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Nuclear Science User Facilities High Performance Computing: Provide a Science Gateway for HPC Users

August 2021

FY 2021 M3UF-21IN0701015 Milestone Report

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SUMMARY

Idaho National Laboratory (INL), supported by the Department of Energy Office of Nuclear Energy (DOE-NE) through the Nuclear Science User Facilities, provides direct access to the Barracuda Virtual Reactor and 18 Multiphysics Object-Oriented Simulation Environment applications via a web-based science gateway developed using Open OnDemand on the INL high performance computing (HPC) systems. This gateway features the computational tools of the Nuclear Computational Resource Center (NCRC) and the computing resources of the INL HPC systems. These computational tools are a key foundation of collaboration and innovation in nuclear energy systems research. HPC resources and INL staff directly support the mission and objectives of DOE-NE.

The Barracuda Virtual Reactor was the first science gateway deployed in January 2021 to support Nuclear Science User Facilities users. In July 2021, the science gateway was expanded to support access to NCRC codes for use across all supported INL HPC systems. The HPC science gateway currently supports 20 total applications. The gateway also includes access to training resources specific to NCRC tools.

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CONTENTS

SUMMARY iii
ACRONYMS vii
1. INTRODUCTION 1
2. SCIENCE GATEWAY CAPABILITY 1
3. CONCLUSIONS 3

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ACRONYMS

DOE-NE	Department of Energy Office of Nuclear Energy
HPC	High Performance Computing
INL	Idaho National Laboratory
MOOSE	Multiphysics Object-Oriented Simulation Environment
NCRC	Nuclear Computational Resource Center

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1. INTRODUCTION

Idaho National Laboratory (INL), supported by the Department of Energy Office of Nuclear Energy (DOE-NE) through the Nuclear Science User Facilities, provides direct access to the Barracuda Virtual Reactor and 18 Multiphysics Object-Oriented Simulation Environment (MOOSE) applications via a web-based science gateway developed using Open OnDemand on the INL high performance computing (HPC) systems. This gateway features the computational tools of the Nuclear Computational Resource Center (NCRC) and the computing resources of the INL HPC systems. These computational tools are a key foundation of collaboration and innovation in nuclear energy systems research. HPC resources and INL staff directly support the mission and objectives of DOE-NE.

2. SCIENCE GATEWAY CAPABILITY

In January 2021, INL launched the Barracuda Virtual Reactor as the first science gateway deployed in INL's Open OnDemand. The Barracuda Virtual Reactor is launched directly from the Open OnDemand dashboard shown in Figure 1.

