INL/MIS-19-56513-Revision-0

Advanced Scientific Computing Nuclear Science User Facilities FY19 Annual Program Review

November 2019

Eric T Whiting

Changing the World's Energy Future

Idaho National Laboratory

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Idaho National Laboratory
Idaho Falls, Idaho 83415

http://www.inl.gov

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Advanced Scientific Computing
Nuclear Science User Facilities
FY19 Annual Program Review

12-13 November 2019

Eric Whiting
Division Director
Advanced Scientific Computing

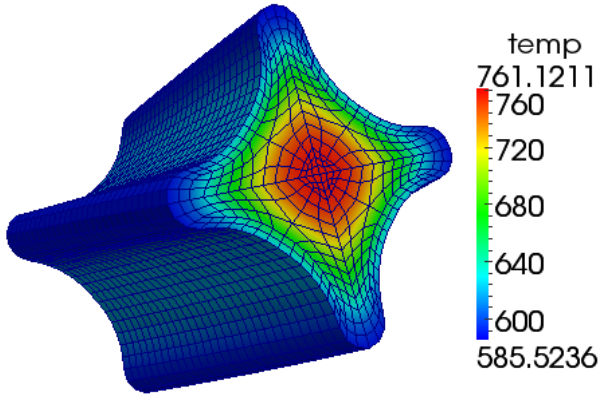
www.inl.gov

Idaho National Laboratory

Idaho National Laboratory

Overview

- Organization
- NSUF FY19 HPC Usage
- Sawtooth
- Collaborative Computing Center (C3)
- Strategy
- Access



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Nuclear Science & Technology

NS&T Associate Lab Director
John Wagner

NS&T Chief Scientist
Jess Gehin

GAIN
John Jackson,
Acting Director

Naval Reactors
Casey Stengel

NS&T Chief Operations Officer
Pete Wells

Integrated Fuel Cycle Solutions
Monica Regalbuto

International Programs
Bonnie Hong

Strategic Planning
Steve Aumeier

NE Senior Technical Advisor
Jon Carmack

NRIC Director
Ashley Finan

C100

Reactor Systems Design & Analysis
Youssef Ballout,
Director

C200

Nuclear Safety & Regulatory Research
Curtis Smith, Director

C400

Fuel Cycle Science and Technology
Terry Todd, Director

C500

Advanced Scientific Computing
Eric Whiting, Director

C600

Nuclear Fuels & Materials
Steven Hayes,
Director

Nuclear Science & Technology

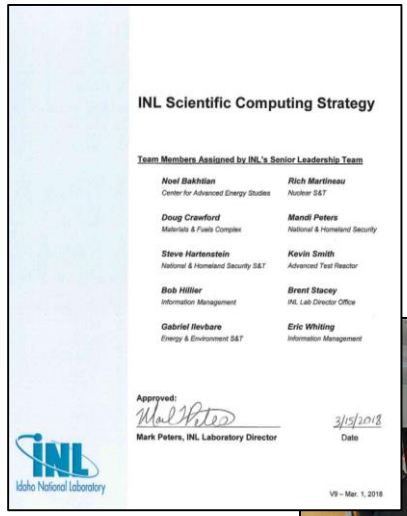
Advanced Scientific Computing – C500
Eric Whiting, Director

Computational Frameworks – C510 (10)
Richard Martineau, Department Manager
David Andrs
Robert Carlsen
Derek Gaston
Joshua Hansel
Casey Icenhour, Grad Fellow
Fande Kong
Matthias Kunick, Post Doc
Alexander Lindsay
Thomas Murphy
Cody Permann
Andrew Slaughter

High Performance Computing and Data Analytics – C520 (21)
Tami Grimmett, Department Manager
Matthew Anderson
Brandon Biggs
Peter Cebull
Garrick Evans
Shane Grover
Scott Jeffery
John Koudelka
Cameron Krome
Kit Menlove
Ben Nickell
Stephanie Parker
Rick Poole
Scott Serr
Jacques LaBranche
Matthew Sgambati
Shad Staples
Jason Weninger
Derek Stucki
Jared Wadsworth
Porter Zohner

"Establish a leadership hierarchy (governance under Nuclear S&T) for scientific computing as a critical INL capability"

2018 INL Scientific Computing Strategy action N9


INL Scientific Computing Strategy

Team Members Assigned by INL's Senior Leadership Team

Noel Bakhtian, Center for Advanced Energy Studies
Rich Martineau, Nuclear S&T
Doug Crawford, Materials & Fuels Complex
Mandi Peters, National & Homeland Security
Steve Hartenstein, National & Homeland Security S&T
Kevin Smith, Advanced Test Reactor
Bob Hillier, Information Management
Brent Stacey, INL Lab Director Office
Gabriel Ilevbare, Energy & Environment S&T
Eric Whiting, Information Management

