MetaCentrum NGI

For scientific computations, collaborative research and its support services

Jiří Vorel

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vorel@cesnet.cz meta@cesnet.cz

4. 6. 2026

MetaCentrum in a nutshell

https://www.cesnet.cz/ https://www.metacentrum.cz/

https://www.e-infra.cz/ https://docs.metacentrum.cz/

- MetaCentrum is
  - The activity of the CESNET association
  - Part of the e-INFRA CZ e-infrastructure
  - A national grid infrastructure (NGI)
  - A provider of computational resources, application software (both commercial and free/open source) and data storage
  - Available to the entire academic and research community (employees and students) in the Czech Republic
  - Free of charge (users 'pay' by acknowledging the project 'e-INFRA CZ ID:90254' in their publications)

https://docs.metacentrum.cz/en/docs/access/terms#acknowledgements-and-publications

MetaCentrum in a nutshell

- MetaCentrum offers
  - Access to all resources without submitted projects (with one exception)
  - The possibility to apply for membership at any time
  - Immediate access to hardware resources and licences (once an application has been approved)
  - CPU/GPU resources, CLI access, GUI applications, Kubernetes and cloud services, etc.
  - Various application software (commercial, free and open source)
  - Data sharing

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☝ *Collaborating industry users and foreign research partners can also get access to MetaCentrum. This includes only non-profit and public research. They can do so upon individual request.*

MetaCentrum in a nutshell

- MetaCentrum cannot help with
  - Purely commercial research
  - Allocating resources for a fee
  - Long-term and secure storage of valuable data (i.e. data archiving) https://du.cesnet.cz
  - Processing sensitive data (Kubernetes Sensitive Cloud within e-INFRA CZ, coordinated by CERIT-SC)
  - Tools whose installation or use would violate the licence terms
  - Windows OS

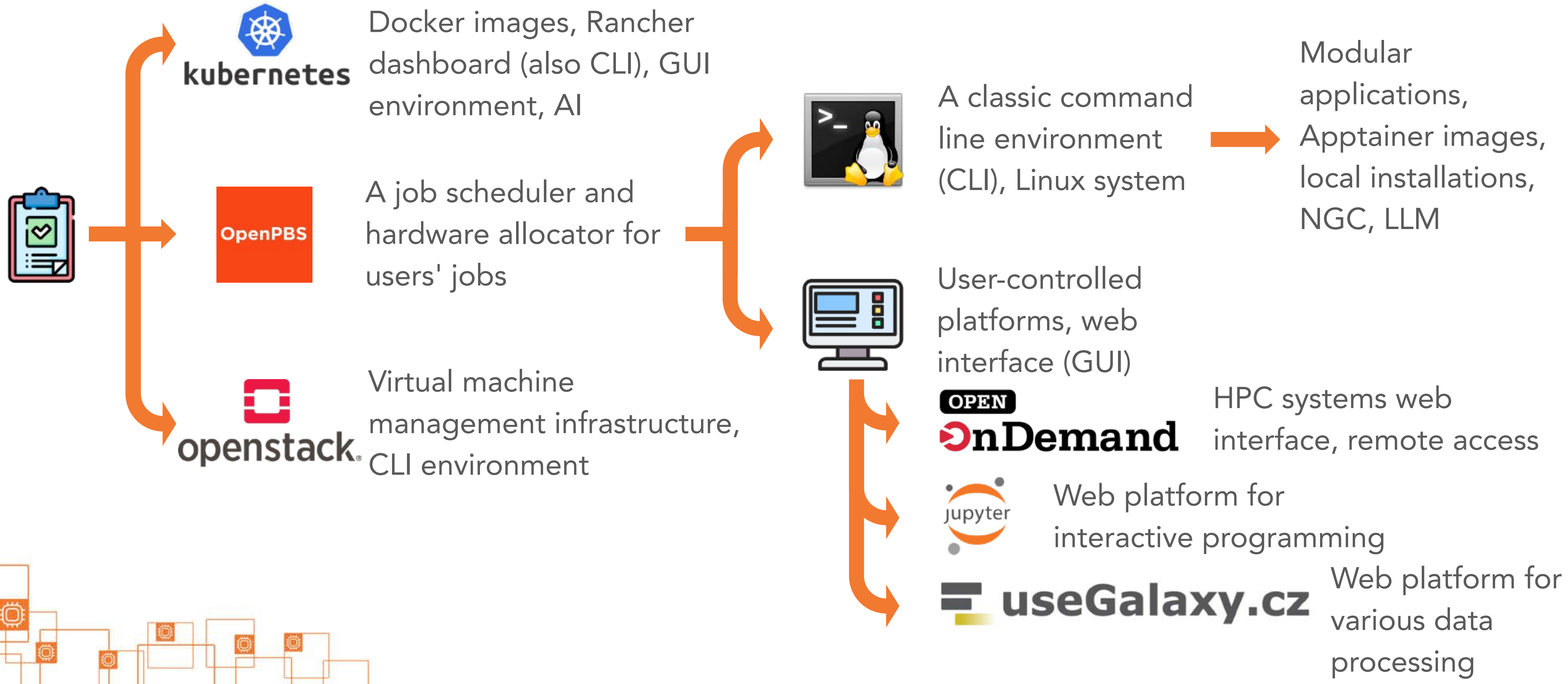
cesnet datacare

https://www.cerit-sc.cz/

ONE APPLICATION TO RULE THEM ALL

One application to rule them all

https://docs.metacentrum.cz/en/docs/welcome



kubernetes

Kubernetes orchestrator of Docker images, Rancher dashboard (also CLI), GUI environment, AI

OpenPBS

A job scheduler and hardware allocator for users' jobs

openstack

Virtual machine management infrastructure, CLI environment

A classic command line environment (CLI), Linux system

Modular applications, Apptainer images, local installations, NGC, LLM

User-controlled platforms, web interface (GUI)

OPEN OnDemand

HPC systems web interface, remote access

jupyter

Web platform for interactive programming

useGalaxy.cz

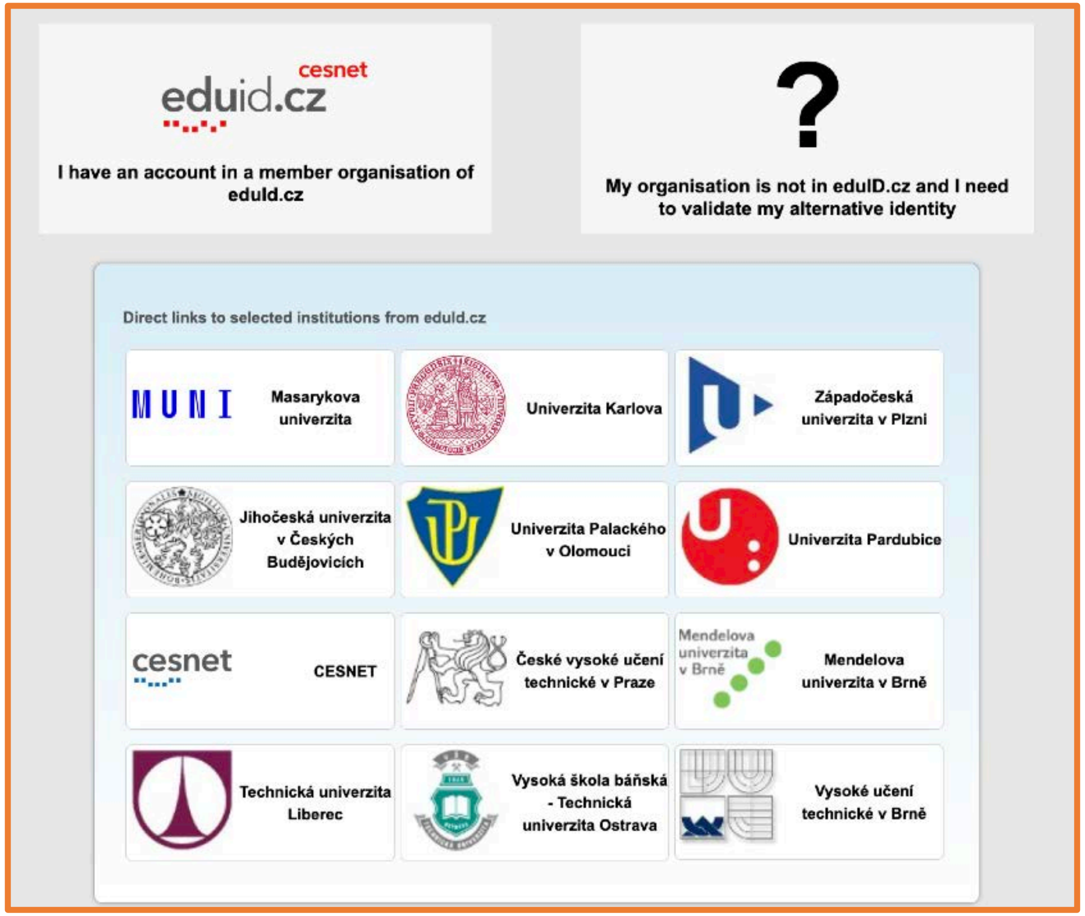
Web platform for various data processing

https://docs.metacentrum.cz/en/docs/access/account

https://docs.metacentrum.cz/en/docs/access/terms

Submitting an application

- Anytime during the year, manual approval
- Log in through the institution (i.e. local name and password) from the eduID federation
- Accounts expire on 2 February each year and must be renewed in January
- Immediate access to hardware resources



I have an account in a member organisation of eduId.cz

My organisation is not in eduID.cz and I need to validate my alternative identity

