OPEN OnDemand

User Group Meeting
PEARC23 BoF

Alan Chalker

Ohio Supercomputer Center

University at Buffalo Center for Computational Research

MGHPCC Massachusetts Green High Performance Computing Center

Virginia Tech

University of Colorado Boulder

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openondemand.org/pearc23

User Group Meeting Agenda

About Open OnDemand

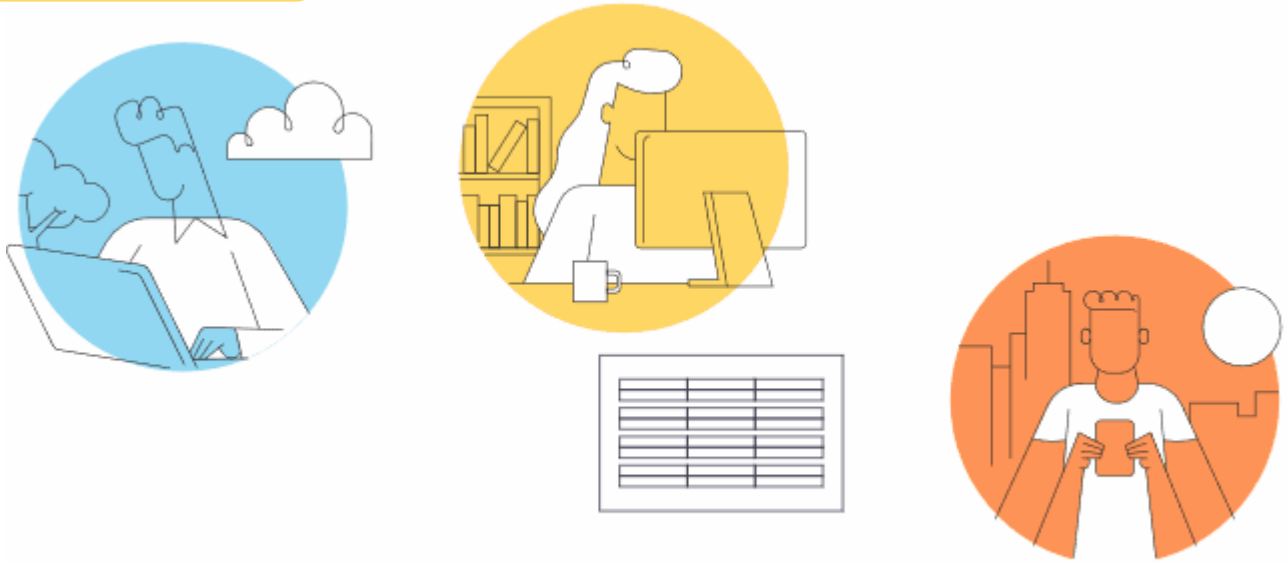
3.0 Updates

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

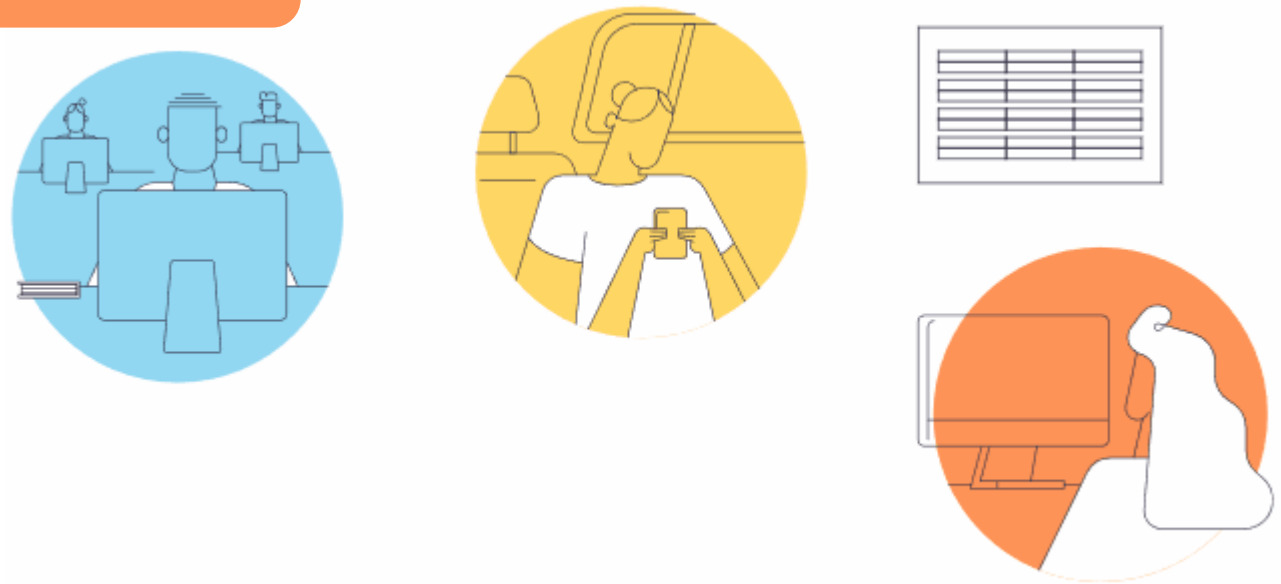
Launch on any device with a browser—even a mobile phone or tablet.

