

# OPEN ONDEMAND

Roman Leontovýč<sup>1,2</sup>

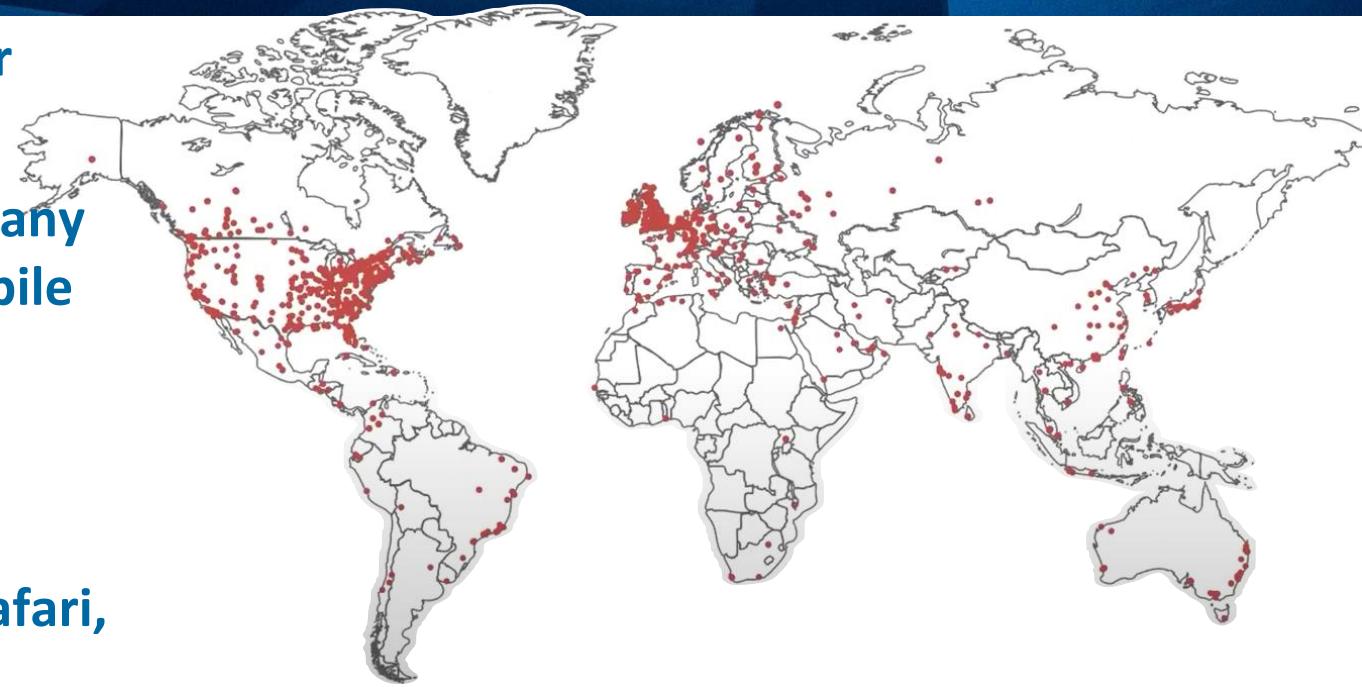
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# Open OnDemand - introduction

- Graphical, web-based cluster interface
- Web access to clusters from any device (desktop, laptop, mobile phone, tablet...)
- No installation needed
- Any modern web browser supported (Chrome, Edge, Safari, Opera...)
- Easy to use
- Developed in 2013, Ohio Supercomputing centre

