User Group Meeting Agenda

About Open OnDemand

3.0 Updates

Key Items of Note

Open Floor Discussion

Run Open OnDemand

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.
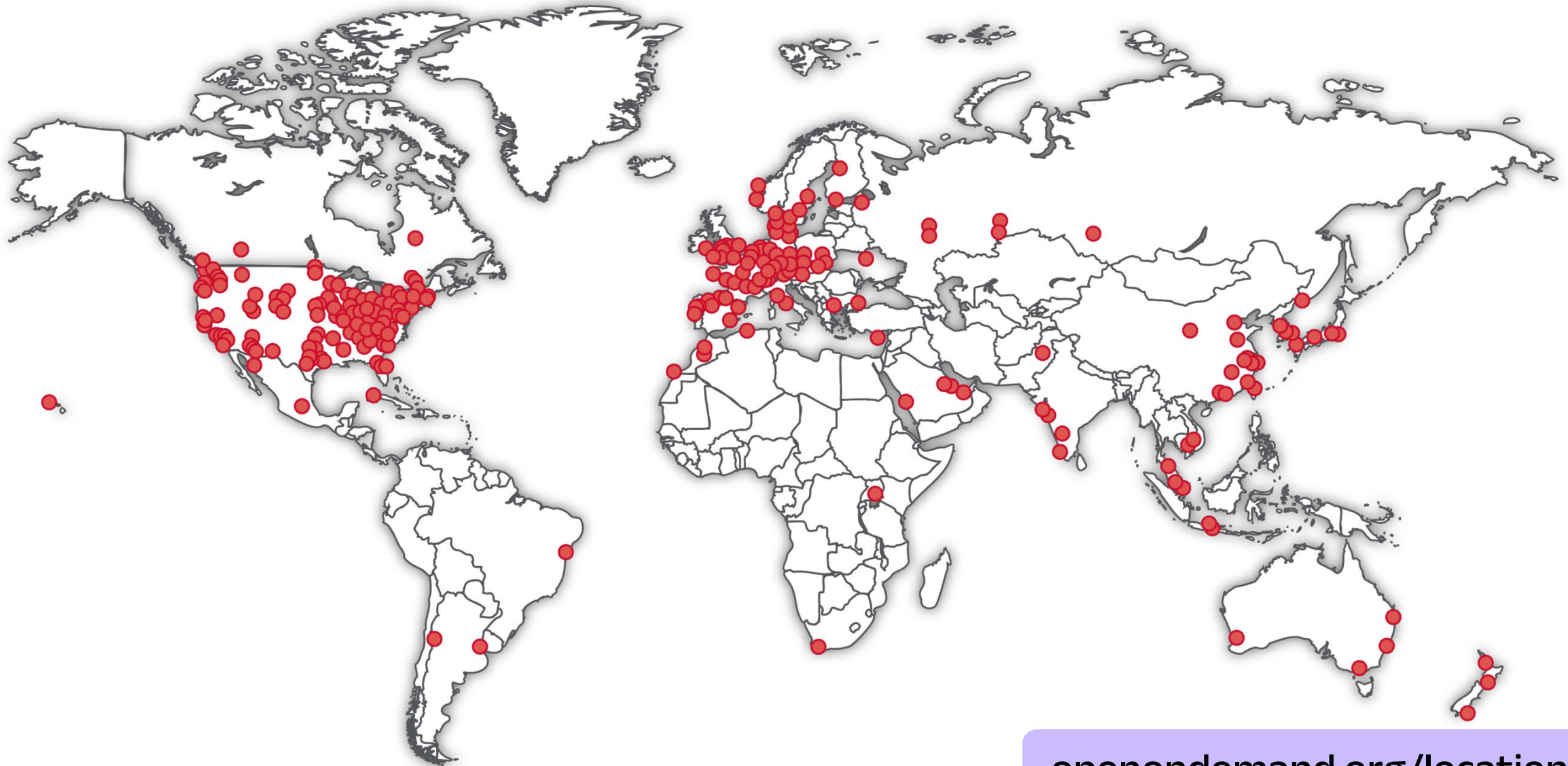
Free and open source

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

OPEN OnDemand

openondemand.org/locations

Example Deployments

Don't see your organization?