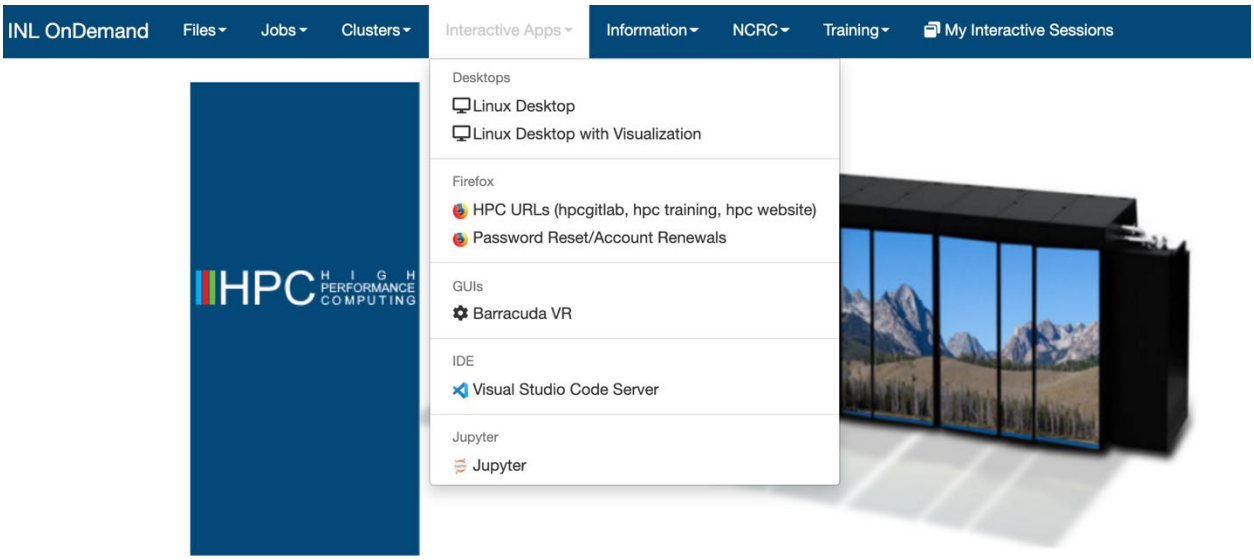

Figure 1. The Interactive Apps dropdown menu from the INL Open OnDemand dashboard. The option "Barracuda VR" corresponds to the Barracuda Virtual Reactor (see Figure 2), which is launched directly on an INL HPC compute node by selecting this science gateway option.

Figure 2. The Barracuda Virtual Reactor science gateway when launched from INL's Open OnDemand dashboard.

The Barracuda Virtual Reactor has been launched 59 times since it was deployed.

Following the success of the Barracuda VR science gateway, 18 additional application gateways were added to OnDemand. Their selection was determined by user demand and support from the NCRC. These application gateways are found in the "NCRC" dropdown menu in the Open OnDemand dashboard, shown in Figure 3.

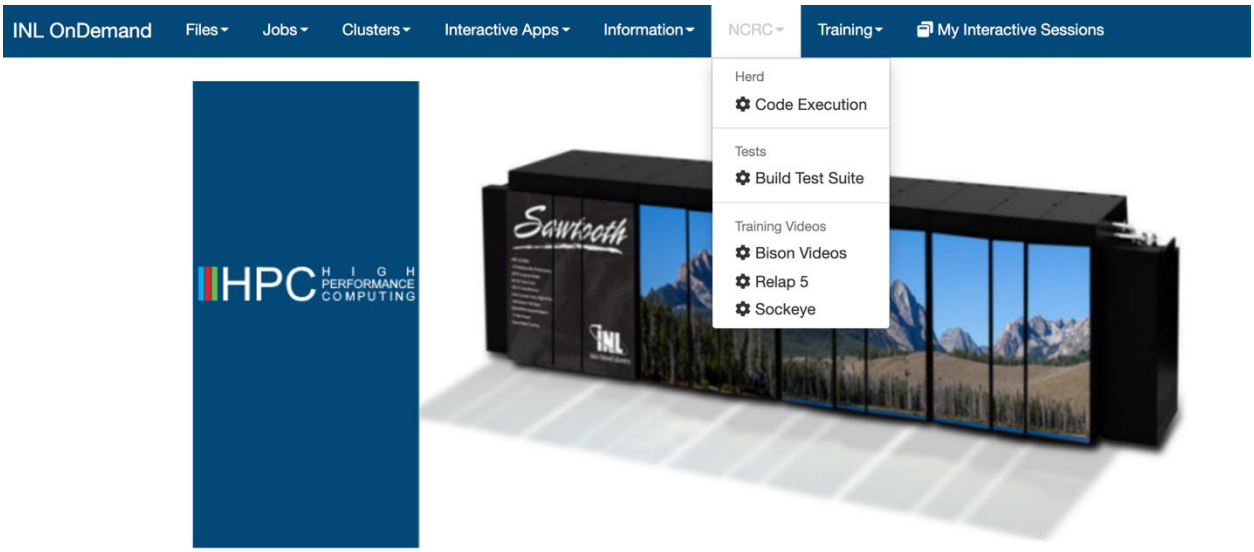

Figure 3. Access to the MOOSE science gateway is via the NCRC dropdown menu in INL's Open OnDemand. The 18 MOOSE herd apps available include Bighorn, Bison, Bison limited, Bluecrab, Direwolf, Griffin, Grizzly, Mammoth, Marmot, Pebbed, Pronghorn, Rattlesnake, Relap5, Relap7, Sabertooth, Sam, Sockeye, and Yellowjacket.

The available science gateway applications available via OnDemand include Bighorn, Bison, Bison limited, Bluecrab, Direwolf, Griffin, Grizzly, Mammoth, Marmot, Pebbed, Pronghorn, Rattlesnake, Relap5, Relap7, Sabertooth, Sam, Sockeye, and Yellowjacket. Test suites and limited training videos are available in the same dropdown menu as access to the science gateway.