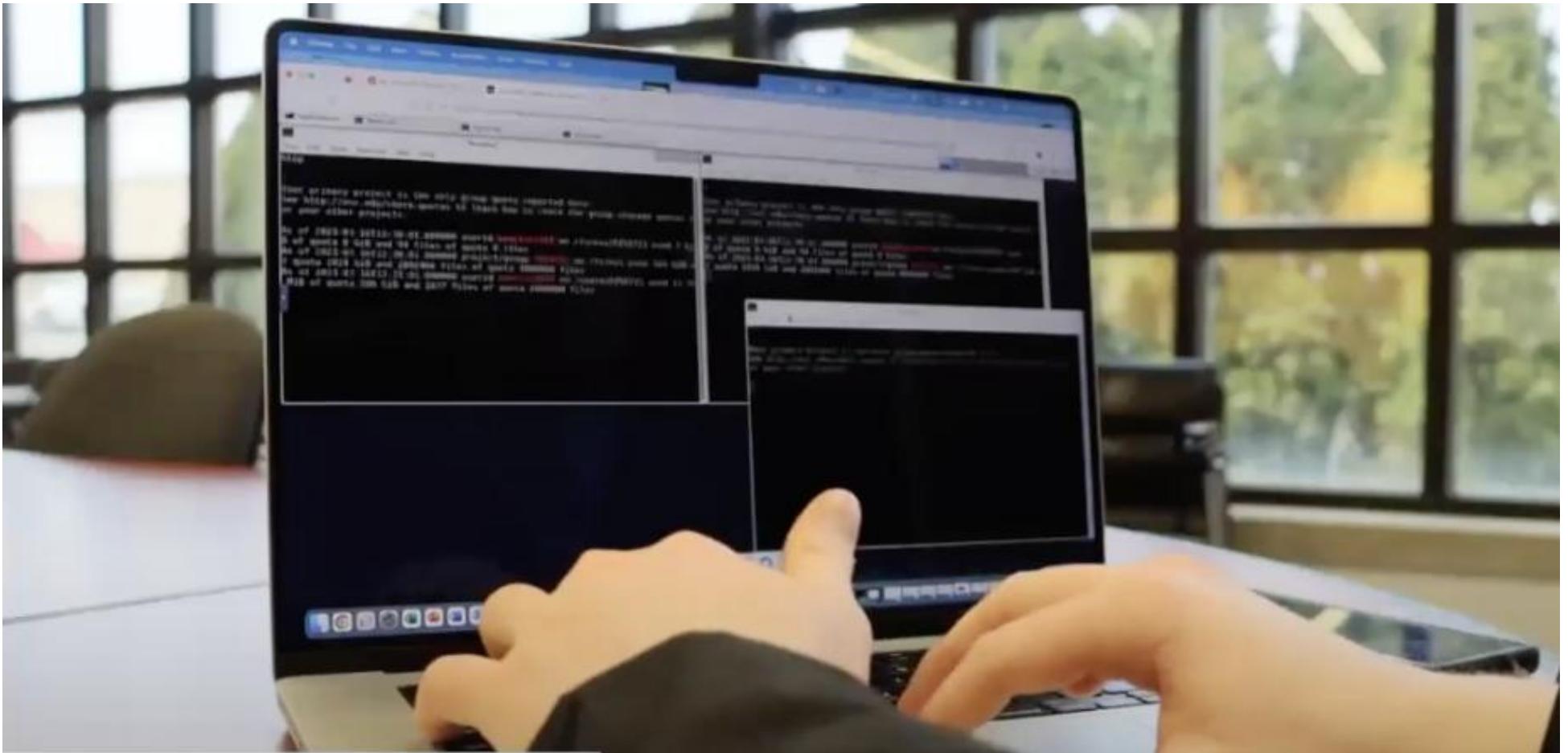


Deployed in 400 HPC centres

2100+  
locations

100  
countries

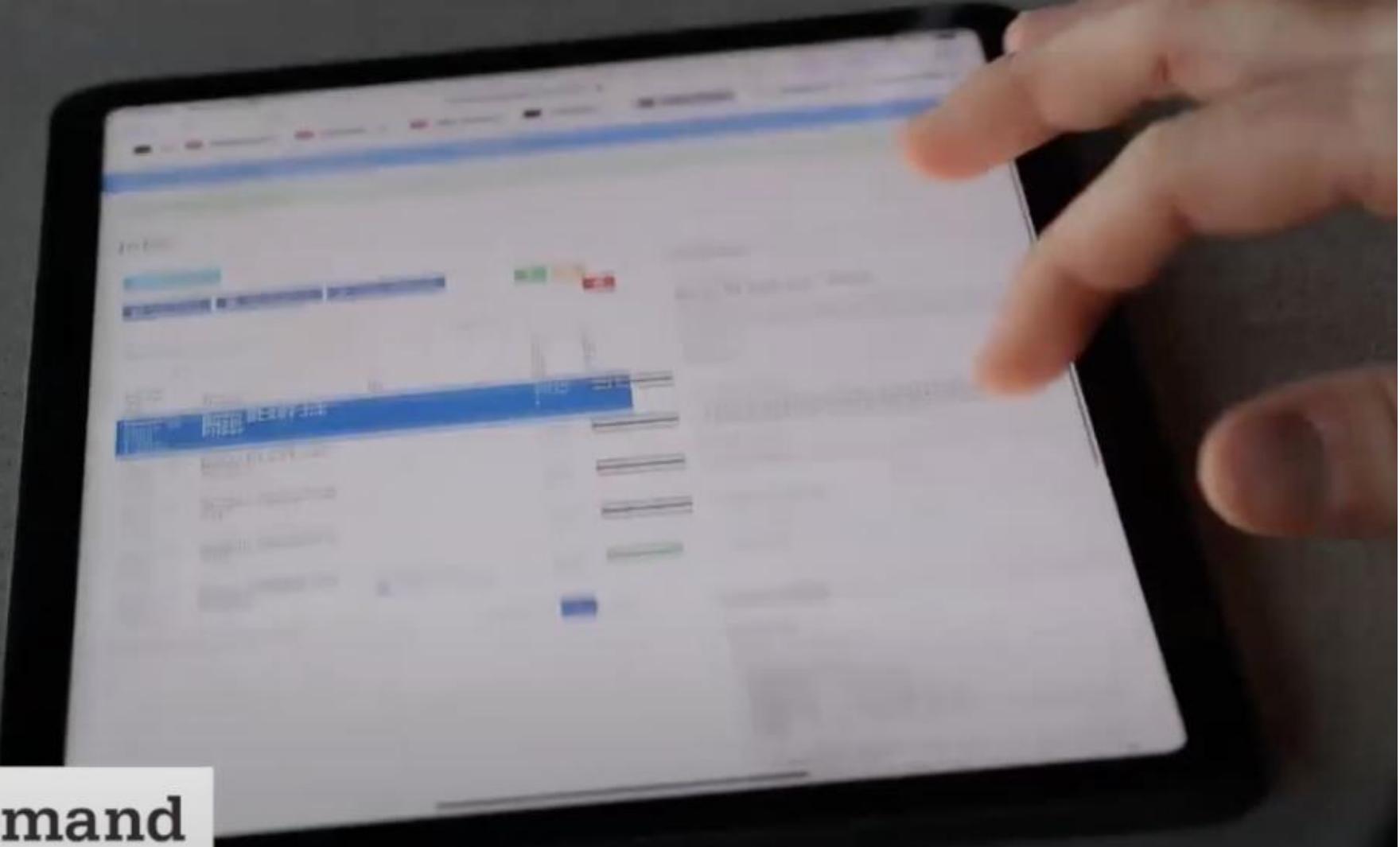
6  
continents



OPEN