openondemand.org/run

Install Open OnDemand

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.

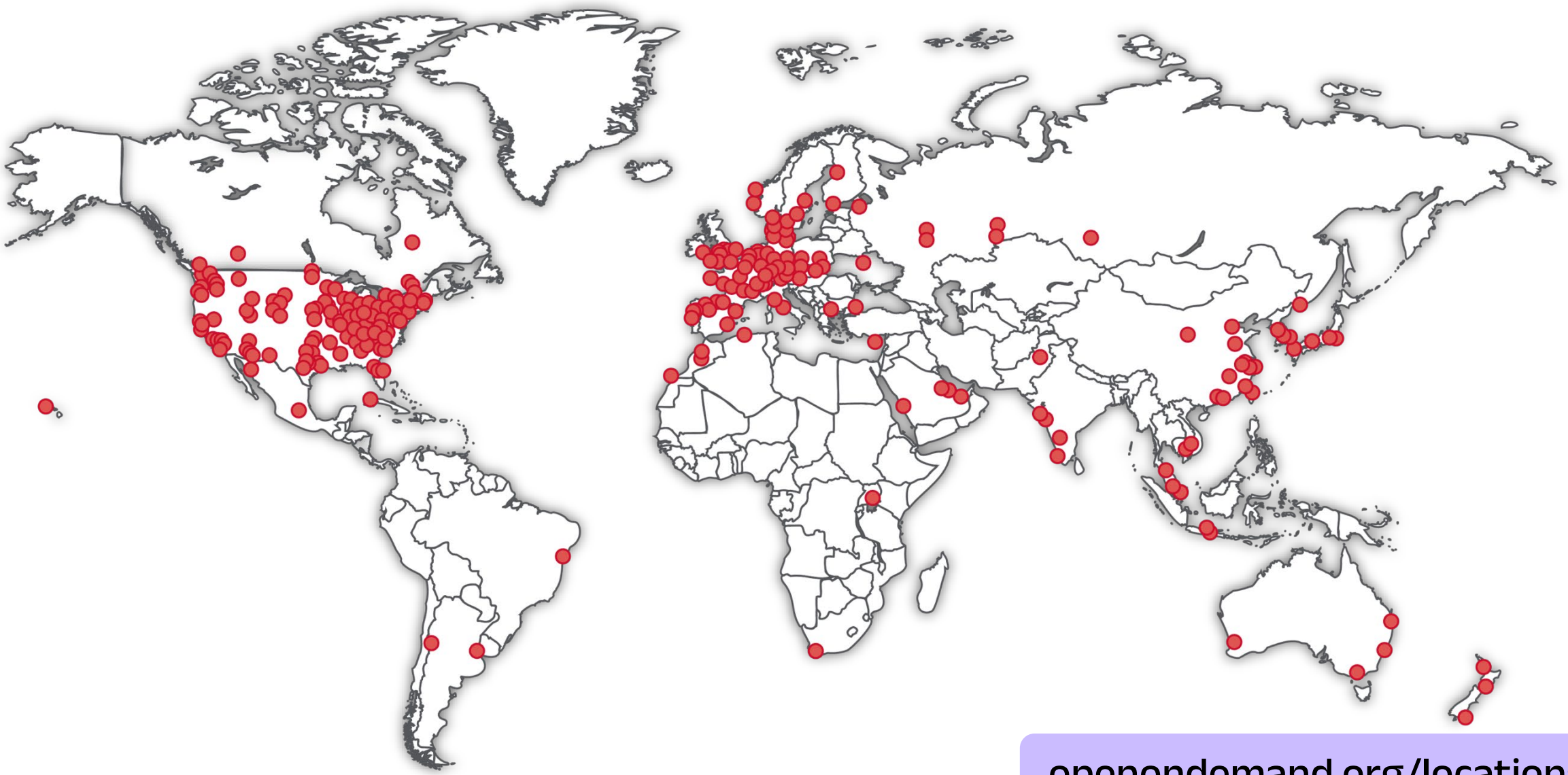
Configurable and flexible

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

openondemand.org/install

Deployed Worldwide

OPEN OnDemand



openondemand.org/locations

Example Deployments

OPEN OnDemand

Agency for Science, Technology and Research
A*STAR Website

Alto Neuroscience
Alto Neuroscience Website

Amazon Web Services
AWS Website

Argonne National Laboratory
Argonne National Laboratory Webiste

Aristotle University of Thessaloniki
Aristotle University Website

Arizona State University
ASU Website

Australian Academic and Research Network
aarnet Website

Boise State University
Boise State University Website

Boston University
Boston University Website

Don't see your organization?

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

USC Website

University of Wisconsin-Eau Claire
UWEC Website

Vanderbilt University
Vanderbilt University Website

Virginia Tech
Virginia Tech Website

Wageningen University & Research
Wageningen University Website

Wayne State University
WSU Website

West Virginia State University
WVU Website

Wright State University
Wright State University Website

XSEDE
XSEDE Website

Yale University
Yale University Website

openondemand.org/orgs

Enabled Utilities & Apps

OPEN OnDemand

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

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

Videos & Publications

OPEN OnDemand

11.13.23
SC23 Exhibiter
Conference site >

10.30.23
Gateways23 Exhibiter
Conference site >

Publication
07.24.23
PEARC23 Preso: HPC toolset
Download >

07.24.23
PEARC23 Exhibiter
Conference site >

Publication
05.02.23
Project Paper: Sector examples
Download >

Video
04.06.23
Tips Webinar: Version 3.0
Watch >

Video
03.02.23
Tips Webinar: Amazon Web Services
Watch >

Video
02.02.23
Tips Webinar: Dynamic forms
Watch >

Video
06.01.23
Tips Webinar: Customizations
Watch >

Publication
05.24.23
ISC23 Preso: User group meeting
Download >

05.21.23
ISC23 Exhibiter
Conference site >

Publication
05.21.23
ISC23 Preso: HPC toolset
Download >

Publication
01.26.23
NVIDIA SAE Preso: Overview
Download >

Publication
01.15.23
Project Paper: Production deployments
Download >

Video
12.01.22
Tips Webinar: SC22 recap
Watch >

Publication
11.15.22
SC22 Preso: User group meeting
Download >

Publication
05.16.23
RMACC HPC 23 Preso: Walkthrough