Approved:
Mark Peters, INL Laboratory Director
3/15/2018
Date

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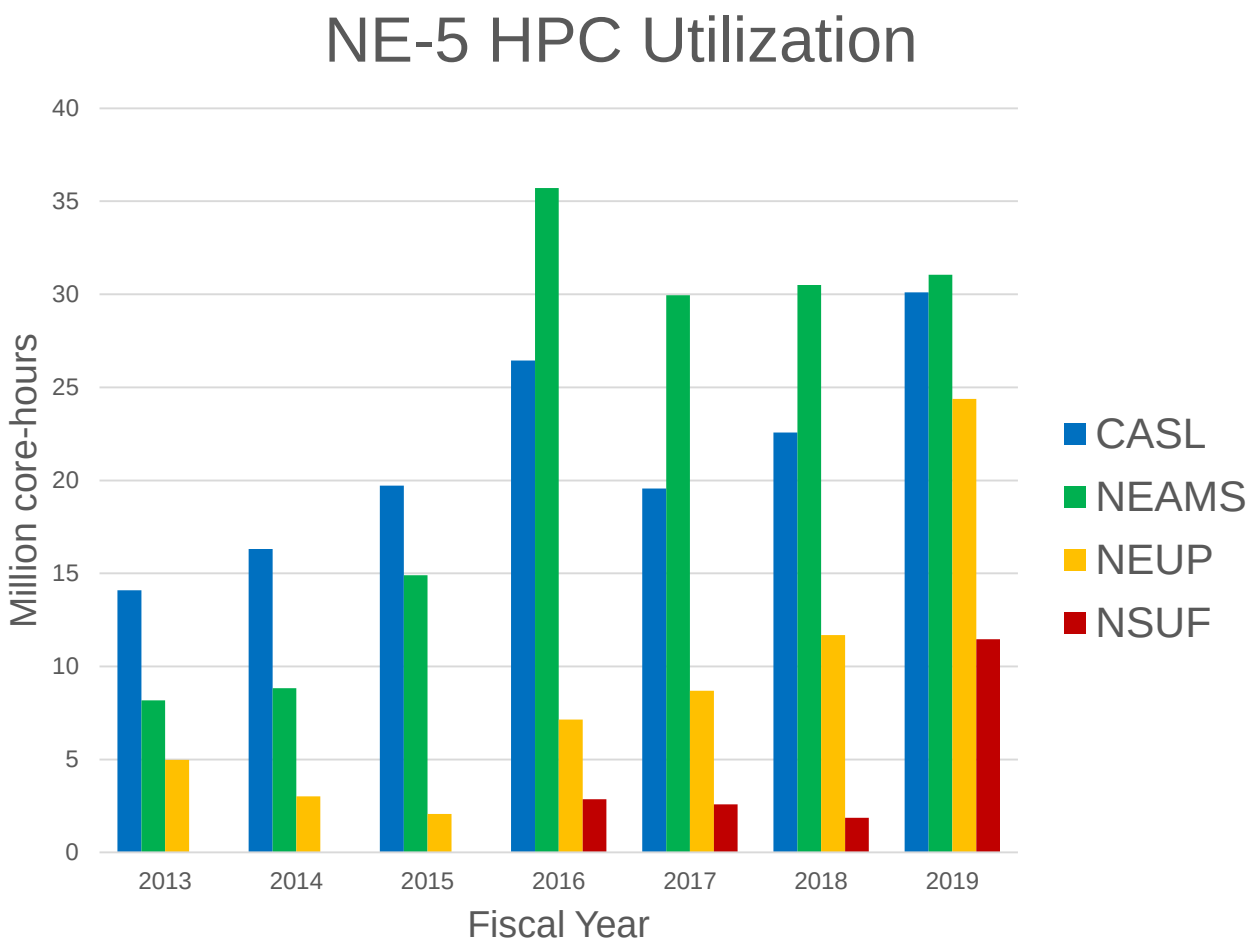
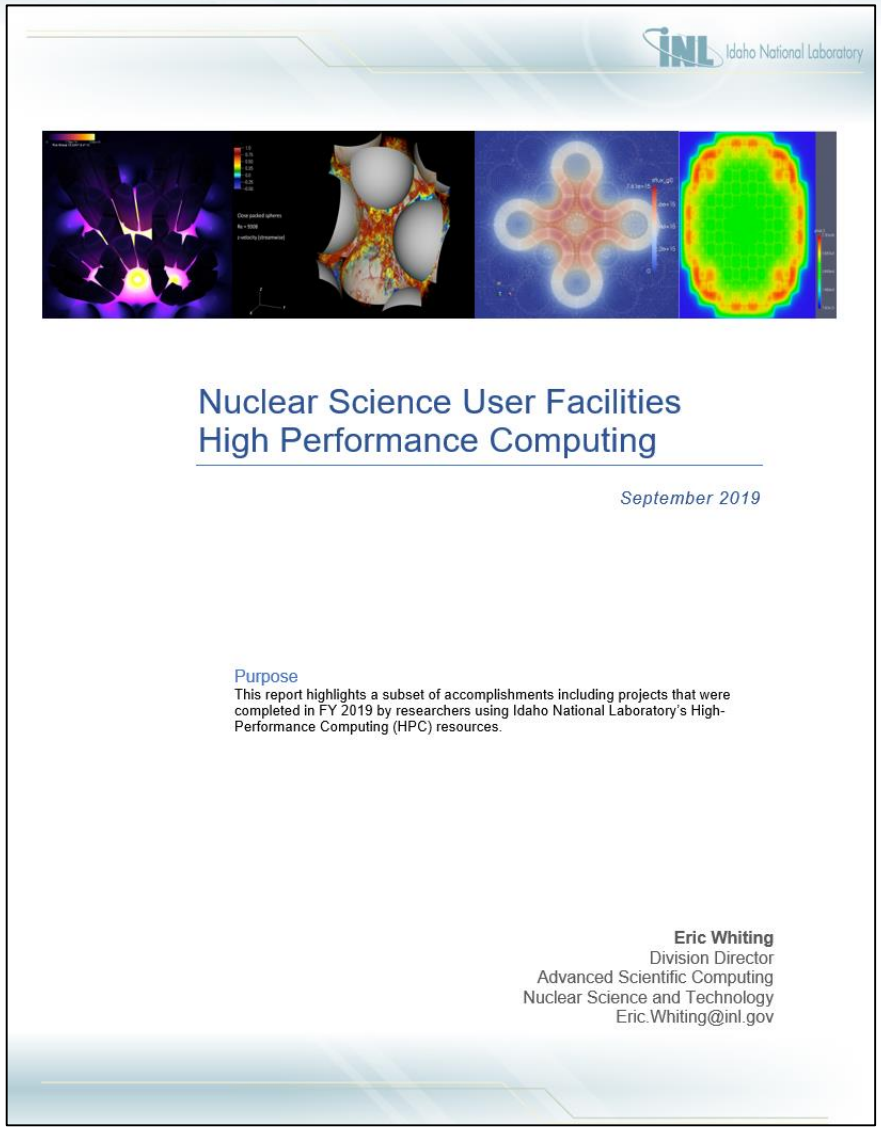
V9 – Mar. 1, 2018

NSUF Usage





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Nuclear Science User Facilities
High Performance Computing

September 2019

Purpose

This report highlights a subset of accomplishments including projects that were completed in FY 2019 by researchers using Idaho National Laboratory's High-Performance Computing (HPC) resources.

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Nuclear Science and Technology
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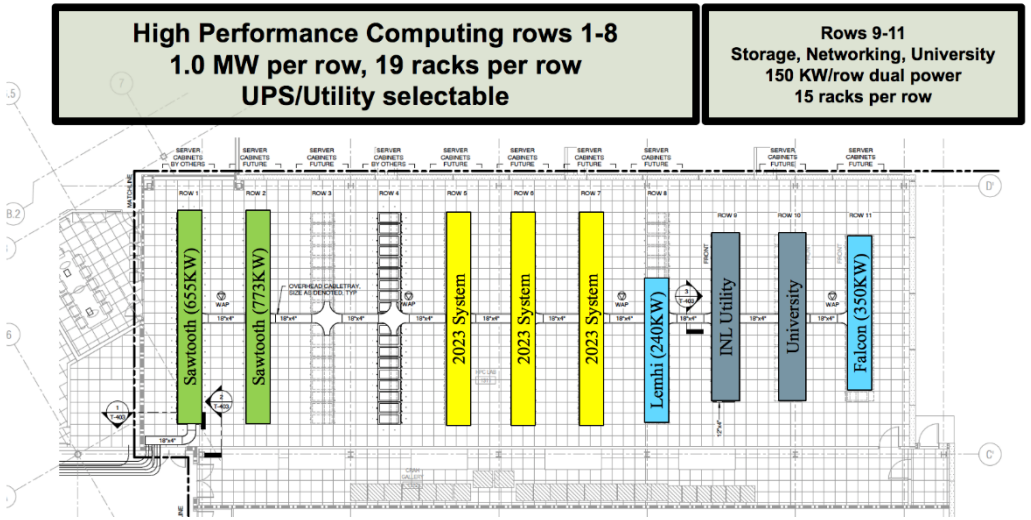
Sawtooth