OnDemand

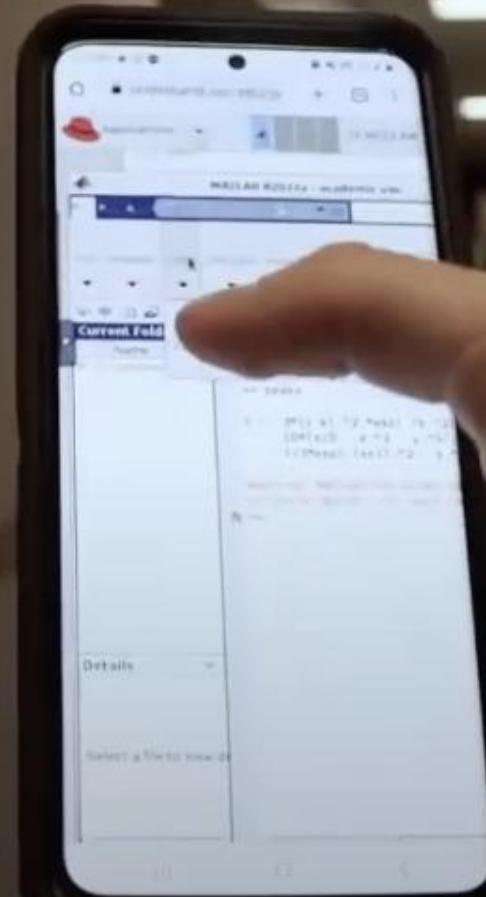
laptop

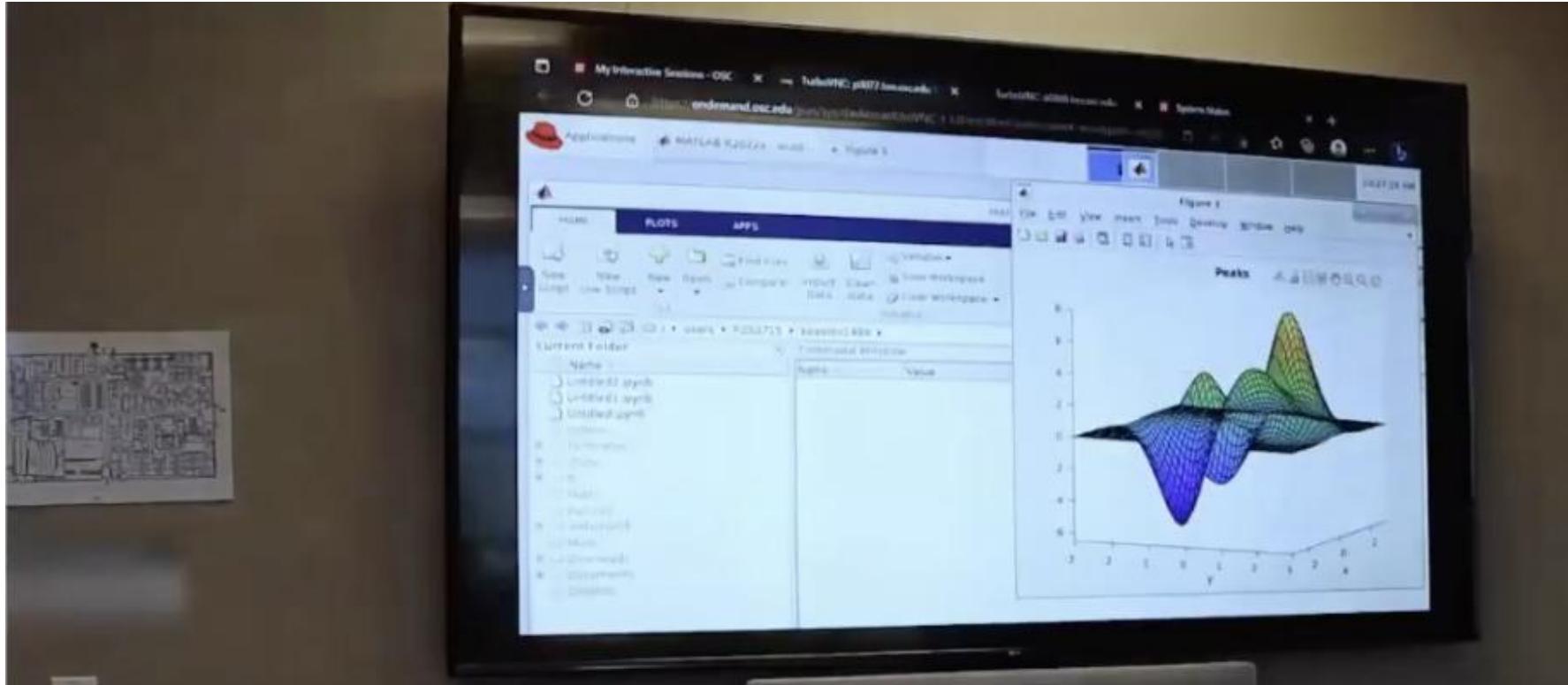


**OnDemand**  
tablet

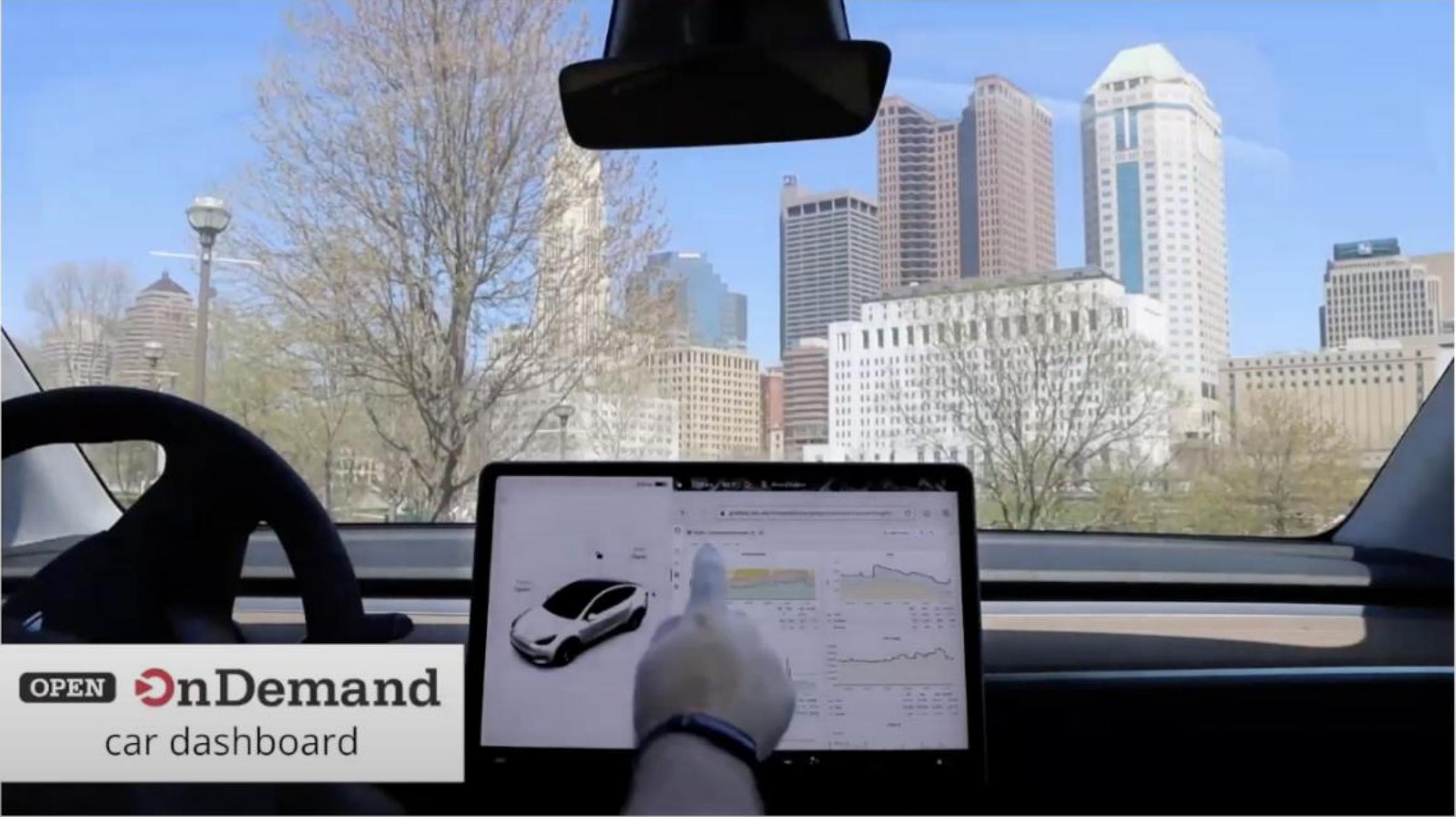
