cesnet
metacentrum

OPEN ONDEMAND

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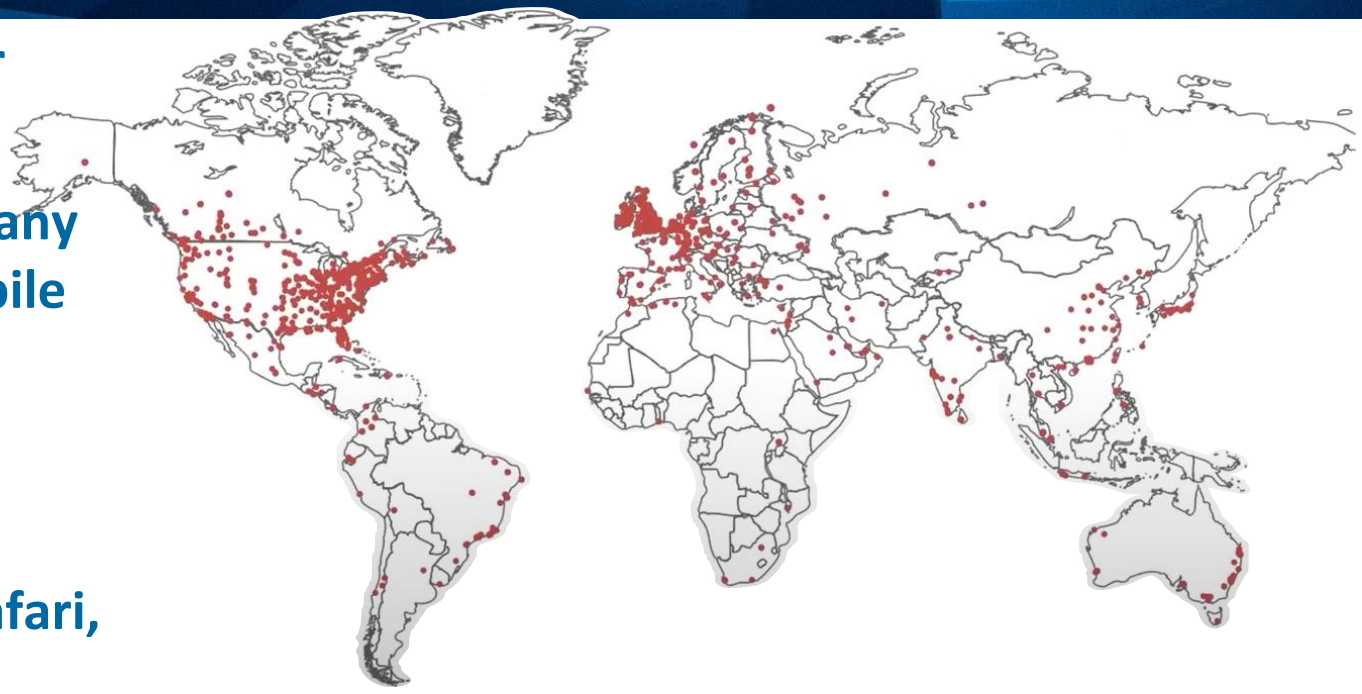
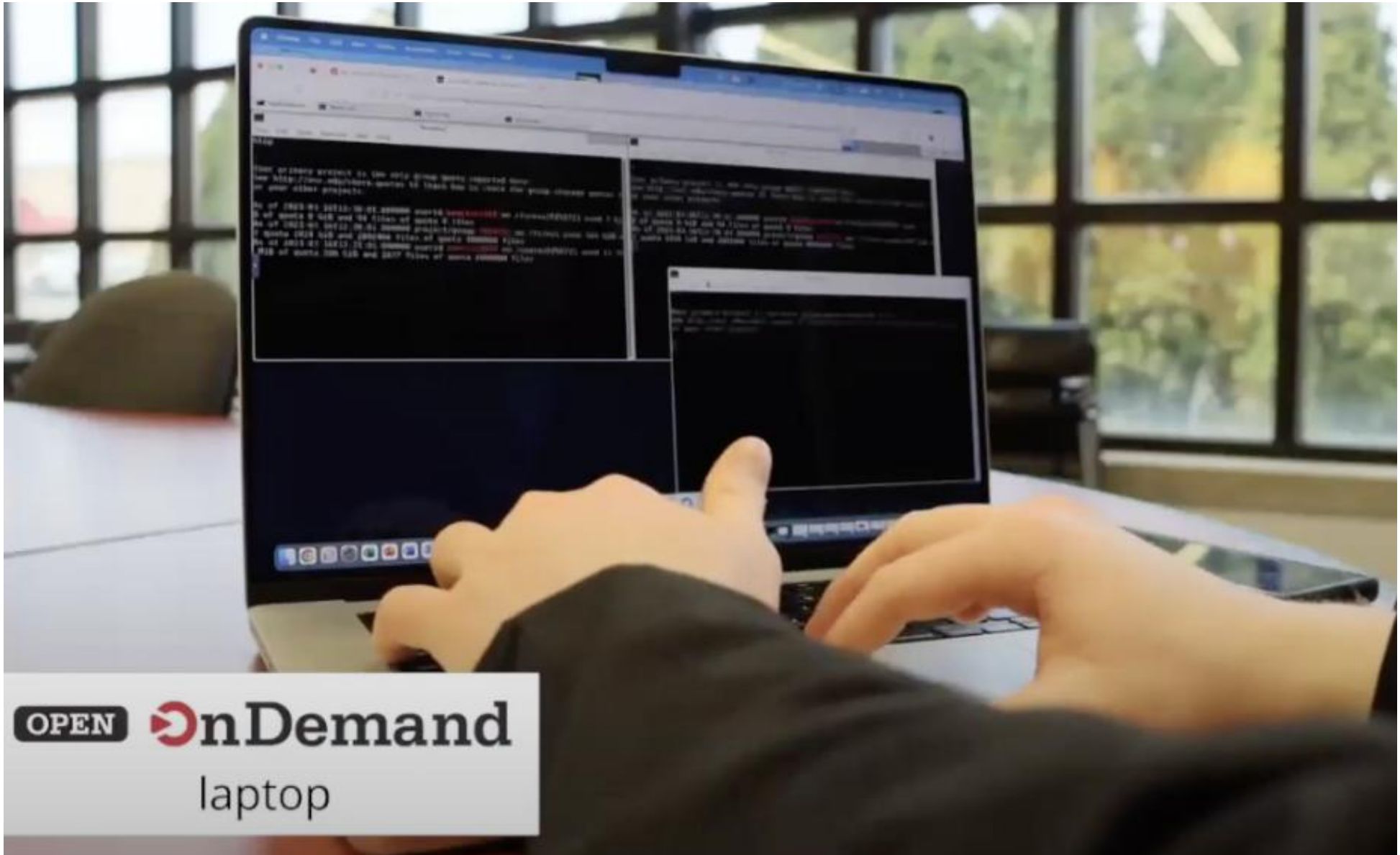
Open OnDemand - introduction

