

OPEN ONDEMAND

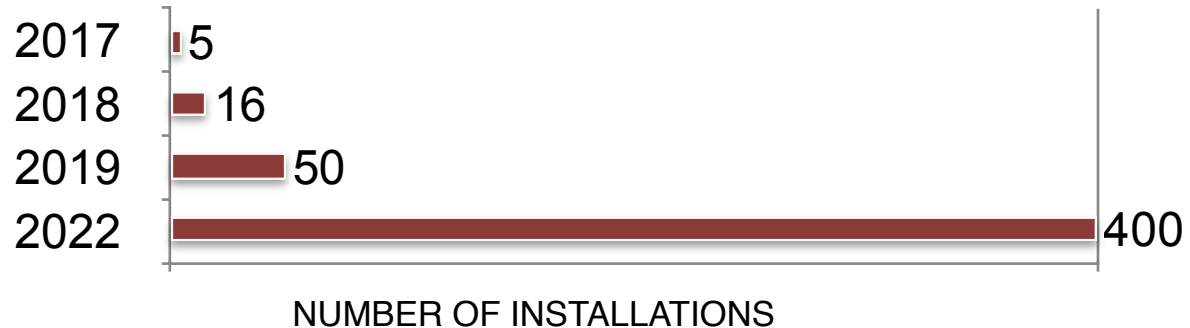
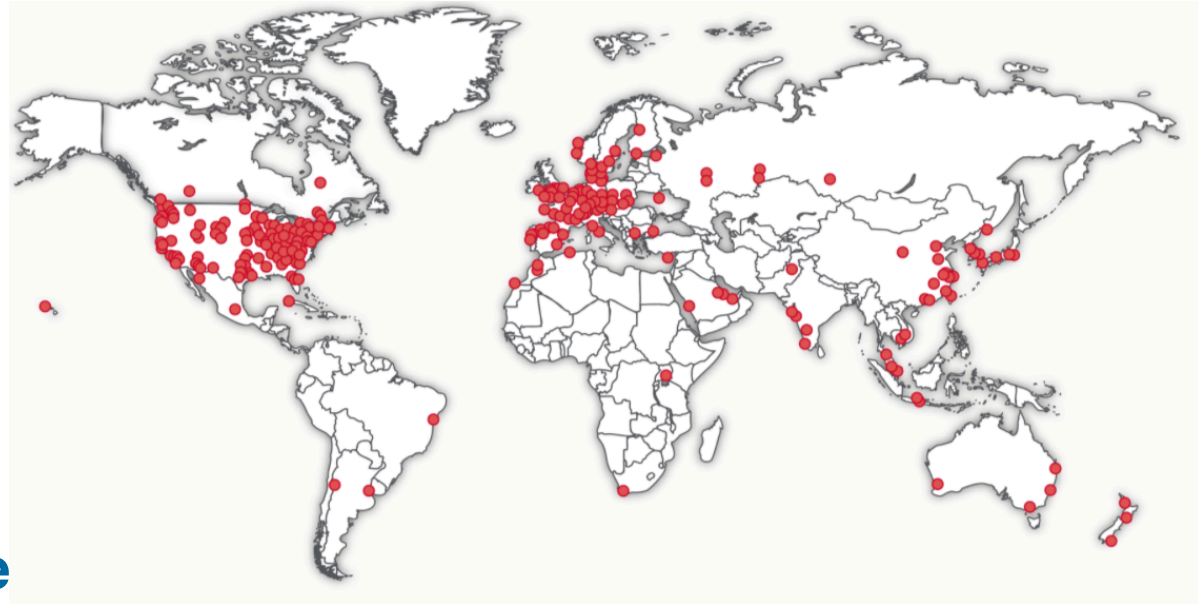
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Open OnDemand - introduction

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



Open Ondemand on Metacentrum

- 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

<https://ondemand.metacentrum.cz>

Přihlášení k účtu ondemand.grid.cesnet.cz:443

Vaše přihlašovací údaje budou odeslány zabezpečeně.

leontovyc_roman

.....