**OPEN**

**OnDemand**  
cell phone





**OPEN**  **OnDemand**  
gaming console



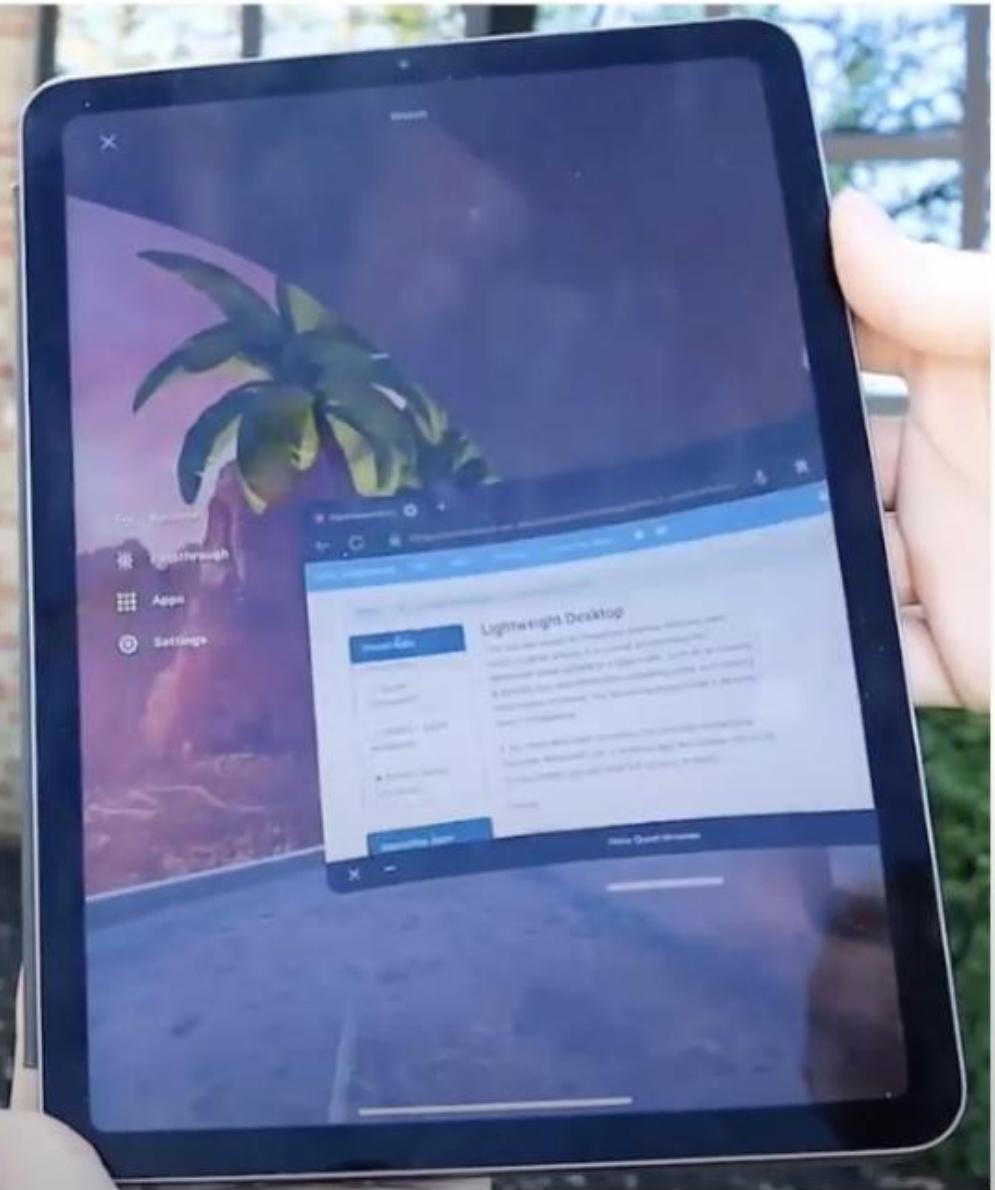
OPEN  **OnDemand**  
car dashboard



OPEN