- **Procurement:**
  - 22 April 2019 – RFP released
  - 19 August 2019 – Award
  - 2 December 2019 – Delivery
- **Overview:**
  - Six times faster than current Falcon/Lemhi systems
  - Four-year lease-to-own; approximately $19.2M total cost
  - 100,000 compute cores with overall LINPACK performance of ~6 Petaflops/s (PF)
  - System will include GPU capabilities (0.56 PF)
  - Room-neutral water cooling with direct water on processors
  - Installation in the new Collaborative Computing Center (C3)
- **Schedule:**
  - Dec 2019-Feb 2020: Installation/acceptance window
  - March 2020: System operational
  - Falcon and Lemhi will move to C3



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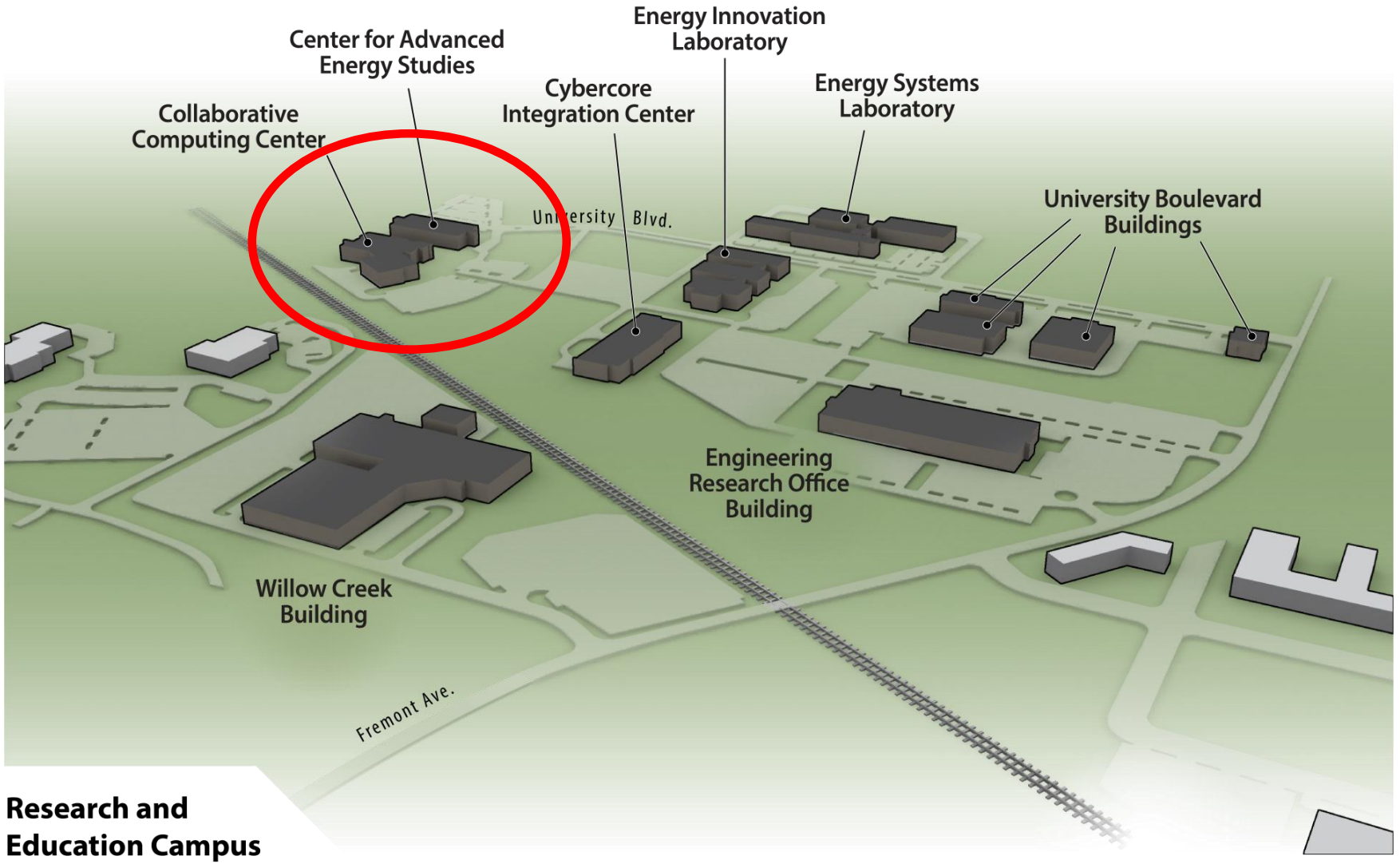
Expansion of Research and Education Campus



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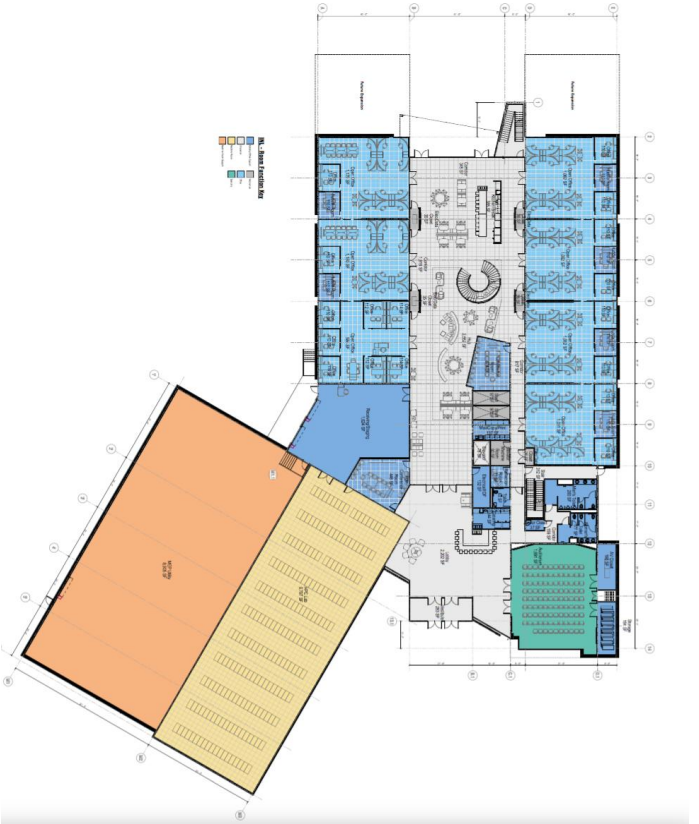
Collaborative Computing Center (C3)