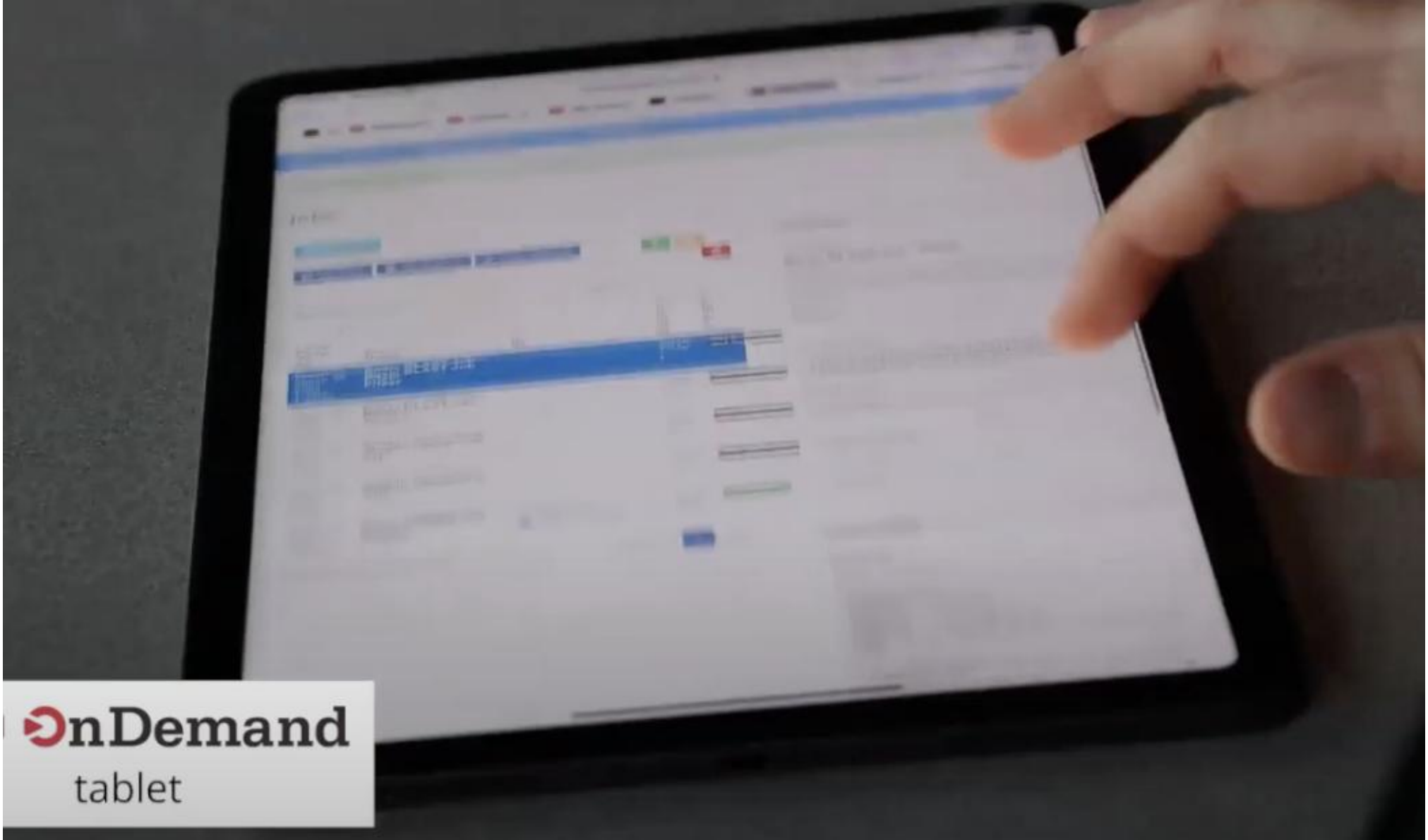
- Graphical, web-based cluster interface
- Web access to clusters from any device (desktop, laptop, mobile phone, tablet…)
- No installation needed
- Any modern web browser supported (Chrome, Edge, Safari, Opera…)
- Easy to use
- Developed in 2013, Ohio Supercomputing centre