Download >

Publication
05.11.23
I2 CommEX 23 Preso: CloudCluster
Download >

Publication
05.04.23
Project Paper: General brochure
Download >

Video
05.04.23
Tips Webinar: MATLAB
Watch >

Publication
11.15.22
SC22 Paper: ERN cryo-EM
Download >

11.15.22
SC22 Exhibitor
Conference site >

Video
11.03.22
Tips Webinar: Quantifying impact
Watch >

10.18.22
Gateways22 Exhibitor
Conference site >

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

OPEN OnDemand

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

OPEN OnDemand

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

OPEN OnDemand

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

OPEN OnDemand

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

OPEN OnDemand

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

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~~3.0 Updates~~

Key Items of Note

Open Floor Discussion

OnDemand for a Decade

OPEN OnDemand

OSC OnDemand: A Web Platform Integrating Access to HPC Systems, Web and VNC Applications

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ABSTRACT
In this paper, we describe the OnDemand web platform for providing OSC users integrated access to HPC systems, web applications and VNC services. We present the user experience and implementation of OnDemand and compare it with existing science gateway approaches.

Categories and Subject Descriptors
I.6.7 [**Simulation and Modeling**]: Simulation Support Systems – *environments*

General Terms
Design, Reliability, Security, Human Factors.

Keywords
Web platform, OpenID, REST, High Performance Computing, Virtual Organizations, Cyberinfrastructure.

1. INTRODUCTION
The web has become the dominant access mechanism for remote compute services in every computing area except HPC. In HPC, web applications primarily exist in the form of science gateways. However, the majority of work is performed via HPC system access provided through SSH for text-based access and (occasionally) VNC for visualization access. This separation between web and system functionality inhibits the impact of HPC. Web applications (gateways) have not truly proliferated in HPC due to the development and administrative overheads required for each individual gateway. Meanwhile, traditional SSH interfaces represent a barrier to entry for new users who must locate acceptable client software and learn command-line interfaces for file editing and job control.

