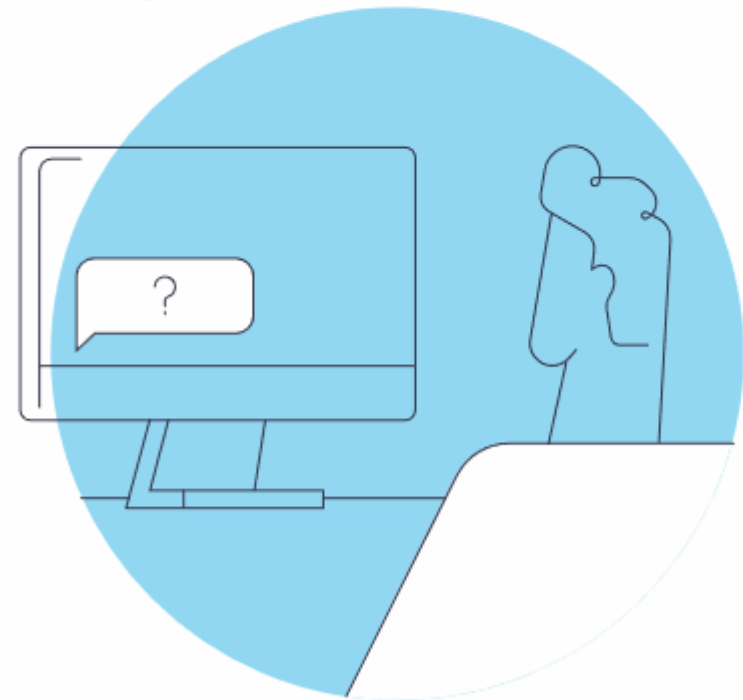


Overview for NVIDIA SAE Team

Alan Chalker, Ph.D.



Ohio Supercomputer Center

Meeting Agenda

About Open OnDemand

Technical Details

Key Items of Note

Open Floor Discussion



Run Open OnDemand

Access your organization's supercomputers through the web to compute from anywhere, on any device.



Zero installation

Run Open OnDemand entirely in your browser. No client software installation required.

Easy to use

Start computing immediately. A simple interface makes Open OnDemand easy to learn and use.

Compatible with any device

Launch on any device with a browser—even a mobile phone or tablet.

openondemand.org/run

Install Open OnDemand

Administer remote web access to your supercomputers to transform the way users work and learn.



Low barrier to entry

Empower users of all skill levels by offering an alternative to command-line interface.

Free and open source

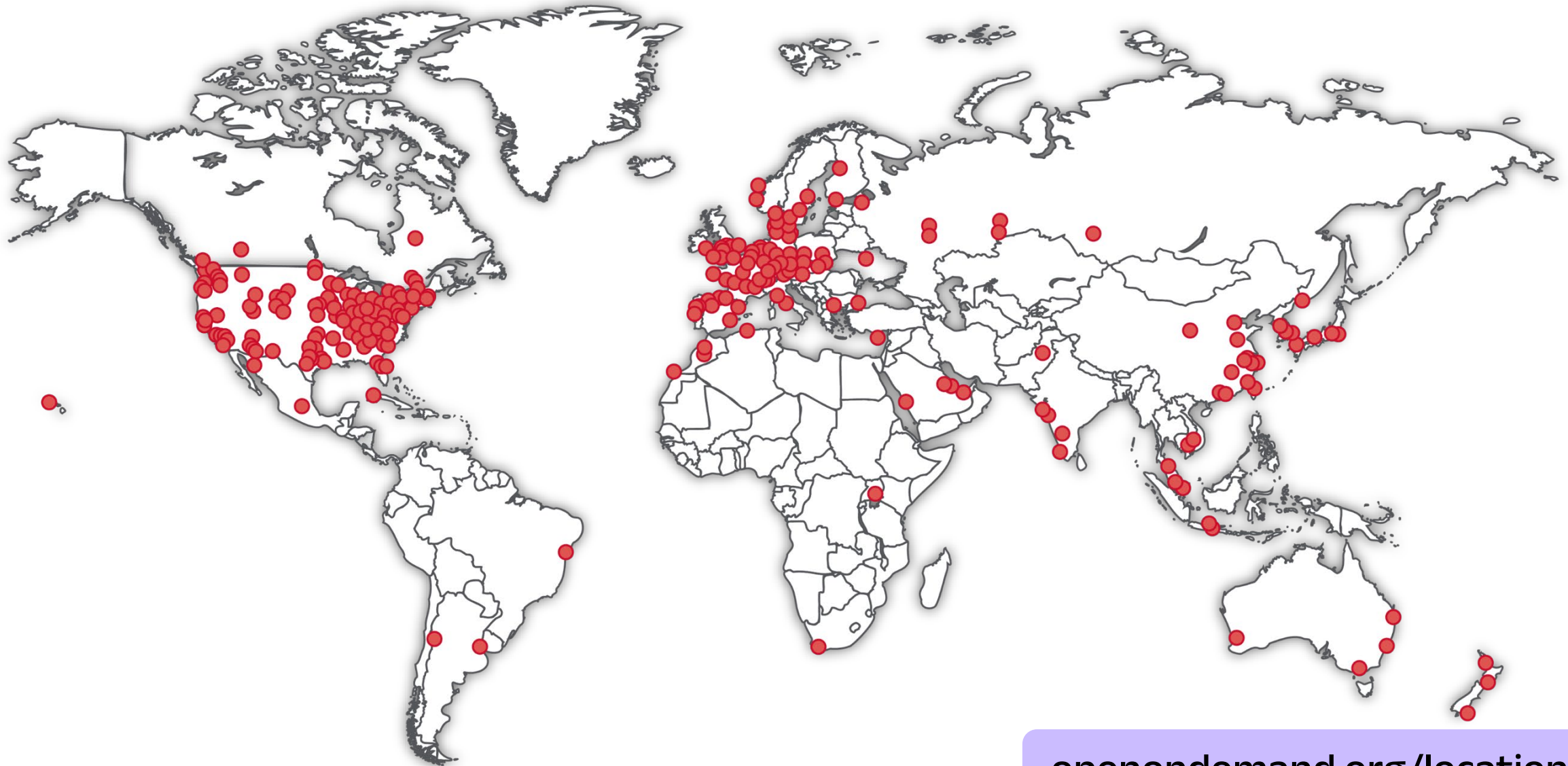
Install Open OnDemand for free, and gather knowledge from our large open-source community.