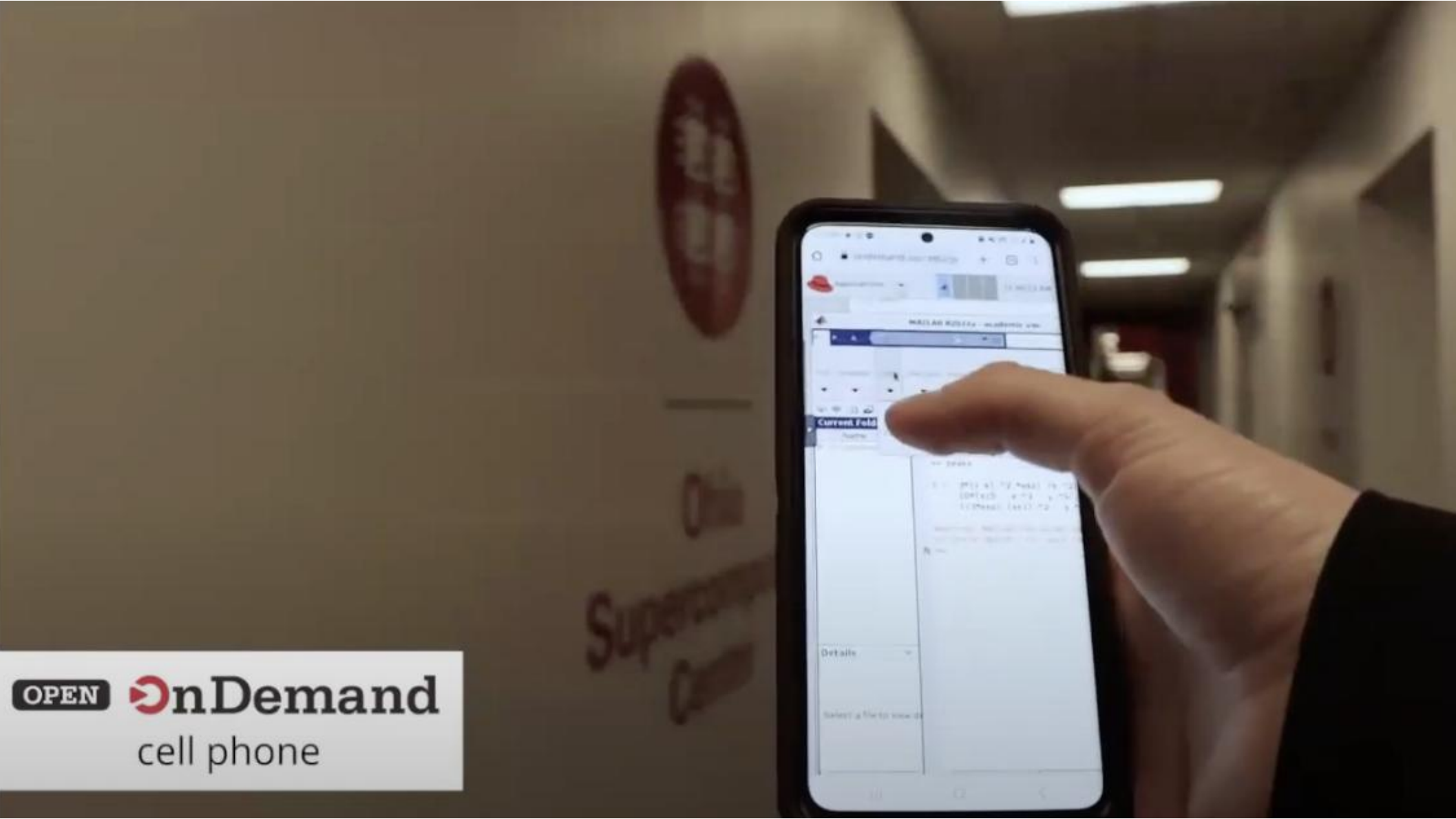


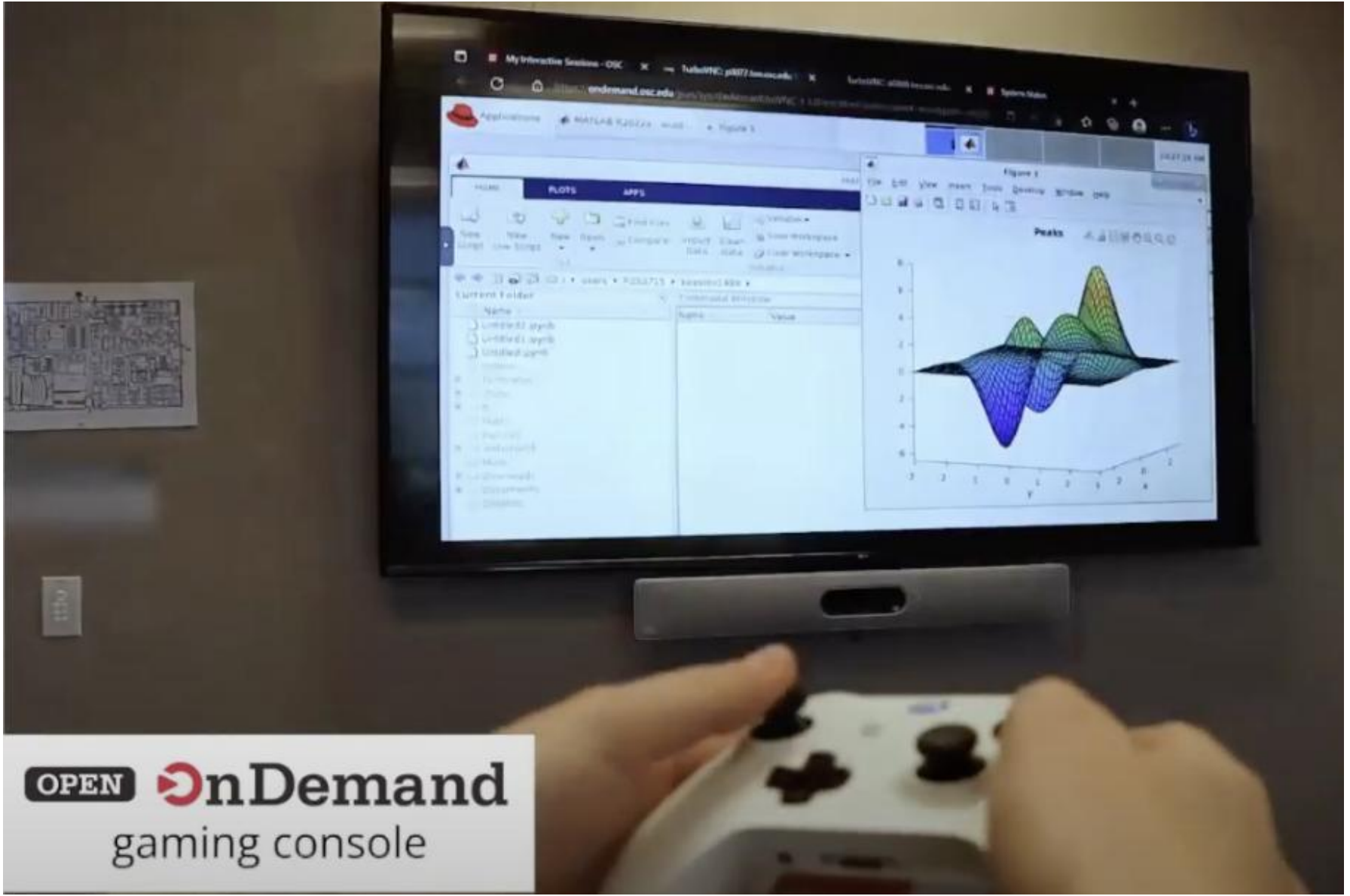
Deployed in 400 HPC centres

2100+	100	6
locations	countries	continents

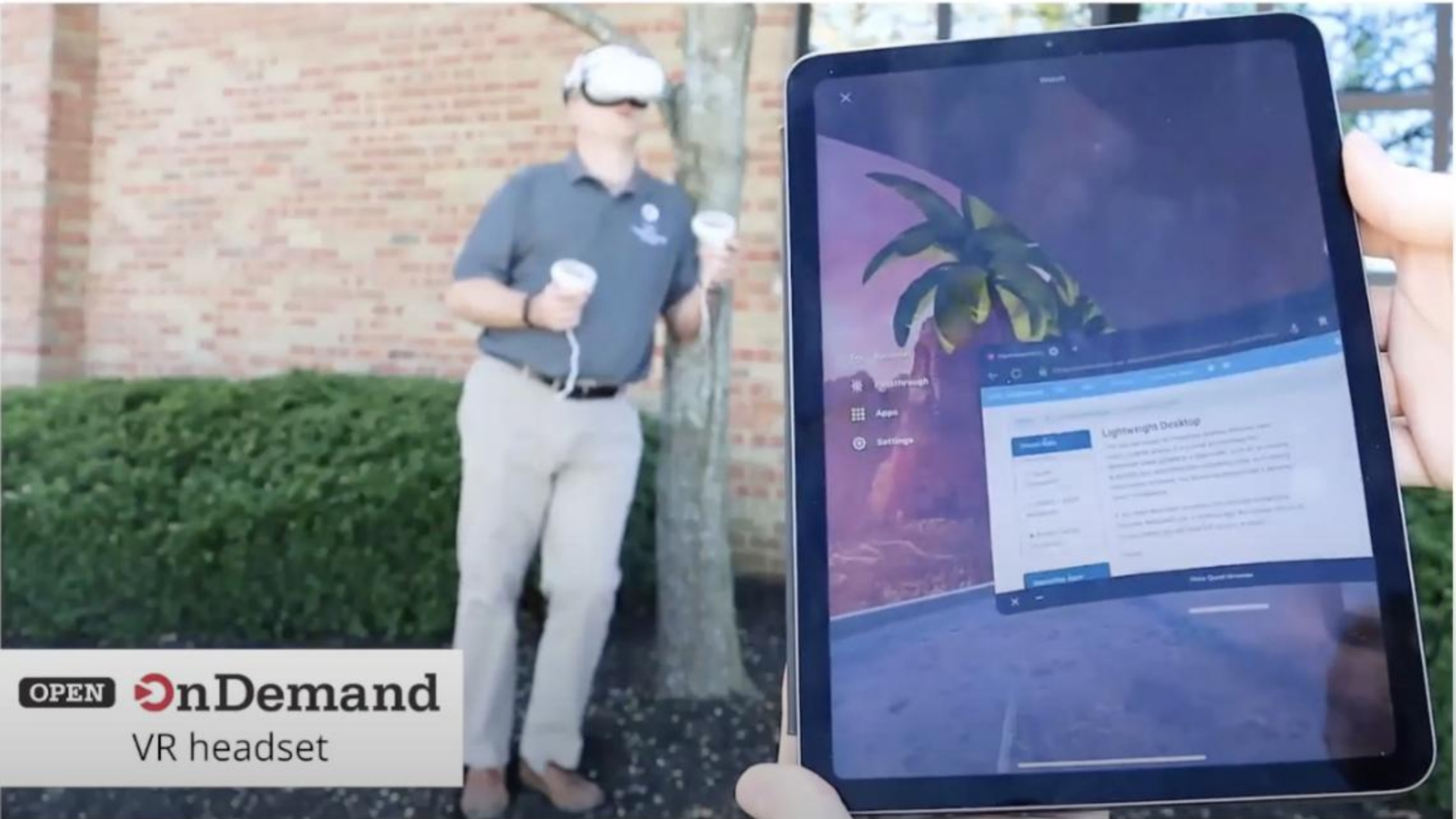

OPEN
OnDemand
laptop


OnDemand
tablet


OPEN
OnDemand
cell phone


OPEN OnDemand