196 max occupancy
~120 current occupancy

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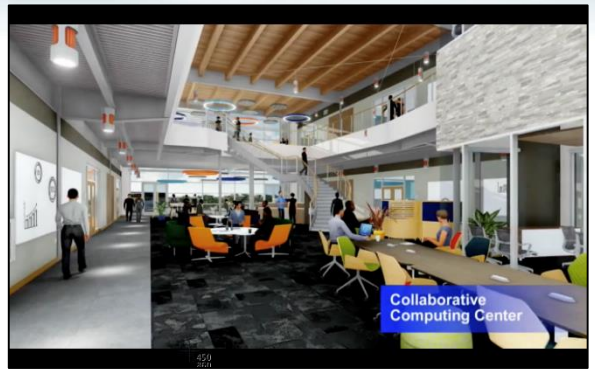
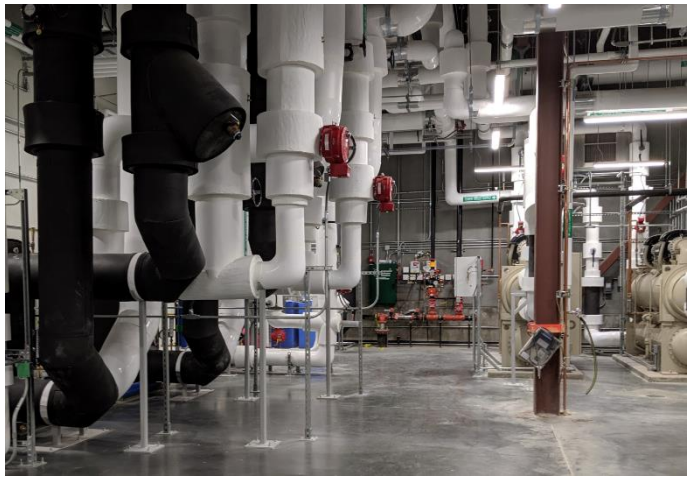
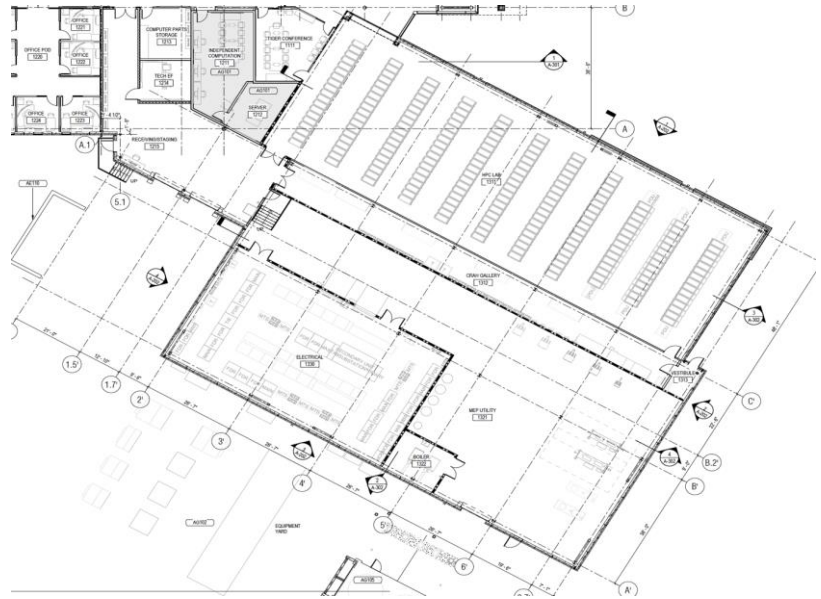
C3 Data Center Quick Facts

- Data center significantly expands upon current INL computing infrastructure:
  - **2x** the computer floor space (7,000 vs 3,700 sq. ft)
  - **4x** the number of computer racks (200 vs 50 racks)
  - **8x** the initial power deployed (4.0 vs 0.5 MW)
  - **16x** the full power build out after future C3 expansion (8.5 MW vs 0.5 MW)







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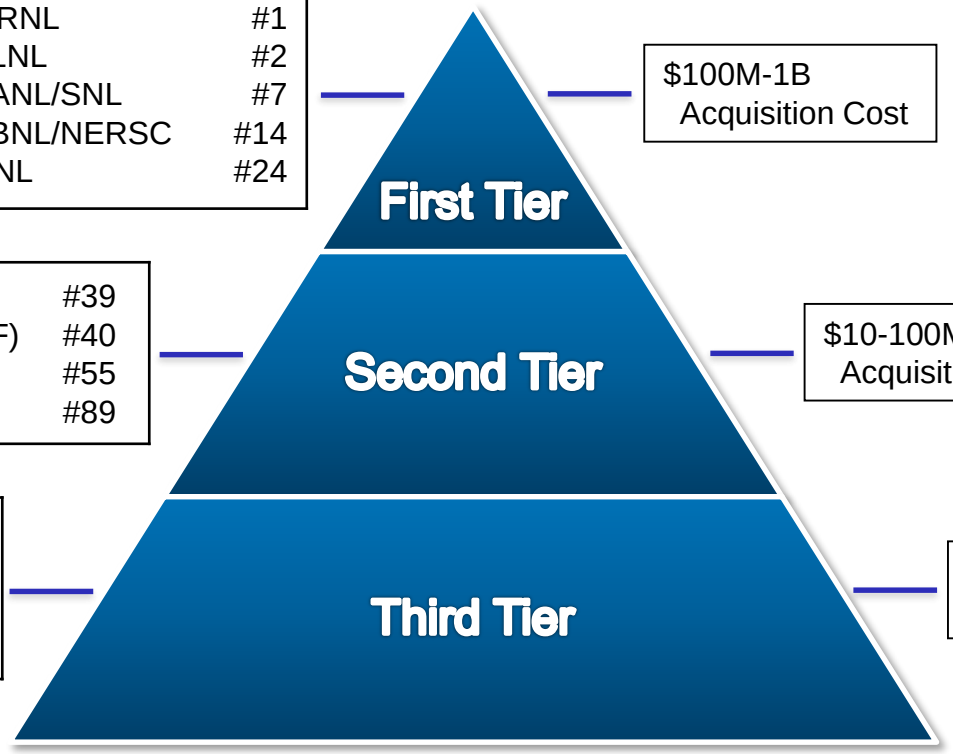
DOE Ecosystem – HPC systems

ORNL	#1
LLNL	#2
LANL/SNL	#7
LBNL/NERSC	#14
ANL	#24

NREL	#39
NCAR (NSF)	#40
NETL	#55
PNNL	#89

INL Falcon	#456
INL Lemhi	#500+
Bettis	#500+
Knolls	#500+



$100M-1B Acquisition Cost

$10-100M Acquisition Cost

$1-10M Acquisition Cost

June 2019 Top500 Rankings

INL's next system 'Sawtooth' will move into the second tier ($10M+) in order to meet program/mission needs