Direct links to selected institutions from eduId.cz

Masarykova univerzita

Univerzita Karlova

Západočeská univerzita v Plzni

Jihočeská univerzita v Českých Budějovicích

Univerzita Palackého v Olomouci

Univerzita Pardubice

CESNET

České vysoké učení technické v Praze

Mendelova univerzita v Brně

Technická univerzita Liberec

Vysoká škola báňská - Technická univerzita Ostrava

Vysoké učení technické v Brně

Choose your home institution

http

http

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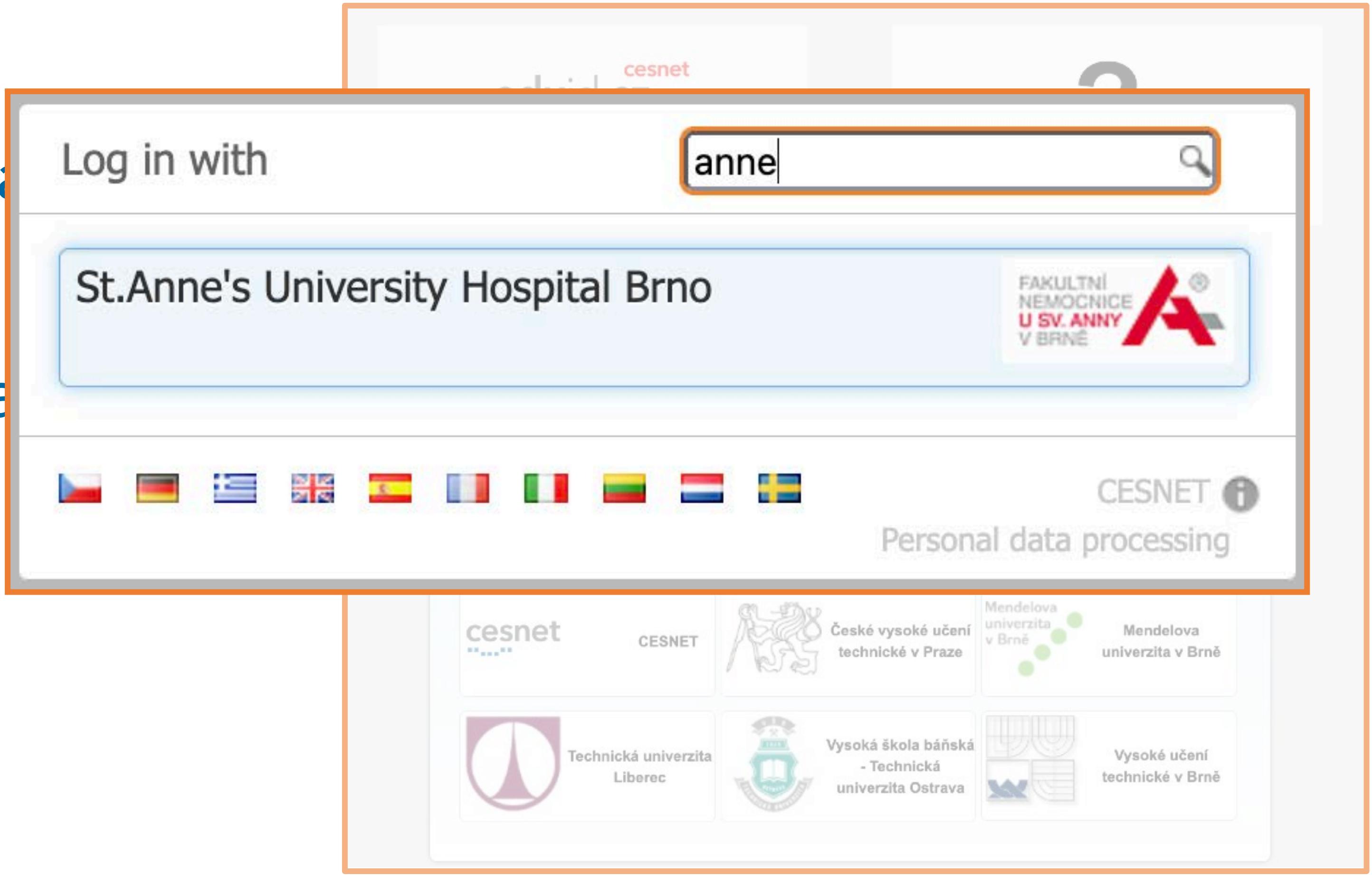
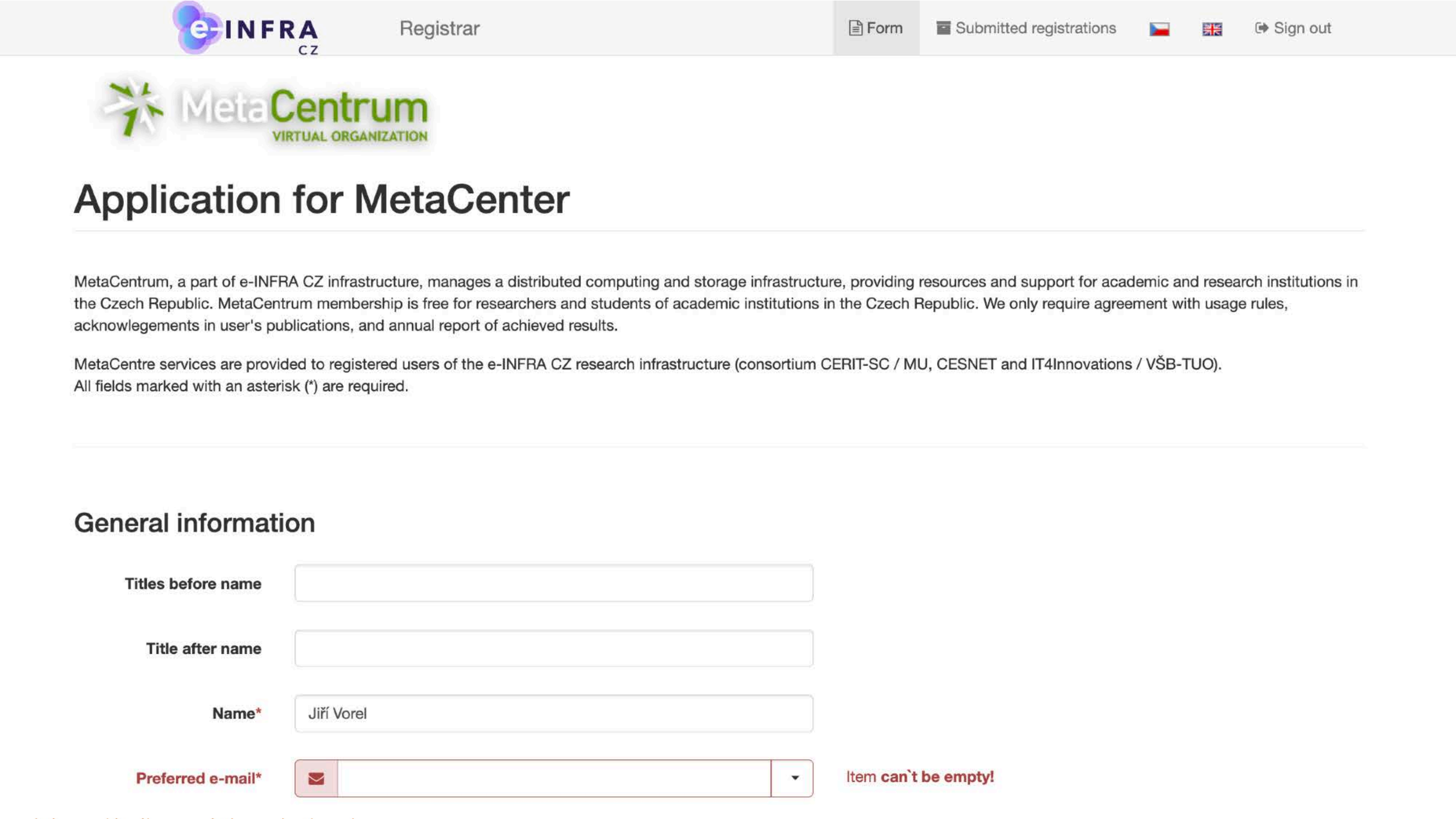
- Accounts expire on 2 Febru
  year and must be renewed i
- Immediate access to hardwa
  resources



Log in with

anne

St.Anne's University Hospital Brno



Application for MetaCenter

MetaCentrum, a part of e-INFRA CZ infrastructure, manages a distributed computing and storage infrastructure, providing resources and support for academic and research institutions in the Czech Republic. MetaCentrum membership is free for researchers and students of academic institutions in the Czech Republic. We only require agreement with usage rules, acknowlegements in user's publications, and annual report of achieved results.

MetaCentre services are provided to registered users of the e-INFRA CZ research infrastructure (consortium CERIT-SC / MU, CESNET and IT4Innovations / VŠB-TUO).
All fields marked with an asterisk (*) are required.

General information

Titles before name		
Title after name		
Name*	Jiří Vorel	
Preferred e-mail*	✉ ▾	Item **can`t be empty!**

MetaCentrum provides access to hundreds of software tools giving thousands of individual modules

Licence models

- We can run almost anything that doesn't violate the licence terms and is for Linux
- Most application software is open source, but…

https://docs.metacentrum.cz/en/docs/software


Paid licence

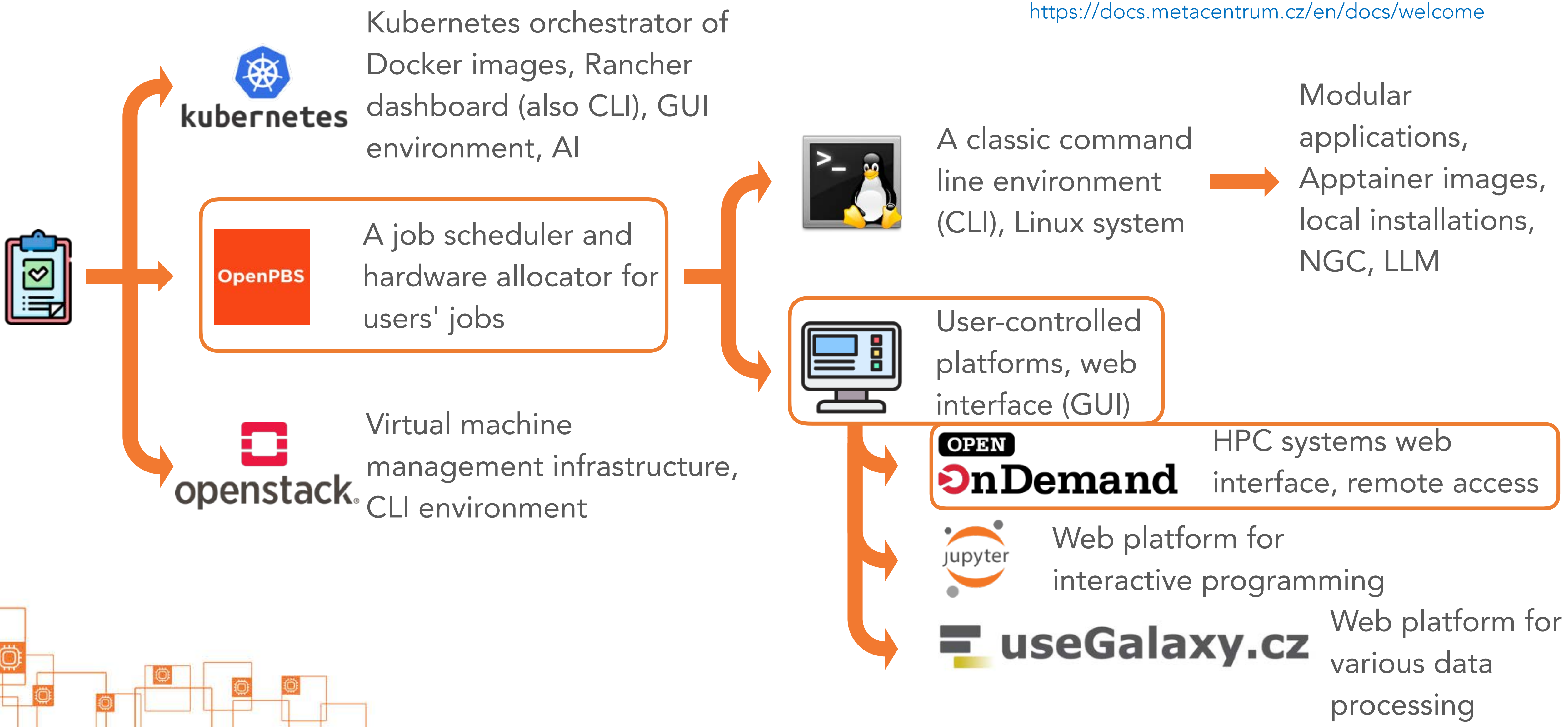
For registered individuals

For all users

Free licence

How to use it

https://docs.metacentrum.cz/en/docs/welcome



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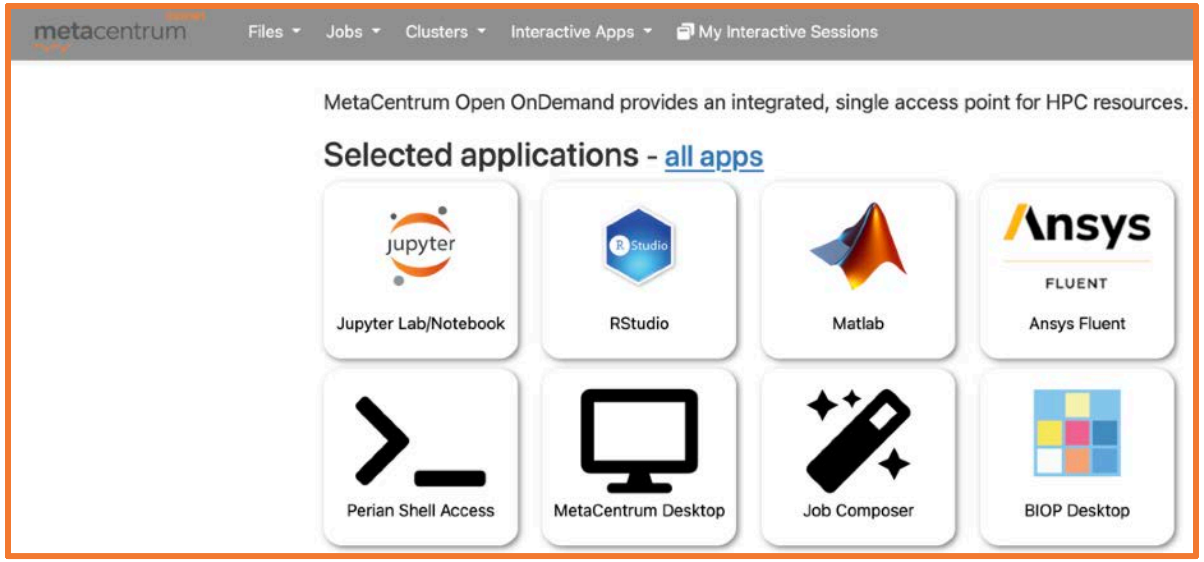
Open OnDemand

- Open OnDemand

  https://ondemand.metacentrum.cz/

  - Web application on top of OpenPBS scheduler
  - Running (not only) GUI applications



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

Selected applications - all apps

Open OnDemand

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  https://ondemand.metacentrum.cz/

  - Web application on top of OpenPBS scheduler
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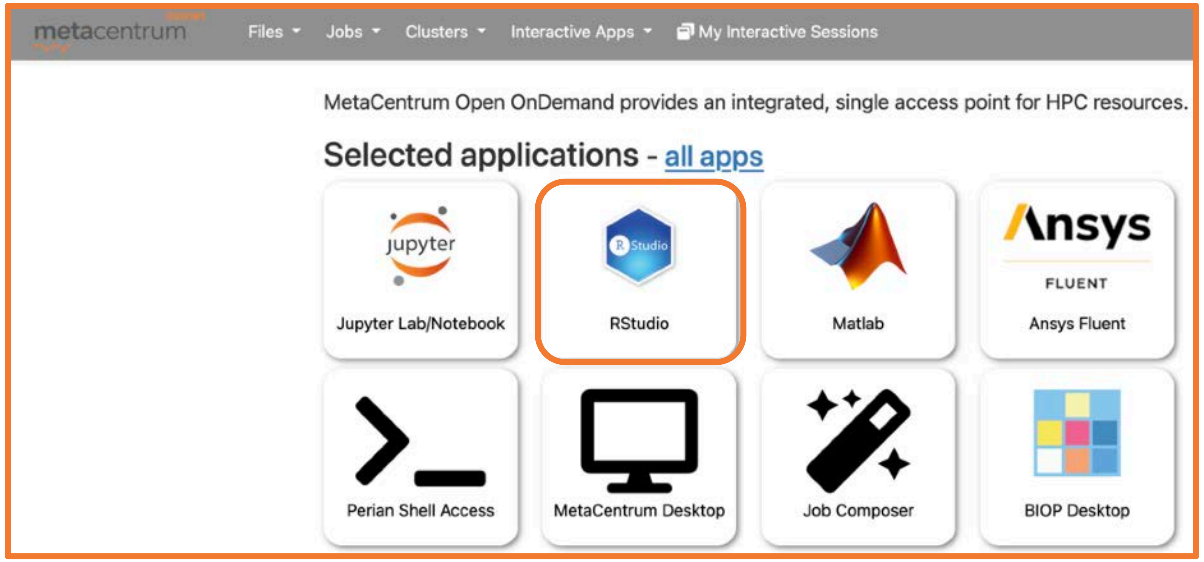


MetaCentrum Open OnDemand provides an integrated, single access point for HPC resources.