When a user attempts to launch a science gateway application, they provide an input file and specify the resource request needed to run the job entirely from within the gateway. They can be notified by email when the request data are available for viewing, and data can be accessed from within Open OnDemand as part of the science gateway. Figure 4 provides the information requested when launching the relap-5 science gateway.

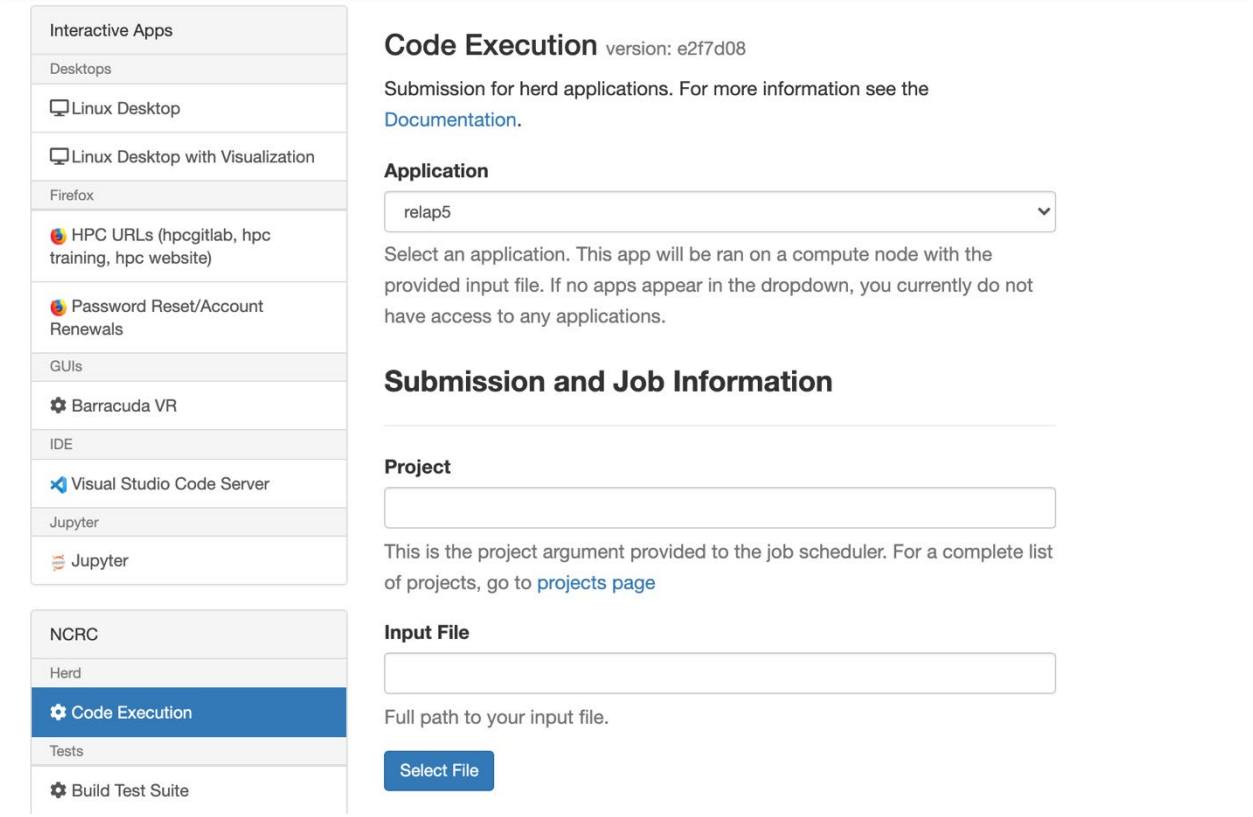

Figure 4. Form for launching the relap-5 science gateway from INL's Open OnDemand.

The MOOSE herd science gateways have been launched 45 times since deployment in July 2021.

3. CONCLUSIONS

The INL HPC-developed science gateway for HPC users based on Open Ondemand provides a channel whereby researchers can deploy science-as-a-service workflows via their web browser without having to directly interact with or compile on the supercomputing resource. This science gateway provides a roadmap for future science-as-a-service deployments and an ongoing delivery mechanism for nuclear engineering applications in support of DOE-NE.