Configurable and flexible

Create and deploy your own applications to meet your users' unique needs.

openondemand.org/install

Deployed Worldwide



openondemand.org/locations

Example Deployments



Don't see an organization?
The more the merrier!
Let us know any that belong on the list



openondemand.org/orgs

Community Events



Tips and tricks calls

Hosted by the larger Open OnDemand community, tips and tricks webinars share best practices for setting up and using Open OnDemand. They take place on the first Thursday of every month at 1 p.m. ET.



Open office hours

Hosted by our development team, Zoom open office hours are the perfect opportunity to ask questions or make a suggestion. They are held on the second Tuesday of every month from 11:15 a.m. to 12:45 p.m. ET.

openondemand.org/events

Meeting Agenda

~~About Open OnDemand~~

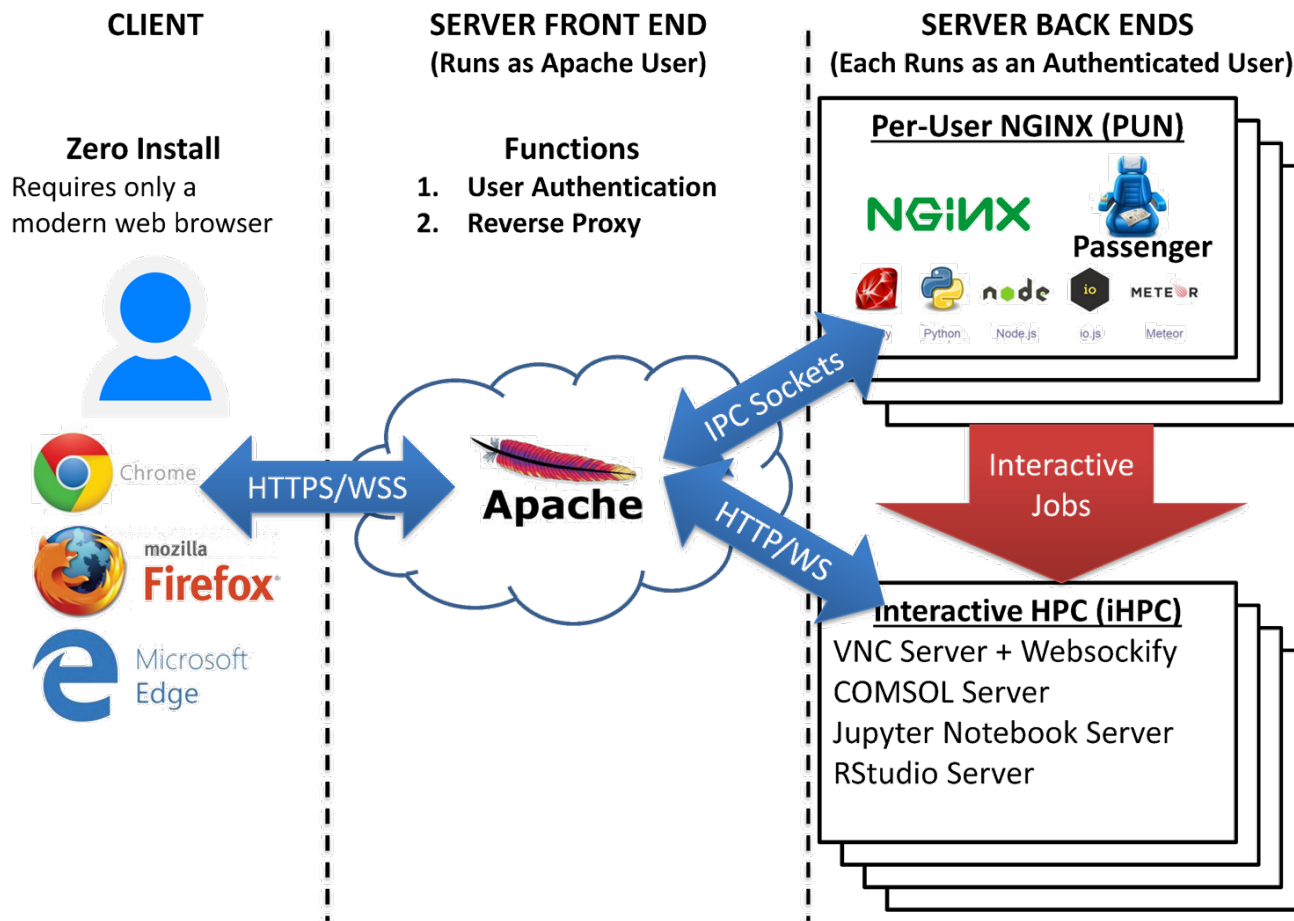
Technical Details

Key Items of Note

Open Floor Discussion



Architecture



Requirements

RedHat/CentOS/Rocky/Ubuntu

Software Collections repos

Lsof

Sudo

Nmap-ncat

TurboVNC

websockify

Enabled Applications

Abaqus
ANSYS
COMSOL
Coot
CSD
Galaxy
Grace
Grafana
Grid Engine
IDL
Jupyter
Kubernetes