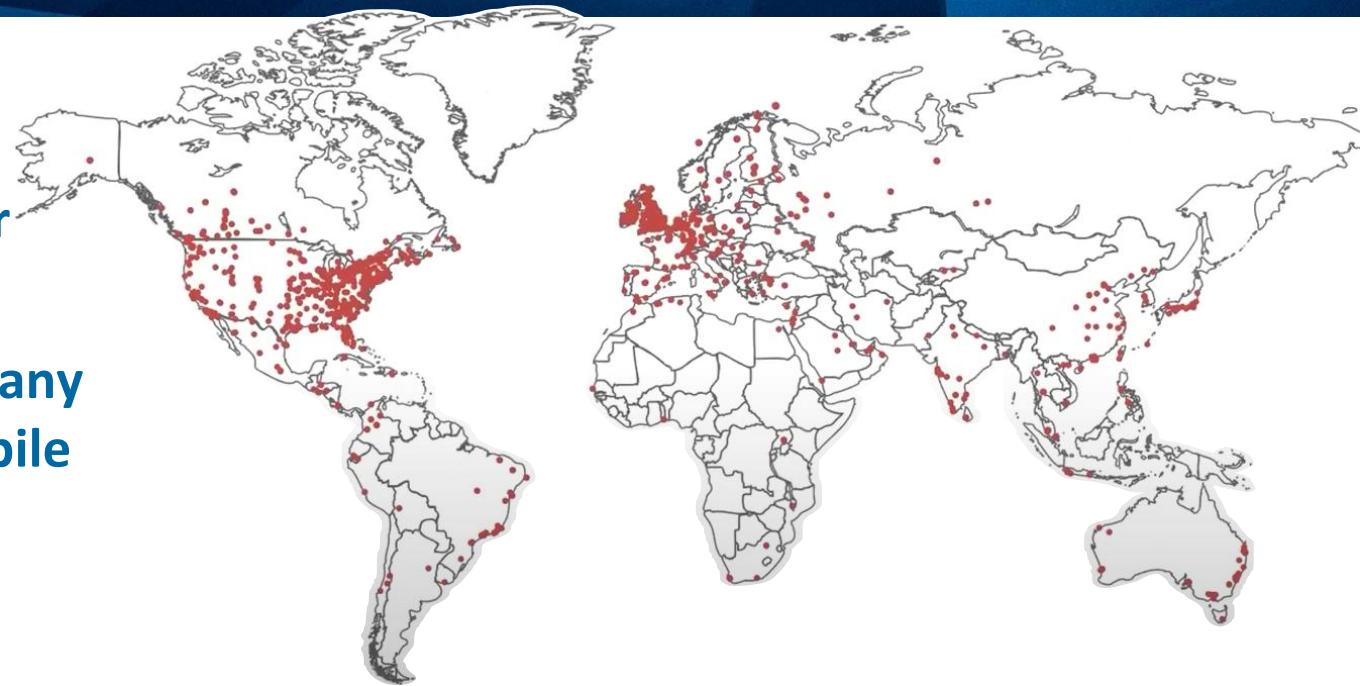
OnDemand

VR headset



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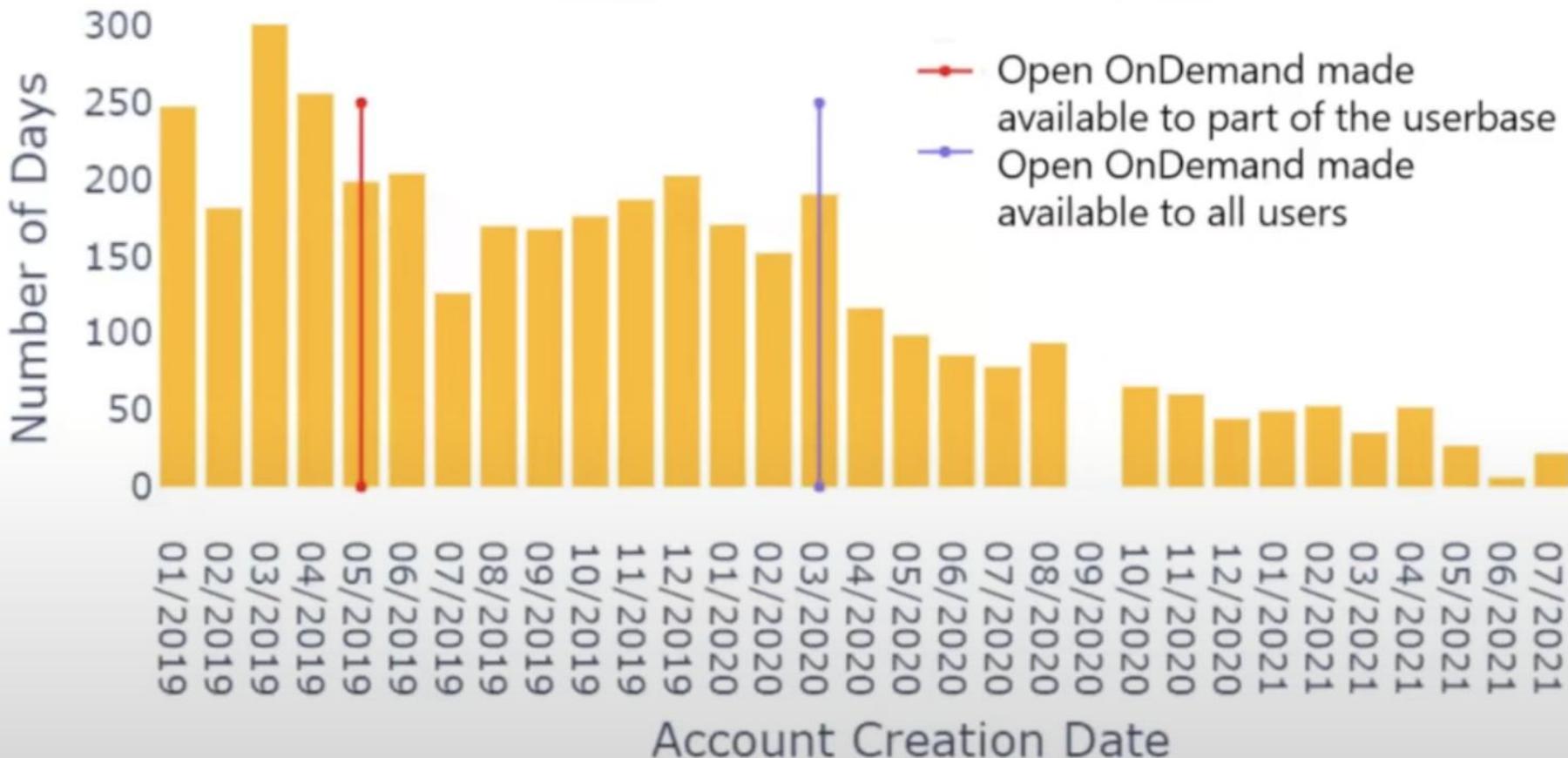
2100+  
locations