We created OSC OnDemand to be a unified web platform where users could access science gateway-styleweb applications, VNC applications, HPC center filesystems and login node terminals. The user has to know only three things: the URL (ondemand.osc.edu), their username and their password. Once logged into OnDemand, the user is presented with a dashboard showing a set of applications for filesystem access, job construction and monitoring, login node terminal access, visualization node access via VNC and science gateways.

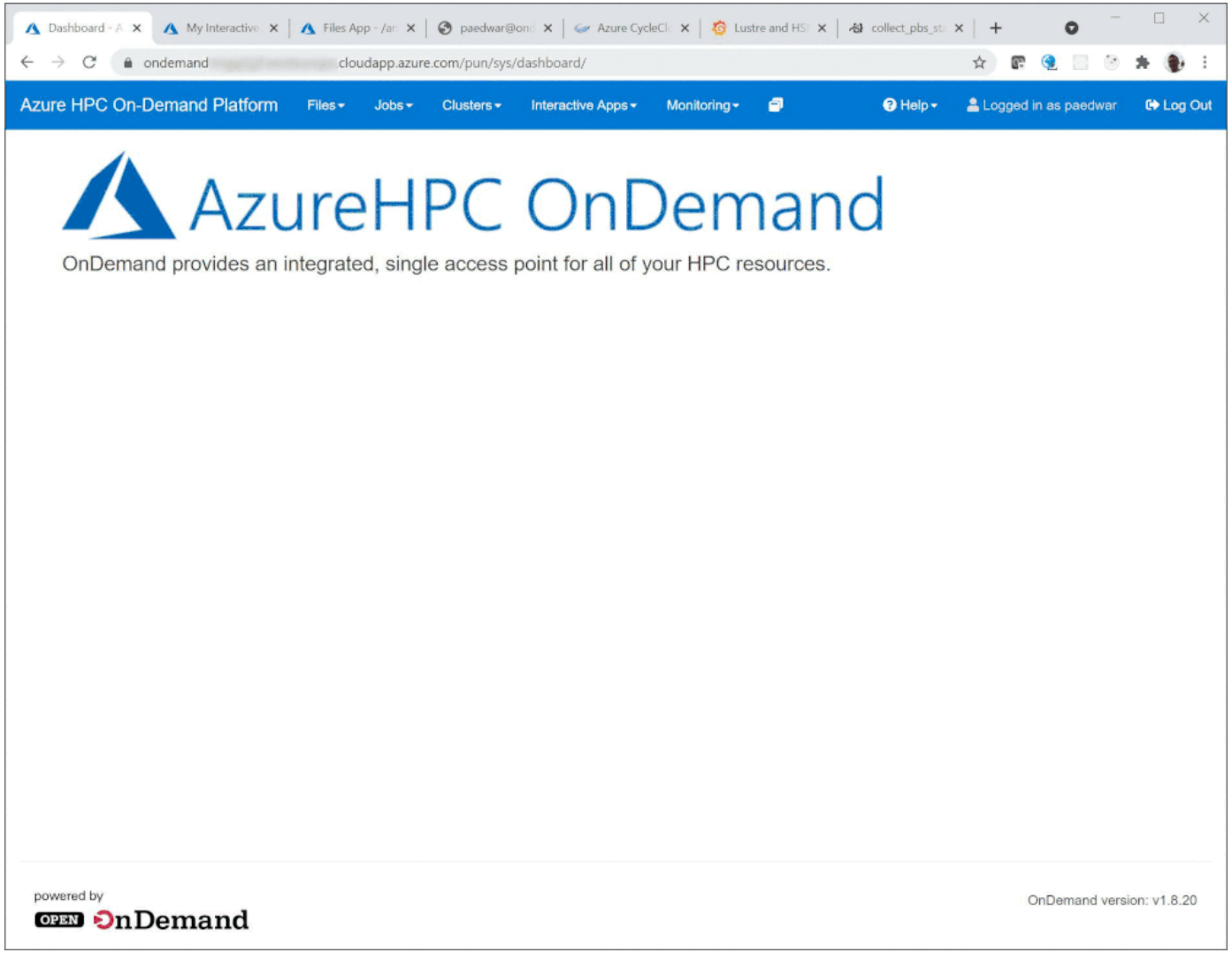
XSEDE '13, July 22 - 25 2013, San Diego, CA, USA

