OPEN OnDemand

User Group Meeting
SciPy24 BoF

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MGHPCC Massachusetts Green High Performance Computing Center

Virginia Tech

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This work is supported by the National Science Foundation of the United States under the awards 1534949, 1835725, 2138286, and 2303692

openondemand.org/scipy24

Quick Survey

OPEN OnDemand

Go to

www.menti.com

Enter the code

6144 2392

Or use QR code

User Group Meeting Agenda

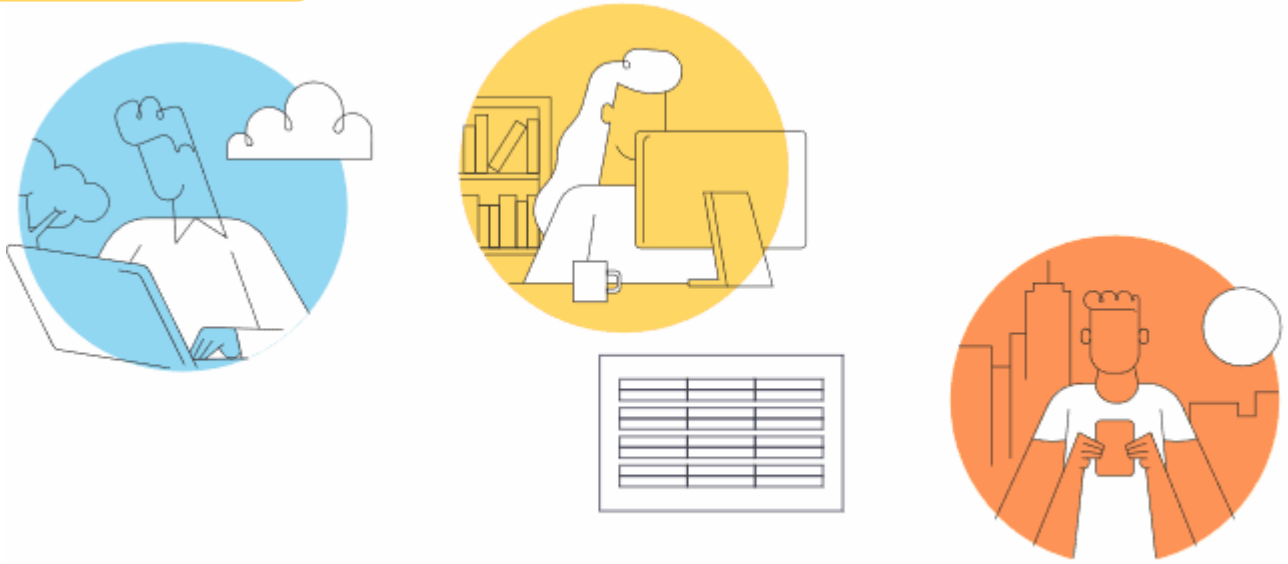
About Open OnDemand

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.