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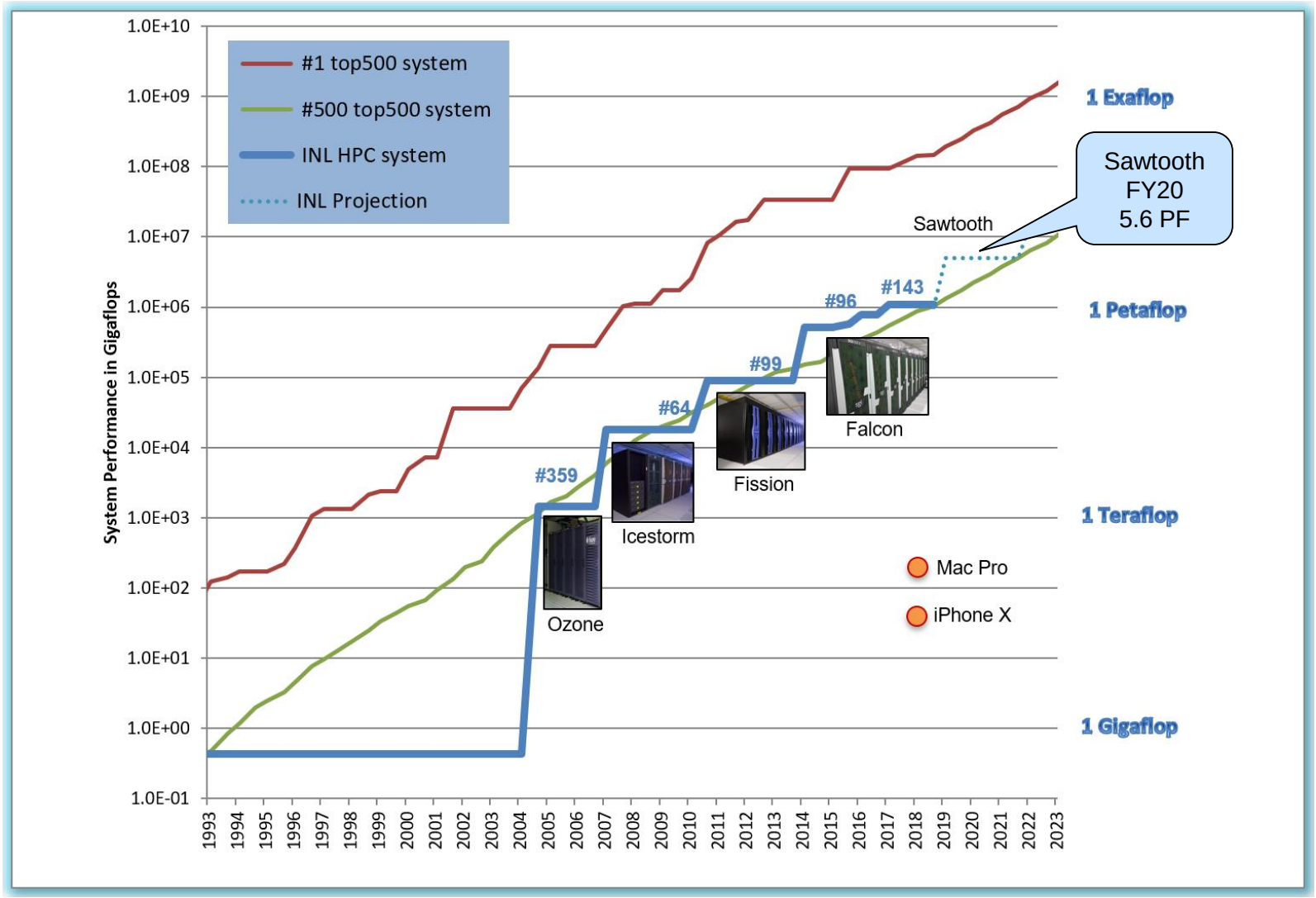
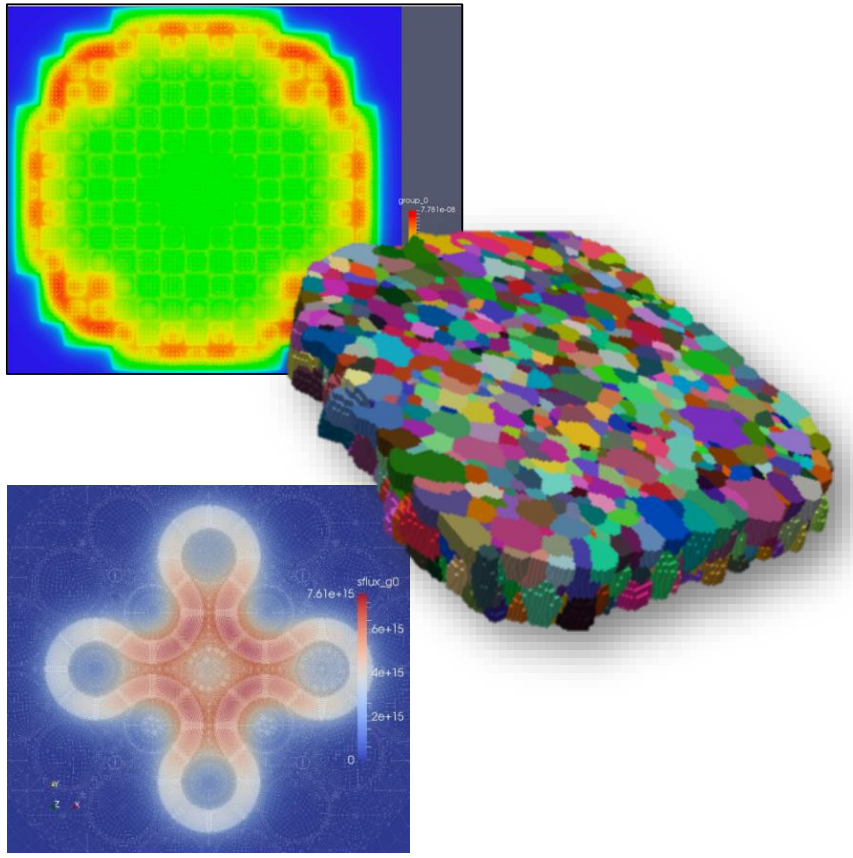
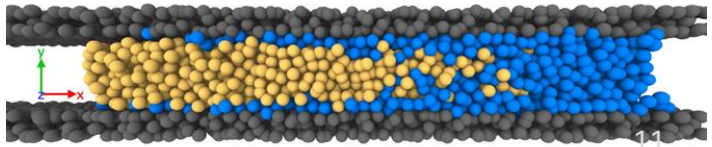
INL HPC History