gaming console

OPEN
OnDemand
car dashboard


OPEN
OnDemand
VR headset
Lightweight Desktop
Apps
Settings

Open OnDemand - introduction

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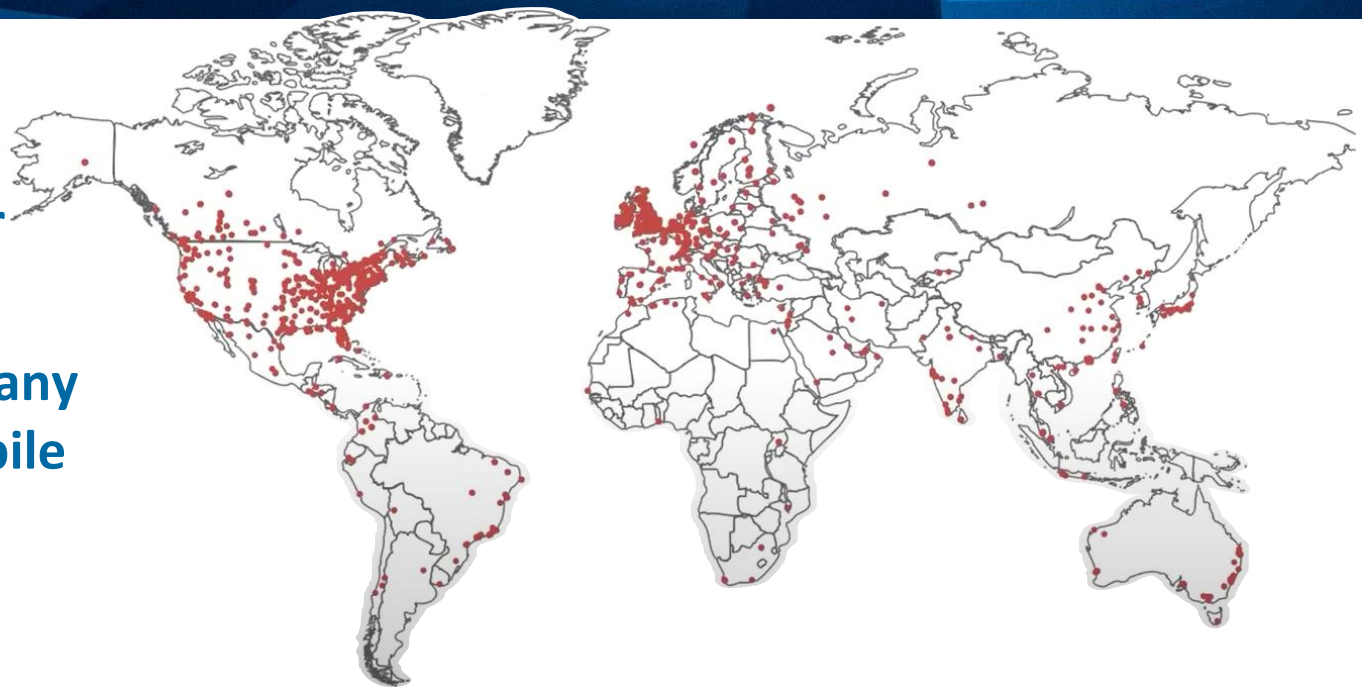
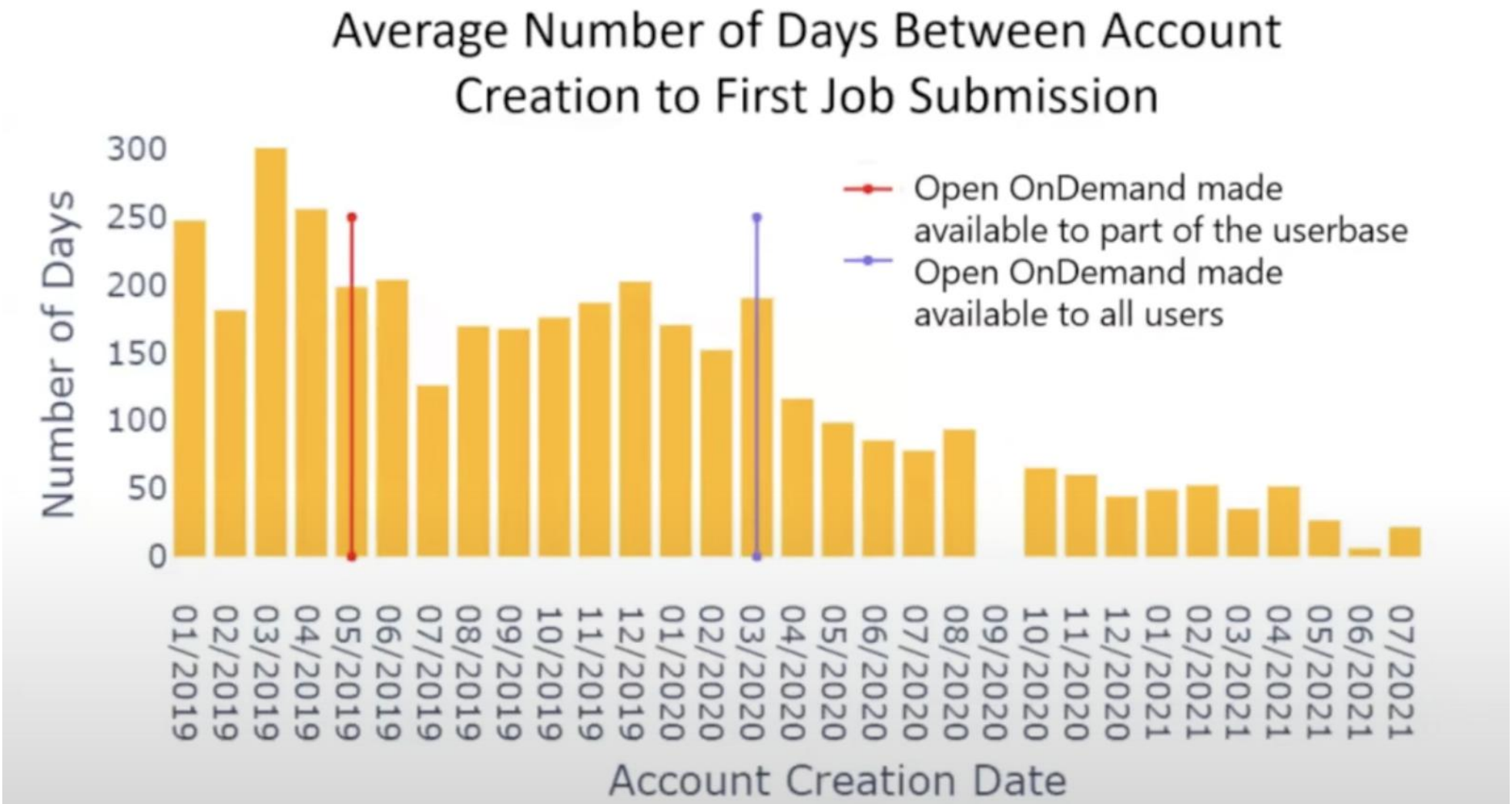