The more the merrier! Let us know if you belong on the list

openondemand.org/orgs

Enabled Utilities & Apps

OPEN OnDemand

Abaqus	LSF	RELION
ANSYS	Lumerical	RStudio
COMSOL	Mathematica	SAS
Coot	MATLAB	Shiny
CSD	Meshroom	Slurm
Galaxy	NAGIOS	Spark
Grace	Octave	STATA
Grafana	Open XDMoD	Tensorboard
Grid Engine	Ovito	Torque
IDL	Paraview	VISIT
Jupyter	PBS Professional	Visual Studio Code
Kubernetes	QGIS	VMD

openondemand.org/apps

Community Events

OPEN OnDemand

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

Support

Discuss on Discourse

The Get Help thread on our Discourse forum features user and admin questions and answers. Browse recent questions or leave one of your own.

Documentation

Our documentation outlines installation steps, app development guidelines, release notes, and more. Search for a specific topic or browse for general info.

openondemand.org/support

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Administrative Changes

Documentation

Restructured to group sections more logically.

Dependency updates

Ruby 3.0, NodeJS 14, Python 3

Dex location

Defaults to behind Apache reverse proxy.

Autoloading deprecated

Impacts any initializers.

openondemand.org/releasenotes

Customization Features

Navbar configurations

Nearly every aspect can be customized.

Custom landing pages

Dedicated URLs can directly access them.

Profile support

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

openondemand.org/releasenotes

App Features

Quick launch apps

All parameters are hard-coded.

Recently used apps

Automatically generated quick launch apps.

Running sessions widget

Displayed directly on dashboard.

openondemand.org/releasenotes

General Features

Remote files

Rclone integration in files app (CSC Finland).

Help ticket integration

Email support staff directly from session cards.

Additional OS support

New packages for EL and Ubuntu.

openondemand.org/releasenotes

Future Releases

Semi-Annual minor releases

Smaller and more frequent

Community input needed

Help us prioritize features

Example Features

System status widget

User favorites

New proxy

First class file picker

Documentation in dashboard

New job composer

Customize session cards

openondemand.org/roadmap

User Group Meeting Agenda
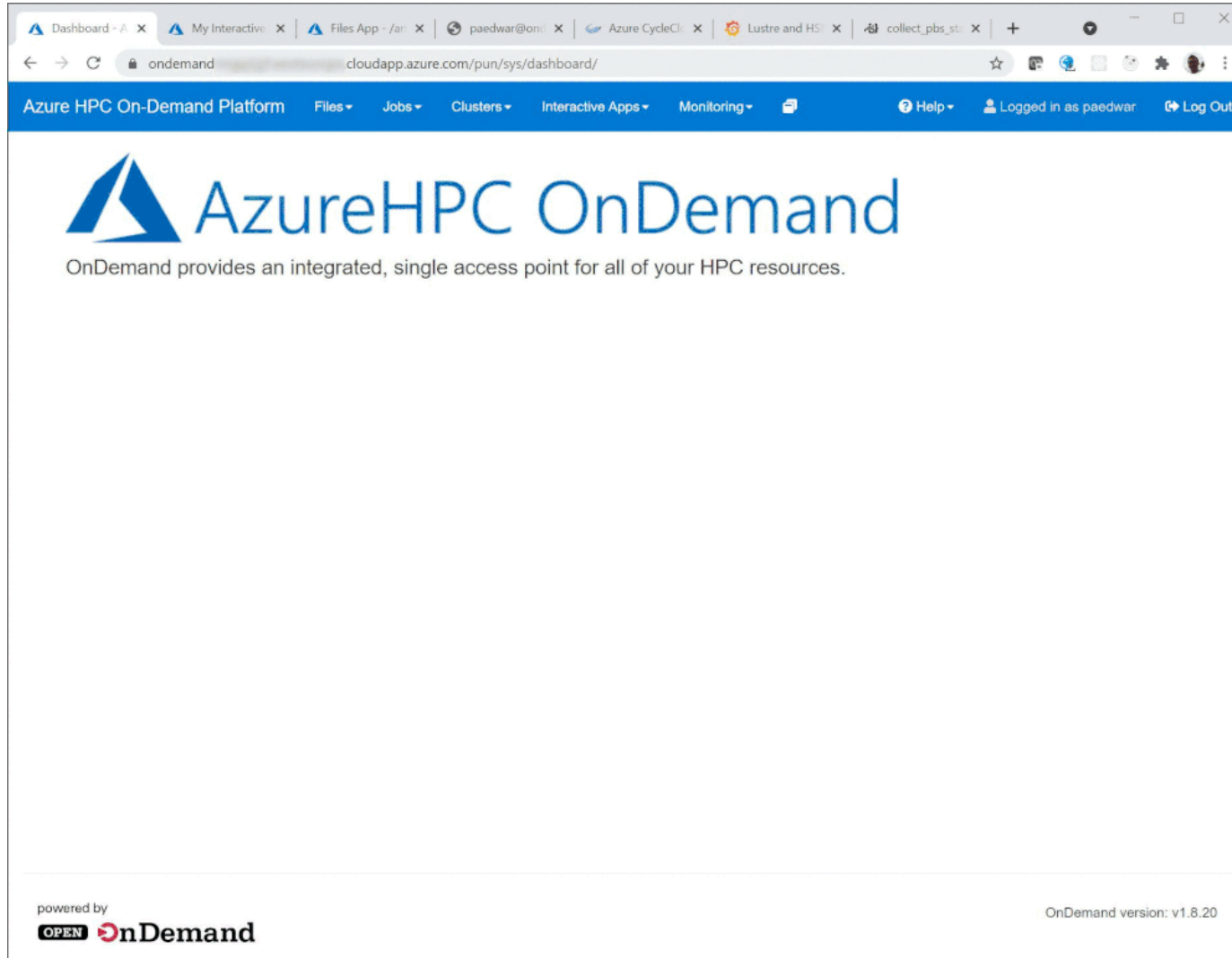
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Commercial Cloud

