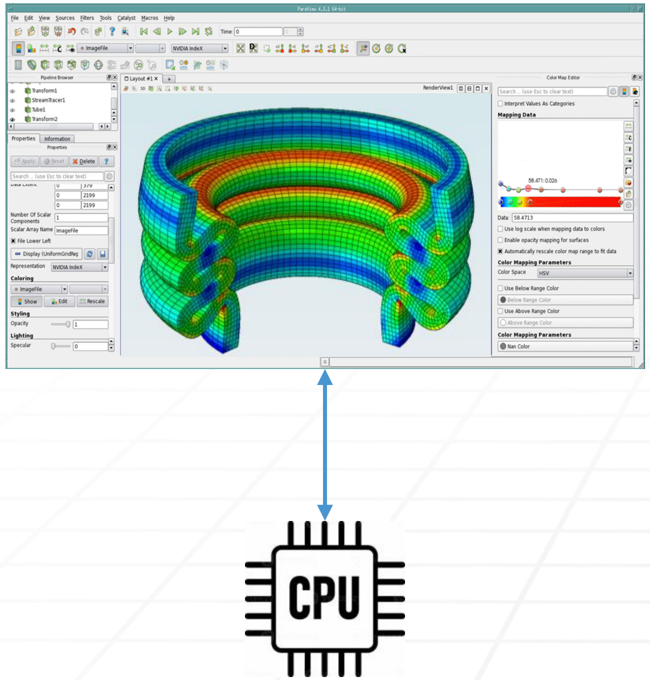
- HPC systems also support artificial intelligence and visualization specific systems:
- Hoodoo
  - 44 A100 GPUS
  - Open for users: 2 Feb 2021
  - Expanded to 116 A100 GPUs
  - Expansion open to users: 15 Jan 2024
- Viz
  - 9 Compute nodes; 864 cores; 2 TB/node
  - 18 A40 48GB GPUs
  - Open to users: 15 Dec 2023

Hoodoo

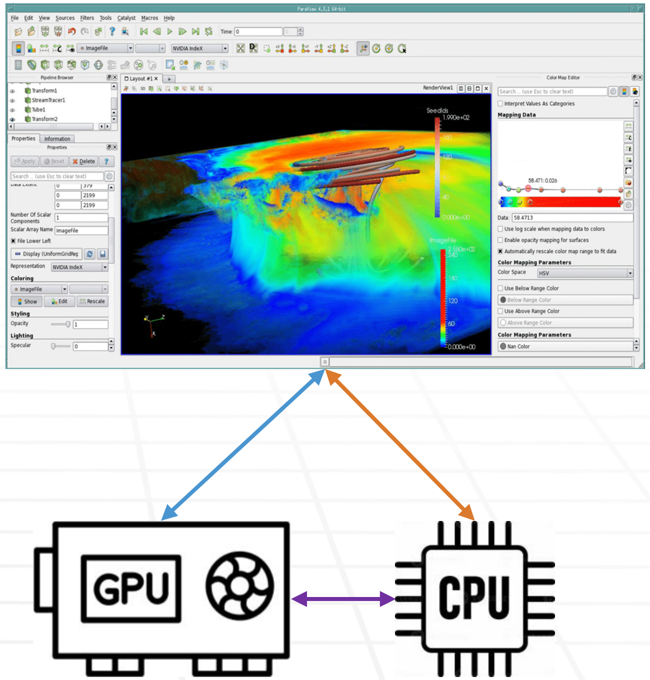


INL Open OnDemand (HPC OnDemand and OnDemand) Desktop vs. Desktop with Visualization