2. RELATED WORK
There has been a large and impressive body of work completed to support grid services and science gateways. The Globus Toolkit [5], [6] provides fundamental technologies for identification, authentication, authorization and service discovery. For example, the Computational Chemistry Grid project created and maintains the GridChem science gateway, [4] using Globus technologies. GridChem users from multiple institutions can securely access services from multiple resource providers. GridChem is also illustrative of the use of science gateways to form *virtual organizations*, where participants from multiple physical institutions can perform calculations and share data via a common web platform, thus forming a single virtual organization. This model has proven popular. Presently, XSEDE supports twenty-nine individual science gateways, many of them supporting discipline-specific virtual organizations [15]. The XSEDE User Portal (XUP) (portal.xsede.org) provides integrated GSI-SSH job status, machine status and account management. OnDemand includes similar functions but adds file browsing and editing, job control (job submission and deletion) and VNC application access. In addition, the nanoHUB project [9] has released the HUBzero [10] software distribution for the creation of virtual organizations at the institutional (or even the laboratory) level. The Open Science Grid also supports non-browser applications for submitting HPC jobs from desktops, like BoSCO [16]. UNICORE [17] supports web portals through its Portal Task Force [18]. Current efforts address basic services, security, and workflow management.

Our team began designing web applications in 2008, including examples in remote instrumentation [2] and data-intensive biomedical science [7]. These applications, like many XSEDE science gateways, are built as standalone web applications that provide user separation at the application level and are deployed in community accounts, i.e., a single HPC account holding all gateway users' data. We encountered two major problems with scaling this approach: first, the increasing overhead of managing gateway deployments and accounts on a per-gateway basis and second, an inability to effectively support use cases in which a user required both gateway functionality as well as system-level access to their data (e.g., access at the command line). In order to solve the overhead problem, we experimented successfully with multiple services reachable from a single entry point that relied on common authentication [8]. In order to solve the second problem, we invented a new mechanism for web server deployment that is used in OnDemand (see section 4).