Selected applications - all apps

https://docs.metacentrum.cz/en/docs/software/sw-list/rstudio

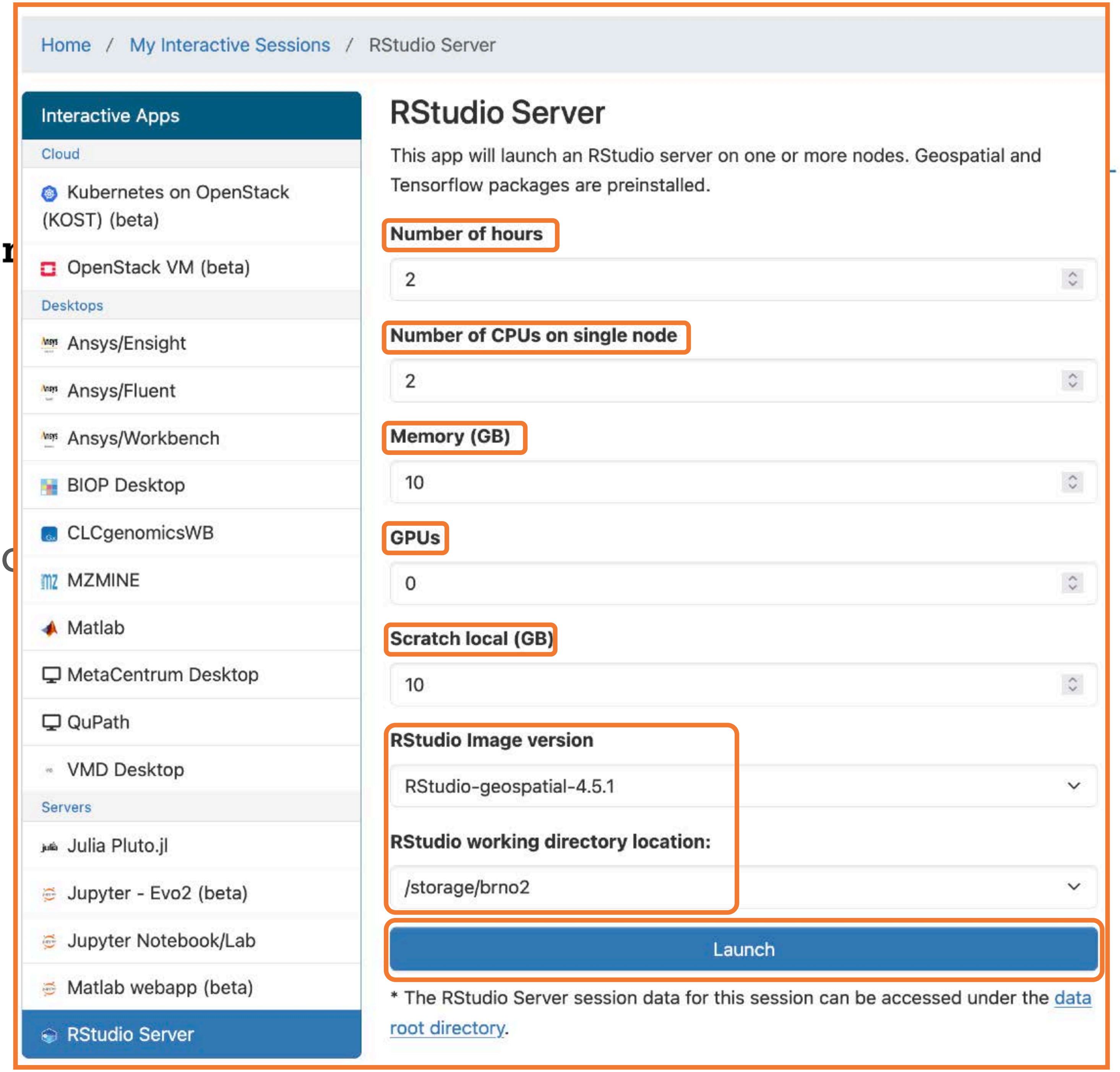
https://docs.metacentrum.cz/en/docs/software/sw-list/r

R is a software environment for statistical computing and graphics

- Open OnDemand

  https://ondemand.metacentrum.cz/

  - Web application on top of OpenPBS scheduler
  - Running (not only) GUI applic



Home / My Interactive Sessions / RStudio Server

RStudio Server

This app will launch an RStudio server on one or more nodes. Geospatial and Tensorflow packages are preinstalled.

Number of hours

2

Number of CPUs on single node

2

Memory (GB)

10

GPUs

0

Scratch local (GB)

10

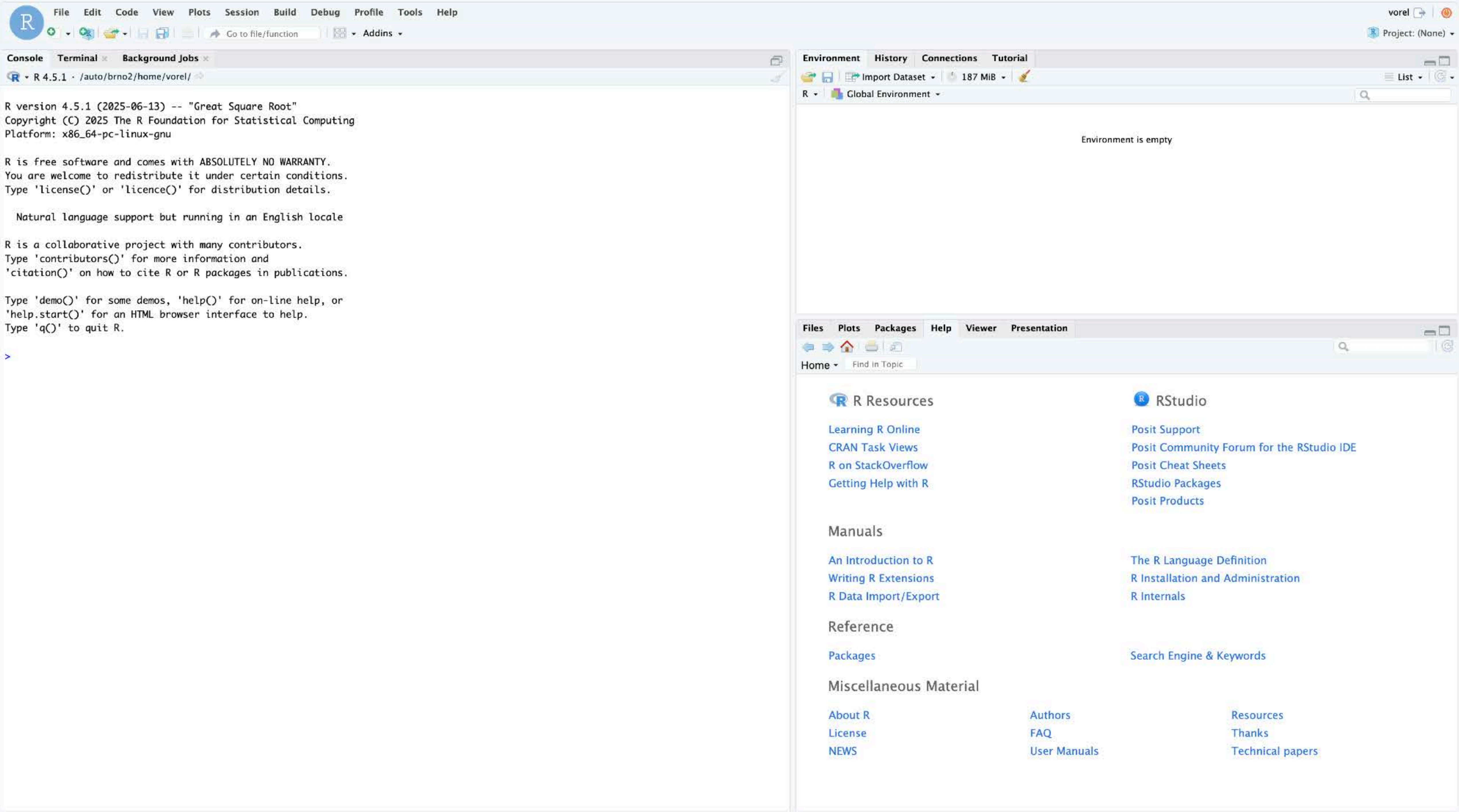
RStudio Image version

RStudio-geospatial-4.5.1

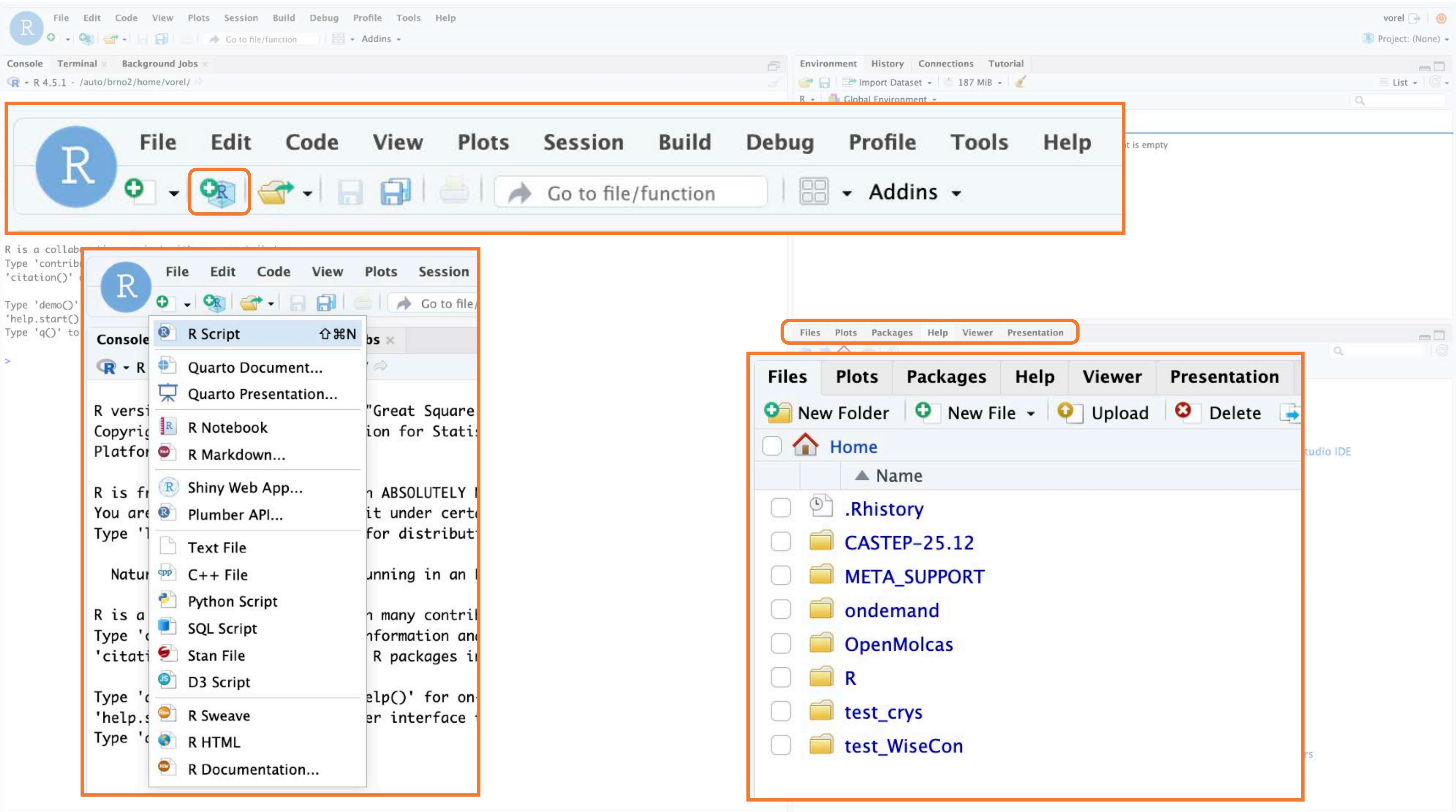
RStudio working directory location:

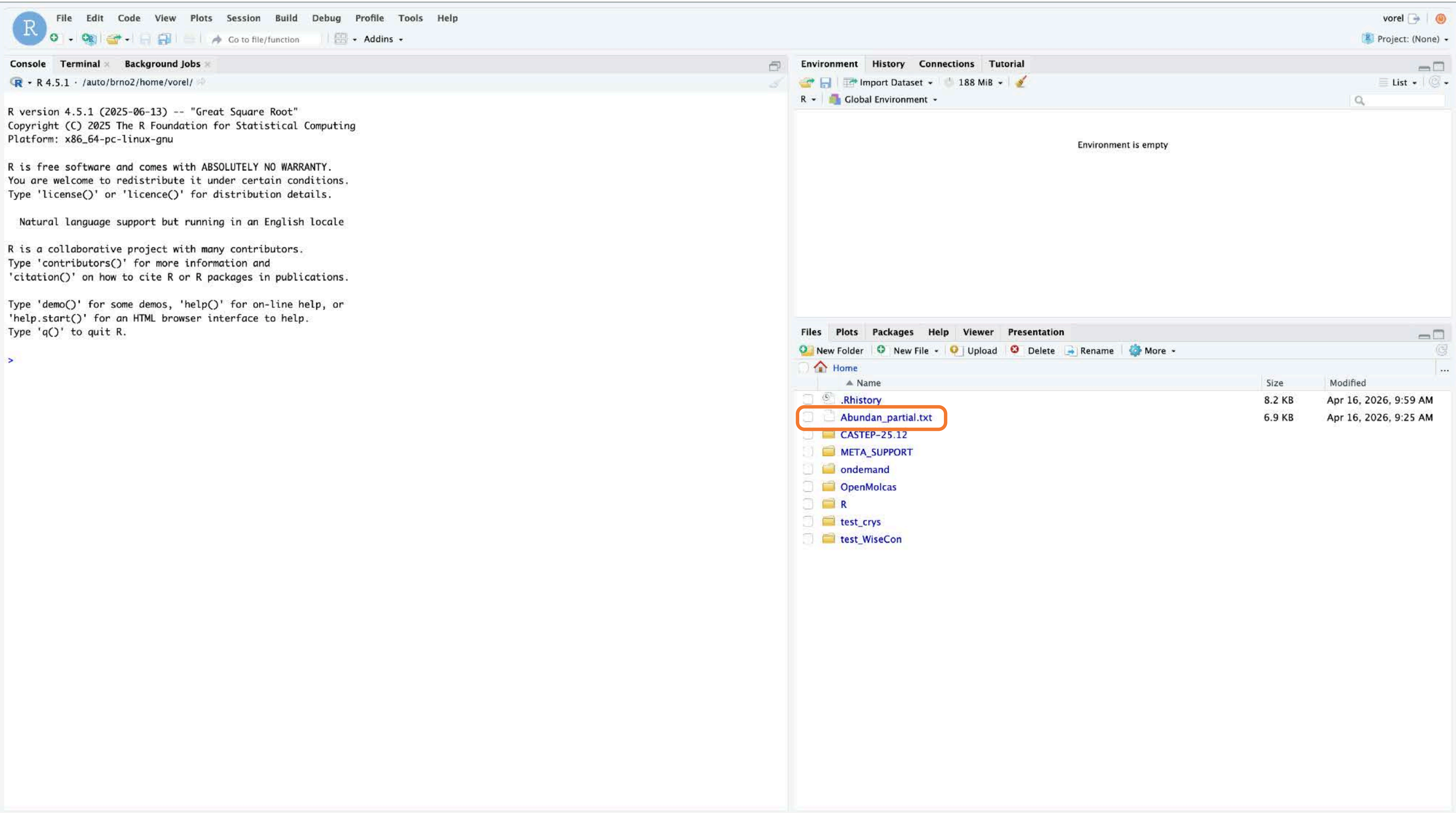
/storage/brno2

* The RStudio Server session data for this session can be accessed under the data root directory.



```
R version 4.5.1 (2025-06-13) -- "Great Square Root"
Copyright (C) 2025 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu

R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

  Natural language support but running in an English locale

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

>
```


File
Edit
Code
View
Plots
Session
Build
Debug
Profile
Tools
Help
Go to file/function
Addins
vorel
Project: (None)
Console
Terminal
Background Jobs
R 4.5.1 · /auto/brno2/home/vorel/
Environment
History
Connections
Tutorial
Import Dataset
187 MiB
List
Global Environment
R Script ⇧⌘N
Quarto Document...
Quarto Presentation...
R Notebook
R Markdown...
Shiny Web App...
Plumber API...
Text File
C++ File
Python Script
SQL Script
Stan File
D3 Script
R Sweave
R HTML
R Documentation...
Files
Plots
Packages
Help
Viewer
Presentation
New Folder
New File
Upload
Delete
Home
Name
.Rhistory
CASTEP-25.12
META_SUPPORT
ondemand
OpenMolcas
R
test_crys
test_WiseCon



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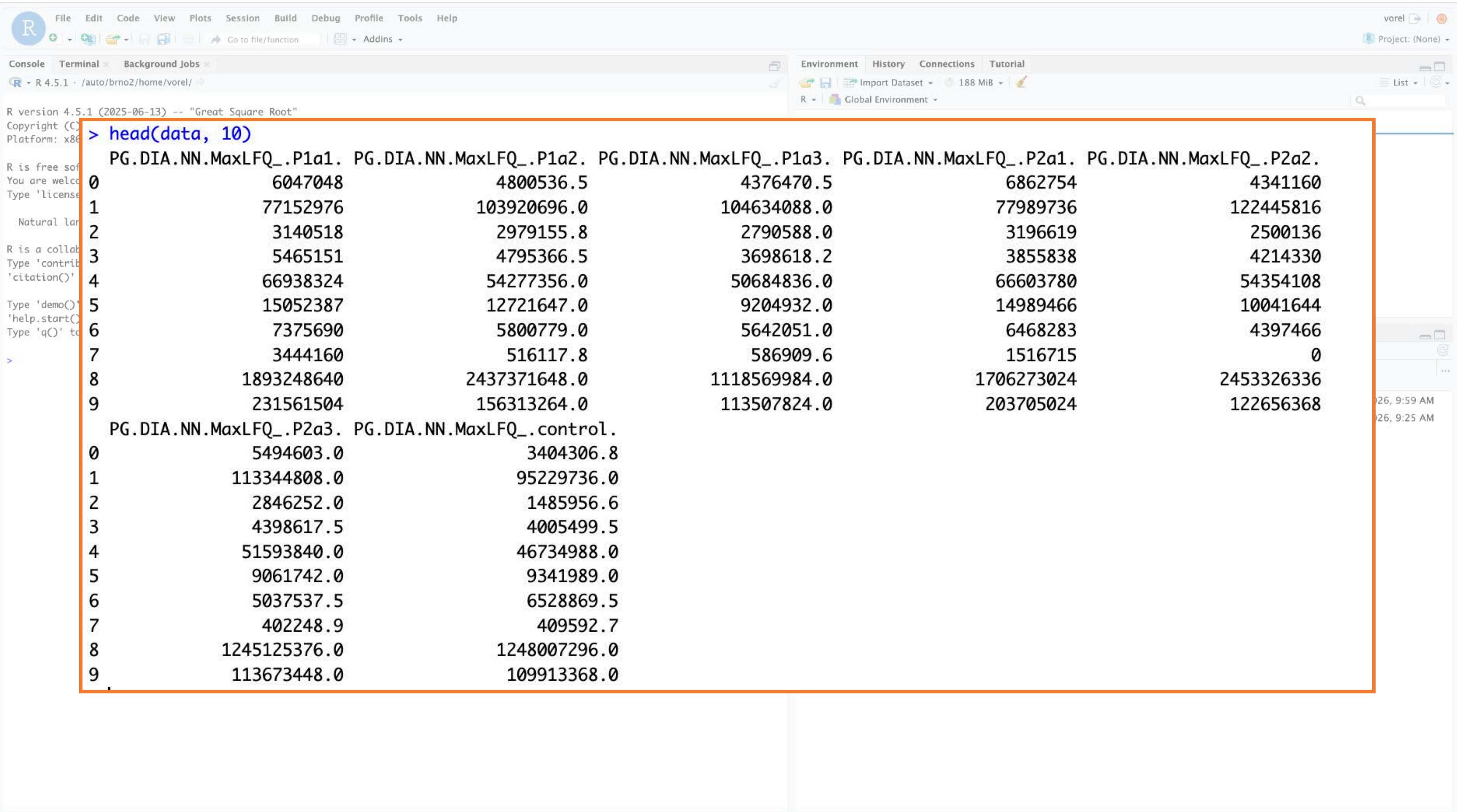
```

Name	Size	Modified
.Rhistory	8.2 KB	Apr 16, 2026, 9:59 AM
Abundan_partial.txt	6.9 KB	Apr 16, 2026, 9:25 AM
CASTEP-25.12		
META_SUPPORT		
ondemand		
OpenMolcas		
R		
test_crys		
test_WiseCon		



```
R version 4.5.1 (2025-06-13) -- "Great Square Root"
Copyright (C)
Platform: x86

R is free sof
You are welco
Type 'license

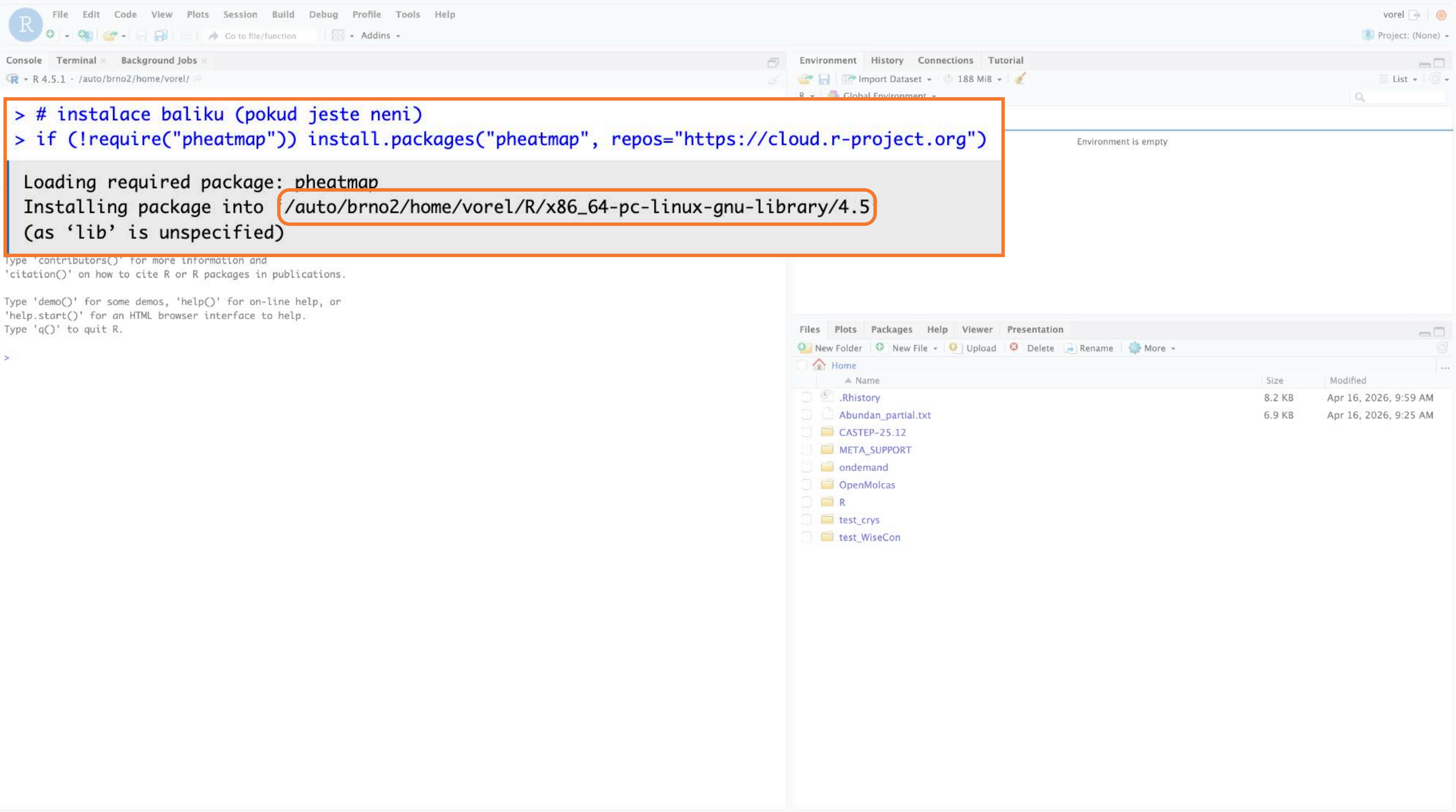
  Natural lar

R is a collab
Type 'contrib
'citation()'