Desktop



Desktop with Visualization



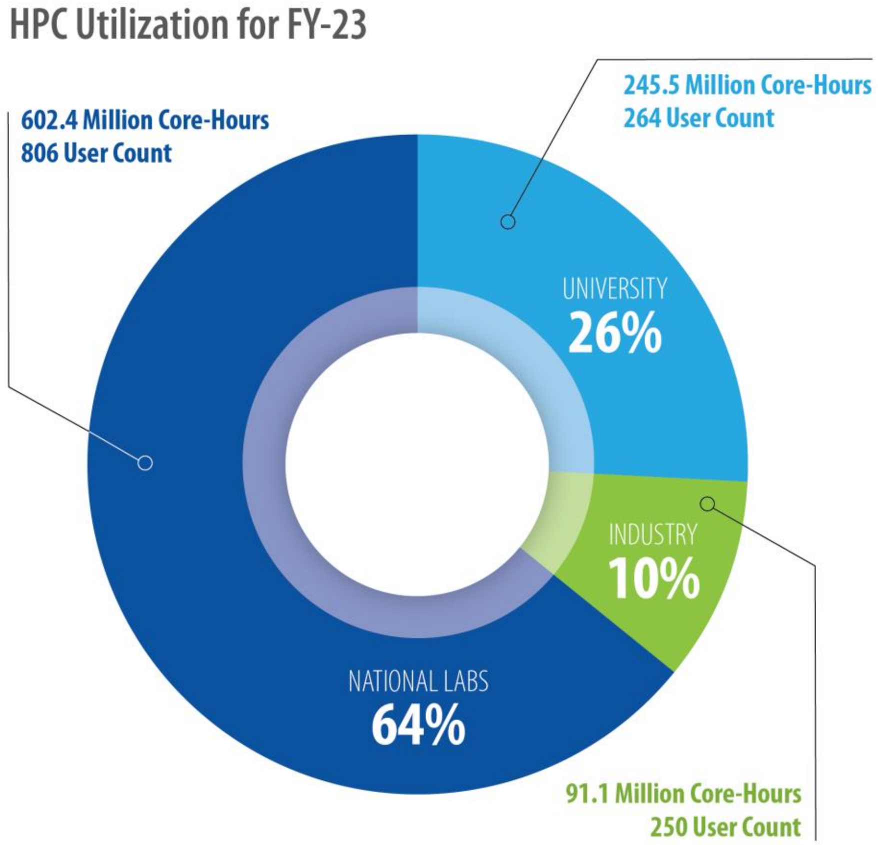
Bitterroot
Bridge to Teton

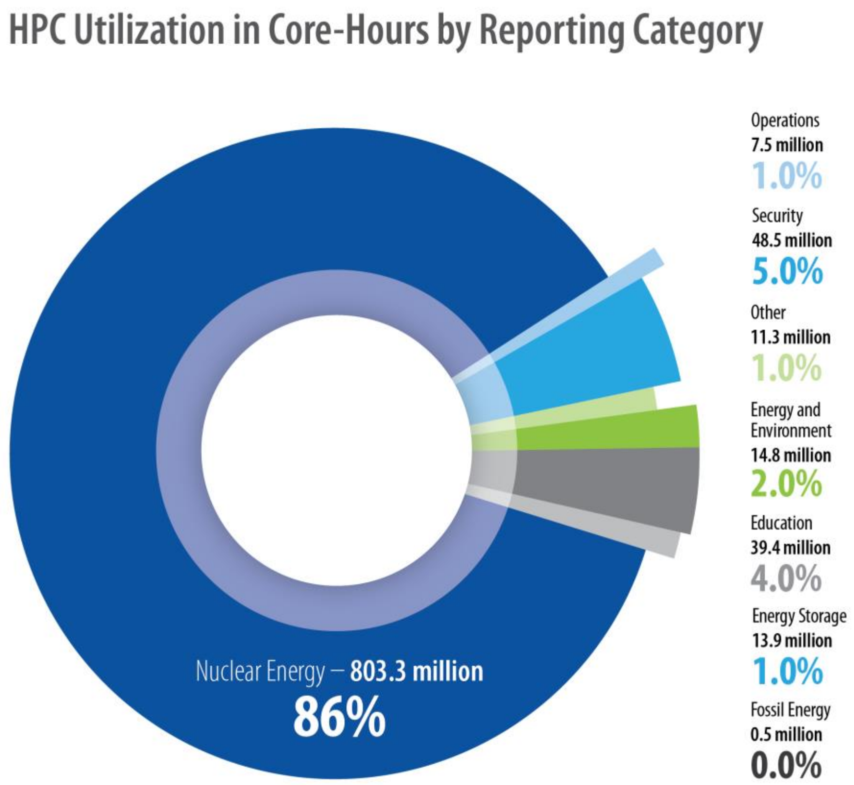
- 384 Nodes
  - Node specs
    - 2 Sapphire Rapids 56 core CPUs
    - 256 GB RAM
  - 48 nodes with HBM
- 41,888 cores
- 200 Gb/s OmniPath network
- Will complement existing systems (Sawtooth, Lemhi, Hoodoo, Viz)
- Expected power-on 16 April 2024
- Release date target of June 2024

Commodity Technology Systems-2 (CTS-2)
Deployed at LLNL & Sandia
Photo credit: Garry McLeod.

HPC User Statistics

- **In FY-23:**
  - Total number of users: **1320**
  - Million Core-Hours Delivered: **939**





Institutions with largest number of users

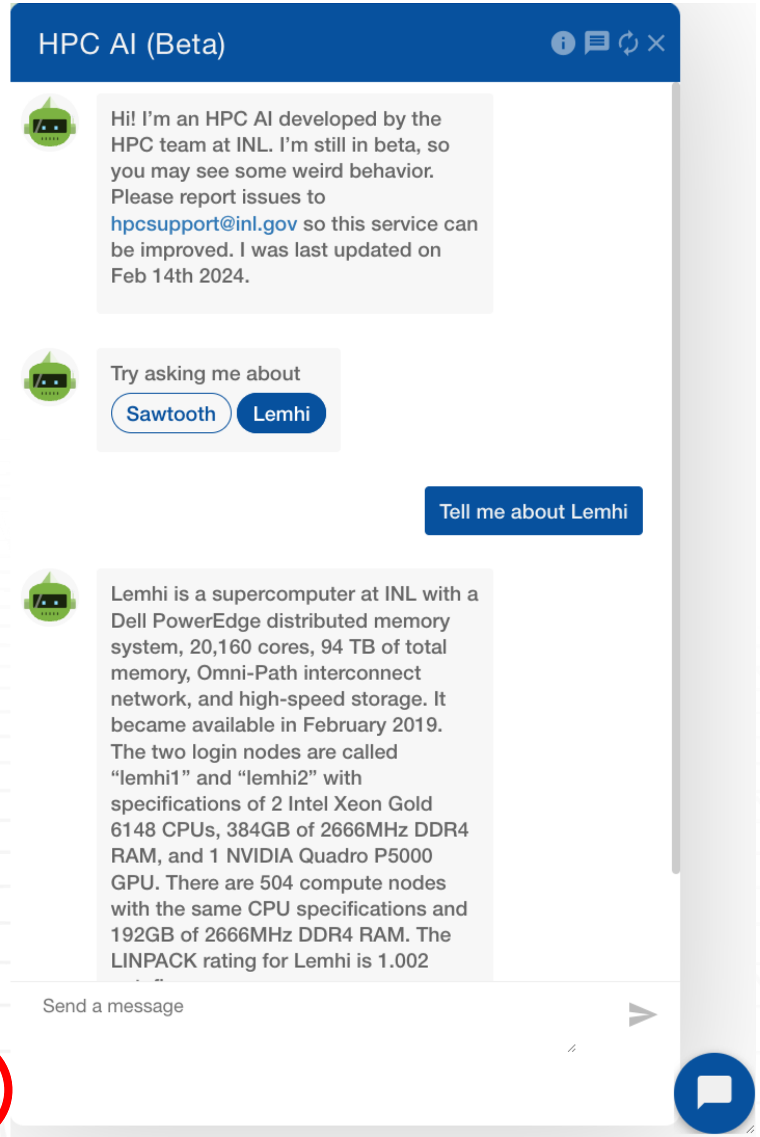
Institution	User Count	Million Core-Hours
Idaho National Laboratory	405	481.4
Naval Nuclear Laboratory	86	23.2
Argonne National Laboratory	32	22.2
MPR Associates	27	20.9
Oak Ridge National Laboratory	25	66.5
Westinghouse Electric Company	22	16.8
North Carolina State University	22	97.6
University of Tennessee Knoxville	16	11.0
Texas A&M University	14	12.2
Georgia Institute of Technology	14	2.6
Pennsylvania State University	13	2.6
Nuclear Regulatory Commission	12	19.0
University of Wisconsin-Madison	12	6.2
Idaho State University	10	5.2
Oregon State University	10	9.6
Massachusetts Institute of Technology	10	15.1
TerraPower	9	3.3
Los Alamos National Laboratory	9	6.0
University of Idaho	8	17.6
Rolls-Royce	8	0.0
University of Michigan	7	1.8
University of Illinois Urbana-Champaign	6	2.1
Boise State University	6	7.6
BWX Technologies, Inc	6	3.4
Radiant Industries Incorporated	5	1.8
FPoliSolutions LLC	5	0.0
Analytical Mechanics Associates	5	2.3
University of Florida	5	18.4
Purdue University	4	1.0
The Ohio State University	4	0.0
University of Mississippi	4	11.3
Virginia Commonwealth University	4	9.8