LSF
Lumerical
Mathematica
MATLAB
Meshroom
NAGIOS
Octave
Open XDMoD
Ovito
Paraview
PBS Professional
QGIS





RELION
RStudio
SAS
Shiny
Slurm
Spark
STATA
Tensorboard
Torque
VISIT
Visual Studio Code
VMD

openondemand.org/apps

Customization

 **Ohio Supercomputer Center**
An OH·TECH Consortium Member

Pinned Apps A featured subset of all available apps

 Classroom Jupyter System Installed App	 Classroom RStudio System Installed App	 IQmol System Installed App	 Home Directory System Installed App
--	--	--	---

Helpful Links

[OSU Carmen](#)

[OSU STAT 2480 textbook: *The Analysis of Biological Data*](#)

Message of the Day

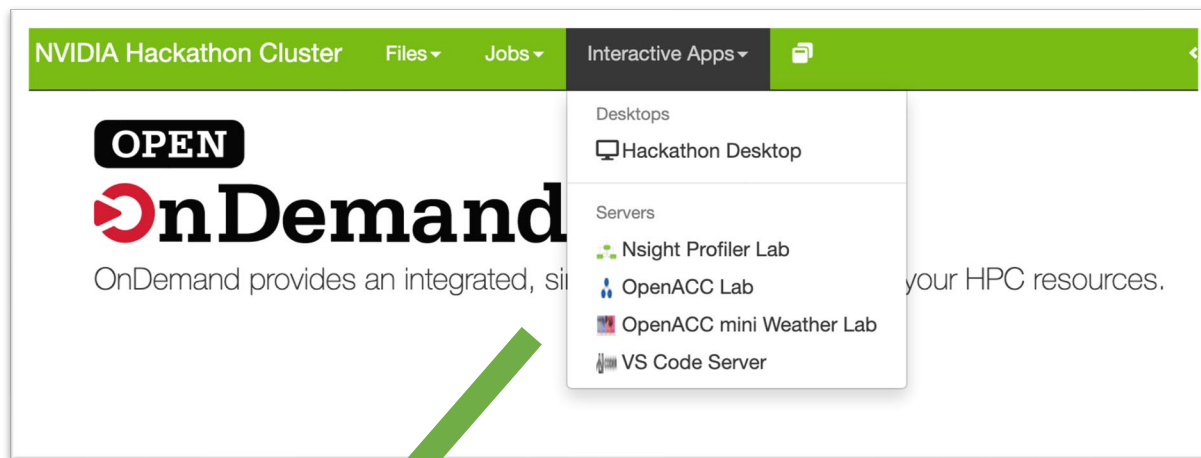
 **ADVANCED RESEARCH COMPUTING TECHNOLOGY SERVICES**
UNIVERSITY OF MICHIGAN

OnDemand provides an integrated, single access point for all of your HPC resources.

Message of the Day

```
*****
* By your use of these resources, you agree to abide by Proper Use of *
* Information Resources, Information Technology, and Networks at the *
* University of Michigan (SPG 601.07), in addition to all relevant *
* state and federal laws. http://spg.umich.edu/policy/601.07 *
*****
```

Desktop Example



NVIDIA Hackathon Cluster Files Jobs Interactive Apps

OPEN
nDemand
OnDemand provides an integrated, simple way to access your HPC resources.

- Desktops
 - Hackathon Desktop
- Servers
 - Nsight Profiler Lab
 - OpenACC Lab
 - OpenACC mini Weather Lab
 - VS Code Server

Hackathon Desktop version: v0.2.2

This app will launch an interactive desktop on one or more compute nodes. You will have full access to the resources these nodes provide. This is analogous to an interactive batch job.

Number of hours
1

Number of nodes
1

Bc Num Gpus
1

I would like to receive an email when the session starts

Launch

* The Hackathon Desktop session data for this session can be accessed under the [data root directory](#).

Hackathon Desktop (7475) 1 node | 8 cores | Running

Host: >_dgn0181 **Delete**

Created at: 2020-11-17 13:54:54 PST

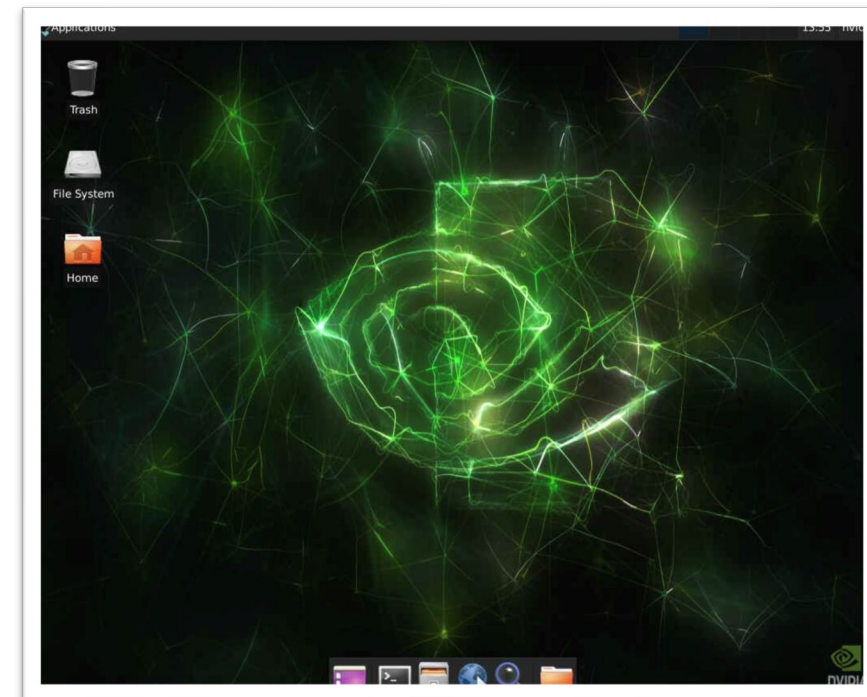
Time Remaining: 59 minutes

Session ID: f681b932-3804-491e-ad1d-988dcf6ad9ef

Compression 0 (low) to 9 (high)

Image Quality 0 (low) to 9 (high)

Launch Hackathon Desktop **View Only (Share-able Link)**



Release 2.1 – February 2023

Quick launch apps

Include preset values to launch with 1 click.