Zapamatovat si heslo

Zrušit


Přihlásit se



Welcome to the MetaCentrum Open OnDemand.


OnDemand provides an integrated, single access point for all of your HPC resources.

Pinned Apps A featured subset of [all available apps](#)




Jupyter Notebook

System Installed App



MetaCentrum Desktop

System Installed App



RStudio Server

System Installed App

Message of the Day

06-03-2023

RStudio has now Geospatial and Tensorflow packages preinstalled.

16-01-2023

We are entering pilot phase of the MetaCentrum OnDemand deployment.

Open OnDemand

Apps ▾

Files ▾

Jobs ▾

Clusters ▾

Interactive Apps ▾



🏠 Home Directory

📁 MetaCentrum /storage/brno2/home/leontovyc_roman

📁 CERIT-SC /storage/brno3-cerit/home/leontovyc_roman

📁 ELIXIR /storage/praha5-elixir/home/leontovyc_roman

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

Files

Open OnDemand Apps ▾ Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾ 



 Open in Terminal

 New File

 New Directory

 Upload

 Download

 Copy/Move

 Delete

Home Directory

MetaCentrum


CERIT-SC

ELIXIR



/ storage / brno2 / home / leontovyc_roman /

 Change directory






 Copy path

Show Owner/Mode

Show Dotfiles

Filter:

Showing 50 of 100 rows - 1 rows selected

Type	Name	Size	Modified at
<input checked="" type="checkbox"/> 	biopython	-	20.12.2019 15:19:45
<input type="checkbox"/> 	brno6		2.12.2021 2:54:48
<input type="checkbox"/> 	brno8		23.9.2021 23:18:12
<input type="checkbox"/> 	CLC_Data		6.4.2023 11:49:57
<input type="checkbox"/> 	Downloads		7.3.2023 13:54:40



 Rename

 Download

 Delete

- **Analogous to a batch job**

- ⌚ Active Jobs

- ✏ Job Composer

- **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

Open OnDemand Apps 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
> 15006011.meta-pbs.metacentrum.cz	Alphafold-OOD-JOB	leontovyc_roman		00:00:00	ondemand	Queued	MetaCentrum	

Showing 1 to 1 of 1 entries

Previous 1 Next

powered by



OnDemand version: 2.0.31

Job composer

+ New Job ▾

☆ Create Template

📄 Edit Files

⚙️ Job Options

📄 Open Terminal

▶ Submit

■ Stop

🗑 Delete

Show 25 entries

Search:

Created	Name	ID	Cluster	Status
April 6, 2023 1:28pm	Alphafold Metacentrum job	14933439.meta-pbs.metacentrum.cz	MetaCentrum	Queued
April 5, 2023 4:24pm	test_ondemand.sh		MetaCentrum	Not Submitted
April 5, 2023 4:15pm	Alphafold Metacentrum job		MetaCentrum	Not Submitted
February 6, 2023	(default) Metacentrum simple	14644331.meta-pbs.metacentrum.cz	MetaCentrum	Completed

```
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 ;
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 Alafold 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/*
```

- Access to command-line interface of 3 different frontends
 - Skirit (MetaCentrum shell access)
 - Elmo (ELIXIR shell access)
 - Zuphux (CERIT-SC access)
- Command line interface in web browser

>_CERIT-SC Shell Access

>_ELIXIR Shell Access

>_MetaCentrum 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  snap  brno11-elixir
4.5P  none  107G   none  8.15k  snap  brno12-cerit
114T  none    0     none    2     snap  brno1-cerit
116T  4.29T 188G   2.5M  132k  snap  brno2
186T  none  48.8G  none  8.06k  snap  brno3-cerit
30T   3.32T 261G   18  2.89k  full  budejovice1
33T   10.4  378M   none  17     -     liberec3-tul
505T  4.29T 4.00T    3M  674k  snap  plzen1
24T   5.36T 1.03T  1.01M 241k  full  praha5-elixir
94T   7.34G  8k     none   3     full  pruhonice1-ibot
211T  2.14T  461G    2M  46.8k  snap  vestec1-elixir