Supported Trainings:

FY-24 Trainings using HPC Resources		
10/01/2023 - 09/30/2024		
Date:	**Training Name:**	**Participant Count:**
23-27 October 2023	2023 IAEA Lise Meitner Programme 2 (LMP2)	33
7-8 November 2023	Bison Training for BWXT	18
4-8 December 2023	International RELAP5-3D User Group Meeting (IRUG)	84
11 December 2023	Griffin Training - NRC	29
18 Decemebr 2023	SAM Training - NRC	29
16-19 January 2024	Bison Fuels Performance Training @MIT January	31
18 January 2024	SAM Training - NRC	24
6-7 February 2024	Canadian Nuclear Laboratories (CNL) Bison Training	11
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	
16-17 July 2024	SHIFT/NEAMS (SCALE-NEAMS) Training	

Chatbot

- HPC deployed an LLM using HPC documentation
- Available in Open OnDemand (https://ondemand.hpc.inl.gov) and (https://hpcondemand.inl.gov)



AI VSCode Plugin

- Local GitHub Copilot like tool

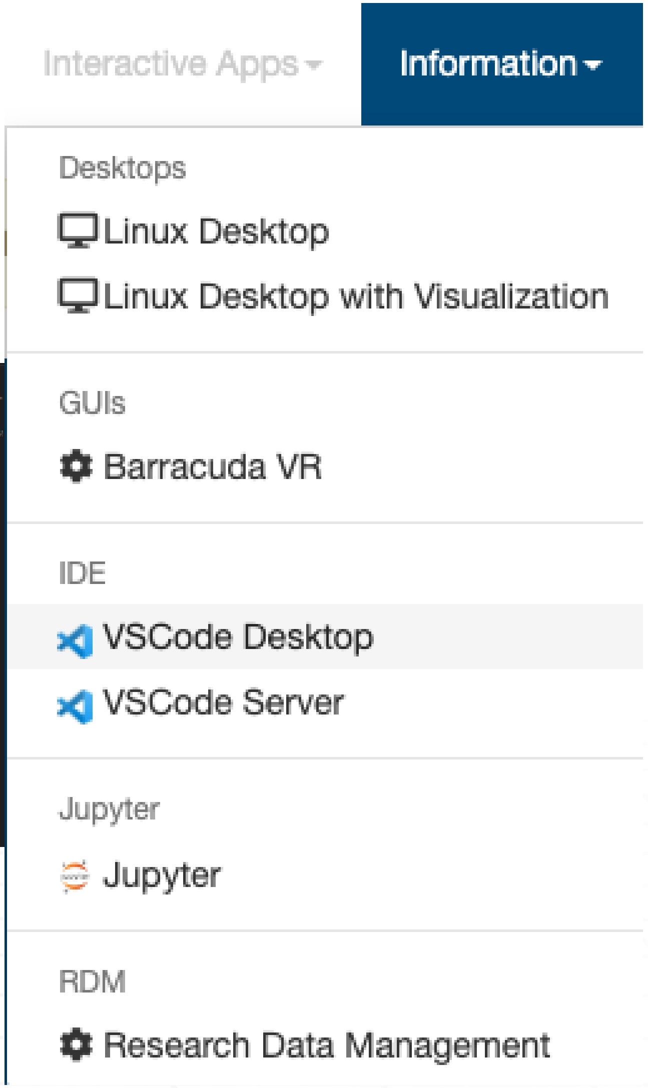
```
hello.py
Accept ⌷ | Reject ⌷ | (^⇧↩/^⇧⌫ to accept/reject all, ^⇧L to retry)
Sure! Here's the code you requested:

Accept ⌷ | Reject ⌷
```python
from fastapi import FastAPI

app = FastAPI()

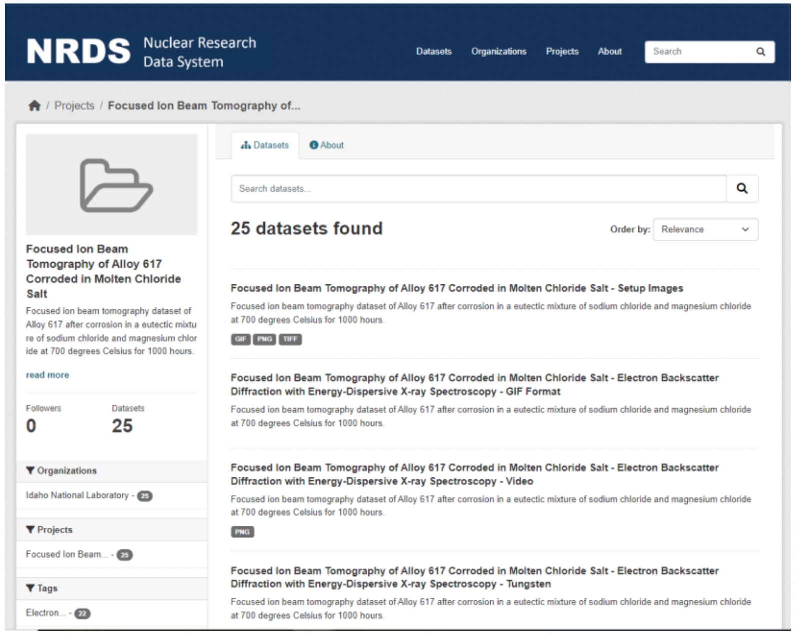
@app.get("/")
def read_root():
    return {"Hello": "World"}