openondemand.org/xsede13

Commercial Cloud



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aws

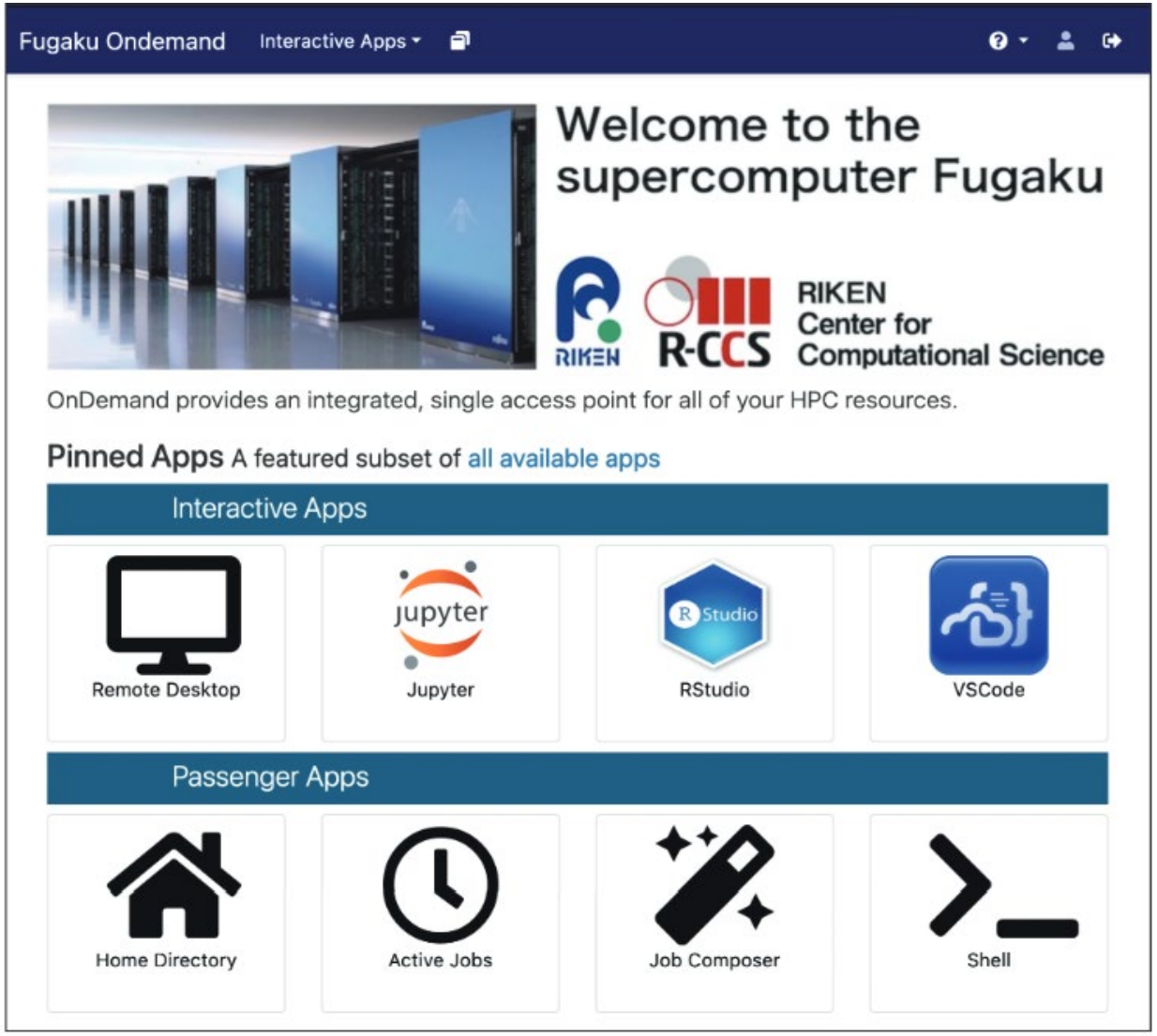
openondemand.org/aws

openondemand.org/azure

Google Cloud

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

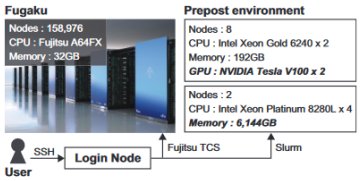


図 1 「富岳」とプリポスト環境の概念図

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[a)] masahiro.nakao@riken.jp

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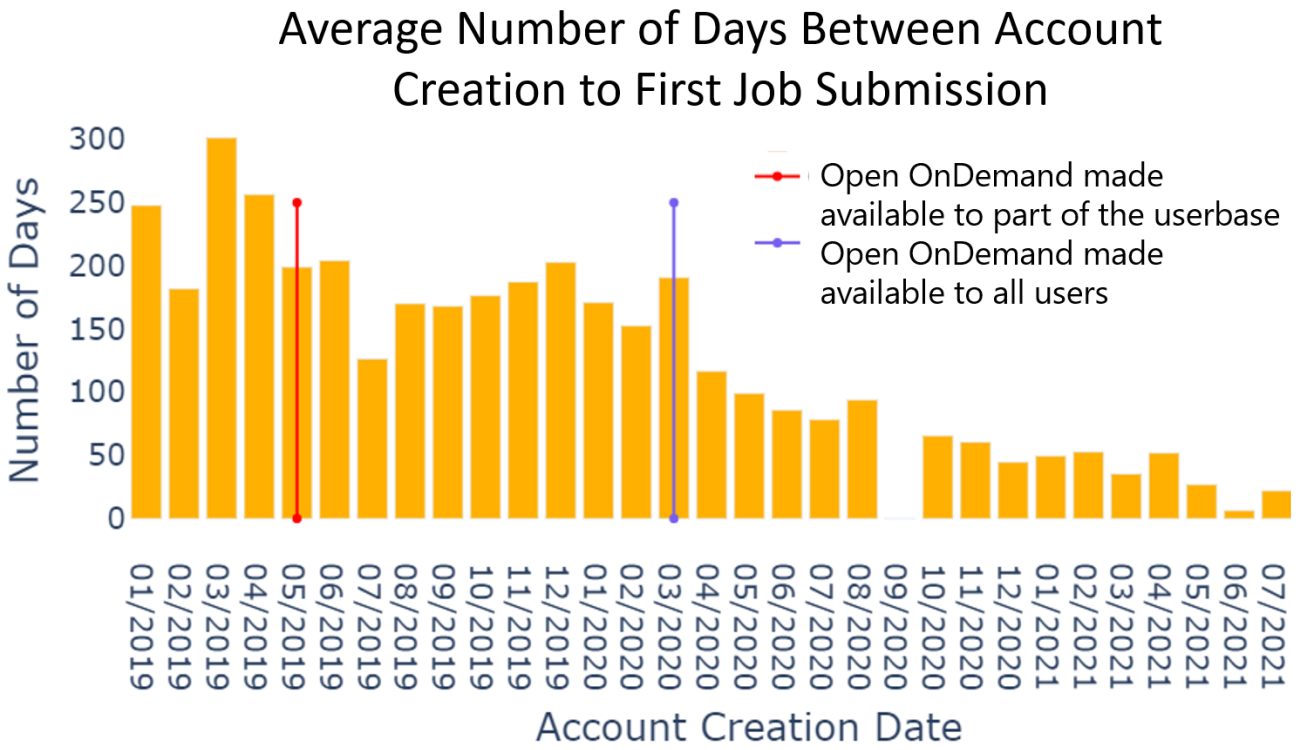
Idaho National Lab