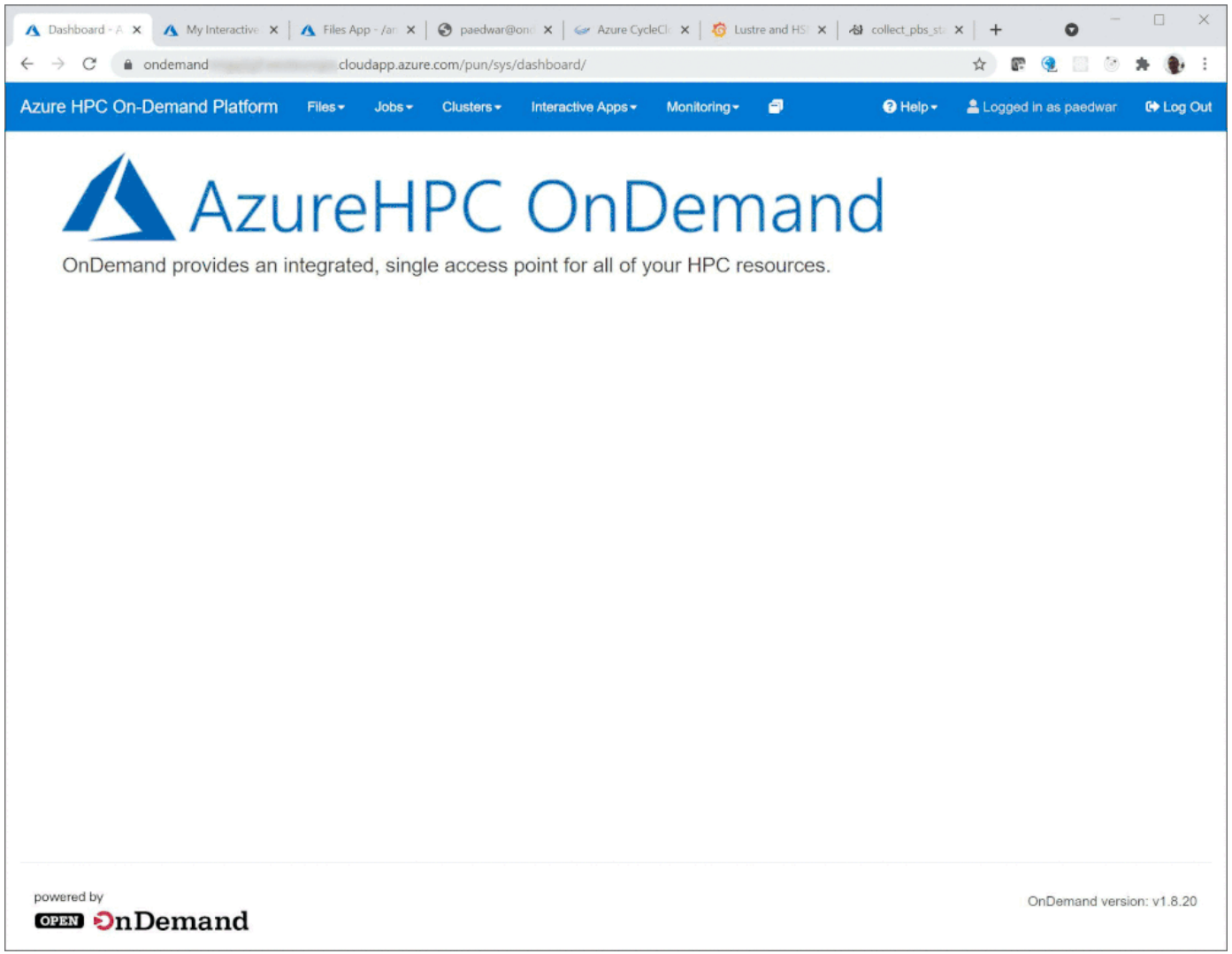
openondemand.org/run

Any Device, Anywhere

OPEN OnDemand

openondemand.org/anydevice

Commercial Cloud



aws

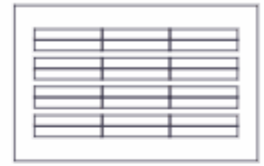
openondemand.org/aws

openondemand.org/azure

Google Cloud

openondemand.org/gcp

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

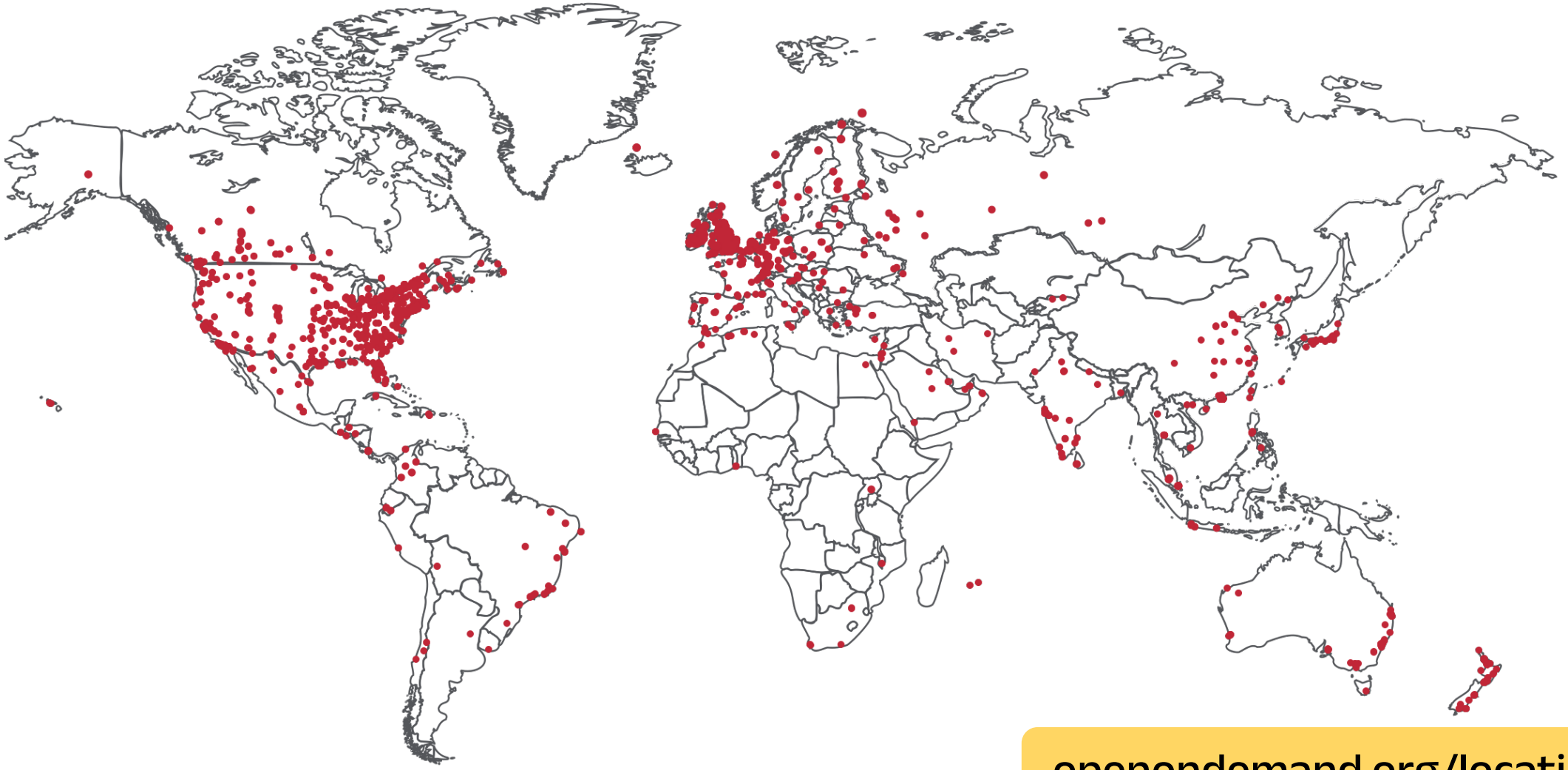
Create and deploy your own applications to meet your users' unique needs.

openondemand.org/install

Deployed Worldwide

OPEN OnDemand

95 Countries | 1,646 Organizations



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

University of Southern California
USC Website

University of Tennessee

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

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 >

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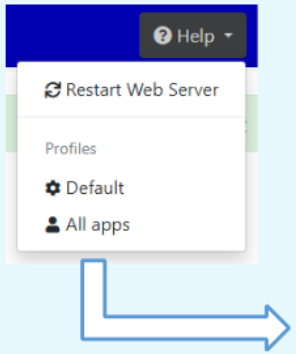
Riken OnDemand

OPEN OnDemand

Some Visualization Applications (OnDemand)

Select **“All apps”** if **“Batch Jobs”** and **“Interactive Apps”** do not appear.



Default
- Recently Used Apps
- Passenger Apps

- **General-Purpose**
  - AVS/Express (Non-OSS)
  - ParaView
  - VisIt
- **Domain Specific**
  - VMD
  - OVITO
  - PyMol
  - …

RIKEN R-CCS 富岳

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LUMI OnDemand

OPEN OnDemand

Introducing a new web interface for LUMI

9.11.2023

A new, easy-to-use web interface for LUMI has been launched at https://www.lumi.csc.fi, providing all the resources and power of the LUMI supercomputer with an easy-access web interface.