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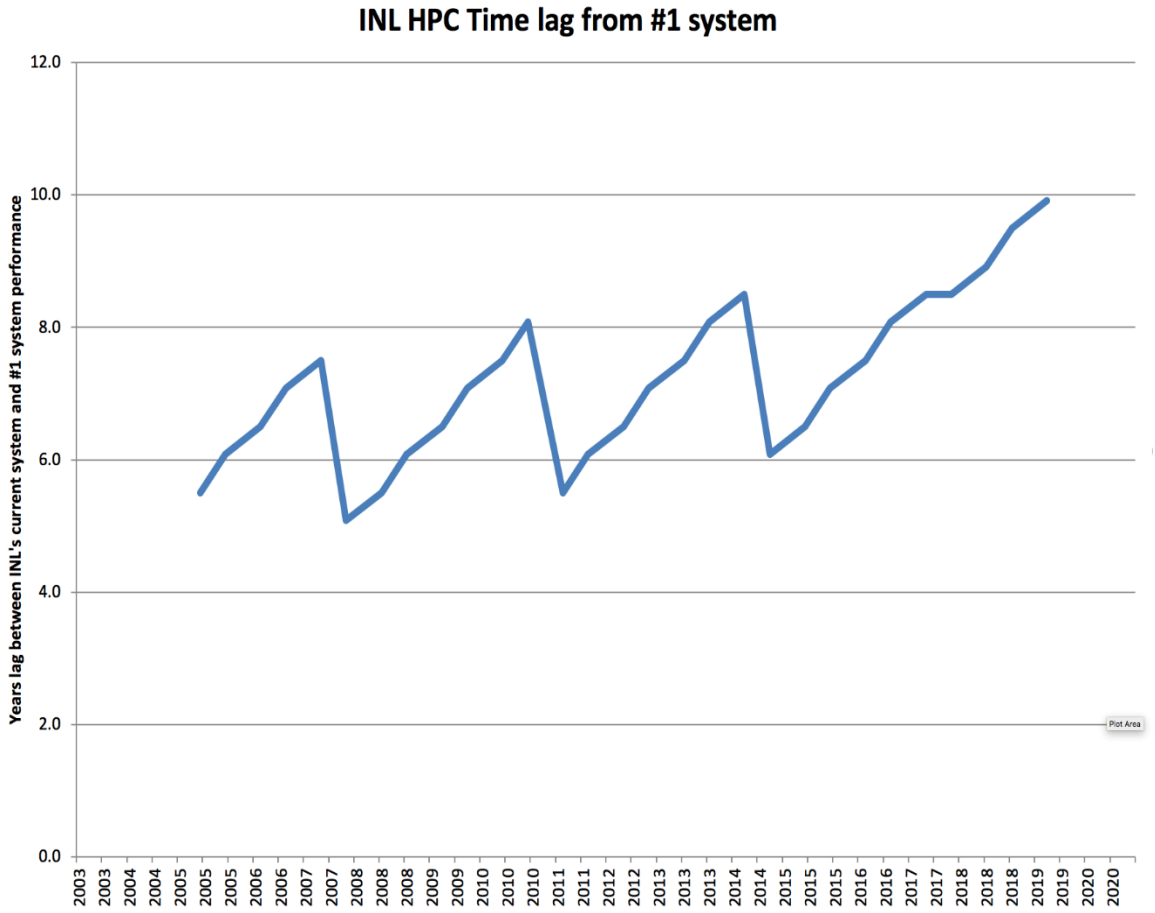
Time Lag between INL HPC System and #1 TOP500 System

INL System	Year	Performance	Prior #1 System with Similar Performance
Ozone 8 racks, $2.1M	June 2005	1.44 TF	June 1999 ASCI RED: Sandia ($46M), 104 racks,1MW, 2.12 TF
Icestorm 4 racks, $2.4M	Nov 2007	17.78 TF	June 2002 Earth Simulator ($556M), 320 racks, 6.4MW, 35.8TF
Fission 14 racks, $3.5M	June 2011	91 TF	June 2005 BlueGene/L (~$200M) LLNL, 104 racks, 136 TF
Falcon 14 racks $9.9M	Nov 2014	511 TF (2014) 1,088 TF (2017 upgrade)	June 2008 Roadrunner LANL ($100M), 296 racks 2.35MW, 1,026TF
Sawtooth (projection) ~40 racks ~$20M	Nov 2019	5-10 PF (projection)	June 2011 K Computer ($1.25B), RIKEN AICS, Japan, 671 racks, 10.0MW, 8,162TF



By taking advantage of technology advances, INL is able to deploy systems that have equivalent #1 performance with a 5-8 year time delay, enabling a huge savings in cost, power, and space

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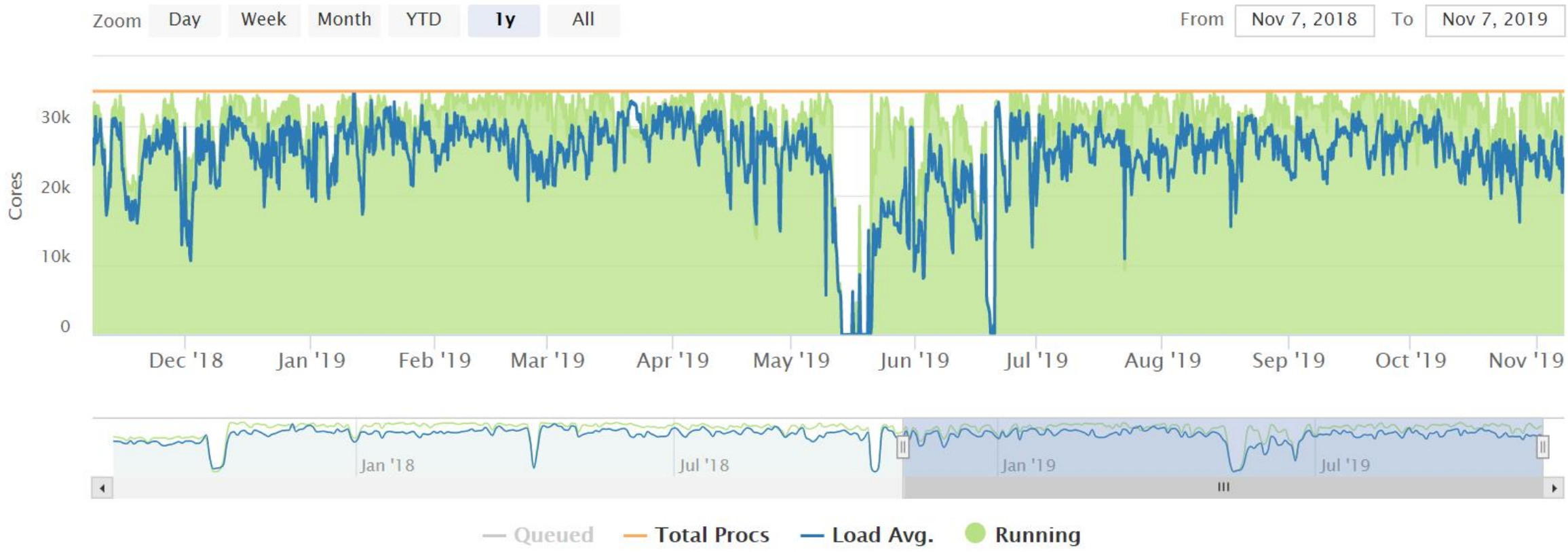
Falcon Usage