OPEN OnDemand

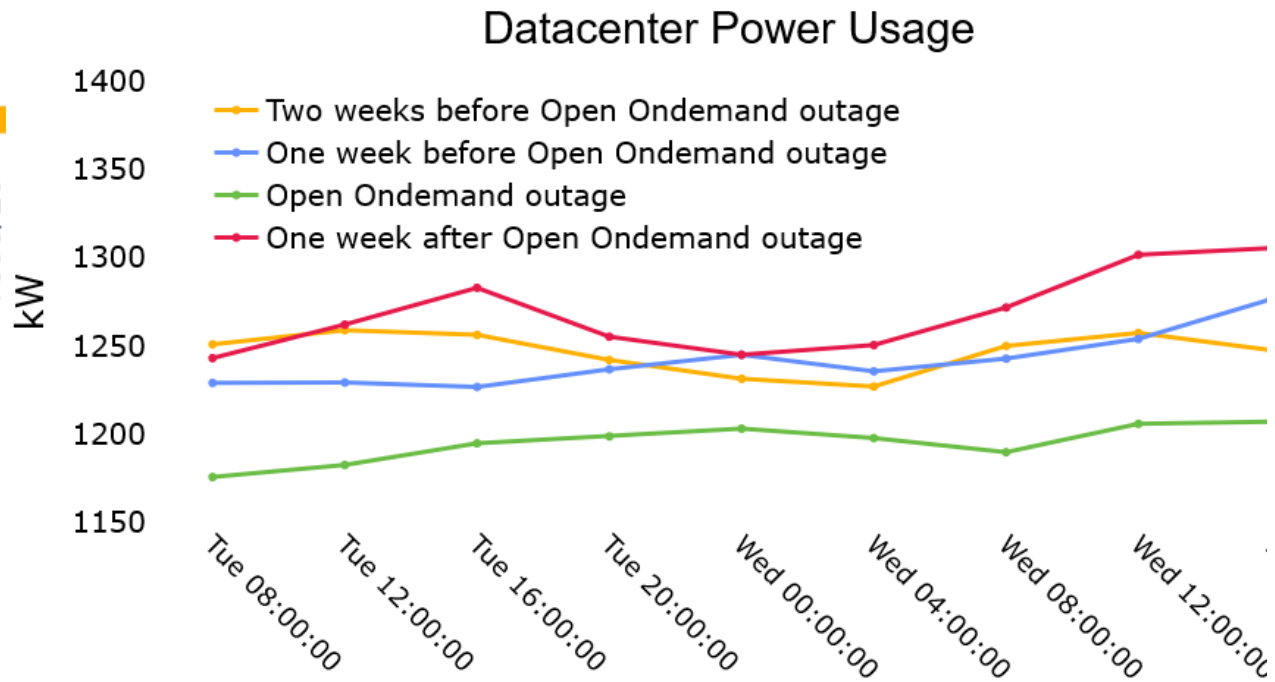


19 times shorter

In days between account creation and first job submission

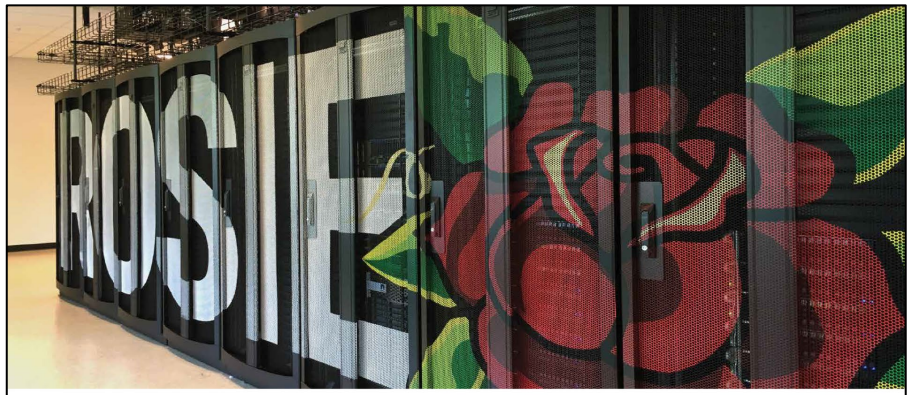
3.7% drop

In power used during an unscheduled 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.

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.

OPEN OnDemand

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.