This new user interface offers something both for less experienced users as well as seasoned power users. The main features are its ability for users to easily launch interactive applications and connect to them seamlessly from the browser. Key highlights include a comprehensive Linux Desktop that offers a rich graphical environment for data visualization and analysis as well as Jupyter environments for Python and Julia. Additionally, users can launch custom containerized environments for, e.g., courses. It also includes VSCode for code development as well as Tensorboard for AI.

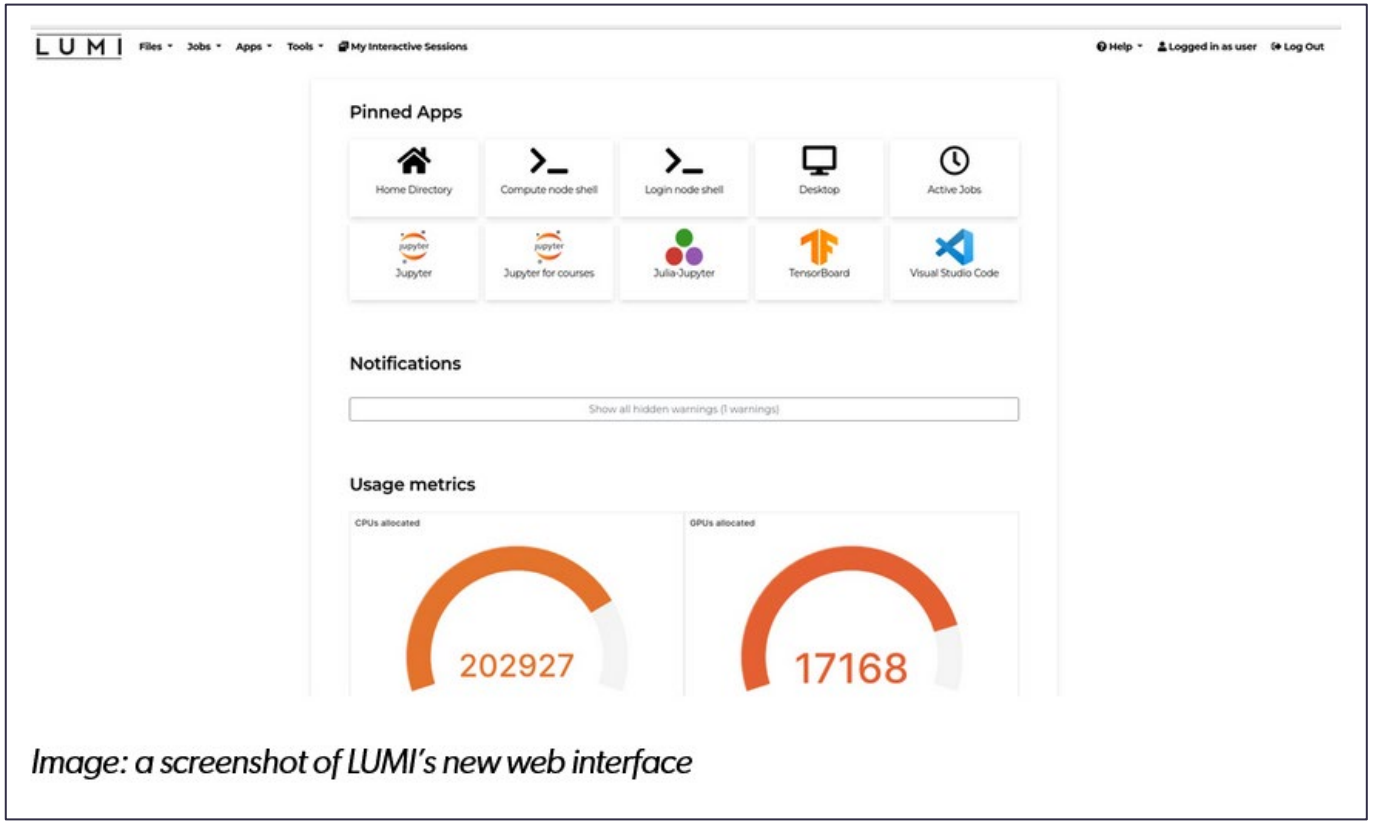


Image: a screenshot of LUMI's new web interface

openondemand.org/lumi

Classroom Computing

OPEN OnDemand

Classroom Computing

Challenge

A professor at The Ohio State University wanted to help more scientists access high performance computing (HPC) resources.