100  
countries

6  
continents

# **Idaho national lab**

## Average Number of Days Between Account Creation to First Job Submission



# Open Ondemand on Metacentrum

- Running version - 3.1.7
- Access to MetaCentrum/CERIT-SC/ELIXIR computational resources and storages via web browser
- Shell (command line) access also possible
- e-INFRA CZ/Metacentrum login and Metacentrum password
- OOD documentation <https://osc.github.io/ood-documentation/latest/>
- Metacentrum documentation <https://docs.metacentrum.cz/ondemand>

<https://ondemand.metacentrum.cz>

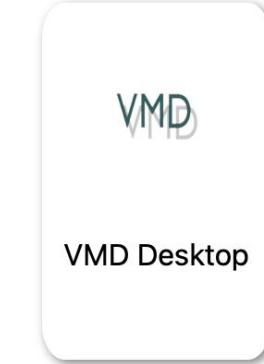
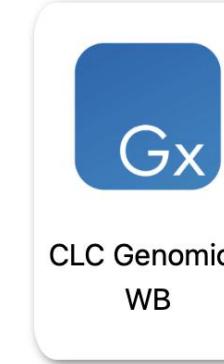
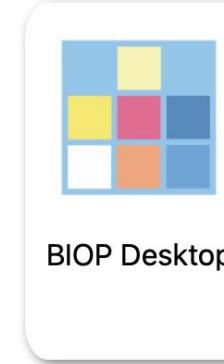
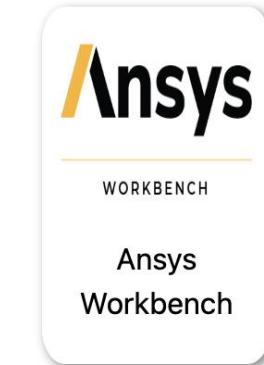
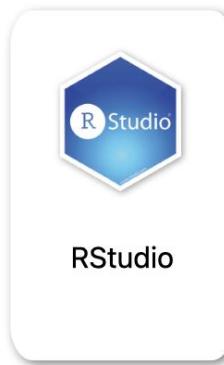
Přihlášení k účtu ondemand.grid.cesnet.cz:443  
Vaše přihlašovací údaje budou odeslány zabezpečeně.

Zapamatovat si heslo

[Zrušit](#) [Přihlásit se](#)

MetaCentrum Open OnDemand provides an integrated, single access point for HPC resources.

## Selected applications - [all apps](#)



# File system in Open Ondemand

The screenshot shows the Open Ondemand web interface. At the top, there is a navigation bar with the 'metacentrum' logo and 'cesnet' text. The navigation items include 'Files', 'Jobs', 'Clusters', 'Interactive Apps', and a folder icon. The 'Files' item is highlighted with a red circle. Below the navigation bar, a sidebar displays a hierarchical list of storage locations under 'Home Directory'. The listed locations are:

- Home Directory
- brno11-elixir /storage/brno11-elixir/home/leontovyc\_roman
- brno12 /storage/brno12-cerit/home/leontovyc\_roman
- brno14-ceitec /storage/brno14-ceitec/home/leontovyc\_roman
- brno2 /storage/brno2/home/leontovyc\_roman
- brno3-cerit /storage/brno3-cerit/home/leontovyc\_roman

- Classical file structure
- Acces to all infrastructure storages
- Manipulation with the files/directories (create, view, rename, edit, delete, upload, download, etc)
- Drag and drop

projects /storage/projects

projects2 /storage/projects2

# Files

metacentrum cesnet

Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾

Action toolbar

Available storages

Home Directory brno2 brno12 praha5-elixir brno11-elixir brno14-ceitec brno3-cerit budejovice1 liberec3 plzen1 praha1

/ storage / brno2 / home / leontovyc\_roman / Change directory Copy path

Show Owner/Mode Show Dottiles Filter: Showing 105 of 175 rows - 0 rows selected

Type	Name	Size	Modified at
Folder	2.3.4	-	27. 5. 2024 12:35:35
Folder	ansys-2024	-	12. 6. 2024 14:45:03
Folder	brno8	-	23. 9. 2021 23:18:12
Folder	colabfold	-	23. 9. 2024 15:12:42

Drop-down menu

The screenshot shows the 'Files' section of the metacentrum web interface. At the top, there's a navigation bar with 'Files', 'Jobs', 'Clusters', 'Interactive Apps', and other links. A red circle highlights the 'Files' link. Below it, a red arrow points from the 'Available storages' heading to the 'Action toolbar'. The toolbar contains buttons for 'Open in Terminal', 'Refresh', 'New File', 'New Directory', 'Upload', 'Download', 'Copy/Move', and 'Delete'. Another red arrow points from the bottom right towards a context menu that appears over a folder entry in the list. This menu includes options like 'Rename', 'Download', and 'Delete'.

# Jobs in Open Ondemand

The screenshot shows the top navigation bar of the Open Ondemand web interface. On the left, there's a logo for 'metacentrum' and 'cesnet'. The top navigation bar includes links for 'Files', 'Jobs' (which is circled in red), 'Clusters', 'Interactive Apps', and a user icon. A tooltip for the 'Jobs' menu is displayed, showing options for 'Active Jobs' and 'Job Composer'. Below the navigation bar, a message states: 'Demand provides an integrated, single access point for HPC resources.'