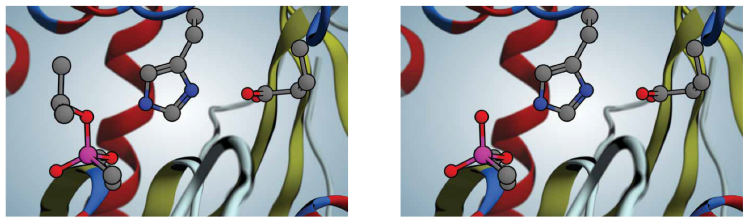
Not only are Hadad's students highly engaged in the classroom, but they also complete research that later may become the basis for their theses.

"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.

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

OPEN OnDemand

openondemand.org/anydevice

Open Positions

OPEN OnDemand

openondemand.org/jobs

User Group Meeting Agenda

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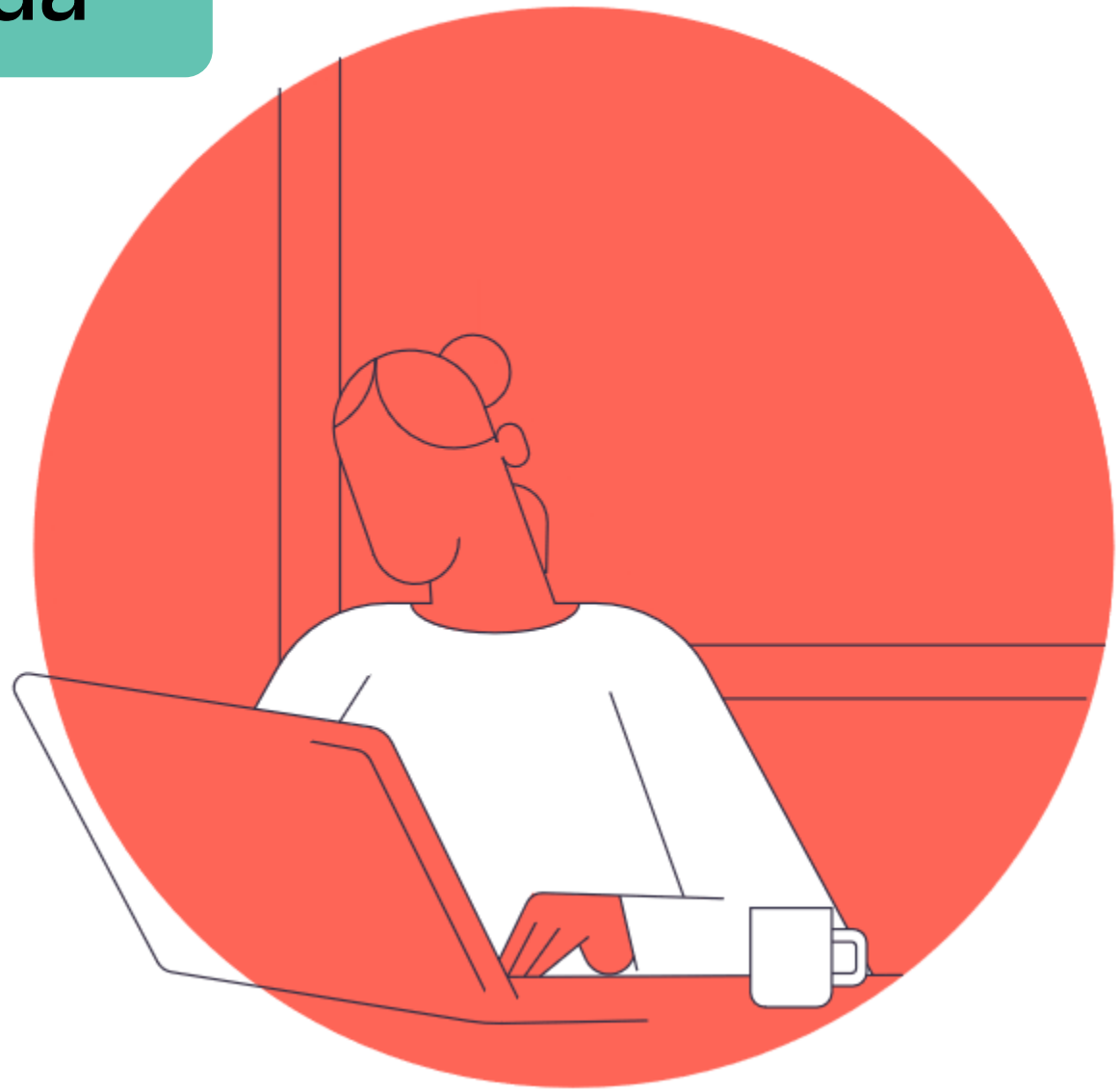
~~3.0 Updates~~

~~Key Items of Note~~

Open Floor Discussion



openondemand.org/discuss