openondemand.org/aws

openondemand.org/azure

openondemand.org/gcp

Fugaku OnDemand

OPEN 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易に利用可能にする 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
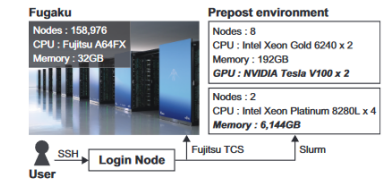
る手順は煩雑である．例えば，JupyterLab のような Web ベースのアプリケーションの場合，次のような手順をアプリケーションを実行する毎に CUI で行う必要がある．(1) SSH でログインノードにログインする．(2) ジョブスケジューラを通して JupyterLab を計算ノード上で実行する．(3) 計算ノードの IP アドレスと JupyterLab が利用するポート番号を取得する．(4) 取得した IP アドレスとポート番号に SSH トンネリングでローカルポートと接続する．(5) ローカルポートを Web ブラウザで開く．このように，多くの手間を要するだけでなく，これらの作業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易に実行できる．ここで，Open OnDemand は様々なスケ

図 1　「富岳」とプリポスト環境の概念図

1

openondemand.org/fugaku

Idaho National Lab

Average Number of Days Between Account Creation to First Job Submission

— Open OnDemand made available to part of the userbase
— Open OnDemand made available to all users
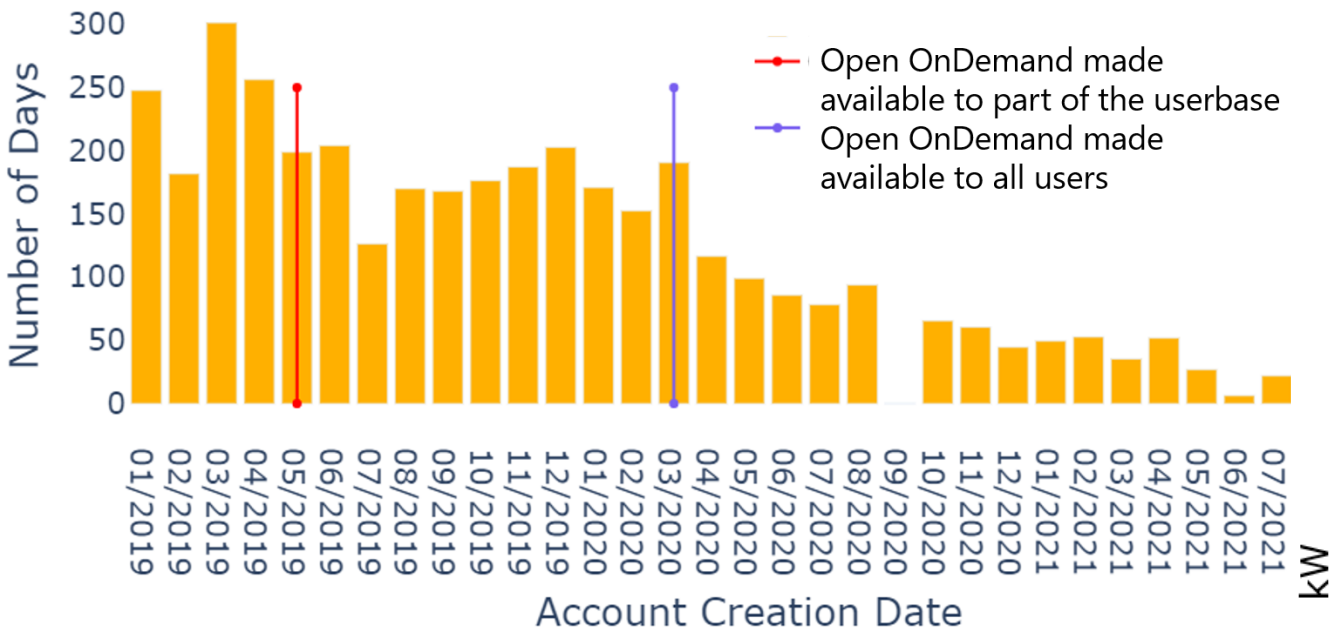
19 times shorter