- Analogous to a batch job
- Active jobs
  - status of submitted jobs (queued, running, completed...)
  - Informations about the job (cluster, walltime, job ID, CPU time, ...)
- Job composer
  - tool for creating and submitting the jobs
    - From templates
    - Run existing previously submitted jobs
  - handling the jobs (submit, delete, edit, stop)

# Active jobs

Your Jobs ▾

All Clusters ▾

## Active Jobs

Show 50 entries

Filter:

ID	Name	User	Account	Time Used	Queue	Status	Cluster	Actions
<a href="#">9163251.pbs-m1.metacentrum.cz</a>	sys-dashboard-sys-bc_desktop-metacentrum	leontovyc_roman		00:21:54	interactive	<span>Running</span>	Perian	

# Job composer

[+ New Job ▾](#)
[★ Create Template](#)
[Edit Files](#)
[Job Options](#)
[Open Terminal](#)
[Submit](#)
[Stop](#)
[Delete](#)

Show 25 entries

Search:

Created	Name	ID	Cluster	Status
May 8, 2024 11:29pm	(default) Metacentrum simple sequential job	9163197.pbs-m1.metacentrum.cz	Perian	Completed
April 29, 2024 9:03am	(default) Metacentrum simple sequential job		Perian	Not Submitted
April 11, 2023 2:40pm	(default) Metacentrum simple sequential job	15005996.meta-pbs.metacentrum.cz	Perian	Completed
April 6, 2023 1:28pm	AlphaFold Metacentrum job	14933439.meta-pbs.metacentrum.cz	Perian	Completed
April 5, 2023 4:24pm	test_ondemand.sh		Perian	Not Submitted
April 5, 2023 4:15pm	AlphaFold Metacentrum job		Perian	Not Submitted
February 6, 2023 8:43pm	(default) Metacentrum simple sequential job	14644331.meta-pbs.metacentrum.cz	Perian	Completed

Showing 1 to 7 of 7 entries

Previous 1 Next

## Job Details

**9163197.pbs-m1.metacentrum.cz**

Job Name:

**(default) Metacentrum simple sequential job**

Submit to:

Perian

Account:

Not specified

Script location:

/storage/brno2/home/leontovyc\_roman/ondemand/data/sys/myjobs/proje

Script name:

main\_job.sh

Submit Script

main\_job.sh

Script contents:

```
#PBS -N hello_world
#PBS -l ncpus=1
#PBS -l walltime=24:00:00
#PBS -l mem=400mb
#PBS -j oe
#PBS -l scratch_local=1g
```

```
cd $PBS_O_WORKDIR
echo "Hello World" > output_file
```

```
echo "Created output_file with 'Hello World'"
```

Folder Contents:

hello\_world.o9163197

main\_job.sh

output\_file

[Open Editor](#)
[Open Terminal](#)
[Open Dir](#)

Save

/storage/brno2/home/leontovyc\_roman/ondemand/data/sys/myjobs/projects/default/3/alphafold\_job.sh

Key Bindings

Default

Font Size

```
1 #PBS -N Alphafold-00D-JOB
2 #PBS -q ondemand
3 #PBS -l select=1:ncpus=8:ngpus=1:mem=100gb:scratch_local=10gb:gpu_cap=cuda75
4 #PBS -l walltime=24:00:00
5 #PBS -m ae
6
7 cd $PBS_O_WORKDIR
8
9 #####
10 #change paths
11 OUTPUTS_DIR=./outputs
12 # here you can set one file, directory or wildcard for files inside dir, e.g. '/dir/ecto/ry/' will process all files in the p
13 FASTA_INPUTS=/storage/brno11-elixir/projects/alphafold/example-fasta/seq.fasta
14 #####
15
16 # multimer example
17 #FASTA_INPUTS=/storage/brno11-elixir/projects/alphafold/example-fasta/multi.fasta
18
19 #choose one of the Alfafold prediction method
20 METHOD="AF_MONOMER_REDUCED_DBs"
21 #METHOD="AF_MULTIMER_FULL_DBs"
22 #METHOD="AF_MULTIMER_REDUCED_DBs"
23
24 # load methods
25 source ./lib.sh
26
27 # execute method
28 $METHOD
29
30 # copy results from scratch
31 mkdir -p $OUTPUTS_DIR
32 cp -r $SCRATCHDIR/* $OUTPUTS_DIR/ && rm -r $SCRATCHDIR/*
```

metacentrum

Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾

Themes: Monokai Remastered

- Access to command-line interface of 5 different frontends
- Command line interface in web browser

>\_ Perian Shell Access  
>\_ Skirit Shell Access  
>\_ Tarkil Shell Access  
>\_ Zenith Shell Access  
>\_ cerit-pbs zuphux Shell Access

Host: skirit.metacentrum.cz

Your Home Directories

Avail	DATA	FILES	Backup	Storage
space	quota	used	quota	used
82T	5.36T	136G	2M	329k
4.5P	none	107G	none	8.15k
114T	none	0	none	2
116T	4.29T	188G	2.5M	132k
186T	none	48.8G	none	8.06k
30T	3.32T	261G	1M	2.89k
33T	10.4	378M	none	17
505T	4.29T	4.00T	3M	674k
24T	5.36T	1.03T	1.01M	241k
94T	7.34G	8k	none	3
211T	2.14T	461G	2M	46.8k

CPUs

Free	Used	Total	Centre
1165	6539	7704	CERIT
1979	989	2968	ELIXIR
3696	15870	19566	META

Contact

E-mail: meta@cesnet.cz  
Web: http://www.metacentrum.cz/

(BULLSEYE)leontovyc\_roman@skirit:~\$



- Different applications able to run interactively
- Installation sw into Open OnDemand on request  
(widely used softwares with potential for global use)
- Selection of the session parameters (walltime, number of CPUs, memory, scratch, ...)