Deployed in 400 HPC centres

2100+	100	6
locations	countries	continents

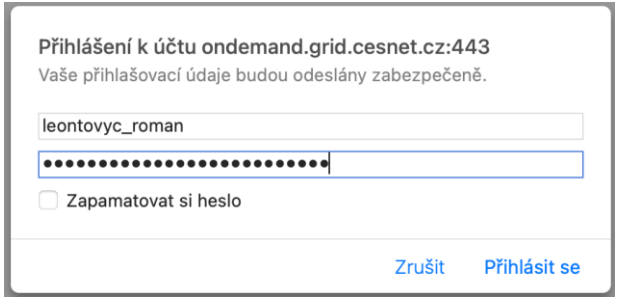
Idaho national lab

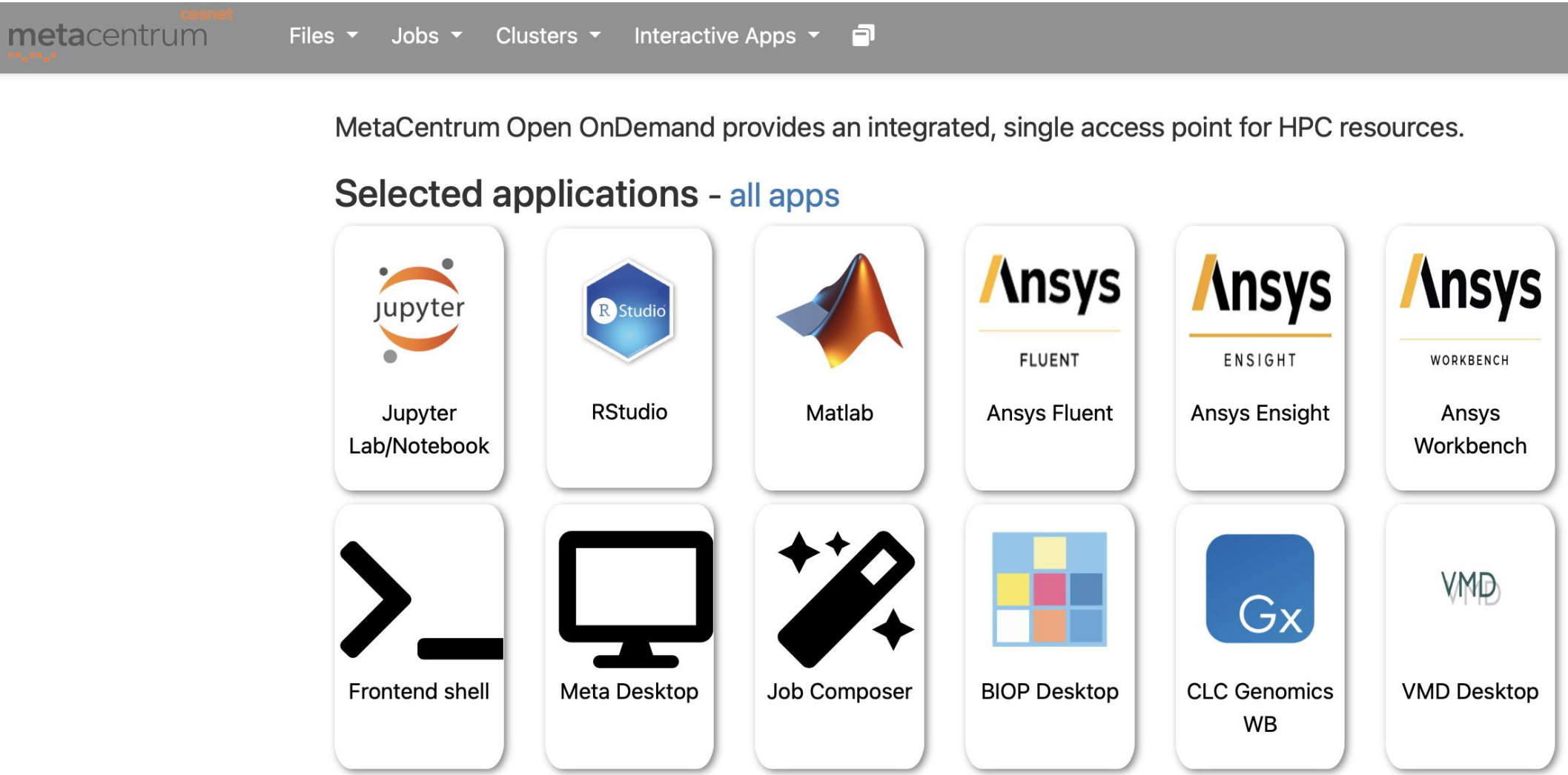


Open Ondemand on Metacentrum

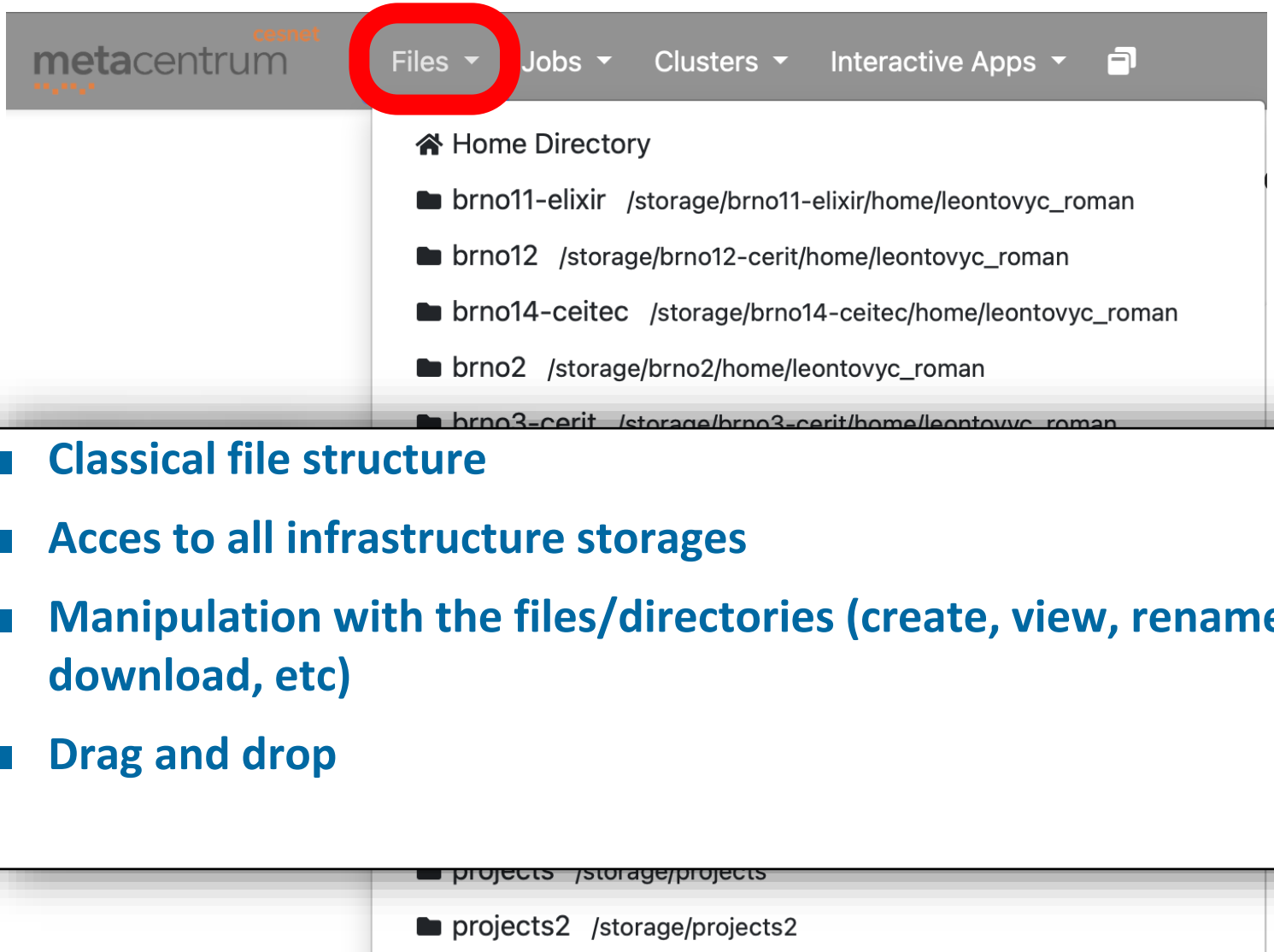
- Running version - 3.1.7
- Access to MetaCentrum/CERIT-SC/ELIXIR computational resources and storages via web browser
- Shell (command line) access also possible
- e-INFRA CZ/Metacentrum login and Metacentrum password
- OOD documentation https://osc.github.io/ood-documentation/latest/
- Metacentrum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

https://ondemand.metacentrum.cz



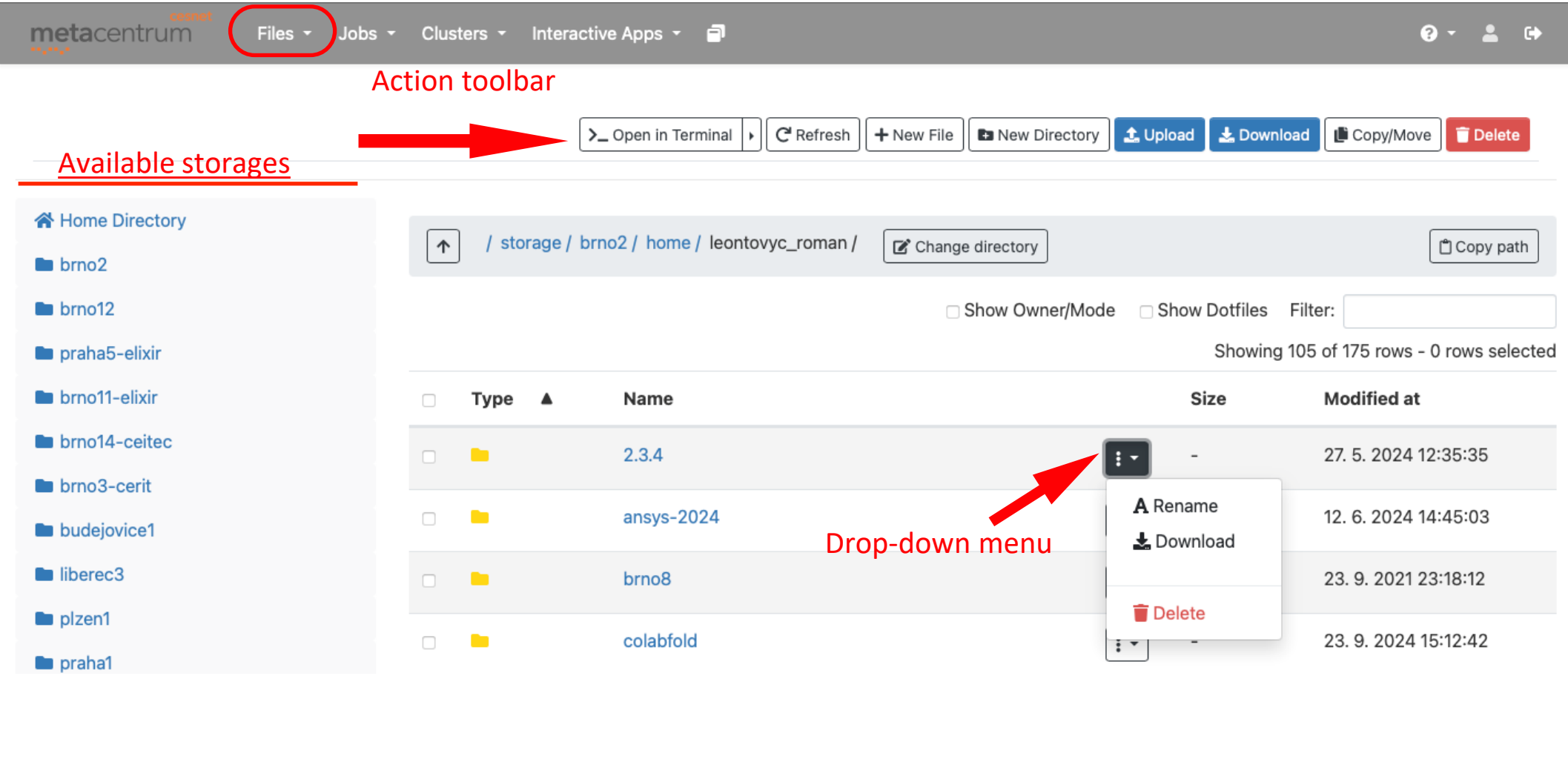

metacentrum
cesnet
Files
Jobs
Clusters
Interactive Apps
MetaCentrum Open OnDemand provides an integrated, single access point for HPC resources.
Selected applications - all apps
Jupyter Lab/Notebook
RStudio
Matlab
Ansys Fluent
Ansys Ensight
Ansys Workbench
Frontend shell
Meta Desktop
Job Composer
BIOP Desktop
CLC Genomics WB
VMD Desktop

File system in Open Ondemand

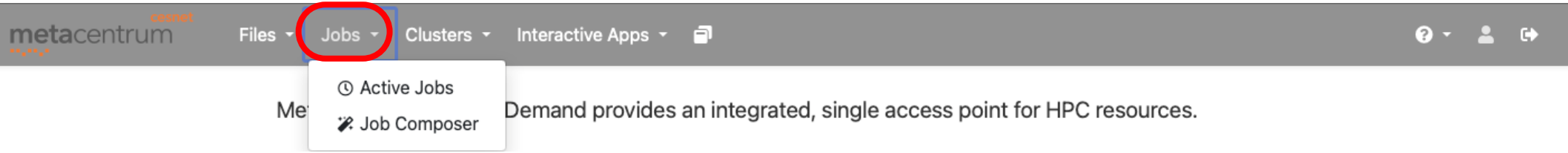


- Classical file structure
- Acces to all infrastructure storages
- Manipulation with the files/directories (create, view, rename, edit, delete, upload, download, etc)
- Drag and drop

Files


metacentrum
Files
Jobs
Clusters
Interactive Apps
Action toolbar
Open in Terminal
Refresh
New File
New Directory
Upload
Download
Copy/Move
Delete
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 Dotfiles
Filter:
Showing 105 of 175 rows - 0 rows selected
Type
Name
Size
Modified at
2.3.4
27. 5. 2024 12:35:35
ansys-2024
12. 6. 2024 14:45:03
brno8
23. 9. 2021 23:18:12
colabfold
23. 9. 2024 15:12:42
Rename
Download
Delete
Drop-down menu