In days between account creation and first job submission

3.7% drop

In power used during an unscheduled Open OnDemand outage

Datacenter Power Usage

— Two weeks before Open Ondemand outage
— One week before Open Ondemand outage
— Open Ondemand outage
— One week after Open Ondemand outage
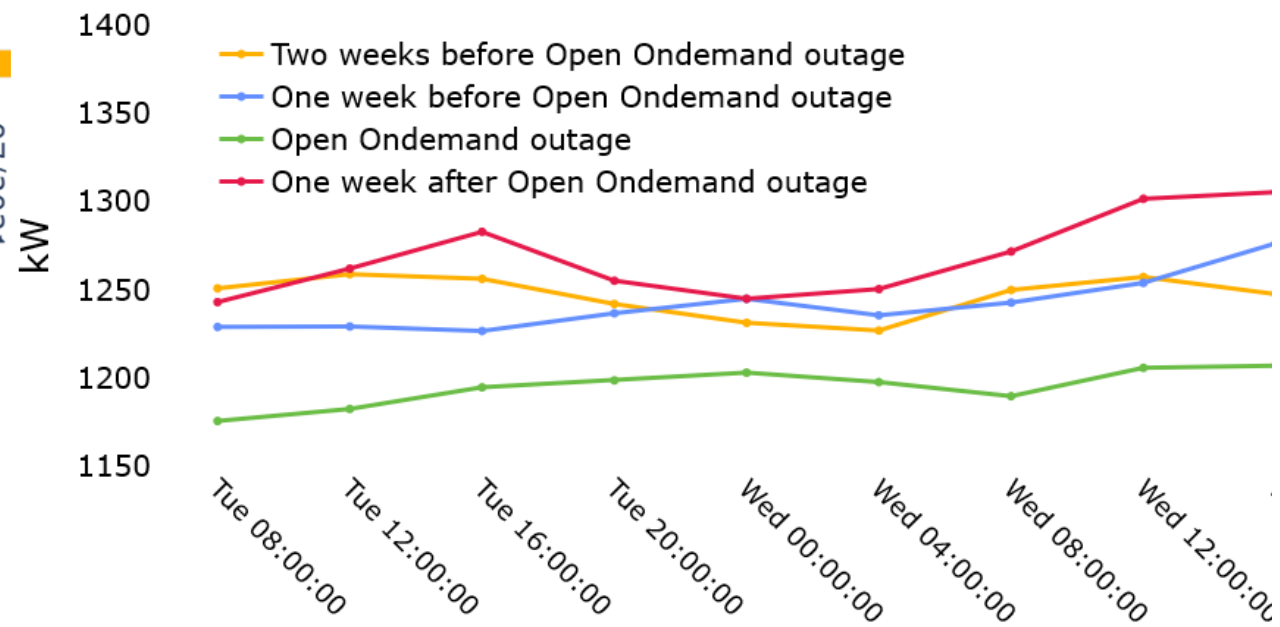
openondemand.org/idaho