Type 'demo()'
'help.start()
Type 'q()' to

>
```

```
> head(data, 10)
  PG.DIA.NN.MaxLFQ_.P1a1. PG.DIA.NN.MaxLFQ_.P1a2. PG.DIA.NN.MaxLFQ_.P1a3. PG.DIA.NN.MaxLFQ_.P2a1. PG.DIA.NN.MaxLFQ_.P2a2.
0                 6047048               4800536.5               4376470.5                 6862754                 4341160
1                77152976             103920696.0             104634088.0                77989736               122445816
2                 3140518               2979155.8               2790588.0                 3196619                 2500136
3                 5465151               4795366.5               3698618.2                 3855838                 4214330
4                66938324              54277356.0              50684836.0                66603780                54354108
5                15052387              12721647.0               9204932.0                14989466                10041644
6                 7375690               5800779.0               5642051.0                 6468283                 4397466
7                 3444160                516117.8                586909.6                 1516715                       0
8              1893248640            2437371648.0            1118569984.0              1706273024              2453326336
9               231561504             156313264.0             113507824.0               203705024               122656368
  PG.DIA.NN.MaxLFQ_.P2a3. PG.DIA.NN.MaxLFQ_.control.
0               5494603.0                  3404306.8
1             113344808.0                 95229736.0
2               2846252.0                  1485956.6
3               4398617.5                  4005499.5
4              51593840.0                 46734988.0
5               9061742.0                  9341989.0
6               5037537.5                  6528869.5
7                402248.9                   409592.7
8            1245125376.0               1248007296.0
9             113673448.0                109913368.0
```



```
> # instalace baliku (pokud jeste neni)
> if (!require("pheatmap")) install.packages("pheatmap", repos="https://cloud.r-project.org")

 Loading required package: pheatmap
 Installing package into /auto/brno2/home/vorel/R/x86_64-pc-linux-gnu-library/4.5
 (as ‘lib’ is unspecified)
```

```
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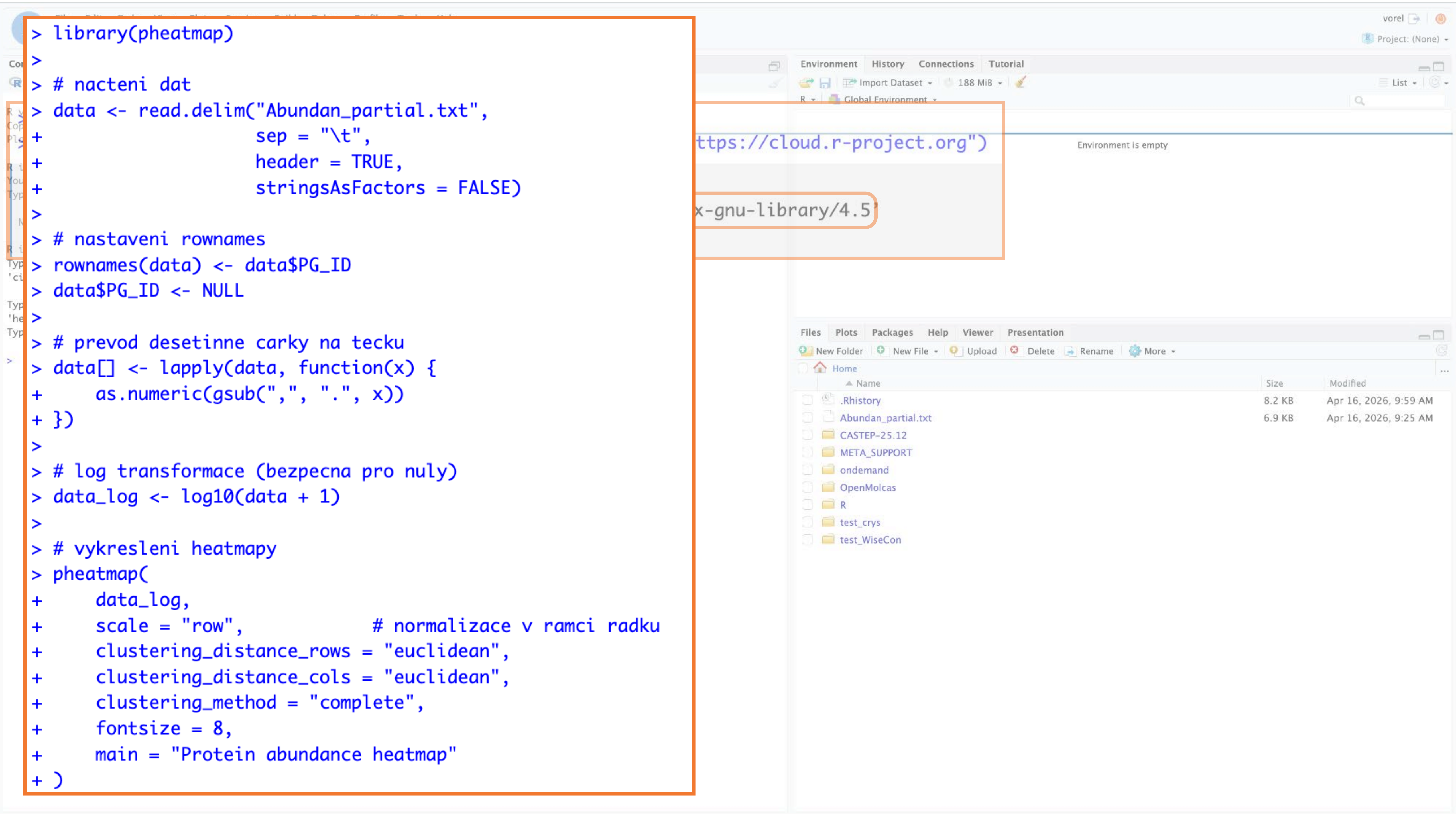

```
> library(pheatmap)
>
> # nacteni dat
> data <- read.delim("Abundan_partial.txt",
+                    sep = "\t",
+                    header = TRUE,
+                    stringsAsFactors = FALSE)
>
> # nastaveni rownames
> rownames(data) <- data$PG_ID
> data$PG_ID <- NULL
>
> # prevod desetinne carky na tecku
> data[] <- lapply(data, function(x) {
+     as.numeric(gsub(",", ".", x))
+ })
>
> # log transformace (bezpecna pro nuly)
> data_log <- log10(data + 1)
>
> # vykresleni heatmapy
> pheatmap(
+     data_log,
+     scale = "row",              # normalizace v ramci radku
+     clustering_distance_rows = "euclidean",
+     clustering_distance_cols = "euclidean",
+     clustering_method = "complete",
+     fontsize = 8,
+     main = "Protein abundance heatmap"
+ )
```

```
ttps://cloud.r-project.org")
x-gnu-library/4.5'
```

Environment is empty

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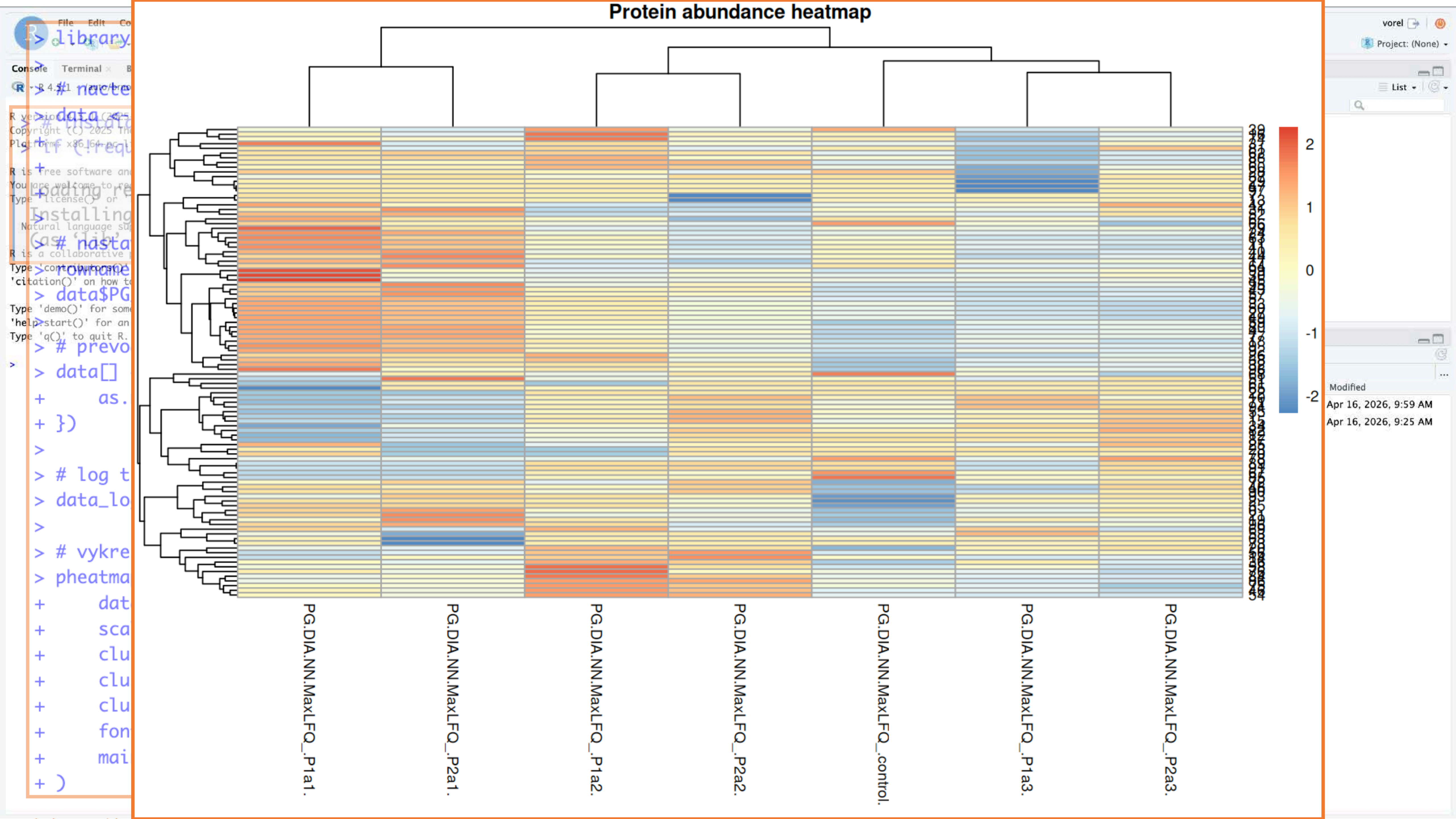
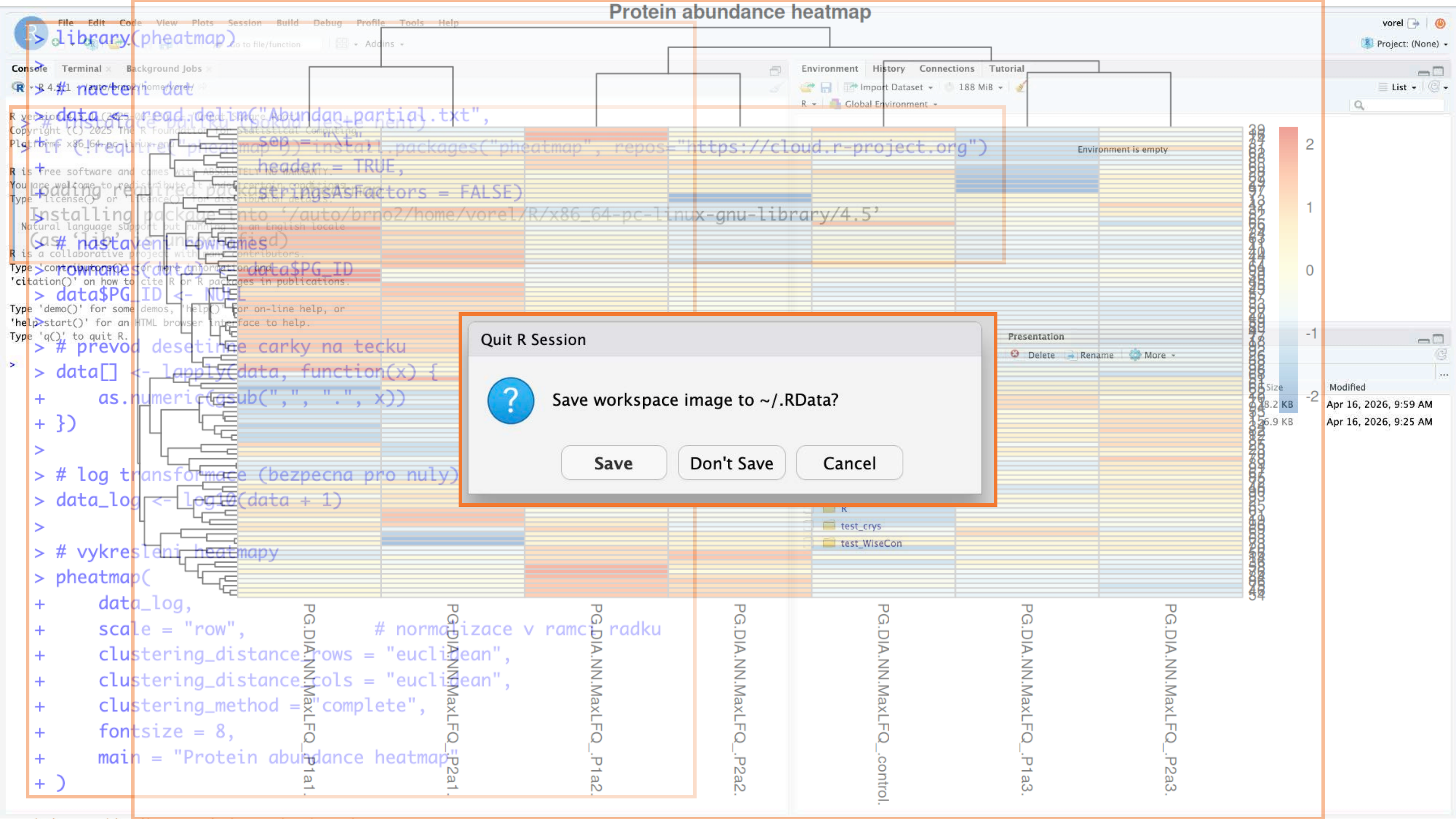


```
> library
>
> # nacte
> data
> # nasta
> if (!requ
+
+
Loading re
Installing
(as 'lib'
> # nasta
> rowname
> data$PG
>
> # prevo
> data[]
+     as.
+ })
>
> # log t
> data_lo
>
> # vykre
> pheatma
+     dat
+     sca
+     clu
+     clu
+     clu
+     fon
+     mai
+ )
```



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Quit R Session

Save workspace image to ~/.RData?