Support tickets

Menu item to submit to a site help desk (Harvard).

Profile support

Includes group profiles, custom navbar, dashboard (Harvard).

Cloud storage

Interfaces to S3, Swift, OneDrive, etc. (CSC – Finland).

Meeting Agenda

~~About Open OnDemand~~

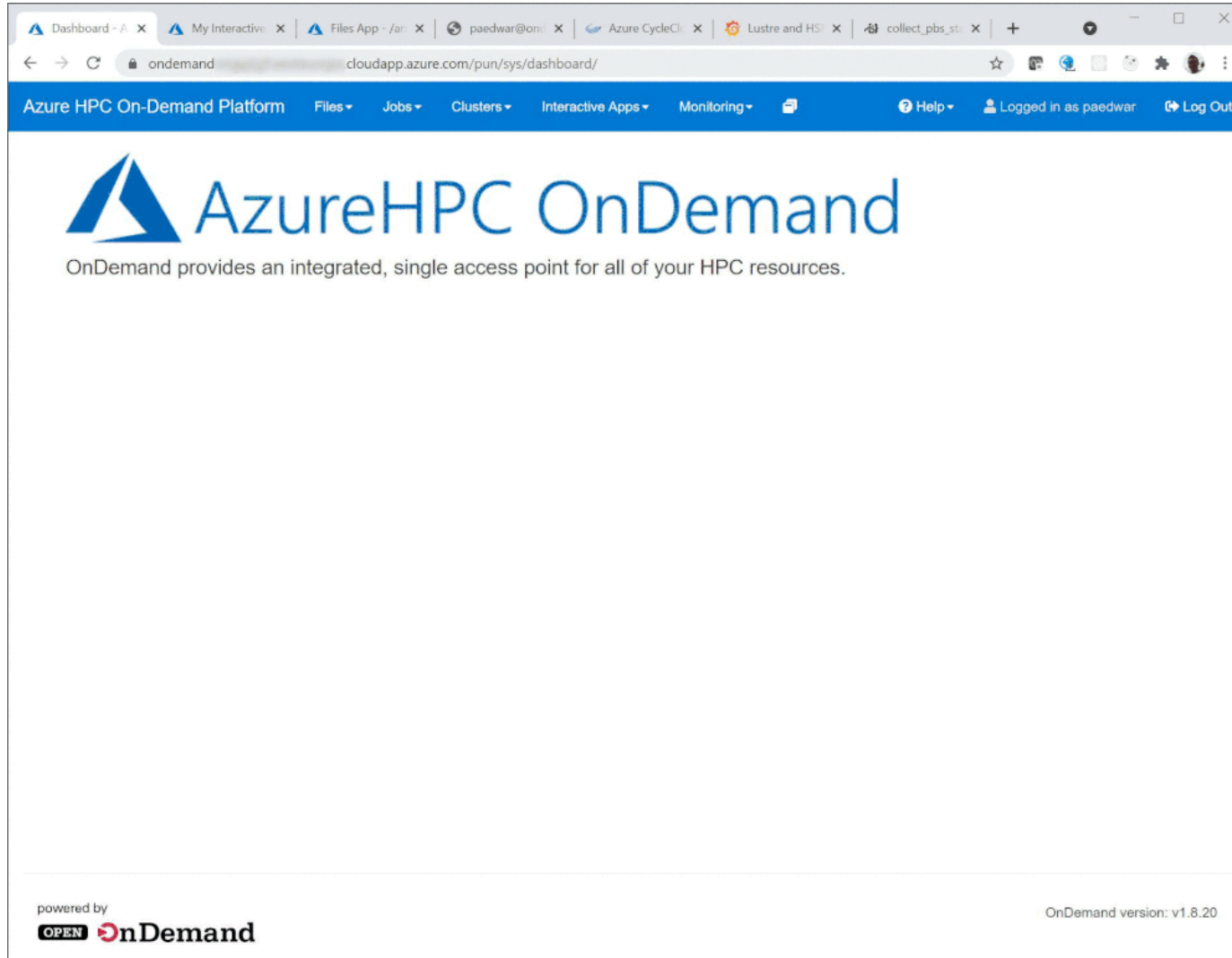
~~Technical Details~~

Key Items of Note

Open Floor Discussion



Commercial Cloud



openondemand.org/aws



openondemand.org/azure



openondemand.org/gcp

Fugaku OnDemand

スーパーコンピュータ「富岳」における HPC クラスタ用 Web ポータル Open OnDemand の導入

中尾 昌広^{1,a)} 三浦 信一¹ 山本 啓二¹

概要：「富岳」などの HPC クラスタの問題点として、HPC クラスタを用いるための前提知識が多いため、初心者にとって利用するまでの学習コストが大きい点が挙げられる。また、近年では、対話的操作を伴う GUI (Graphical User Interface) アプリケーションを計算ノード上で動作させることを望まれているが、その手順は煩雑である。そこで、本稿では HPC クラスタの計算資源を簡単に利用可能にする Web ポータル Open OnDemand を「富岳」に導入する。その導入を実現するため、「富岳」で用いられているジョブスケジューラを Open OnDemand から利用できるアダプタの開発を行った。本稿では、アダプタの開発および「富岳」における Open OnDemand の利用例について述べる。