Approach

The scientist developed a course, "Computational Chemistry," to teach graduate-level students how to use HPC in their research.

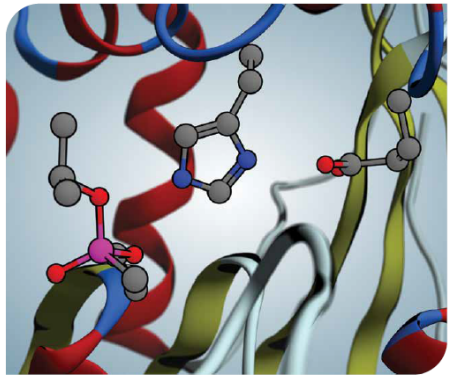
Solution

Over 40 student HPC research projects have been published in different academic journals, including top chemistry journals.

Any Device, Anywhere

"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."

— Chris Hadad, Ohio State professor



Ohio State course helps students use HPC in chemistry research

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.

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— Chris Hadad, Ohio State professor

openondemand.org/hadad

Remote Science

OPEN OnDemand

Remote Science

Challenge

Researchers seek to build an online portal that allows remote use of scientific instruments across the nation.

Approach

With its widespread usage, security measures and adaptability, Open OnDemand serves as a foundation for the project.

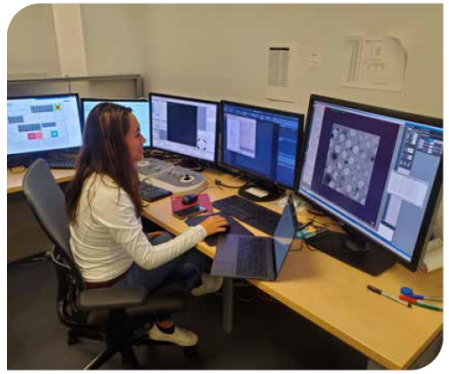
Solution

The team is collaborating with institutions to expand functionality and begin implementation of the portal within the research community.

Any Device, Anywhere

"Open OnDemand is an interface that a lot of researchers are familiar with, which made it an obvious choice for our interface."

— J. Barr von Oehsen, Rutgers University



Ecosystem for Research Networking develops portal for remote instruments

The Ecosystem for Research Networking (ERN), a team consisting of members from Rutgers University, MGHPCC, Omnibond, Virginia Tech, UMass Amherst, Penn State University and Pegasus, is developing a way to use scientific instruments remotely online. The project seeks to improve access to high-cost, specialized equipment to advance national research initiatives.

The ERN Cryo-EM Federated Instrument Pilot Project, in partnership with Rutgers University, is creating a portal, built upon Open OnDemand, that enables the remote control of cryo-electron microscopes and analysis of electron microscopy data.

Cryo-electron microscopy (Cryo-EM) is quickly gaining popularity within the biochemistry

"Open OnDemand is an interface that a lot of researchers are familiar with, which made it an obvious choice for our interface."

— J. Barr von Oehsen, Rutgers University

openondemand.org/ern

Support

Discuss on Discourse

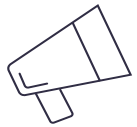
The Get Help category features user and admin questions and answers.
openondemand.org/discourse

Slack Workspace

Communicate and collaborate with the project team and community members.
openondemand.org/slack

Github Documentation

Outlines installation steps, app guidelines, release notes, and more.
openondemand.org/docs



Constant Contact Newsletter

Subscribe to get notices about upcoming events, new releases and user stories.
openondemand.org/newsletter

openondemand.org/support

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.