@app.get("/items/{item_id}")
def read_item(item_id: int, q: str = None):
    return {"item_id": item_id, "q": q}
```


```

NRDS
https://nrds.inl.gov

- Place for data to be:
  - Publicly available
  - FpAIRe
    - Findability
    - Peekable
    - Accessibility
    - Interoperable
      - Stored close to HPC systems
    - Reusable
    - Extensible



Additional Info

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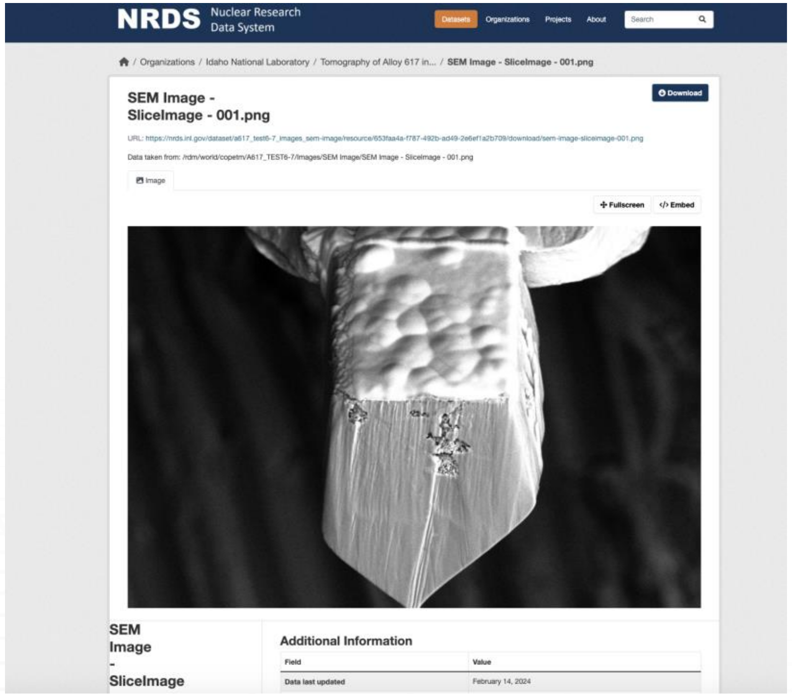
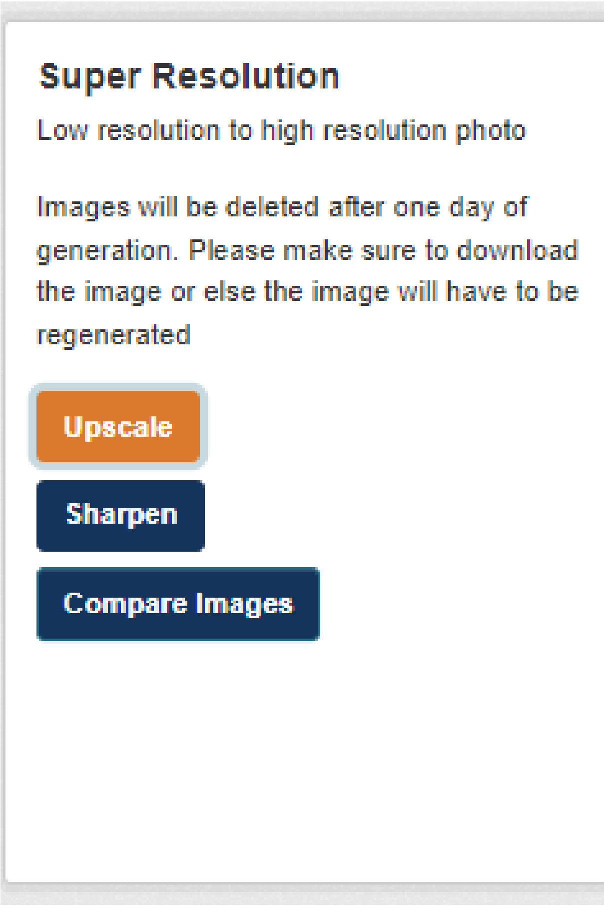
Author	Trishelle Copeland-Johnson
Last Updated	February 27, 2024, 2:04 PM (UTC-07:00)
Created	February 7, 2024, 10:31 AM (UTC-07:00)
OSTI	
DOI Link	https://doi.org/10.48806/2287679
Instrument	FEI G4 Helios Hydra Plasma-FIB
Publication	Copeland-Johnson TM, Murray DJ, Cao G and He L (2022) Assessing the interfacial corrosion mechanism of Inconel 617 in chloride molten salt corrosion using multi-modal advanced characterization techniques. Front. Nucl. Eng. 1:1049693. doi: 10.3389/fnuen.2022.1049693
Slice Offset	100 nm
Statement of Credit	"Focused ion beam tomography of Alloy 617 corroded in molten chloride salt" by Trishelle Copeland-Johnson and Daniel J. J. Murray is licensed under CC BY 4.0 for distribution.