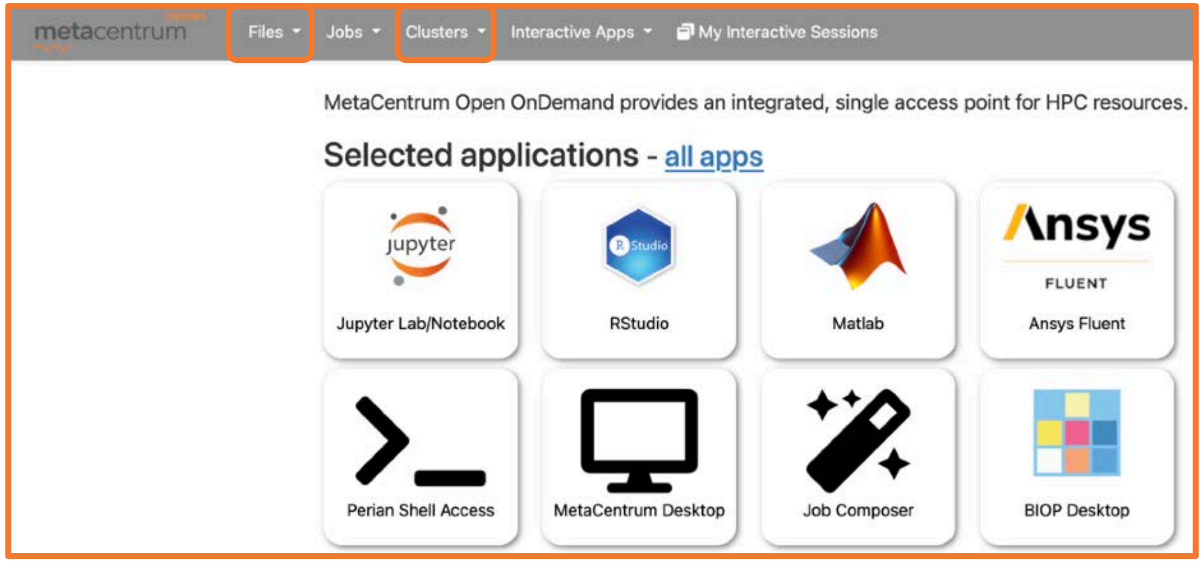
Save | Don't Save | Cancel

Open OnDemand

- Open OnDemand

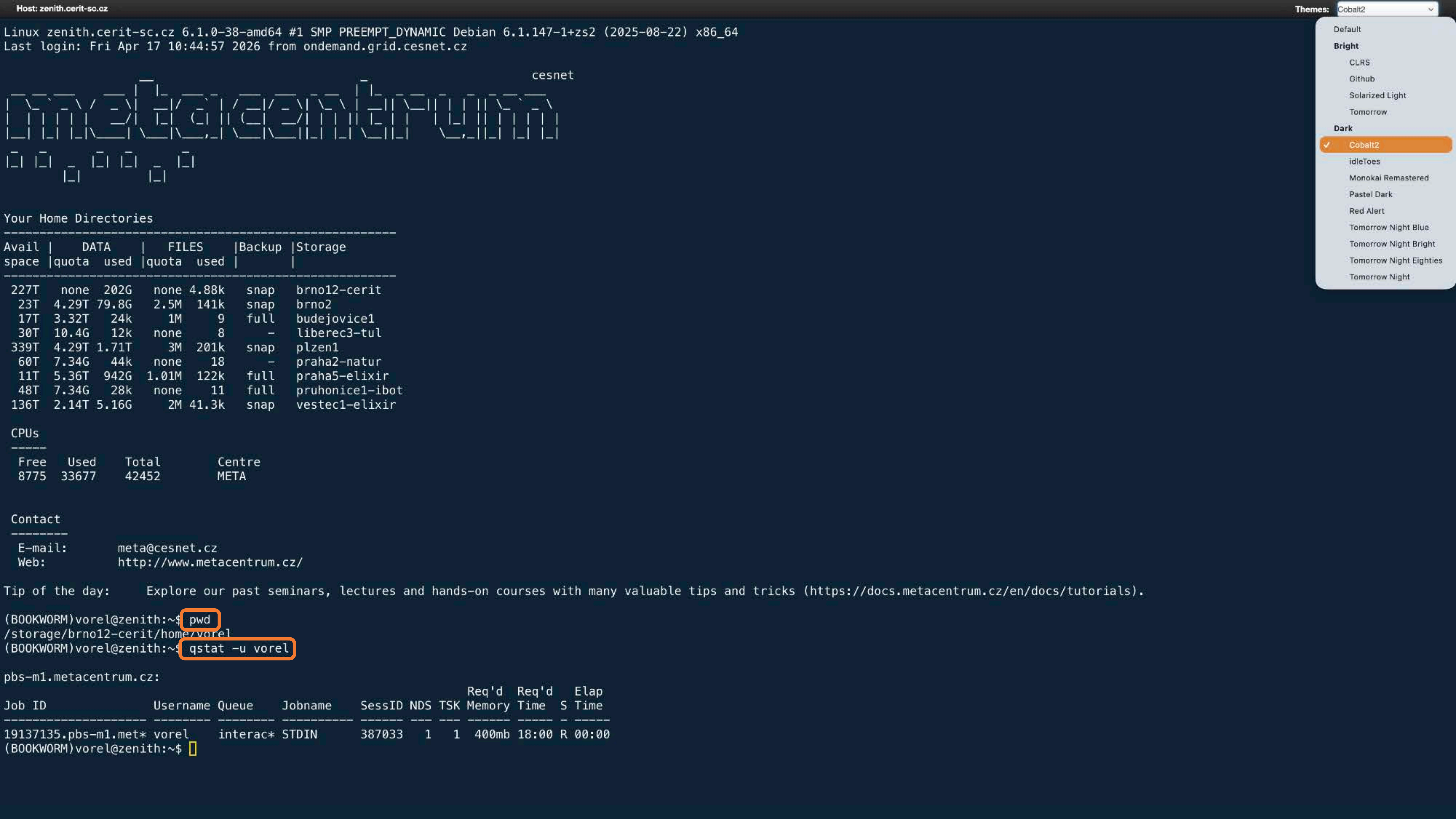
  https://ondemand.metacentrum.cz/

  - Web application on top of OpenPBS scheduler
  - Running (not only) GUI applications
  - Browsing storages (tab 'Files')
  - Launch a virtual desktop (MetaCentrum Desktop app)
  - Create (write) and submit a batch job
  - Command line (tab 'Clusters')



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

Selected applications - all apps



Host: zenith.cerit-sc.cz

Themes: Cobalt2

```
Linux zenith.cerit-sc.cz 6.1.0-38-amd64 #1 SMP PREEMPT_DYNAMIC Debian 6.1.147-1+zs2 (2025-08-22) x86_64
Last login: Fri Apr 17 10:44:57 2026 from ondemand.grid.cesnet.cz

                    __                            _                       cesnet
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|_|  |_|  _   |_| |_|  _   |_|
         |_|          |_|


Your Home Directories
-------------------------------------------------------
Avail |    DATA     |    FILES    |Backup |Storage
space |quota  used |quota  used |       |
-------------------------------------------------------
 227T   none  202G   none 4.88k   snap   brno12-cerit
  23T  4.29T 79.8G   2.5M  141k   snap   brno2
  17T  3.32T   24k     1M     9   full   budejovice1
  30T  10.4G   12k   none     8      -   liberec3-tul
 339T  4.29T 1.71T     3M  201k   snap   plzen1
  60T  7.34G   44k   none    18      -   praha2-natur
  11T  5.36T  942G  1.01M  122k   full   praha5-elixir
  48T  7.34G   28k   none    11   full   pruhonice1-ibot
 136T  2.14T 5.16G     2M 41.3k   snap   vestec1-elixir

 CPUs
 -----
  Free   Used    Total        Centre
  8775   33677   42452        META


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

Tip of the day:     Explore our past seminars, lectures and hands-on courses with many valuable tips and tricks (https://docs.metacentrum.cz/en/docs/tutorials).

(BOOKWORM)vorel@zenith:~$ pwd
/storage/brno12-cerit/home/vorel
(BOOKWORM)vorel@zenith:~$ qstat -u vorel

pbs-m1.metacentrum.cz:
                                                            Req'd  Req'd   Elap
Job ID               Username Queue    Jobname    SessID NDS TSK Memory Time  S Time
-------------------- -------- -------- ---------- ------ --- --- ------ ----- - -----
19137135.pbs-m1.met* vorel    interac* STDIN      387033   1   1  400mb 18:00 R 00:00
(BOOKWORM)vorel@zenith:~$
```
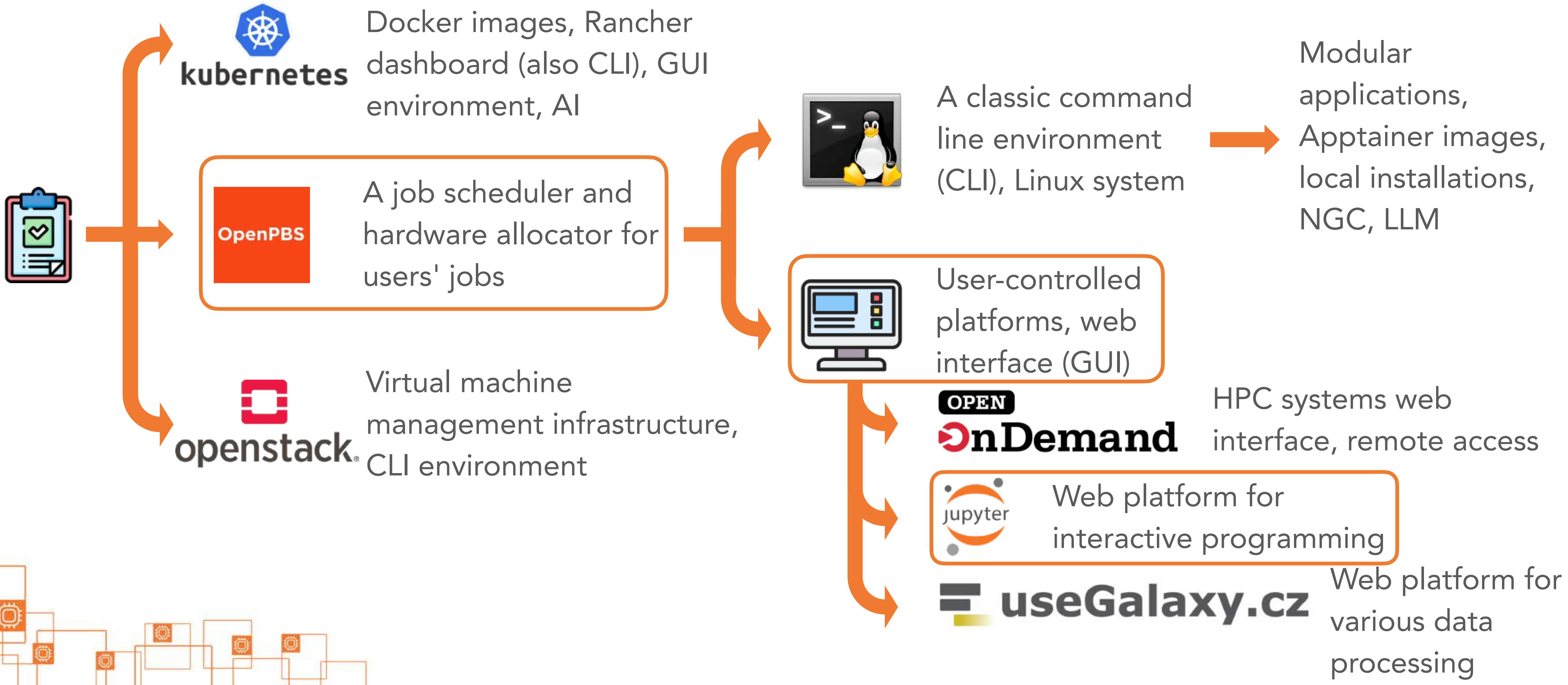