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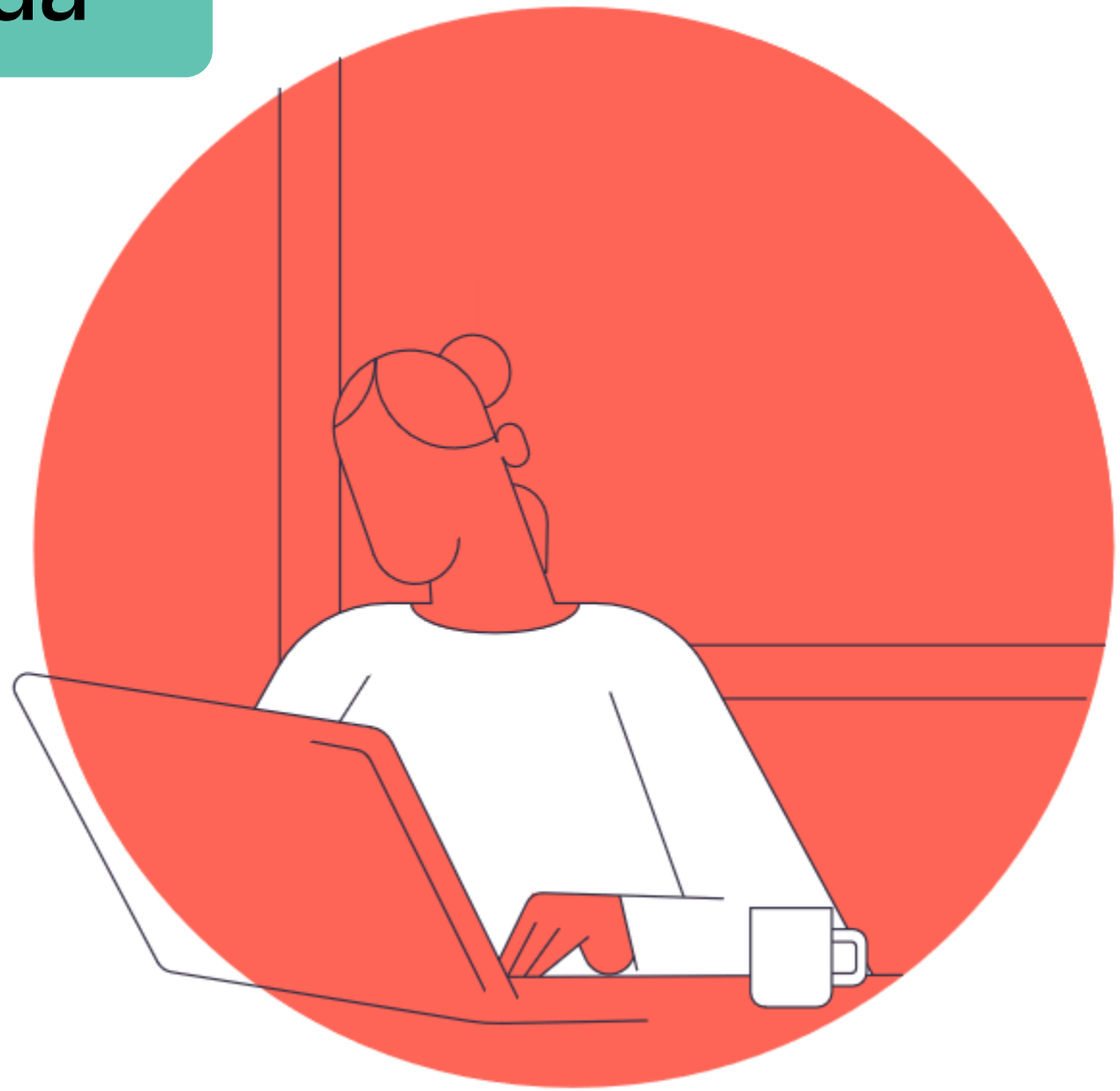

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Questions/Comments

OPEN OnDemand

Ask at the microphone or post on the Menti page!

Go to

www.menti.com

Enter the code

6144 2392

Or use QR code

Thank You!

Emily Moffat Sadeghi

Dev Rel Program Manager

emoffat@openondemand.org

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