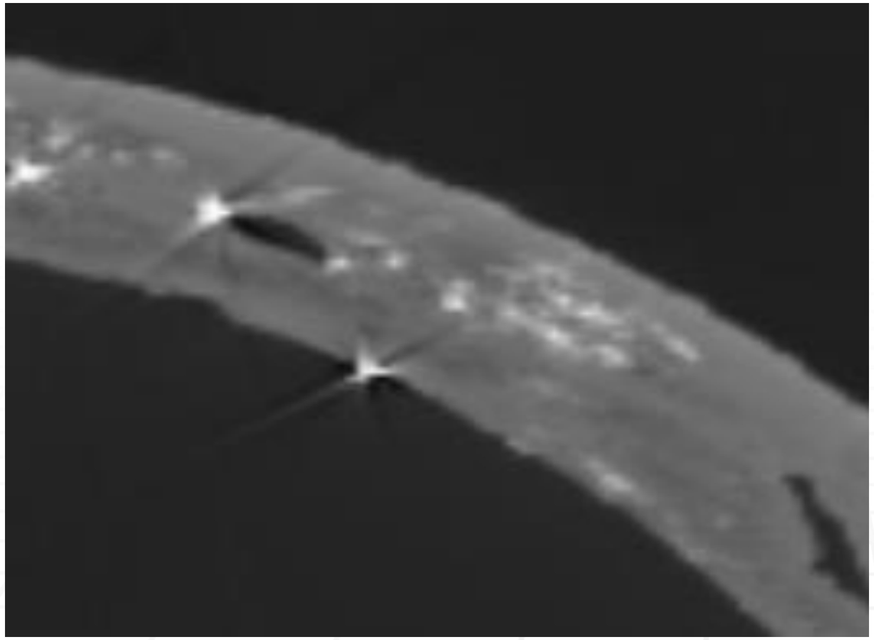


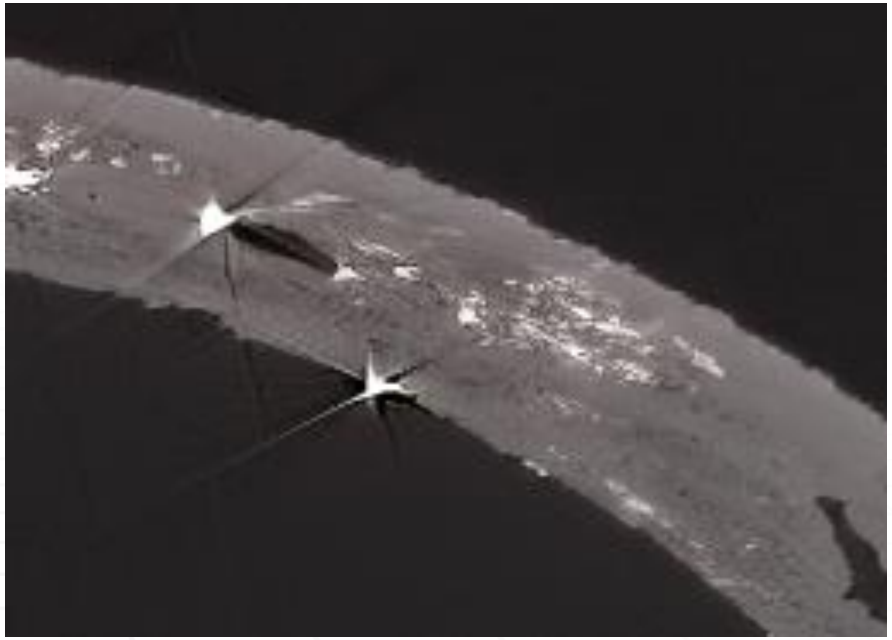
- Funded by the Nuclear Science User Facilities