1. はじめに

理化学研究所 計算科学研究センター (R-CCS : RIKEN Center for Computational Science) [1] は、日本におけるフラッグシップスーパーコンピュータとして「富岳」を運用している [2]。また、R-CCS は「富岳」の利便性を向上させるため、可視化やデータ変換等を行うプリポスト環境も提供している。図 1 に「富岳」とプリポスト環境の概念図を示す。プリポスト環境は、GPU を搭載したノードと大容量メモリを搭載したノードで構成される。ジョブスケジューラは「富岳」とプリポスト環境とで異なり、「富岳」は Fujitsu Software Technical Computing Suite (Fujitsu TCS) [3] であるのに対し、プリポスト環境は Slurm [4] である。各システムの利用手順としては、ユーザはまず Secure Shell (SSH) を用いて共通のログインノードにログインし、次にジョブスケジューラを用いて各システムにジョブを投入する。

「富岳」などの HPC クラスタを利用するためには、Shell による CLI (Command Line Interface)、SSH の鍵ペアの生成と公開鍵の登録、ジョブスケジューラなどの知識が必要であるため、初心者にとって学習コストが大きいという問題点がある。また、近年では、対話的操作を伴う GUI (Graphical User Interface) アプリケーションを HPC アプリケーションとして動作させることを望まれているが、そのようなアプリケーションを HPC クラスタ上で動作させ

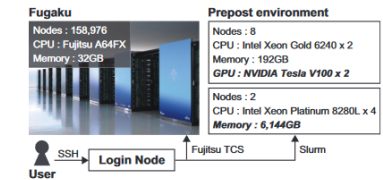


図 1 「富岳」とプリポスト環境の概念図

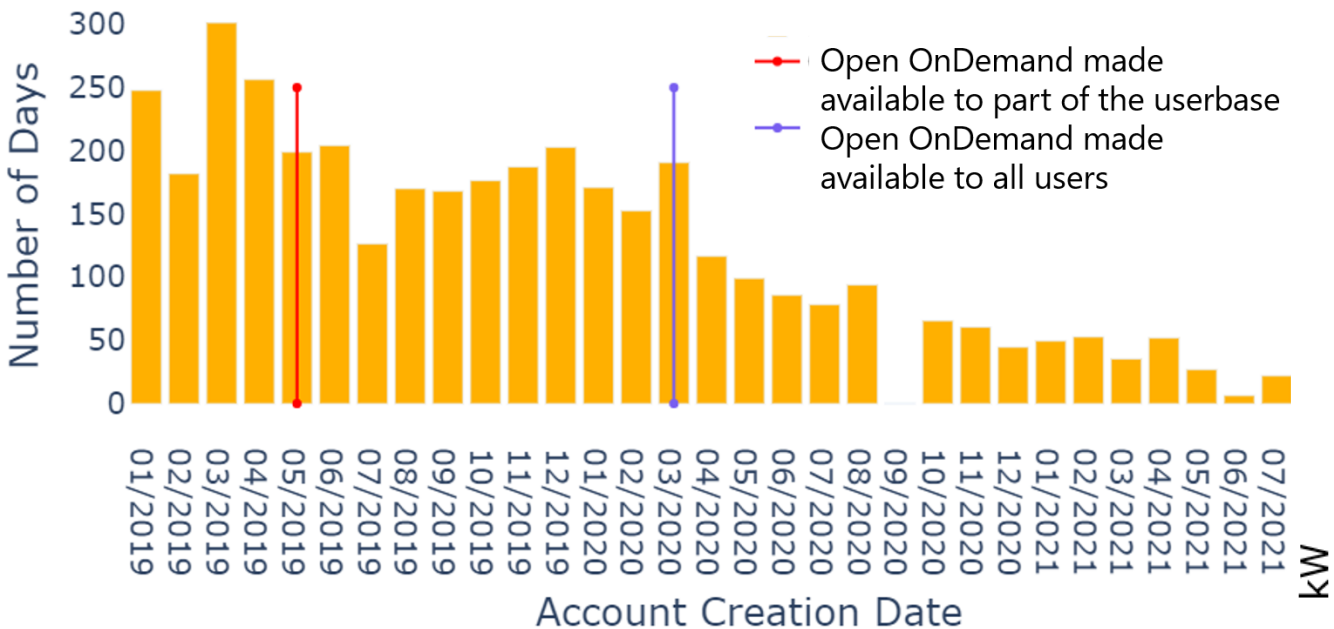
る手順は煩雑である。例えば、JupyterLab のような Web ベースのアプリケーションの場合、次のような手順をアプリケーションを実行する毎に GUI で行う必要がある。(1) SSH でログインノードにログインする。(2) ジョブスケジューラを通して JupyterLab を計算ノード上で実行する。(3) 計算ノードの IP アドレスと JupyterLab が利用するポート番号を取得する。(4) 取得した IP アドレスとポート番号に SSH トンネリングでローカルポートと接続する。(5) ローカルポートを Web ブラウザで開く。このように、多くの手間を要するだけでなく、これらの作業には前述した知識も必要であるため、GUI に慣れたユーザにとって大きな負担となっている。

本稿では HPC クラスタ用の Web ポータル Open OnDemand [5] を「富岳」に導入する。Open OnDemand を用いると、SSH ではなく Web ブラウザから HPC クラスタの計算資源を利用できる。さらに、HPC クラスタの計算ノード上で動作する GUI アプリケーションの対話的操作を簡単に実行できる。ここで、Open OnDemand は様々なスケ