Example Case Studies
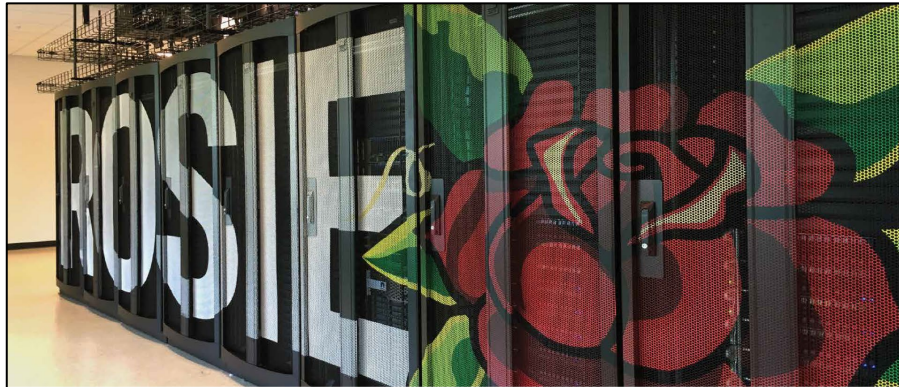
WEB PORTALS

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/r22/msoe

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

14   OHIO SUPERCOMPUTER CENTER

> With the development of OSC's online portal Open OnDemand, much of this complexity has been eliminated, as OnDemand integrates software familiar to the students.

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

CLASSROOM LEARNING

Professor builds Ohio State course around research using the Ohio Supercomputer Center

■ Research Landscape ▲ Energy/Chemical

Chris Hadad has been a client of the Ohio Supercomputer Center (OSC) for over two decades and leads one of the most active accounts. A professor of organic chemistry at The Ohio State University, Hadad is currently developing medical countermeasures against organophosphorus chemical nerve agents used in chemical warfare and as pesticides in agriculture.

More than 20 years ago, Hadad was inspired by the impact of OSC on his research to help others in the scientific community learn about and access high performance computing (HPC) resources.

"The idea I've always had was essentially to help develop expertise in different research groups on how they can use computational methods as a benefit to their experimental studies," he said.

To accomplish this goal, in 1996 Hadad developed a course at Ohio State, "Computational Chemistry," that teaches graduate-level students how to use HPC within their various fields of research.

Today Hadad has taught the course 16 times and has made a significant impact on students' education and careers. "Computational Chemistry" introduces students to real-world research using the HPC resources provided by OSC. The students choose their projects based on what interests them, and Hadad helps them

tailor their use of OSC to find the answers they are seeking.

When Hadad began teaching this course, some students encountered difficulty using OSC, as they first needed to learn Unix commands to interface with the systems, the professor recalled. With the development of OSC's online portal Open OnDemand, much of this complexity has been eliminated, as OnDemand integrates software familiar to the students.

Not only are Hadad's students highly engaged in the classroom, but they also complete research that later may become the basis for their theses.

"Over 40 student projects have actually been published in different journals, many of them in some of the best journals in chemistry," Hadad said.

Hadad's integration of OSC within the classroom has helped disseminate HPC skills throughout educational and research communities.

"I've even had faculty take my class, including some faculty who have then gone on to other institutions to teach a computational chemistry class there," Hadad said.

Read and share online: osc.edu/r22/hadad
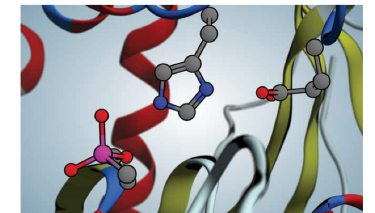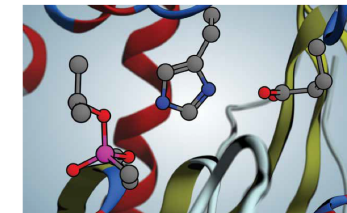
Left: Catalytic active site of OP-inhibited acetylcholinesterase by the nerve agent Sarin as generated in silico from the 5FPQ crystal structure. Right: Catalytic active site of OP-aged acetylcholinesterase by the nerve agent Sarin as generated in silico from the 5FPQ crystal structure.

2021–2022 RESEARCH REPORT / RESEARCH   9

openondemand.org/casestudies

How to Contribute

OPEN **OnDemand**

Spread the word

Mention us on Twitter @open_ondemand—or simply tell your friends!

Make a suggestion

Pitch a new app or feature—or report a bug—to help make Open OnDemand even better.
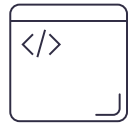
Engage with us

Collaborate with us to make your corporate or higher ed project a reality.