NRDS
AI Analysis

- Currently Available
  - Super Resolution
  - Activity Detection

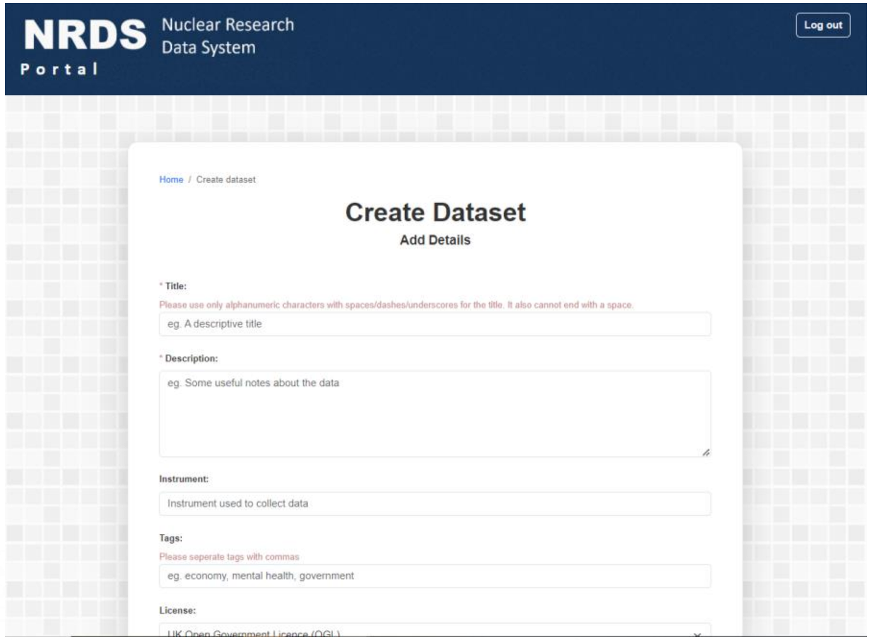


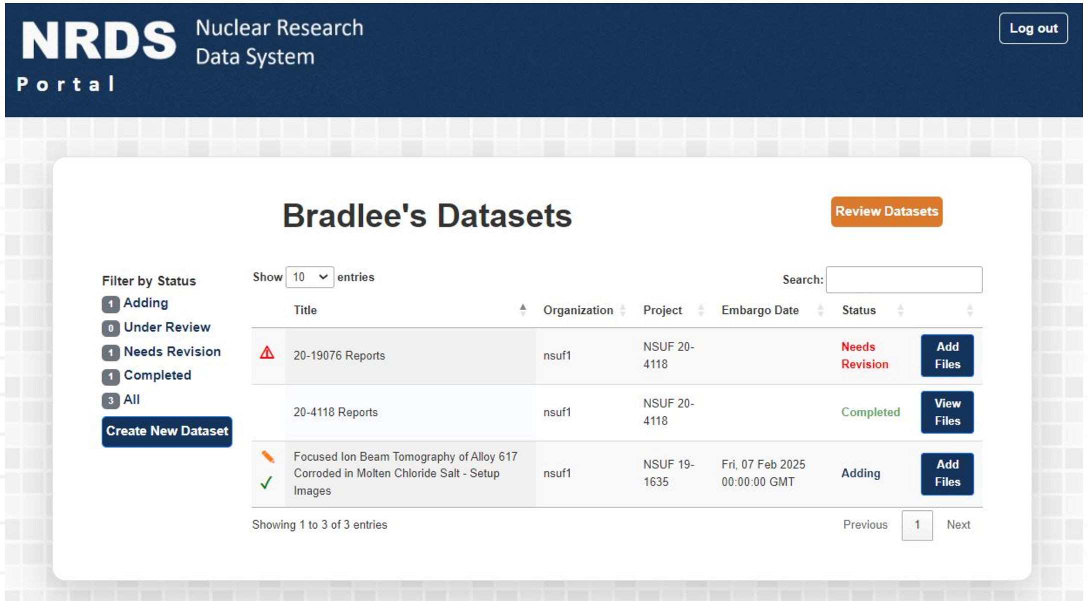


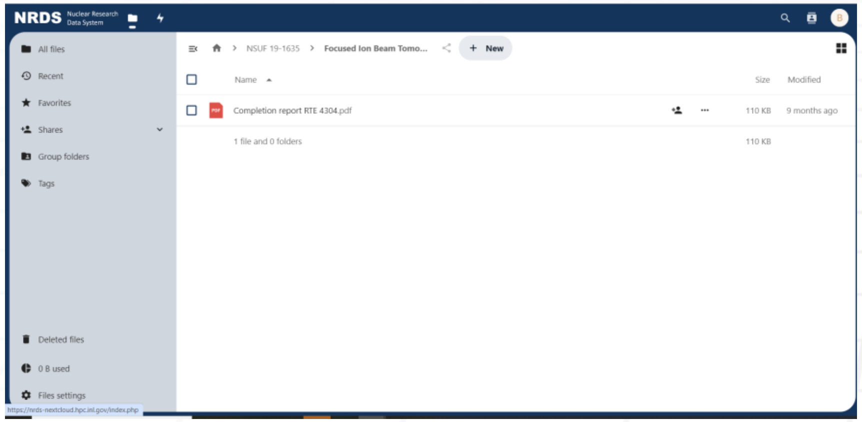


NRDS Portal

- Any researcher within the project can upload data
- Enforced embargo dates
- Allows drop and drag of files
- Collaboration among others in project
- PI approval required before public release







Annual User Report

https://www.osti.gov/biblio/2328595

Hundred’s of user report
Summary of major FY23 accomplishments

B.140 SpaceX Falcon Heavy Mass Constraints as Design Driver for Practical Heat Pipe Stirling Microreactors

Report Participants

Watson, Daniel L[1], Gatchalian, Ronald Daryll E[1], Hsieh, Hui-Yu [1], Bhat, Pramatha [1], Tsvetkov, Pavel [1]
1 Texas A&M University

Scientific Achievement

A nuclear reactor system was designed with a SpaceX Falcon Heavy as the design driver (mass and size constraints). Neutronics, depletion, shielding, and criticality safety analyses were performed with MCNP6.2 on the INL Sawtooth cluster. Ansys was performed on local Texas A&M resources to assess heat-pipe performance.

Significance

The project outcomes delineated the maximum power yields achievable with the current commercial heavy-lift rocketry utilizing a nuclear power system. Acceptable neutron radiation doses were observed at the 300 kWt power range with LiH shielding, however, photon doses surpassed NASA FSP SoW DR-3’s threshold (combined 5 Rem/yr). The reactor, modeled on INL’s “Special Purpose Heat Pipe Microreactor Design A," exhibited safe shutdown margins during oceanic submersion incidents and control drum malfunctions.

Key Publications

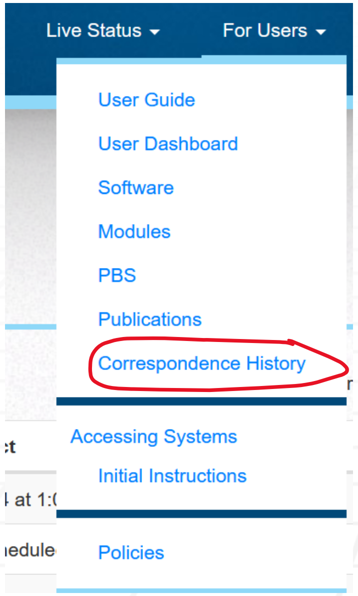
Watson, D. L. P., Gatchalian R. D. E., Hsieh H., Bhat P., & Tsvetkov P. V (2023). SpaceX Falcon Heavy Mass Constraints as Design Driver for Practical Heat Pipe Stirling Micro Reactors. Proceedings of Nuclear and Emerging Technologies for Space (NETS 2023), Idaho Falls, 305-311. doi.org/10.13182/NETS23-41911