¹ 理化学研究所 計算科学研究センター 兵庫県神戸市中央区港島南町 7-1-26
^{a)} masahiro.nakao@riken.jp

Idaho National Lab

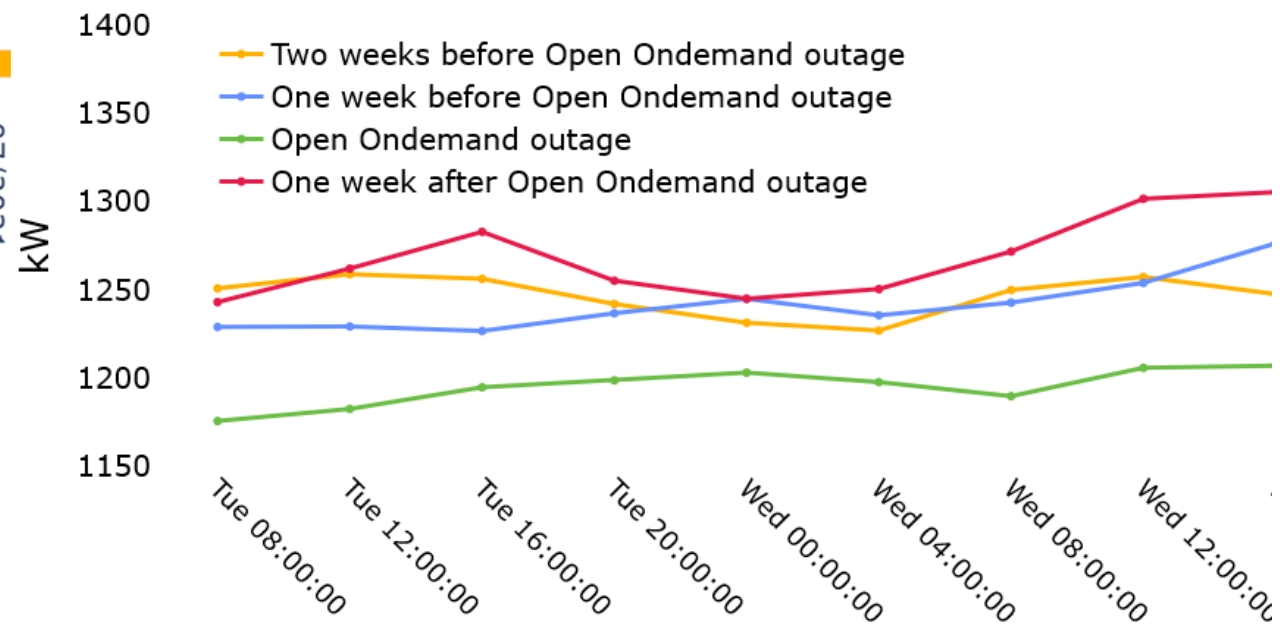
Average Number of Days Between Account Creation to First Job Submission



19 times shorter
In days between account creation and first job submission

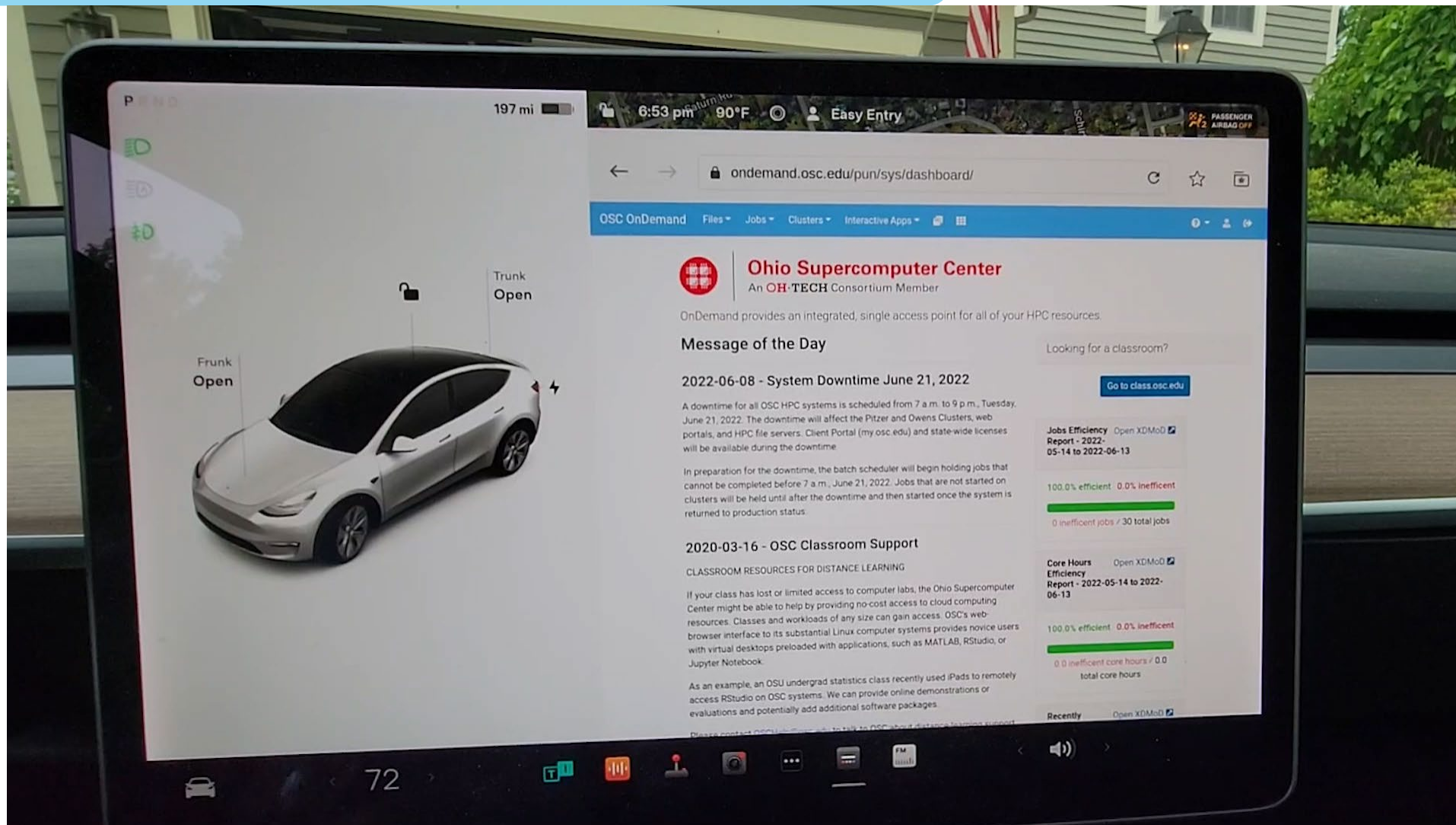
3.7% drop
In power used during an unscheduled Open OnDemand outage

