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Level 3 Milestone Report: April 2020

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HPC Utilization Data for NSUF/NE5 Projects from October 1, 2019, through March 31, 2020

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Idaho National Laboratory (INL)'s High Performance Computing (HPC) resources provide scientific computing capabilities to support INL and DOE-NE's efforts in advanced modeling and simulation. The HPC systems support a wide range of research activities, including performance of materials in harsh environments (including the effects of irradiation and high temperatures), modeling of geomechanical changes in subsurface flow, performance of advanced nuclear reactors, and multiscale analysis of nuclear fuel performance.

The Nuclear Science User Facilities (NSUF) program combines access to nuclear science R&D capabilities and staff expertise with novel ideas provided by external contributors (universities, laboratories, and industry). These collaborations represent the cutting edge of nuclear technology research and stimulate cooperative research among user groups conducting basic and applied research. INL's HPC resources support universities and other external collaborators as part of the NSUF Program.

Current HPC resources include the following:

- **Sawtooth:** INL's newest supercomputer, an HPE SGI 8600 distributed memory system, deployed in March 2020 in the Collaborative Computing Center: 99,792 cores, 395 TB of total memory, and 0.56 PF of GPU capabilities. The current LINKPACK rating for Sawtooth is about 6 petaflops from both CPUs and GPUs. Ranked 37th on November 2019's list of the Top500 fastest supercomputers in the world, it has achieved the highest ranking of any INL supercomputer.
- **Falcon:** an SGI ICE X distributed-memory system: 34,992 cores, 121 TB of total memory, high-speed FDR interconnect network, and high-speed disk storage. The current LINPACK rating for Falcon is 1.087 petaflops.
- **Lemhi:** a Dell PowerEdge distributed-memory system: 20,160 cores, 94 TB of total memory, Omni-Path interconnect network, and high-speed storage. The LINPACK rating for Lemhi is 1.002 petaflops.
- **Galena:** a NVIDIA DGX-1 system for machine learning and artificial intelligence.

INL also leverages visualization resources such as a 3D immersive CAVE environment and various power-wall systems to help researchers understand their data and communicate complex science to stakeholders, as well as to the general public.

The following table shows compute utilization in million core-hours for all machines from October 1, 2019, through March 31, 2020:

Project		Million Core-Hours
ANSUF	ATR NSUF Project (Legacy Project)	0.091
ART	Reactor Engineering	3.145
ATR	Advanced Reactor Technologies	9.396
CASL	Consortium for Advanced Simulation of Light Water Reactors	16.787
EEST	Energy & Environment Science & Technology	31.622
EFRC	Energy Frontier Research Centers	3.981
FCRD	Fuel Cycle Research & Development	6.352
HPC	High Performance Computing support	0.229
ISO	Isotope project	0.074
IUC	Idaho University Consortium	14.845
LDRD	Laboratory Directed Research & Development	6.772
LWRS	Light Water Reactor Sustainability	2.994
MMM	Materials Minimization & Management	5.440
MOOSE	MOOSE-based code development	8.587
NEAMS	Nuclear Energy Advanced Modeling & Simulation	21.269
NEUP	Nuclear Energy University Program	8.881
NHS	National & Homeland Security	3.738
NST	Nuclear Science & Technology	15.531
NSUF	Computer allocation through Nuclear Science User Facilities	4.835
OTHER	-	0.000
STRUC	Structural Analysis / Facilities & Site Services	0.129
TREAT	Transient Reactor Test Facility	4.233
VERA	VERA User Group members	7.247
VTR	Versatile Test Reactor	2.571
WFO	Work for Others	0.144

The following table lists the external organizations with the largest number of active HPC users, along with the number of INL users, as of April 22, 2020.