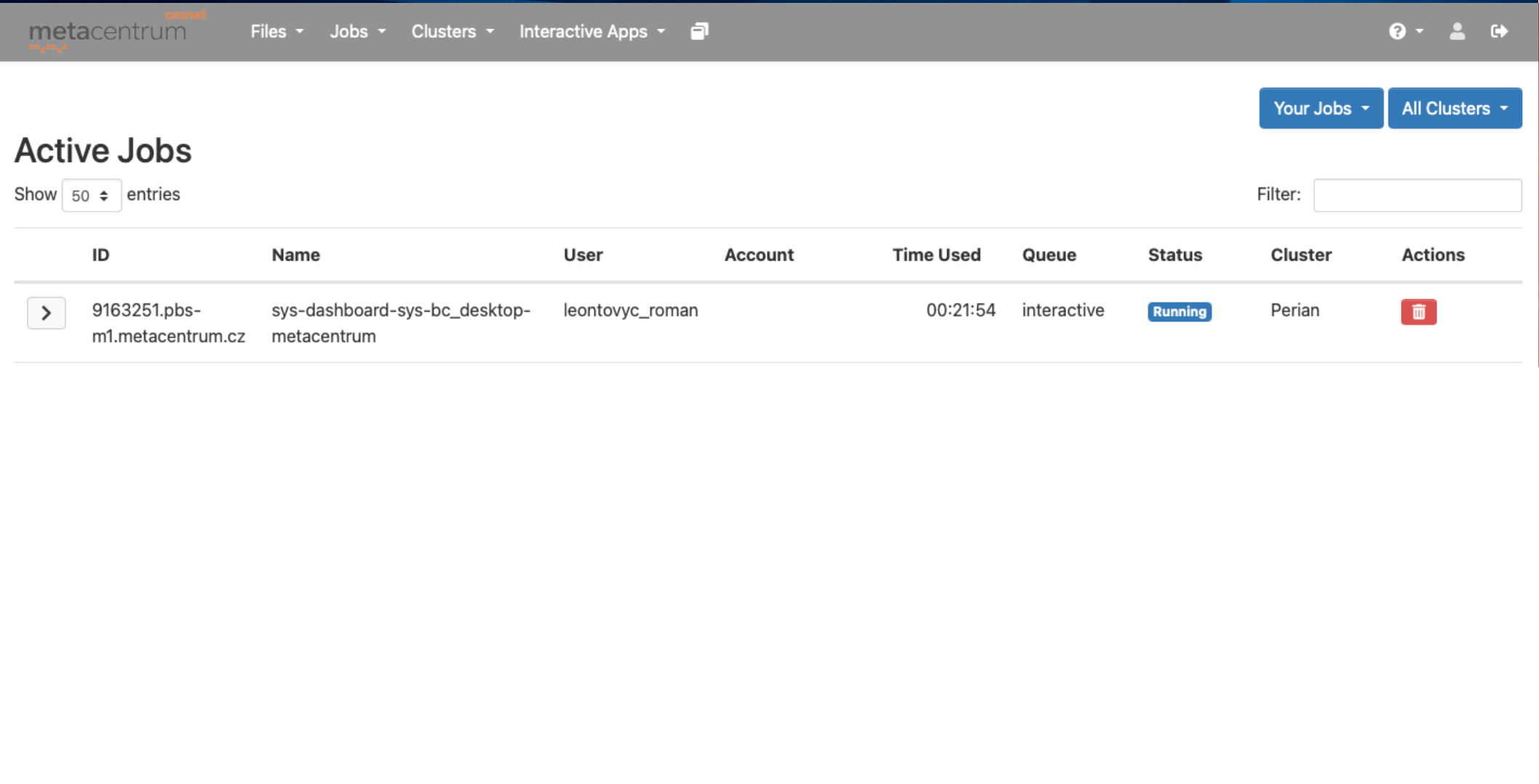
Jobs in Open Ondemand



- 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


metacentrum
cesnet
Files
Jobs
Clusters
Interactive Apps
Your Jobs
All Clusters
Active Jobs
Show 50 entries
Filter:
ID
Name
User
Account
Time Used
Queue
Status
Cluster
Actions
9163251.pbs-m1.metacentrum.cz
sys-dashboard-sys-bc_desktop-metacentrum
leontovyc_roman
00:21:54
interactive
Running
Perian

Jobs

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`

Folder Contents:

- hello_world.o9163197
- **main_job.sh**
- output_file

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'"
```

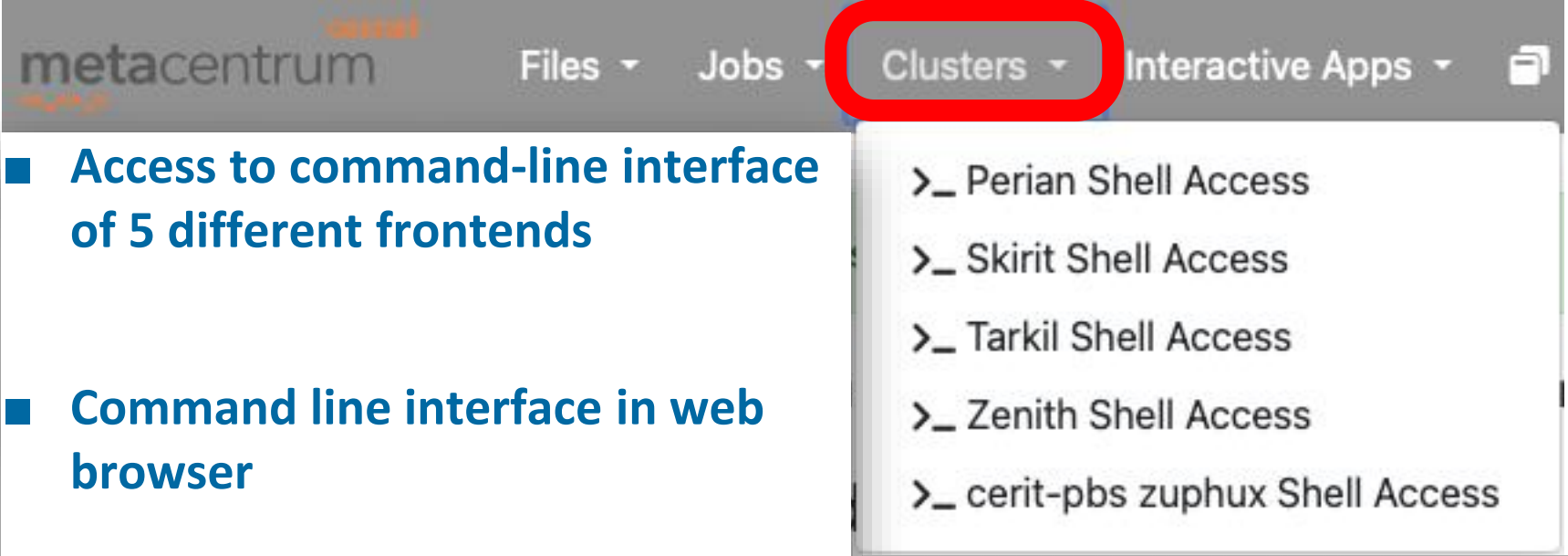
Open Editor | Open Terminal | Open Dir

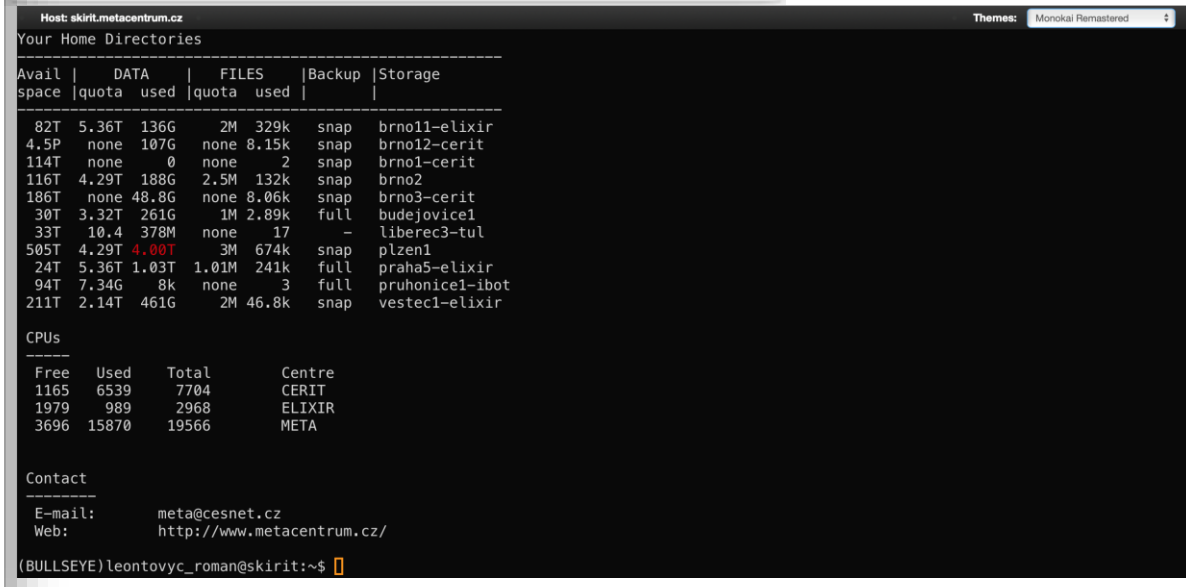
Save /storage/brno2/home/leontovyc_roman/ondemand/data/sys/myjobs/projects/default/3/alphafold_job.sh Key Bindings Default Font Siz

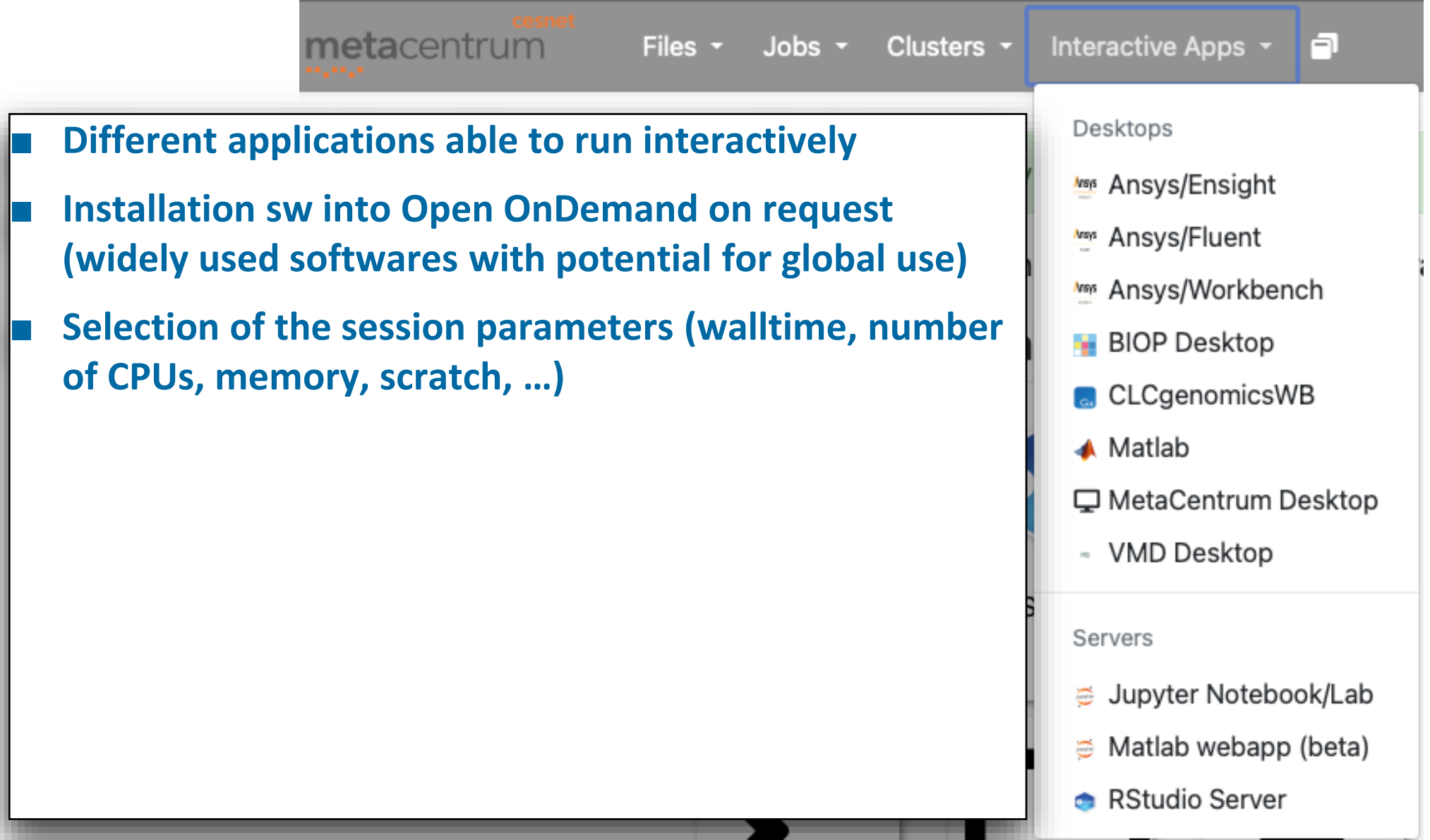
```
#PBS -N Alphafold-OOD-JOB
#PBS -q ondemand
#PBS -l select=1:ncpus=8:ngpus=1:mem=100gb:scratch_local=10gb:gpu_cap=cuda75
#PBS -l walltime=24:00:00
#PBS -m ae

cd $PBS_O_WORKDIR

###############################################
#change paths
OUTPUTS_DIR=./outputs
# 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
FASTA_INPUTS=/storage/brno11-elixir/projects/alphafold/example-fasta/seq.fasta
###############################################

# multimer example
#FASTA_INPUTS=/storage/brno11-elixir/projects/alphafold/example-fasta/multi.fasta

#choose one of the Alfafold prediction method
METHOD="AF_MONOMER_REDUCED_DBS"
#METHOD="AF_MULTIMER_FULL_DBS"
#METHOD="AF_MULTIMER_REDUCED_DBS"