#### Desktops

Ansys/Ensight

Ansys/Fluent

Ansys/Workbench

BIOP Desktop

CLCgenomicsWB

Matlab

MetaCentrum Desktop

VMD Desktop

#### Servers

Jupyter Notebook/Lab

Matlab webapp (beta)

RStudio Server

## Interactive Apps

### Desktops

>Ansys/Fluent Desktop

Matlab Desktop

MetaCentrum Desktop

VMD Desktop

### Servers

Jupyter Notebook

RStudio Server

# Matlab Desktop version: f8a6b5a

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 CPUs on single node

4



Memory (GB)

4



GPUs

0



Scratch local (GB)

10



Session was successfully created.



Home / My Interactive Sessions

## Interactive Apps

### Desktops

Ansys/Fluent

Desktop

Matlab Desktop

MetaCentrum

Desktop

VMD Desktop

### Servers

Jupyter Notebook

## Matlab Desktop (14933502.meta-pbs.metacentrum.cz)

1 node

4 cores

Running

**Host:** halmir2.metacentrum.cz

Delete

**Created at:** 2023-04-06 13:59:46 CEST

**Time Remaining:** 43 minutes

**Session ID:** [802d5c28-0f32-43bd-ba42-84de4baaacd4](#)

Compression



0 (low) to 9 (high)

Image Quality



0 (low) to 9 (high)

**Launch Matlab Desktop**

**View Only (Share-able Link)**

## MATLAB R2022b - academic use

HOME

PLOTS

APPS



Search Documentation



Sign In



New



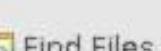
Live Script



New



Open



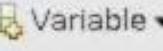
Find Files



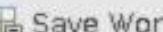
Import Data



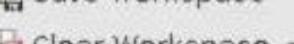
Clean Data



Variable



Save Workspace



Clear Workspace

CODE

SIMULINK

ENVIRONMENT

RESOURCES

FILE

VARIABLE

/ auto &gt; brno2 &gt; home &gt; leontovyc\_roman &gt;

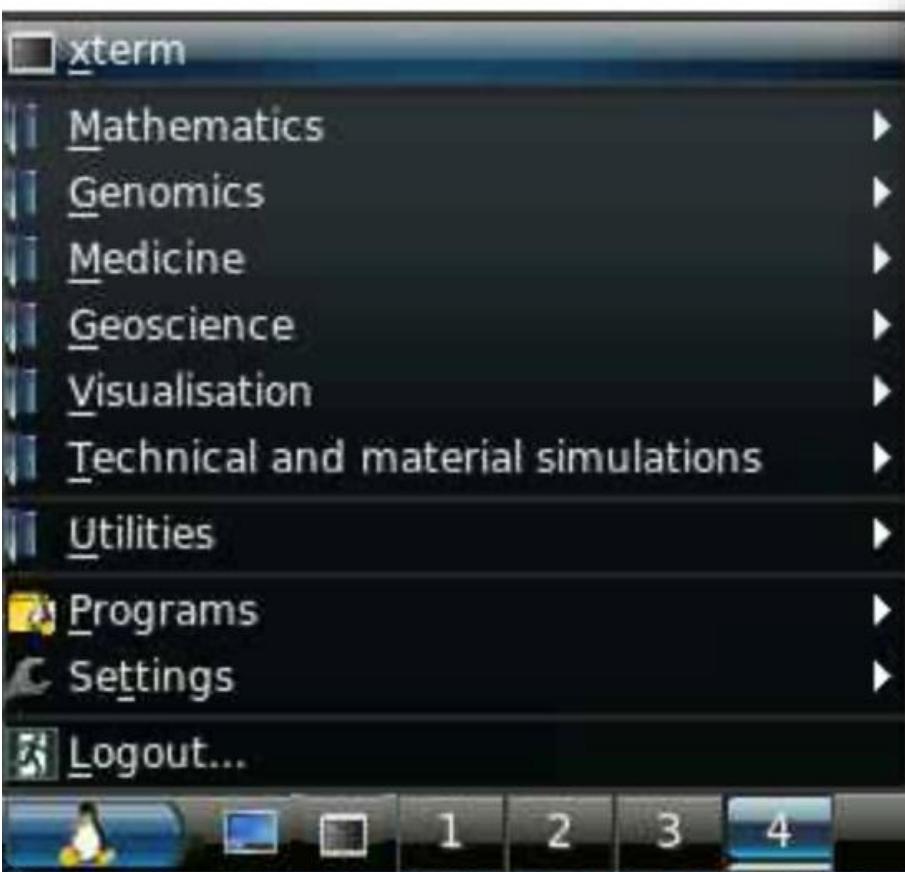
## Current Folder

	Name
+	biopython
+	brno6
+	brno8
	CLC_Data
	Downloads
+	espresso_md
+	gene_enriched
+	hands-on
	high_ethanol_yeast
	high_ethanol_yeast_1
+	Kegg_download
+	korena
+	korena_busco

## Command Window

fx &gt;&gt; |

# Metacentrum desktop



- Analogous to an interactive job
- Access to other GUI applications
  - Sorted by categories
- Command line control option

# All available graphical applications

- **Mathematics**

- Matlab
- Maple
- Wolfram Mathematica
- Scilab
- R

- **Genomics**

- CLCbio Genomic Workbench
- Geneious
- SNP and AFLPPackage for Phylogenetic analysis
- Tablet
- FingerPrinted Contigs
- UEA sRNA Workbench

- **Medicine**

- Freesurfer

- **Geoscience**

- integrated data viewer

- **Visualisation**

- Visit
- XCrysDen

- **Technical and material simulations**

- Ansys 15, 16.1, 16.2, 17.1, 17.2, 18.0, 18.2

# Conclusion



## Command-line

- Pros
  - efficient for experienced users
  - good for large-scale data processing
- Cons
  - high learning curve
  - not GUI applications friendly

## GUI - Open OnDemand

- Pros
  - easy to use
  - GUI applications friendly
  - no installation needed
- Cons
  - not as efficient as the command-line
  - challenging to submit the array jobs

# Demo/Hands on

<https://ondemand.metacentrum.cz>

Thank you for attention