Institution	Active Users
INL	285
Idaho State University	31
Oak Ridge National Laboratory	21
University of Idaho	20
Boise State University	17
Argonne National Laboratory	15

Institution	Active Users
Westinghouse Electric Company	15
MPR Associates	13
North Carolina State University	11
Texas A&M University	11
Naval Nuclear Laboratory	8
Nuclear Regulatory Commission	8
University of Utah	8
Massachusetts Institute of Technology	7
Oregon State University	7
University of Illinois at Urbana-Champaign	7

The following table displays the system utilization in million core-hours for the top 30 organizations using INL HPC systems from October 1, 2019, through March 31, 2020:

Institution	Million Core-Hours
INL	100.894
Boise State University	12.988
Oak Ridge National Laboratory	9.073
University of Idaho	6.931
University of Michigan	6.929
Westinghouse Electric Company	6.549
North Carolina State University	5.469
Los Alamos National Laboratory	2.594
Massachusetts Institute of Technology	2.418
University of Wyoming	2.396
Purdue University	2.378
University of Illinois at Urbana-Champaign	2.144
MPR Associates	1.873
Electric Power Research Institute	1.695
University of New Mexico	1.552
Texas A&M University	1.250
Framatome	1.050
Seoul National University	1.006
Virginia Tech	0.976
University of Texas at Arlington	0.814
Pennsylvania State University	0.724
Idaho State University	0.688
Kairos Power	0.573
University of Nevada, Reno	0.567
University of Utah	0.532

Institution	Million Core-Hours
University of Massachusetts Lowell	0.501
University of Colorado Boulder	0.444
University of South Carolina	0.362
Utah State University	0.357
University of Tennessee	0.310

As a result of the HPC funding provided by NSUF, several journal articles and conference proceedings were published. The following is a list of such published work:

Journals

Jin, M., Cao, P., & Short, M. (2020). Achieving exceptional radiation tolerance with crystalline-amorphous nanocrystalline structures. Acta Materialia 186 587-596. https://doi.org/10.1016/j.actamat.2019.12.058

Jin, M., Cao, P., & Short, M. (2019). Predicting the onset of void swelling in irradiated metals with machine learning. Journal of Nuclear Materials 523 189-197. https://doi.org/10.1016/j.jnucmat.2019.05.054

Liu, Y., Kochunas, B., Martin, W., & Downar, T. (2019). Delayed Fission Energy Effect on LWR Normal Operation and Transients. Annals of Nuclear Energy 128 84-93. 10.1016/j.anucene.2018.12.048

Radaideh, M. (2019). Integrated framework for model assessment and advanced uncertainty quantification of nuclear computer codes under Bayesian statistics. Reliability Engineering & System Safety 189 357-377. https://doi.org/10.1016/j.ress.2019.04.020

Ramirez Ruiz, J. (2019). The influence of plasticity-induced crack closure on creep-fatigue crack growth in two heat-resistance steels. International Journal of Fatigue 125 291-298. https://doi.org/10.1016/j.ijfatigue.2019.04.007

Ramirez Ruiz, J. (2019). Fatigue and creep-fatigue crack growth in alloy 709 at elevated temperatures. Materials at High Temperatures 36 562-574. https://doi.org/10.1080/09603409.2019.1664079

Conferences

Calvin, O., Ortensi, J., Schunert, S., Wang, Y., DeHart, M., & Goluoglu, S. (August 2019). Implementation of Depletion Architecture in the MAMMOTH Reactor Physics Application, ANS Mathematics and Computational Methods 2019, Portland, OR, 2019-08-25.

Chen, J., & Brooks, C. (March 2020). Experiment study of fluid motion and mass

transfer in a cylindrical bubble column, ATH'2020 International Topical Meeting on Advances in Thermal Hydraulics, 2020-03-31.

Chen, J., & Brooks, C. (August 2019). CFD simulation of Xenon removal by Helium bubble sparging in molten salt - effect of material properties, 18th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-18), 2019-08-18.