# load methods
source ./lib.sh

# execute method
$METHOD

# copy results from scratch
mkdir -p $OUTPUTS_DIR
cp -r  $SCRATCHDIR/* $OUTPUTS_DIR/ &&  rm -r $SCRATCHDIR/*
```

- **Access to command-line interface of 5 different frontends**

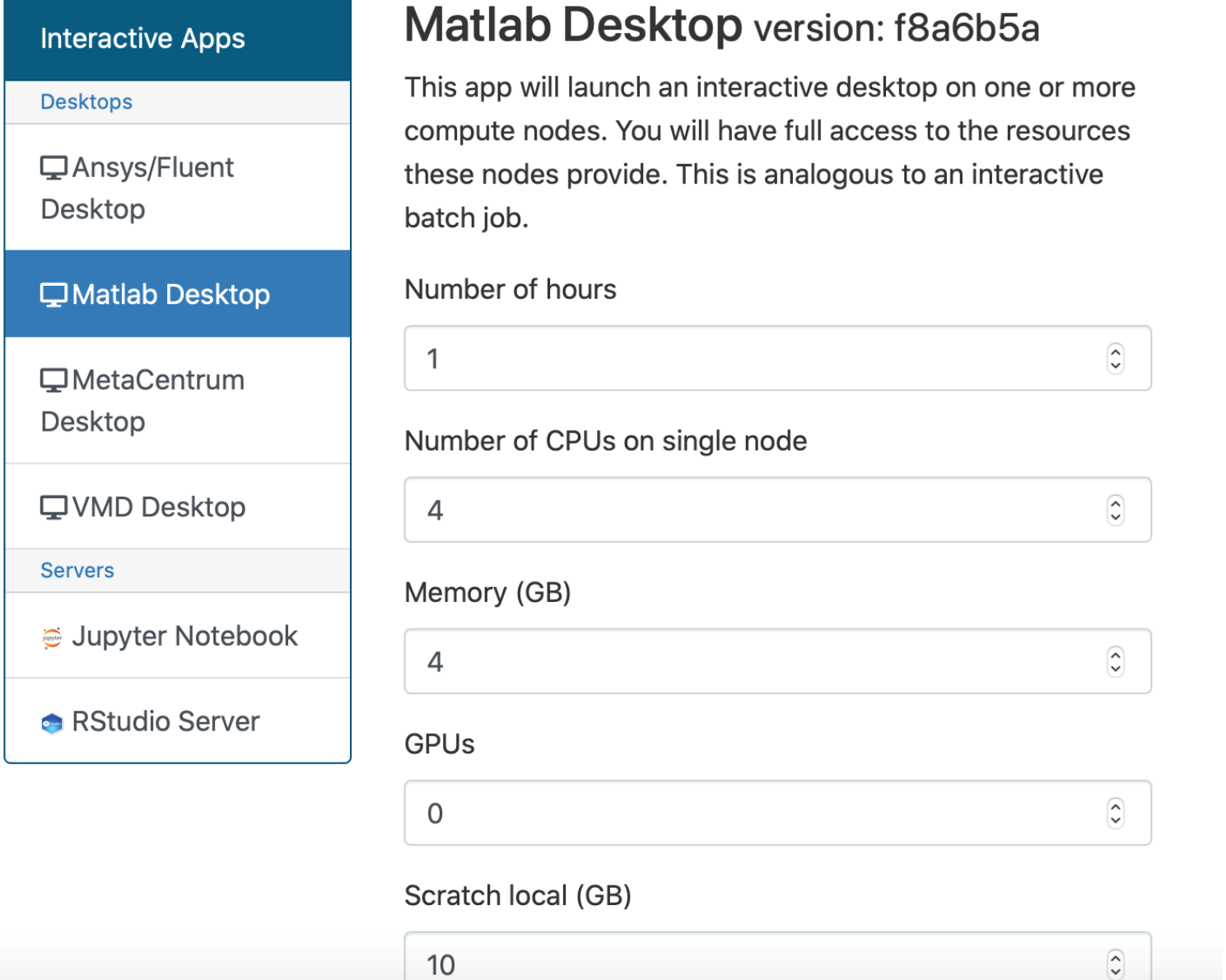
- **Command line interface in web browser**







- 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, …)


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

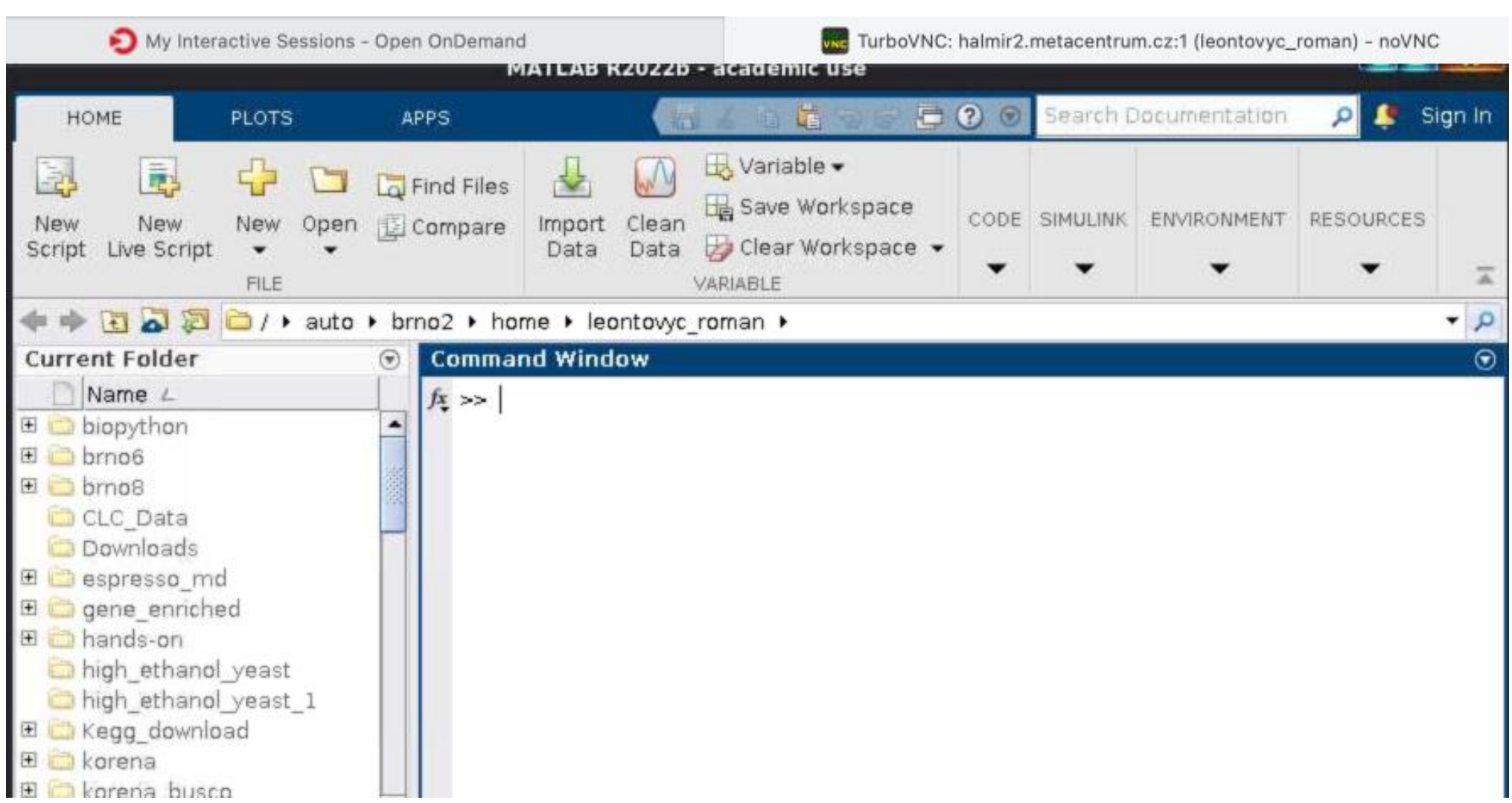
0 (low) to 9 (high)

Image Quality

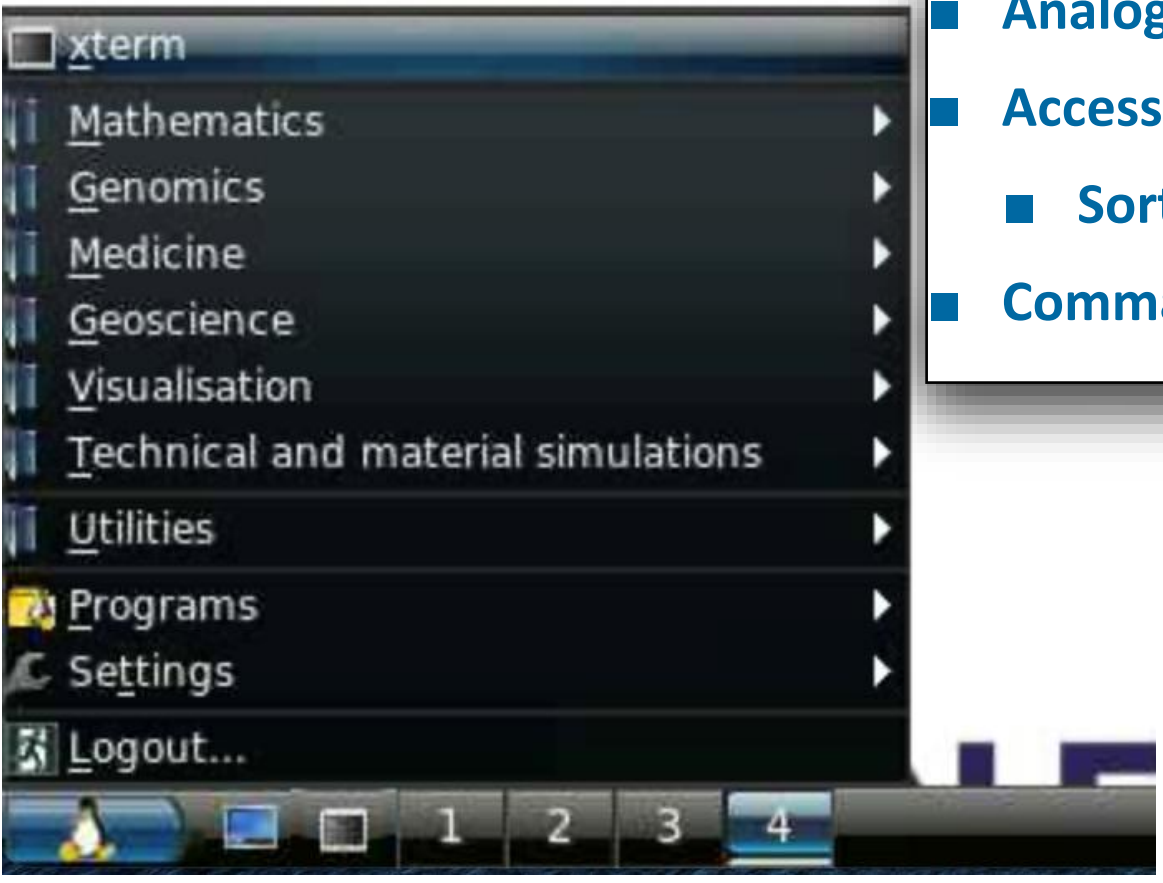
0 (low) to 9 (high)

Launch Matlab Desktop

View Only (Share-able Link)


My Interactive Sessions - Open OnDemand
TurboVNC: halmir2.metacentrum.cz:1 (leontovyc_roman) - noVNC
MATLAB R2022b - academic use
HOME
PLOTS
APPS
Search Documentation
Sign In
New Script
New Live Script
New
Open
Find Files
Compare
FILE
Import Data
Clean Data
Variable
Save Workspace
Clear Workspace
VARIABLE
CODE
SIMULINK
ENVIRONMENT
RESOURCES
/ ▸ auto ▸ brno2 ▸ home ▸ leontovyc_roman ▸
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
>>

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

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Thank you for attention