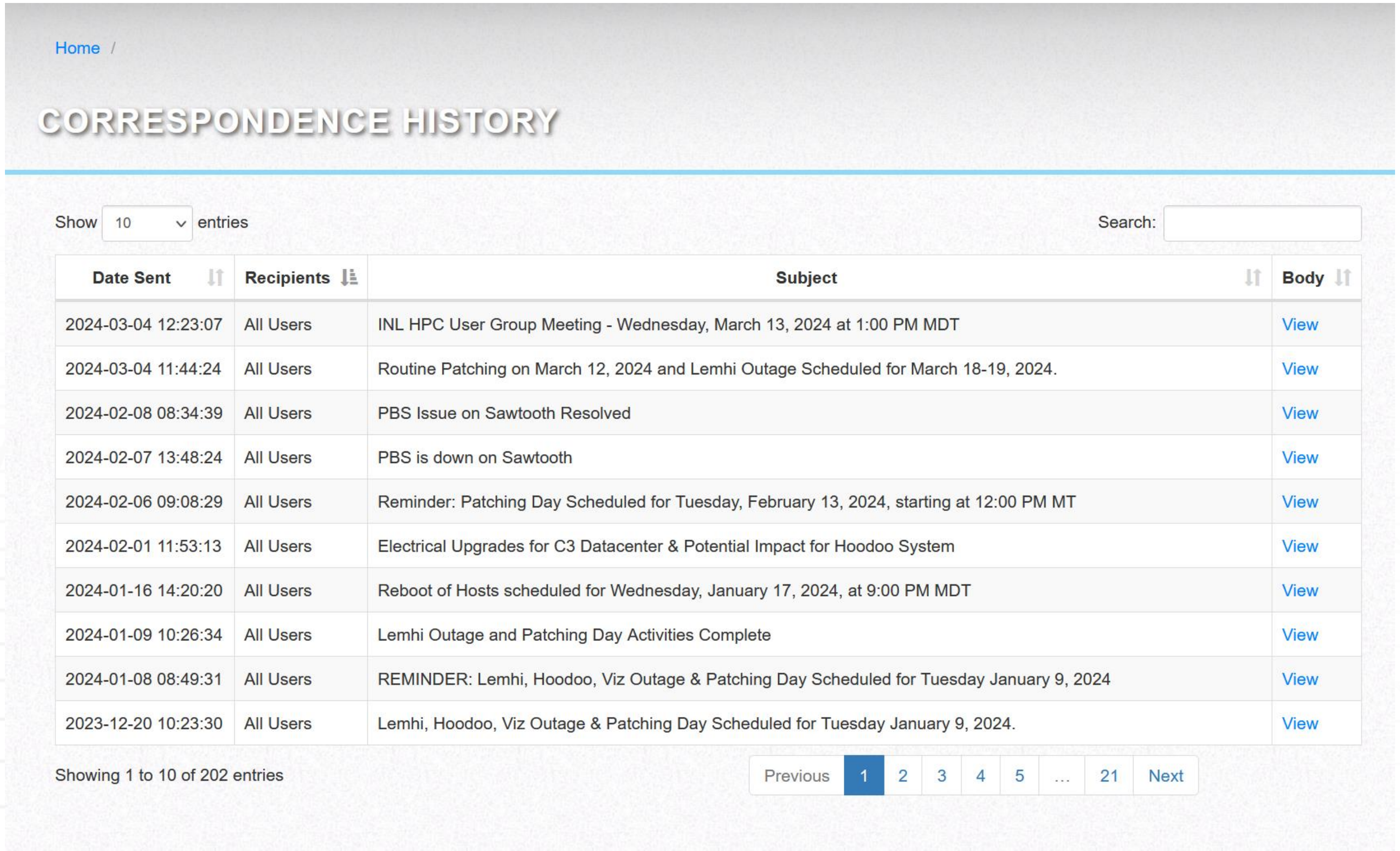
Sponsor/Program

This project was completed as an assignment within a course at Texas A&M University (NUEN610 - Reactor Design). Maturation of the evaluations yielded a conference paper that was accepted to NETS 2023, and ultimately invited to a special (upcoming) publication of Nuclear Technology .

HPCweb
Correspondence History

- A searchable list of emails that have been sent to users





Home /

CORRESPONDENCE HISTORY

Show 10 entries

Search:

Date Sent	Recipients	Subject	Body
2024-03-04 12:23:07	All Users	INL HPC User Group Meeting - Wednesday, March 13, 2024 at 1:00 PM MDT	View
2024-03-04 11:44:24	All Users	Routine Patching on March 12, 2024 and Lemhi Outage Scheduled for March 18-19, 2024.	View
2024-02-08 08:34:39	All Users	PBS Issue on Sawtooth Resolved	View
2024-02-07 13:48:24	All Users	PBS is down on Sawtooth	View
2024-02-06 09:08:29	All Users	Reminder: Patching Day Scheduled for Tuesday, February 13, 2024, starting at 12:00 PM MT	View
2024-02-01 11:53:13	All Users	Electrical Upgrades for C3 Datacenter & Potential Impact for Hoodoo System	View
2024-01-16 14:20:20	All Users	Reboot of Hosts scheduled for Wednesday, January 17, 2024, at 9:00 PM MDT	View
2024-01-09 10:26:34	All Users	Lemhi Outage and Patching Day Activities Complete	View
2024-01-08 08:49:31	All Users	REMINDER: Lemhi, Hoodoo, Viz Outage & Patching Day Scheduled for Tuesday January 9, 2024	View
2023-12-20 10:23:30	All Users	Lemhi, Hoodoo, Viz Outage & Patching Day Scheduled for Tuesday January 9, 2024.	View

Showing 1 to 10 of 202 entries

Previous 1 2 3 4 5 … 21 Next

HPC Container Strategy

- HPC developed and published a high performance computing container strategy based on layering
- Adopted by development teams at Sandia, Naval Nuclear Laboratories, ATR, and Relap5.

Software Quality Assurance for High Performance Computing Containers

MATTHEW SGAMBATI and MATTHEW ANDERSON, Idaho National Laboratory, USA

Software containers are a key channel for delivering portable and reproducible scientific software in high performance computing (HPC) environments. HPC environments are different from other types of computing environments primarily due to usage of the message passing interface (MPI) and drivers for specialized hardware to enable distributed computing capabilities. This distinction directly impacts how software containers are built for HPC applications and can complicate software quality assurance efforts including portability and performance. This work introduces a strategy for building containers for HPC applications that adopts layering as a mechanism for software quality assurance. The strategy is demonstrated across three different HPC systems, two of them petaflops scale with entirely different interconnect technologies and/or processor chipsets but running the same container. Performance consequences of the containerization strategy are found to be less than 5-14% while still achieving portable and reproducible containers for HPC systems.