Datacenter Power Usage



openondemand.org/idaho

Any Device, Anywhere



Example Case Studies



WEB PORTALS

Open OnDemand aids engineering school's supercomputing curriculum

■ Research Landscape ▲ Invention/Discovery

In 2019, the Milwaukee School of Engineering (MSOE) unveiled a major addition to its campus: the Dwight and Dian Diercks Computational Science Hall, featuring Rosie the supercomputer. The facility opened in the wake of the launch of MSOE's bachelor's degree in computer science, with a curriculum focused on the growing field of artificial intelligence.

Alumnus Dwight Diercks, who along with his wife Dian donated \$34 million for the facility, has worked for the technology company NVIDIA since 1994 and today serves as its senior vice president of software engineering. MSOE worked closely with the company on assembling the necessary hardware and software for the supercomputer, which features NVIDIA graphics processing units (GPUs).

NVIDIA recommended that MSOE adopt Open OnDemand, an open-source high performance computing portal developed by the Ohio Supercomputer Center (OSC). Open OnDemand is used by researchers and college students around the world to access supercomputing resources anywhere from any device.

Derek Riley, a professor and program director for electrical engineering and computer science

at MSOE, reports that most of the jobs run on Rosie use the Open OnDemand portal. MSOE established the supercomputer primarily as a teaching tool for undergraduates studying machine learning and data science, and Open OnDemand has made it easy for them to directly access Rosie, Riley said. Students can avoid time-consuming technical setups and instead gain more experience using the supercomputer to answer a variety of scientific and engineering questions.

"It can't be overstated how important it is for students to focus on the problems we want them to learn," he said.

MSOE's approach to supercomputing also reflects the work environment that many students will find themselves in after graduation, as most employers have engineering teams that handle the more technical aspects of supercomputer setup and maintenance while the data scientists conduct analyses, Riley said.

Not only has Open OnDemand been beneficial for undergraduates to use, but MSOE's own system administrators have found it easy to learn and manage, Riley said.

"We've had a really great experience using it—we've been really happy with it," he said. "We've been able to use it primarily out of the box, and it's the main entry point for students and faculty to the cluster."

Read and share online: osc.edu/27/msoe

Above: Rosie the supercomputer supports the Milwaukee School of Engineering's computer science program. Image courtesy of Milwaukee School of Engineering.

OHIO SUPERCOMPUTER CENTER

"In order to learn from millions and millions of chemical structures, we need a lot of computational power," Ning said.

The Ohio Supercomputer Center (OSC) is integral to the project. Each model requires the use of one graphical processing unit (GPU) and 96 GB of RAM for the data generated, Ning noted.

Alumnus Dwight Diercks, who along with his wife Dian donated \$34 million for the facility, has worked for the technology company NVIDIA since 1994 and today serves as its senior vice president of software engineering. MSOE worked closely with the company on assembling the necessary hardware and software for the supercomputer, which features NVIDIA graphics processing units (GPUs).

ARTIFICIAL INTELLIGENCE

Accelerating drug discovery with AI

■ BIOLOGICAL SCIENCES | ▲ INVENTION/DISCOVERY

Xia Ning has a large portfolio of research projects at The Ohio State University that focus on understanding how artificial intelligence can be used to solve issues in health care.

Discovering new drugs to treat disease is one of Ning's goals. Traditional research methods, which call for lengthy trials with animal models, have disadvantages.

"To find a single drug is costly and time consuming," said Ning, an associate professor who holds joint appointments in Ohio State's College of Medicine and College of Engineering.

Ning is drawing on her expertise in computer science and biomedical informatics to create a new path to drug discovery. Her lab examines millions of small molecules and uses that information to create novel models that could be strong candidates for drugs.

"In order to learn from millions and millions of chemical structures, we need a lot of computational power," Ning said.

The Ohio Supercomputer Center (OSC) is integral to the project. Each model requires the use of one graphical processing unit (GPU) and 96 GB of RAM for the data generated, Ning noted.

Compared to the conventional central processing units (CPUs) researchers may use in their labs, GPUs offer a significant boost in computing power. OSC features GPUs across its systems to allow clients to efficiently process large amounts of data, and consistently upgrades its hardware to ensure access to the most cutting-edge technologies.