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:~$
```



- **Applications able to run interactively**
 - **Ansys/Fluent**
 - **Matlab**
 - **VMD (Visual Molecular Dynamics)**
 - **Jupyter Notebook**
 - **RStudio**
- **Selection of the session parameters (walltime, number of CPUs, memory, scratch, ...)**

Desktops

 Ansys/Fluent Desktop Matlab Desktop MetaCentrum Desktop VMD Desktop

Servers

 Jupyter Notebook 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



Number of CPUs on single node



Memory (GB)



GPUs



Scratch local (GB)




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 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

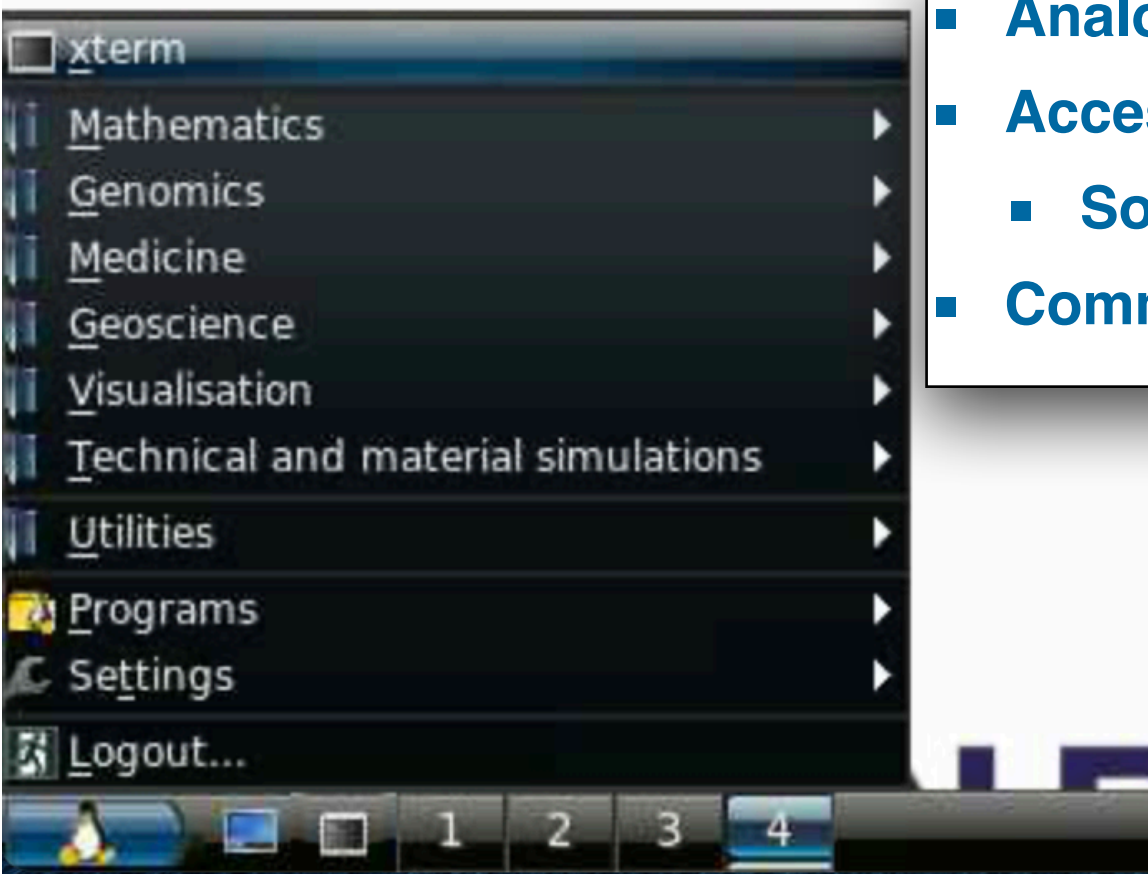
Name

- 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

```
fx >> |
```

Metacentrum desktop



- Analogous to an interactive batch 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

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

Thank you for attention