Max Running: 35698
Avg Running: 29996

Max Load: 34932
Avg Load: 25557

Max Queued: 1389896
Avg Queued: 71788

Data Export: 8/7/2019

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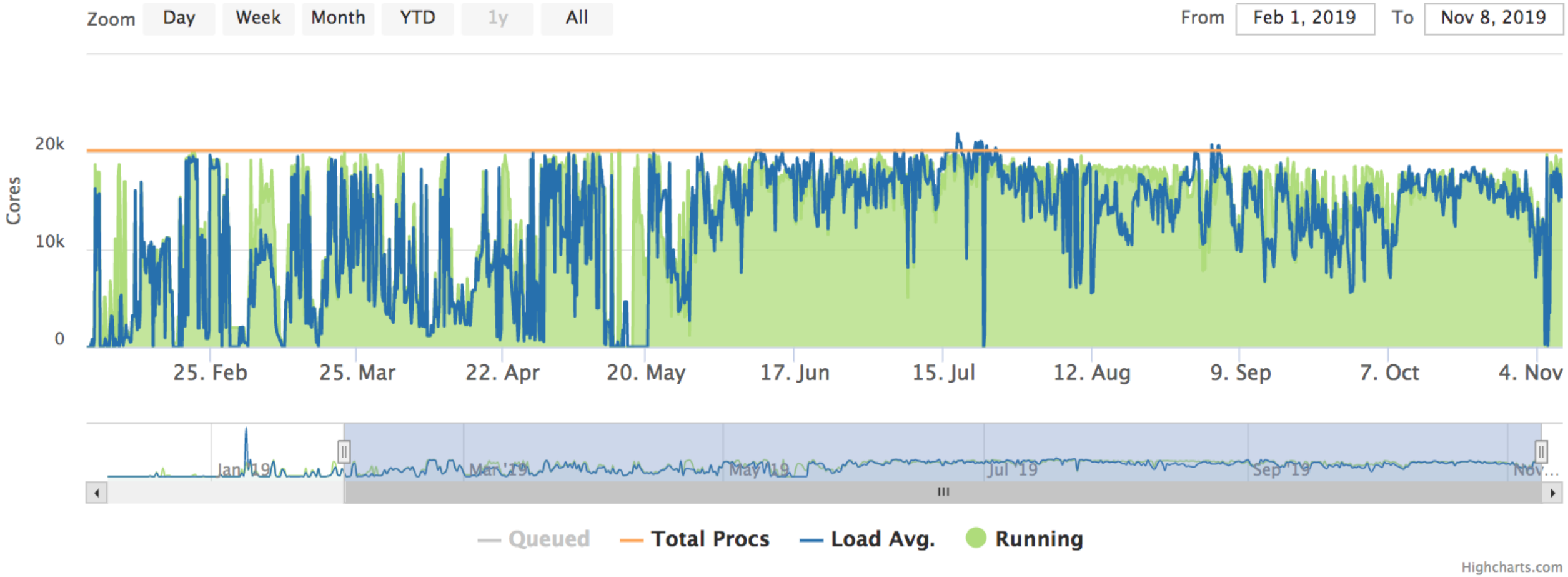
Lemhi Usage



Max Running: 20160
Avg Running: 13550

Max Load: 23384.35
Avg Load: 12259

Max Queued: 93504241
Avg Queued: 47761

Data Export: 8/7/2019

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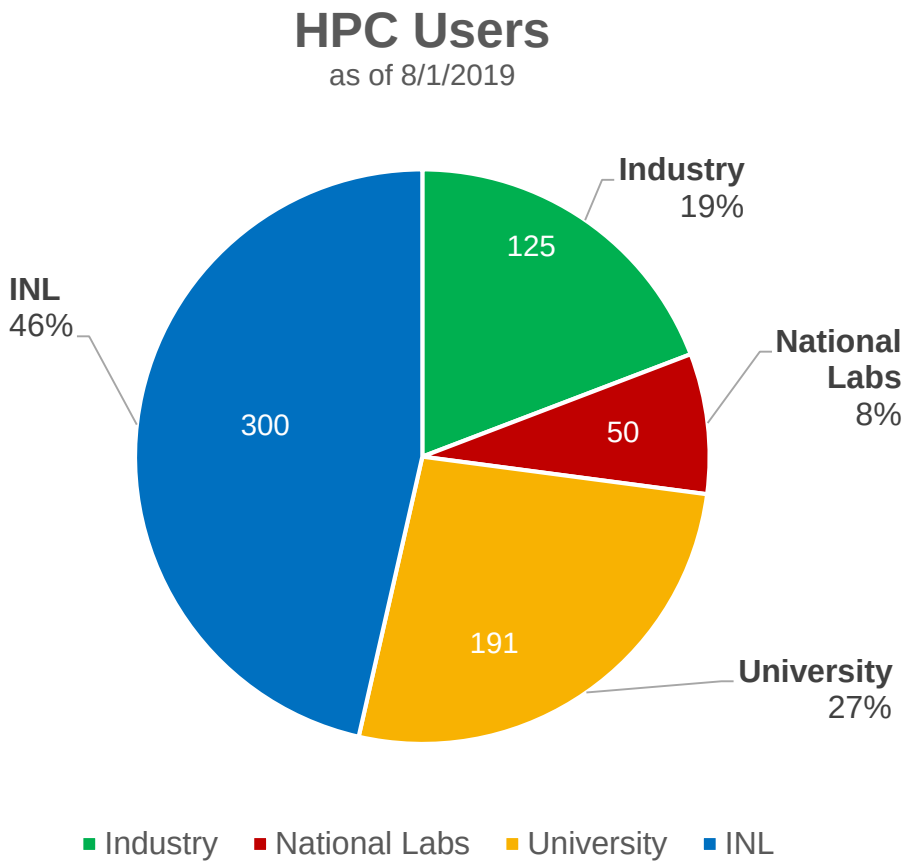
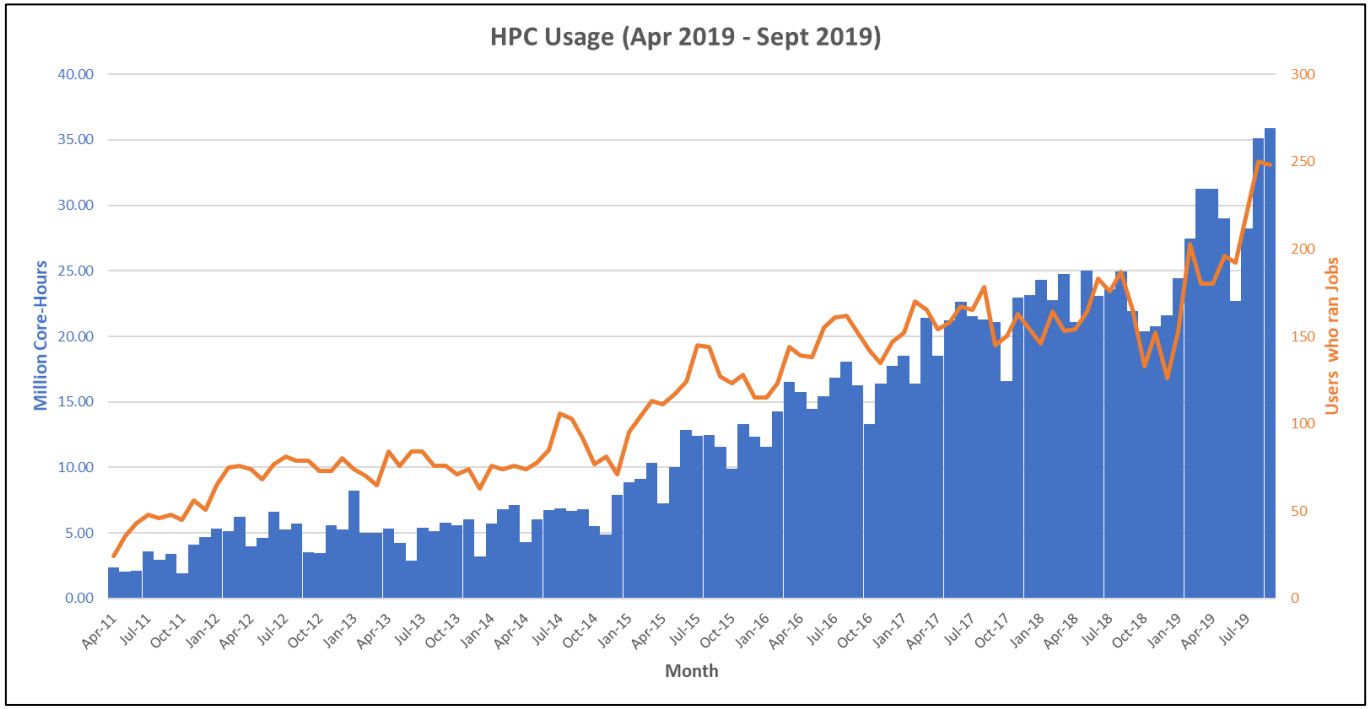
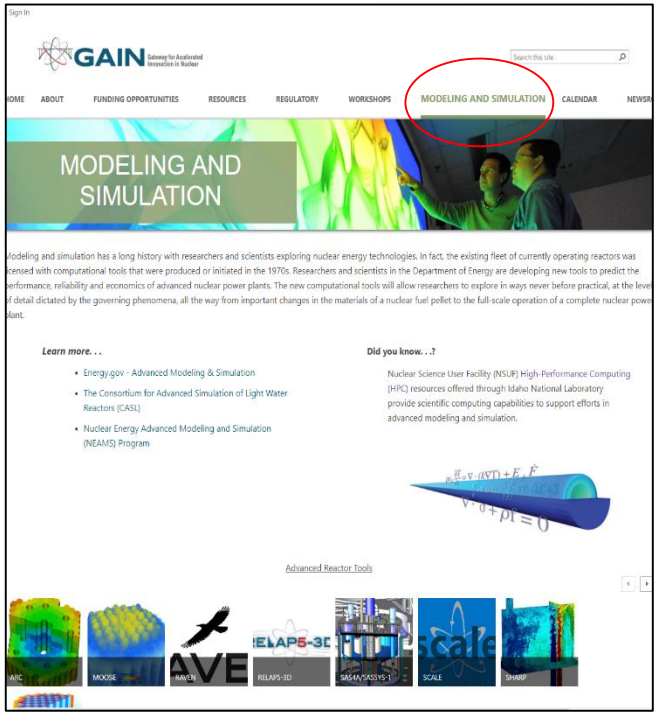
High Demand for Computational Support