How to use it

https://docs.metacentrum.cz/en/docs/welcome



Kubernetes orchestrator of Docker images, Rancher dashboard (also CLI), GUI environment, AI

A job scheduler and hardware allocator for users' jobs

Virtual machine management infrastructure, CLI environment

A classic command line environment (CLI), Linux system

Modular applications, Apptainer images, local installations, NGC, LLM

User-controlled platforms, web interface (GUI)

HPC systems web interface, remote access

Web platform for interactive programming

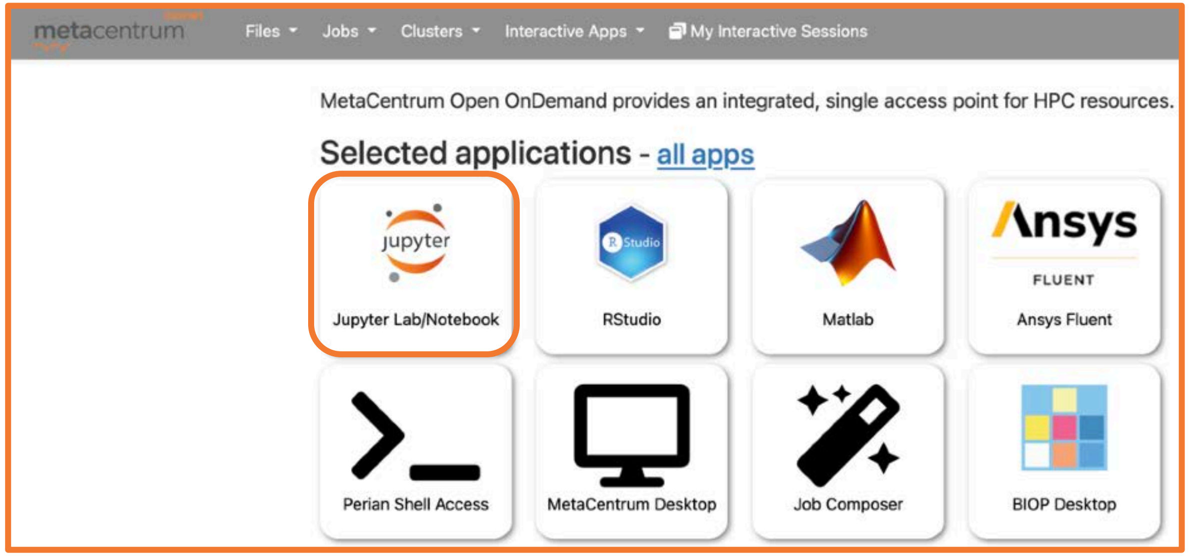
Web platform for various data processing

Jupyter Notebook in Open OnDemand

- Jupyter Notebook

  https://ondemand.metacentrum.cz/

  - Web-based interactive environment mixing code, text, and visuals
  - Excellent for step-by-step data analysis, machine learning, and prototyping
  - Supports many languages (Python, R, Julia)
  - Embeds plots, widgets, and equations directly
  - Promotes reproducible, shareable work via version control and exports
  - Also accessible in the Kubernetes service (with Claude Code)



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

Selected applications - all apps

https://docs.cerit.io/en/docs/web-apps/jupyterhub

Jupyt

- Jupyter Notebook

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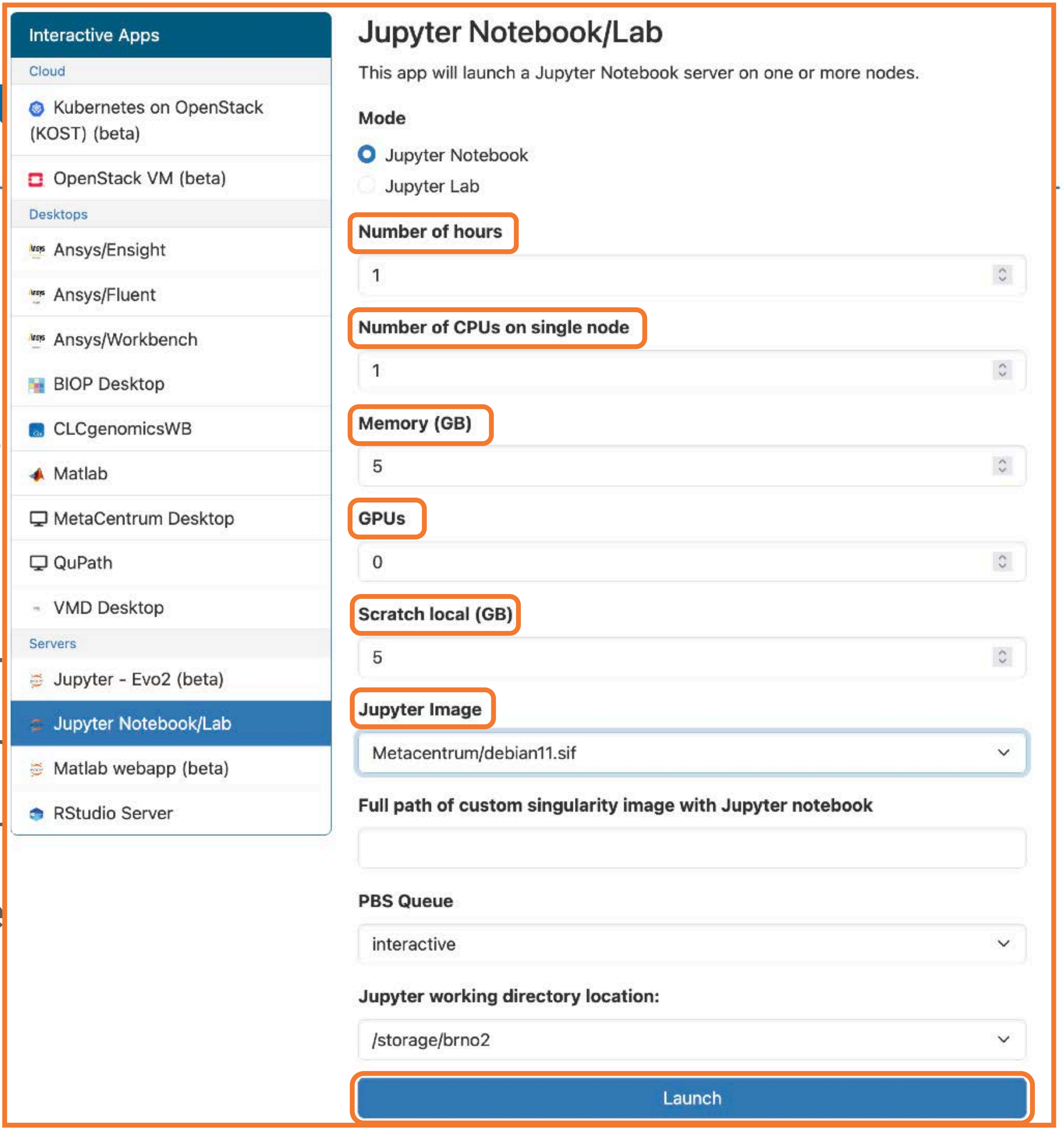


Jupyter Notebook/Lab

This app will launch a Jupyter Notebook server on one or more nodes.

Mode

● Jupyter Notebook
○ Jupyter Lab

Number of hours: 1

Number of CPUs on single node: 1

Memory (GB): 5

GPUs: 0

Scratch local (GB): 5

Jupyter Image: Metacentrum/debian11.sif

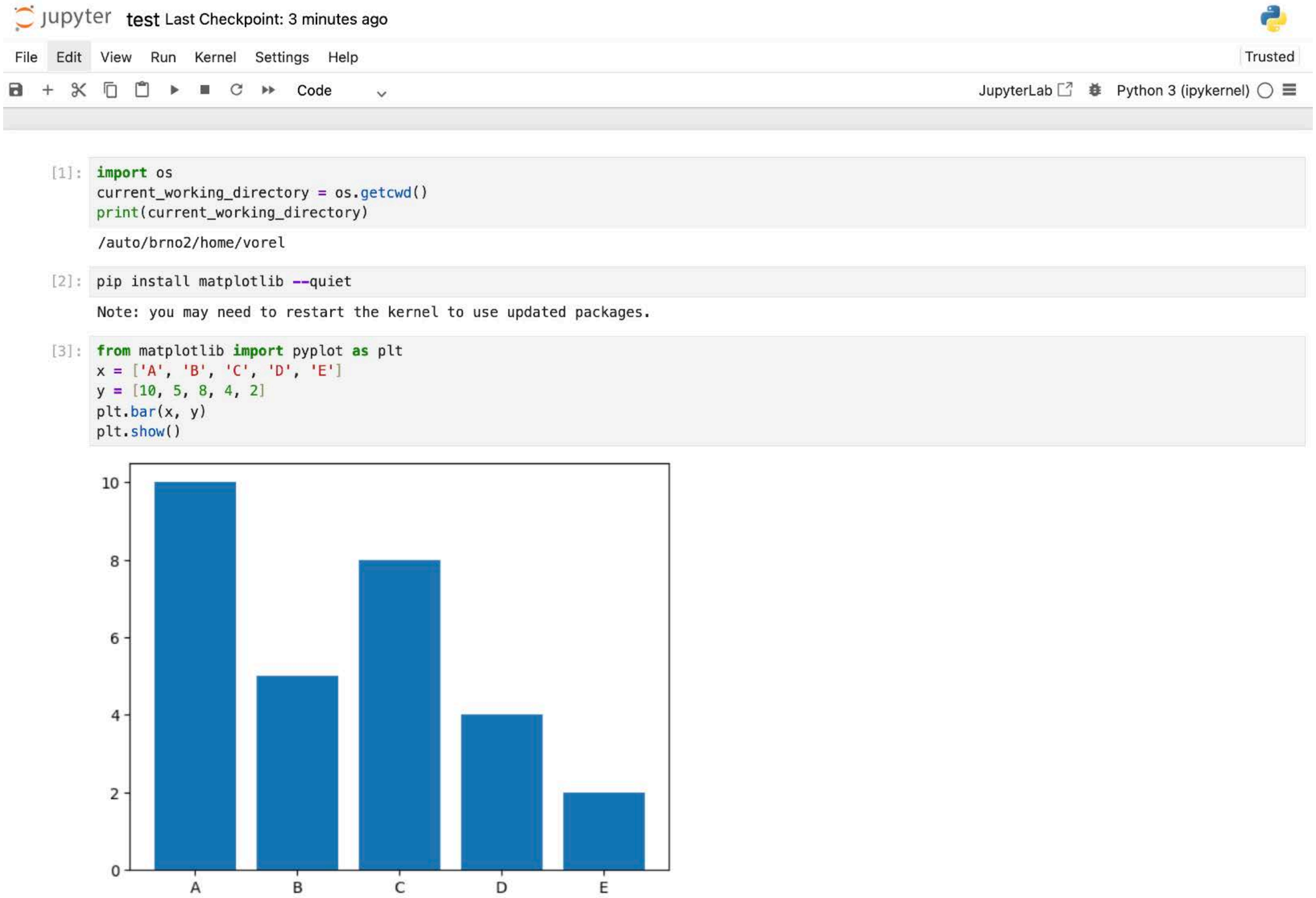
Full path of custom singularity image with Jupyter notebook:

PBS Queue: interactive

Jupyter working directory location:: /storage/brno2

Select items to perform actions on them.