Write documentation

Draft documentation for a new app or feature, or help us revise existing docs.

Write code

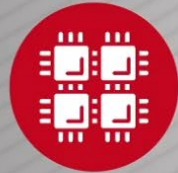Write code for a new app or feature, and share it with our community.

Fund the project

Provide monetary support to our development team or one of our partners. Every gift helps!

openondemand.org/contribute

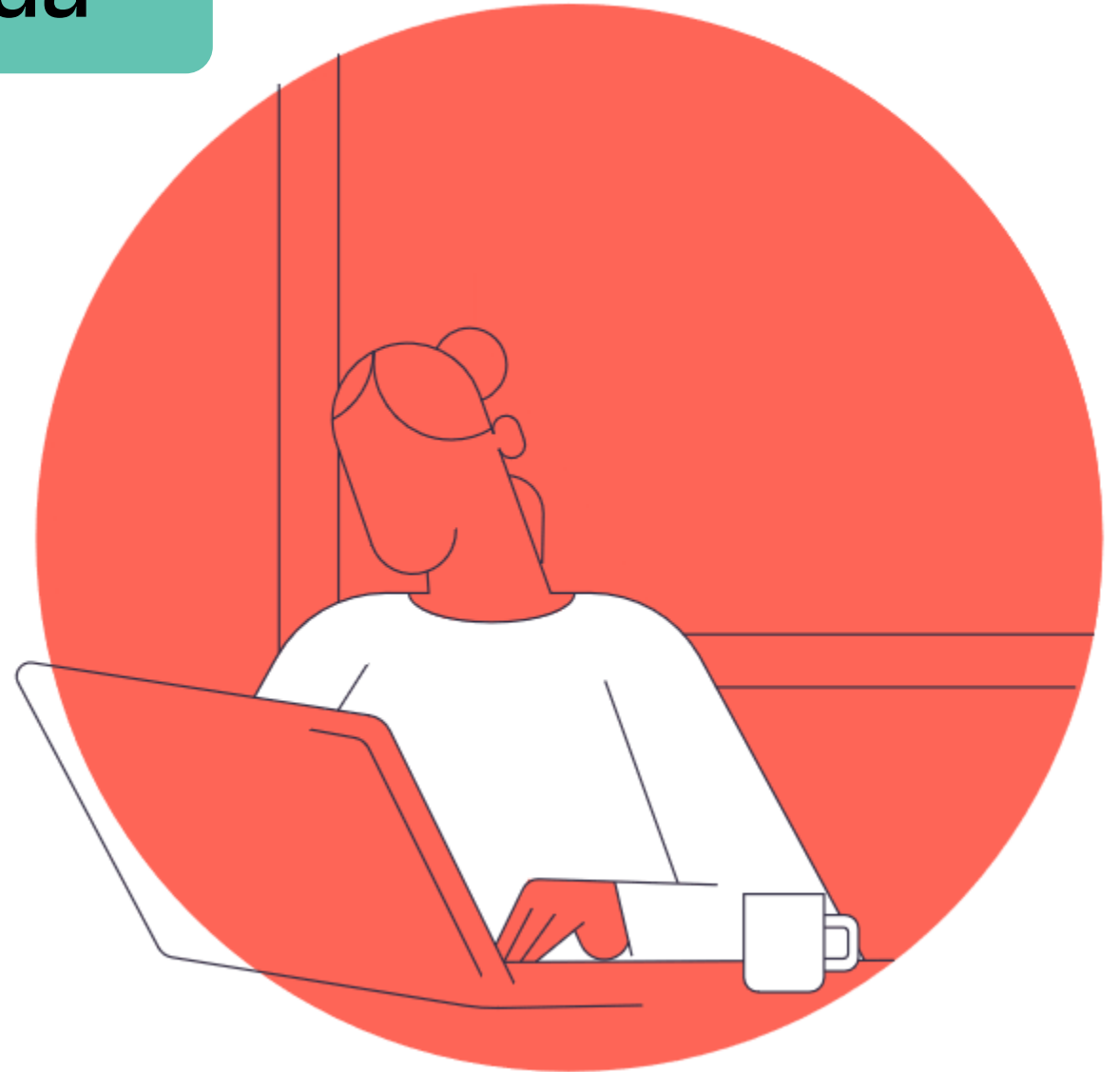# Any Device, Anywhere

openondemand.org/anydevice

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openondemand.org/discuss