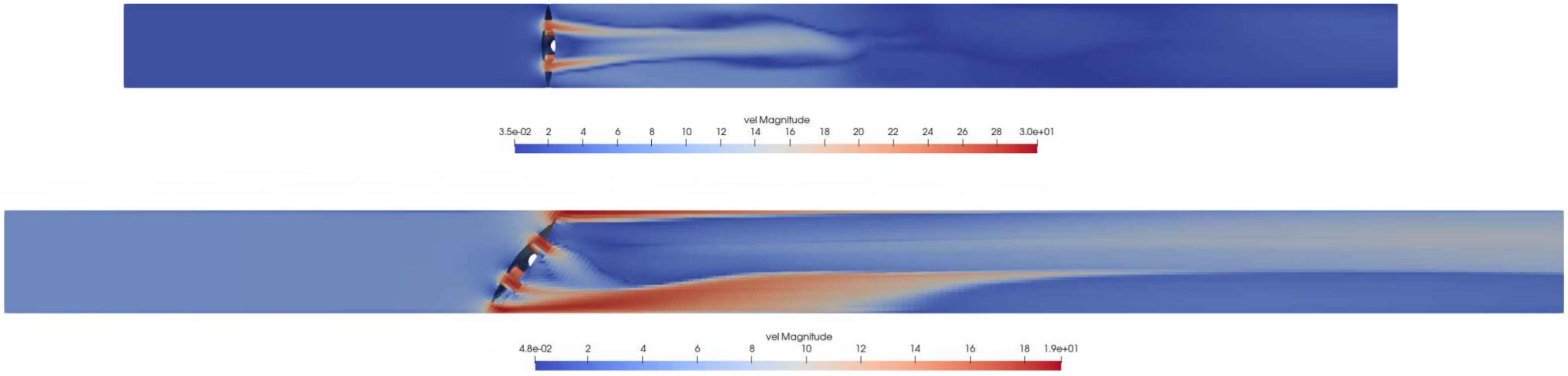
Additional Key Words and Phrases: singularity, containers, message passing interface, software quality assurance

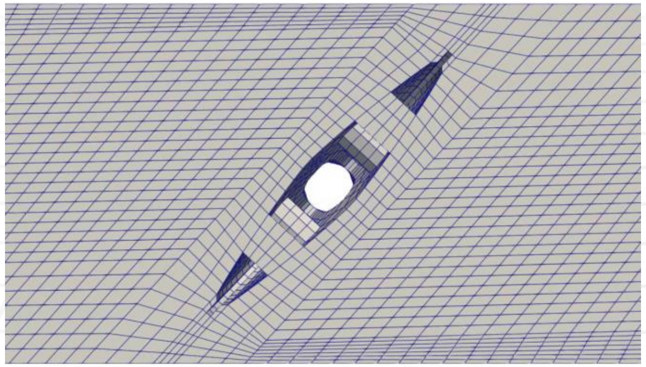
https://doi.org/10.1145/3569951.3593596

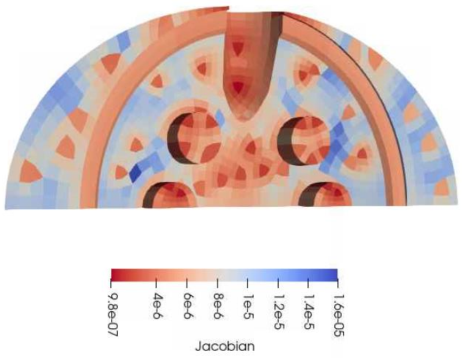
Verification and Validation Efforts for key MOOSE software

ATR Butterfly Valve

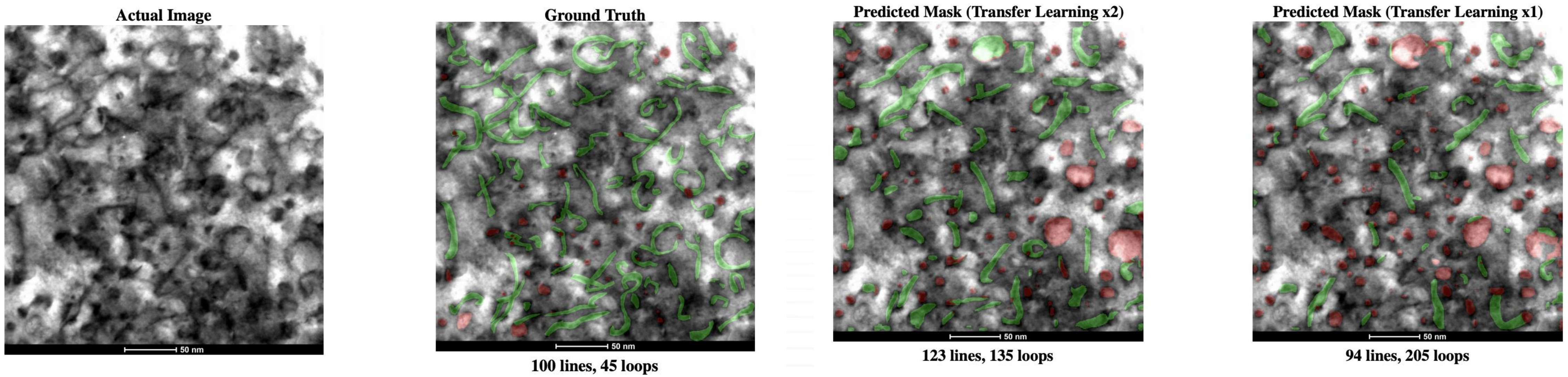
Interoperability with STAR-CCM+







Automated Dislocation Defect Detection



Soon to appear in NRDS…

Questions