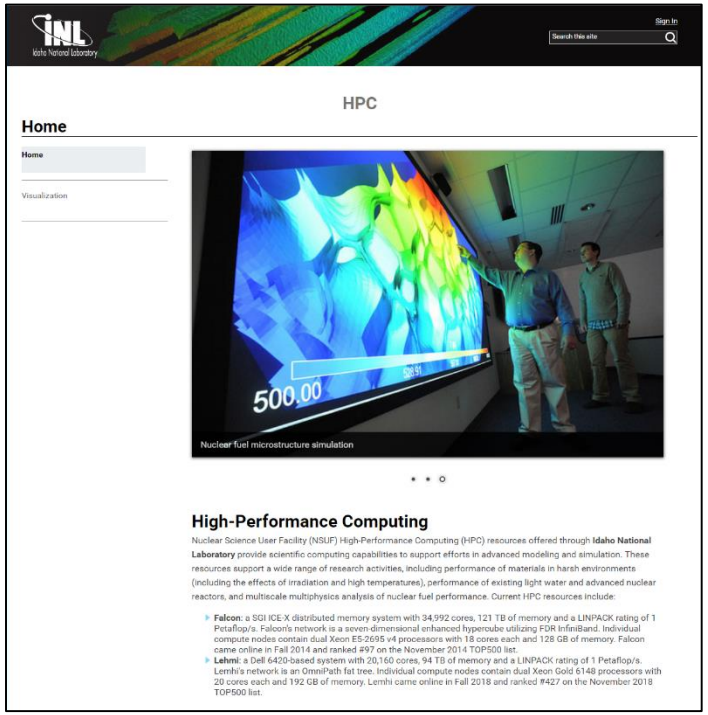


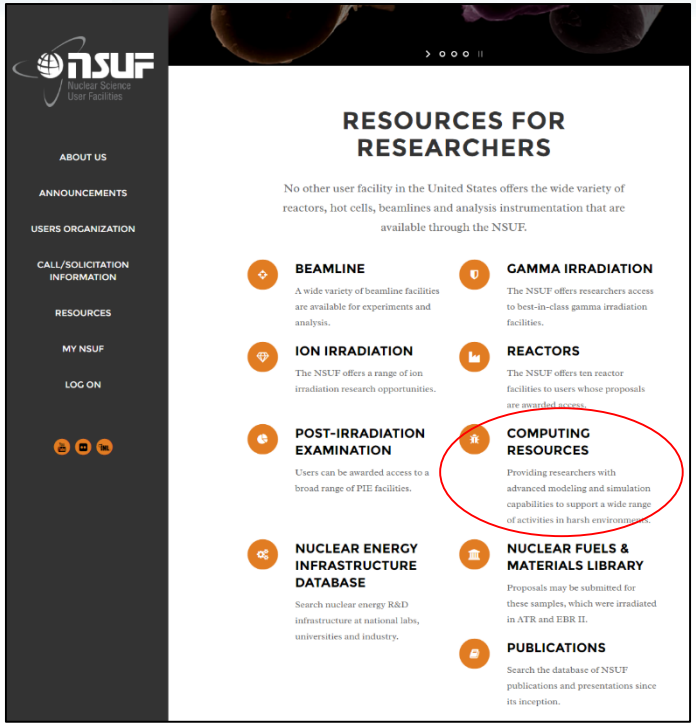
Access to INL HPC systems



https://gain.inl.gov

https://hpc.inl.gov





https://nsuf.inl.gov

HPC Access Policy

Justifications for high-priority use of the DOE-NE sponsored computer systems:

1. US-based industry, DOE national laboratory, US-based university, or other federal agency user requesting access associated with nuclear-related DOE/federal programs or a DOE/federal award.
2. US-based Industry or US-based university user requesting access for nuclear-related research that generates openly published results for the benefit to DOE and INL missions.

Justifications for standard-priority use of the systems:

3. INL staff requesting access for non-nuclear research and development
4. US-based University user requesting access for INL collaborative research supporting education or workforce development with an INL connection such as the INL National University Consortium, the Idaho education ecosystem or other strategic relationship.
5. Director discretionary access for activities such as: response to DOE-NE direction, code testing and calibration, or system/software support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