Hallee, B. (November 2019). Non-parametric Statistical Safety Analysis Tools to Support ATR Conversion to LEU, Reduced Enrichment for Research and Test Reactors, Zagreb, Croatia, 2019-10-06. Chicago, IL: https://www.rertr.anl.gov/RERTR40/pdfs/S13-P1_Hallee_paper.pdf

Khuwaileh, B., & Turinsky, P. (August 2019). Bayesian Calibration of Cross-sections Using Plant Operating Data, M&C 2019 Topical Meeting, Portland, OR, 2019-08-26.

Lee, Y., Gryazin, Y., & Gonzales, R. (May 2019). Scalable high-resolution algorithms for landmine imaging problem, SPIE Defense + Commercial Sensing 2019 Exhibition, Baltimore, 2019-04-16. https://doi.org/10.117/12.2519782

Liu, W. (September 2019). Top Fuel 2019, BISON APPLICATION TO THE ANALYSIS OF LWR FUEL RESPONSES UNDER ACCIDENT CONDITIONS, Seattle, USA, 2019-09-22.

Liu, W. (September 2019). Top Fuel 2019, BISON AS A PCI SCREENING TOOL – PCI FAILURE MODEL DEVELOPMENT, Seattle, USA, 2019-09-22.

Liu, Y. (August 2019). Development of Simplified Methods for Ex-core Detector Response in MPACT, The International Conference on Mathematics and Computational Methods applied to Nuclear Science and Engineering (M&C 2019), 2019-08-25. Portland, OR.

Liu, Y., & et. al., (March 2020). An improved energy deposition model in MPACT and explicit heat generation coupling with CTF, Physor 2020, United Kingdom, 2020-03-29.

Liu, Y. (August 2019). Development of Simplified Methods for Ex-core Detector Response in MPACT, M&C 2019, Portland, OR , 2019-08-25.

Mohamed, W., Ozaltun, H., & Roh, H. (July 2019). Proceeding of the ASME 2019 Power Conference, ASME 2019 Power Conference, 2019-07-14.

Mohamed, W., Ozaltun, H., & Roh, H. (July 2019). ASME 2019 Power conference, Effect of Zr diffusion barrier properties on the irradiation performance of u-10mo monolithic fuel plate, Snowbird, 2019-07-14. UT:

Ozaltun, H., Roh, H., & Mohamed, W. (July 2019). Proceedings of the ASME 2019 Power Conference, ASME 2019 Power Conference, 2019-07-14.

Paladino, T., Nicholson, B., & Nawotniak, S. (December 2019). AGU Conference

Proceedings, Quantifying Wind Driven Collapse Scenarios of Explosive Eruption Plumes, 2019-12-09.

Patel, D. (March 2019). Studying the Calcium-dependent Albumin Conformation to Improve Osteoblast Cell Adhesion in Bone Repair and Regeneration, Biophysical Society (BPS) Conference, 2019-03-03.

Patel, D. (November 2019). Paired Simulations and Experimental Investigations into the Calcium-Dependent Bioactivity of Albumin, AIChE, 2019-11-14.

Rezwan, A., Jokisaari, A., & Tonks, M. (April 2019). Modeling Fracture due to Thermal Expansion of Polycrystalline Alpha Uranium at Room Temperature, MRS Spring Meeting and Exhibits, Phoenix, 2019-04-22

Roh, H., Mohamed, W., & Ozaltun, H. (July 2019). ASME 2019 Power conference, Effects of fission profiles on the performance of a U-10Mo fuel plate, Snowbird, 2019-07-14. UT:

Rykhlevskii, A., O'Grady, D., Kozlowski, T., & Huff, K. (November 2019). Transactions of American Nuclear Society, The Impact of Xenon-135 on Load Following Transatomic Power Molten Salt Reactor, Washington D.C., 2019-11-17.

Wang, X., Liu, Y., Martin, W., & Stimpson, S. (August 2019). Implementation of gamma transport capability in MPACT, M&C 2019, Portland, OR, 2019-08-25.