Those computing resources have helped Ning reach important milestones in her drug discovery work. Research findings from the project have been accepted for publication in the prestigious journal Nature Machine Intelligence and also have attracted new grant funding to the lab.

Ning has been a heavy user of high performance computing centers since her days as a faculty member at Indiana University. She joined Ohio State in 2018.

"The first thing I did here was look for similar resources," Ning recalled. "I didn't think about having my own cluster—that would have taken me a lot of effort."

In addition to OSC's capabilities and technical support, Ning appreciates its availability to her lab members. OSC offers Open OnDemand, an interface funded by the National Science Foundation that allows users to remotely access the Center resources online from any device.

"(OSC) provides a very nice Open OnDemand tool that we can access through the web," Ning said. "I believe all of my students are using it. It's very easy for us to use, and we don't need to worry about maintenance or software installation."

Ning also employs OSC for teaching Python programming in her biomedical course. The Center creates a class project through which her students can quickly access computational resources and see results immediately through the OSC web portal, she said.

Over the next year, Ning will continue to work with OSC on the drug discovery project, as well as on research on predicting peptides that could be used for vaccine development.

"As long as we're doing research," Ning said, "we'll rely on OSC." •

Website: u.osu.edu/ning.104

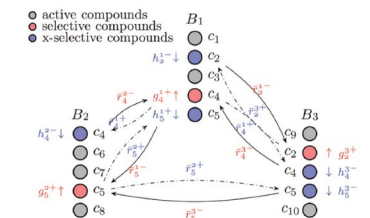


Figure: Advanced AI and large-scale computing enabling multi-purpose drug discovery.

OHIO SUPERCOMPUTER CENTER

12

openondemand.org/casestudies

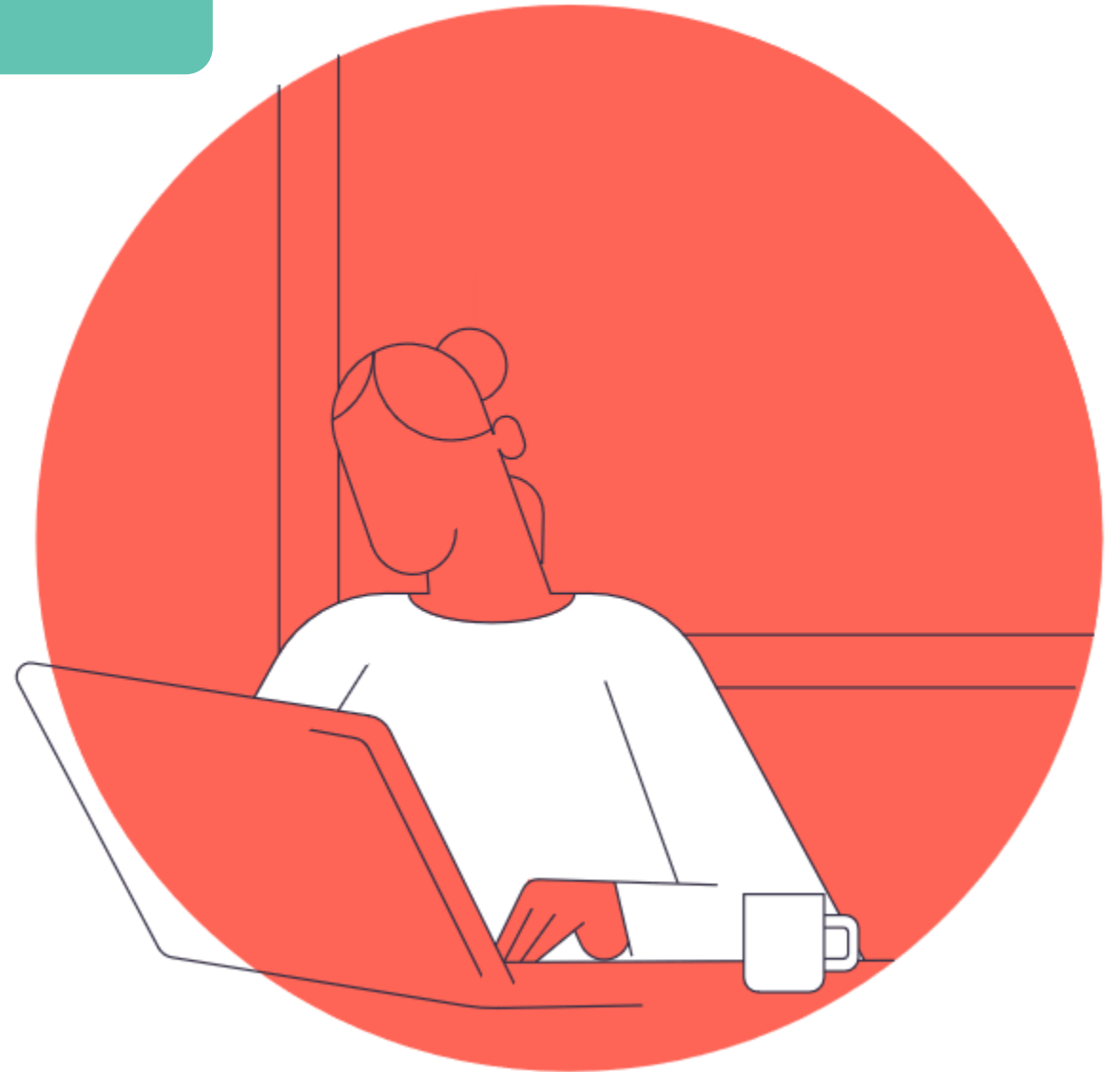
Meeting Agenda

~~About Open OnDemand~~

~~Technical Details~~

~~Key Items of Note~~

Open Floor Discussion



openondemand.org/discuss