Name		
CASTEP-25.12		
META_SUPPORT		
ondemand		
OpenMolcas		
test_crys		
Untitled.ipynb	před hodinou	4.98 kB



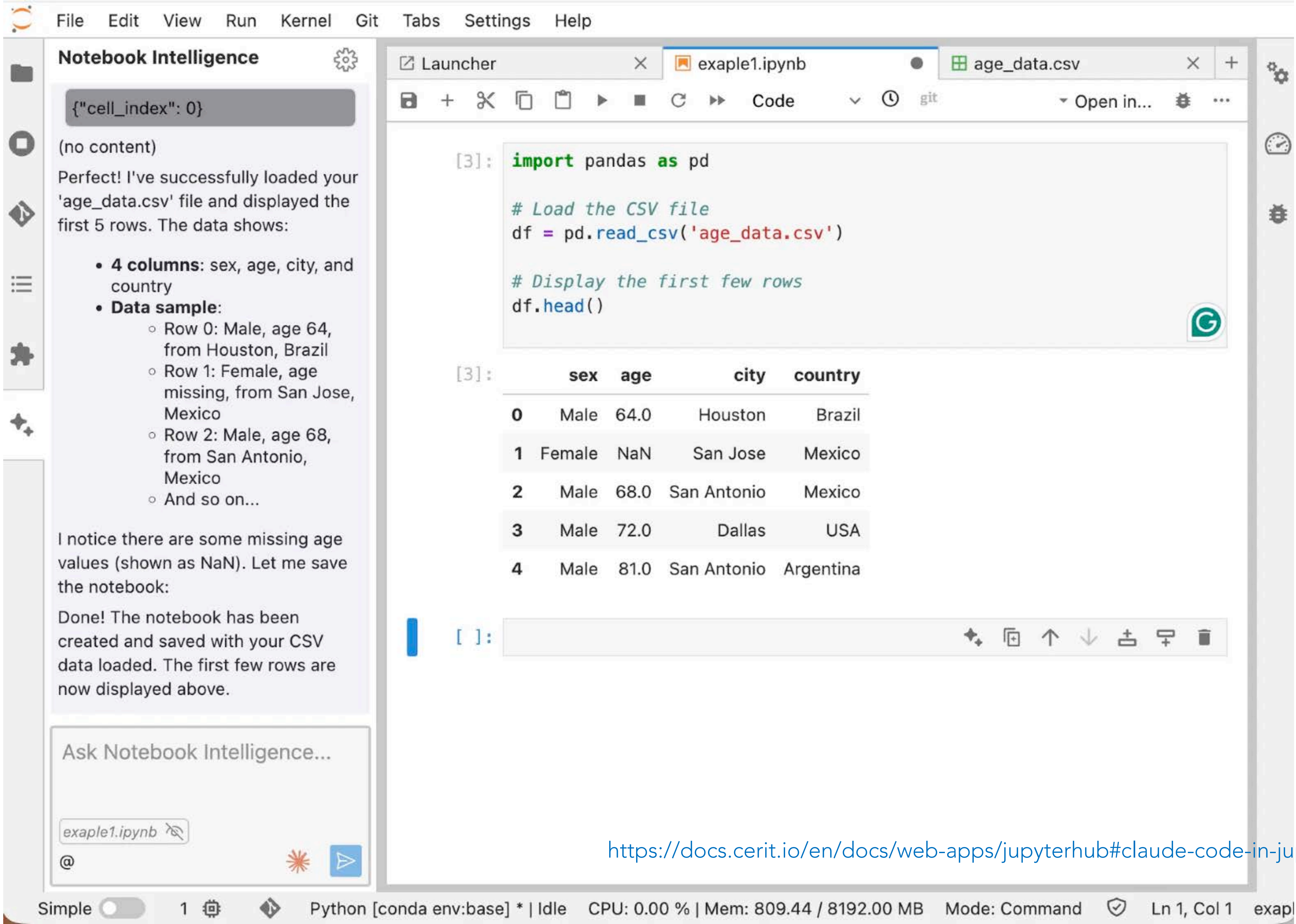
```
import os
current_working_directory = os.getcwd()
print(current_working_directory)
```

```
/auto/brno2/home/vorel
```

```
pip install matplotlib --quiet
```

```
Note: you may need to restart the kernel to use updated packages.
```

```
from matplotlib import pyplot as plt
x = ['A', 'B', 'C', 'D', 'E']
y = [10, 5, 8, 4, 2]
plt.bar(x, y)
plt.show()
```



{"cell_index": 0}

(no content)

Perfect! I've successfully loaded your 'age_data.csv' file and displayed the first 5 rows. The data shows:

- **4 columns**: sex, age, city, and country
- **Data sample**:
  - Row 0: Male, age 64, from Houston, Brazil
  - Row 1: Female, age missing, from San Jose, Mexico
  - Row 2: Male, age 68, from San Antonio, Mexico
  - And so on...

I notice there are some missing age values (shown as NaN). Let me save the notebook:

Done! The notebook has been created and saved with your CSV data loaded. The first few rows are now displayed above.

[3]:

```python
import pandas as pd

# Load the CSV file
df = pd.read_csv('age_data.csv')

# Display the first few rows
df.head()
```

[3]:

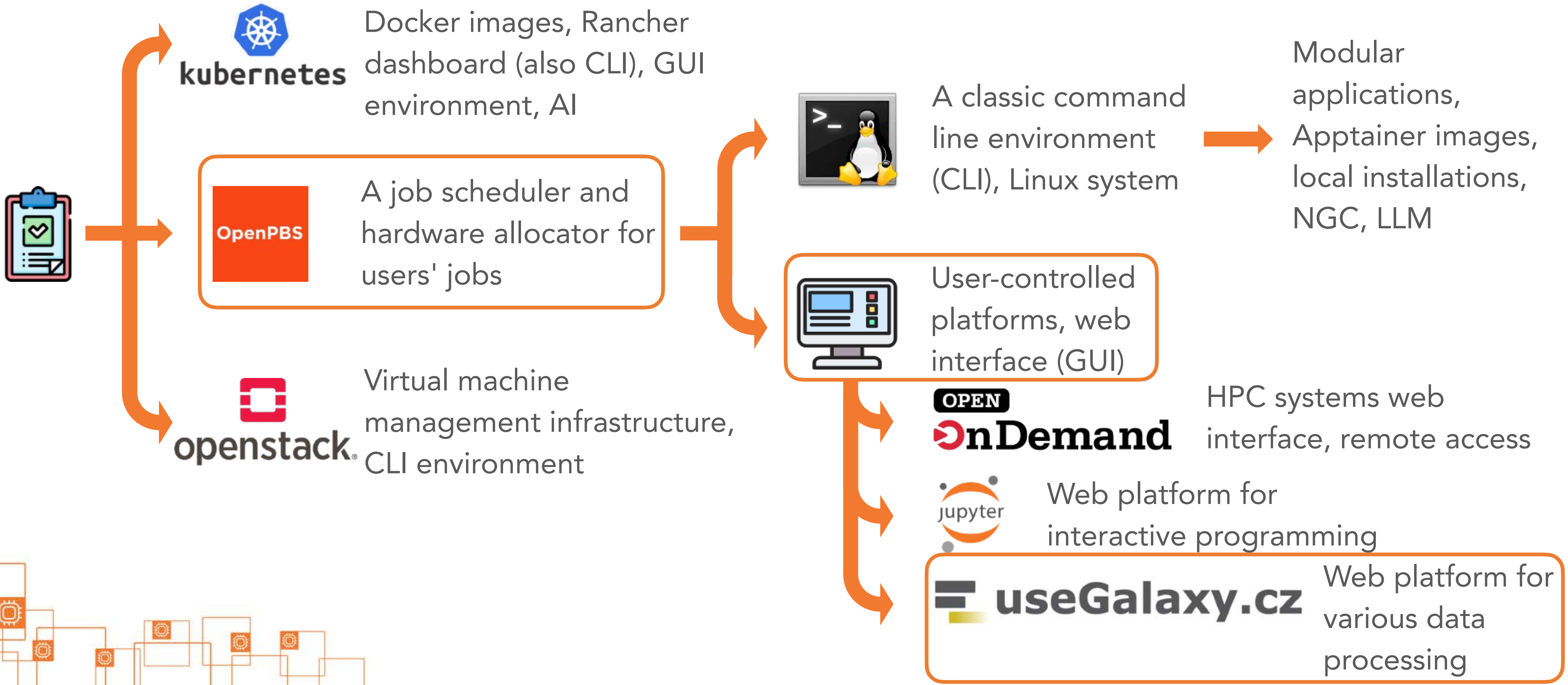
	sex	age	city	country
0	Male	64.0	Houston	Brazil
1	Female	NaN	San Jose	Mexico
2	Male	68.0	San Antonio	Mexico
3	Male	72.0	Dallas	USA
4	Male	81.0	San Antonio	Argentina

[ ]:

https://docs.cerit.io/en/docs/web-apps/jupyterhub#claude-code-in-jupyter-notebook

How to use it

https://docs.metacentrum.cz/en/docs/welcome



kubernetes Kubernetes orchestrator of Docker images, Rancher dashboard (also CLI), GUI environment, AI

OpenPBS A job scheduler and hardware allocator for users' jobs

- A classic command line environment (CLI), Linux system → Modular applications, Apptainer images, local installations, NGC, LLM
- User-controlled platforms, web interface (GUI)
  - **OPEN OnDemand** HPC systems web interface, remote access
  - **jupyter** Web platform for interactive programming
  - **useGalaxy.cz** Web platform for various data processing

openstack Virtual machine management infrastructure, CLI environment

Galaxy

- Galaxy useGalaxy.cz

  https://usegalaxy.cz/

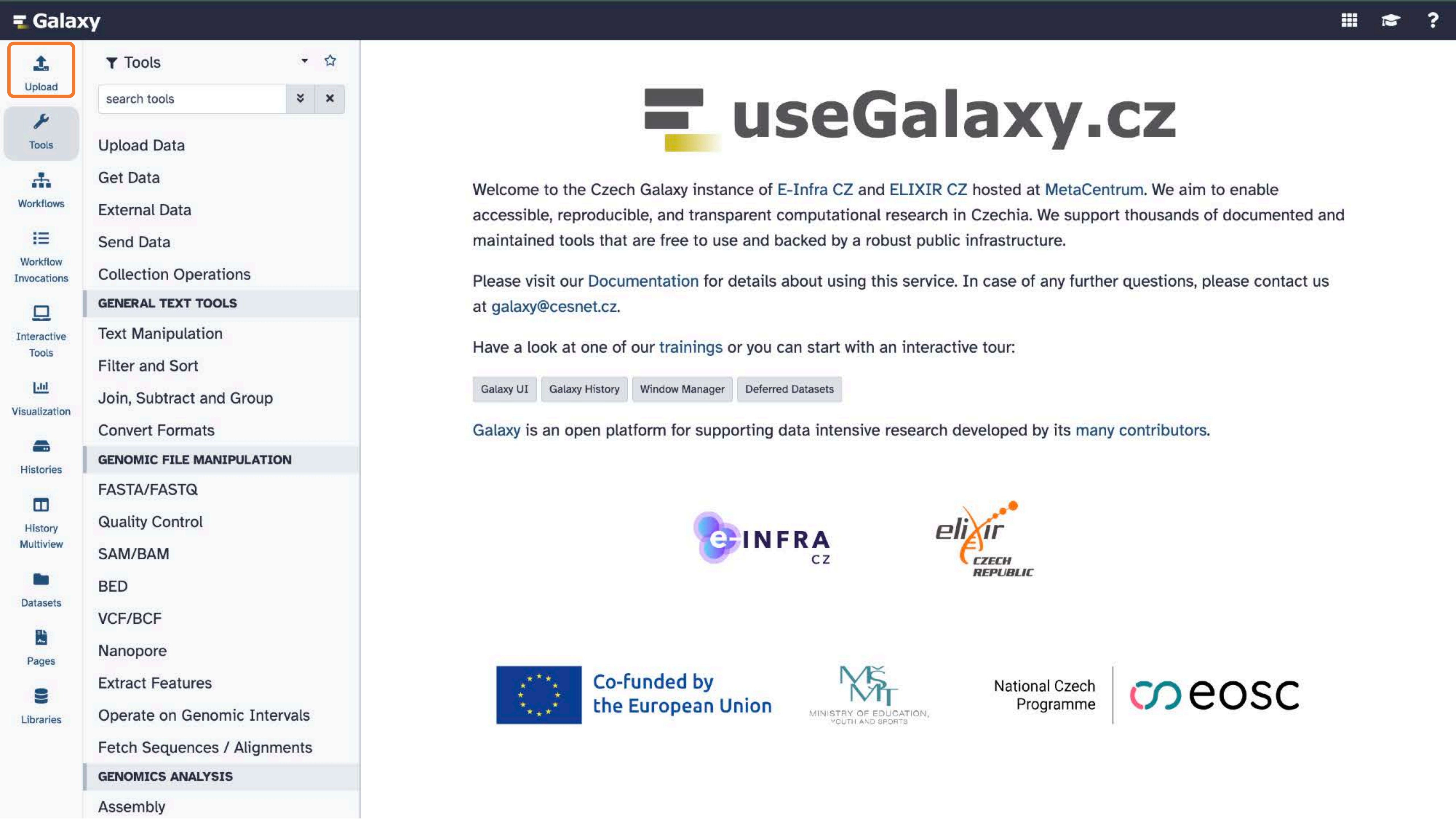
  - National instance hosted by MetaCentrum
  - Web application based on OpenPBS
  - A system for complex data analysis, workflow creation and sharing and teaching
  - Processing of '-omic' data, LLM, ML, material science, ecology, chemistry, statistical analysis and humanities studies, and more
  - Users do not need to worry about hardware reservation
  - No programming required

Welcome to the Czech Galaxy instance of E-Infra CZ and ELIXIR CZ hosted at MetaCentrum. We aim to enable accessible, reproducible, and transparent computational research in Czechia. We support thousands of documented and maintained tools that are free to use and backed by a robust public infrastructure.

Please visit our Documentation for details about using this service. In case of any further questions, please contact us at galaxy@cesnet.cz.

Have a look at one of our trainings or you can start with an interactive tour:

Galaxy is an open platform for supporting data intensive research developed by its many contributors.



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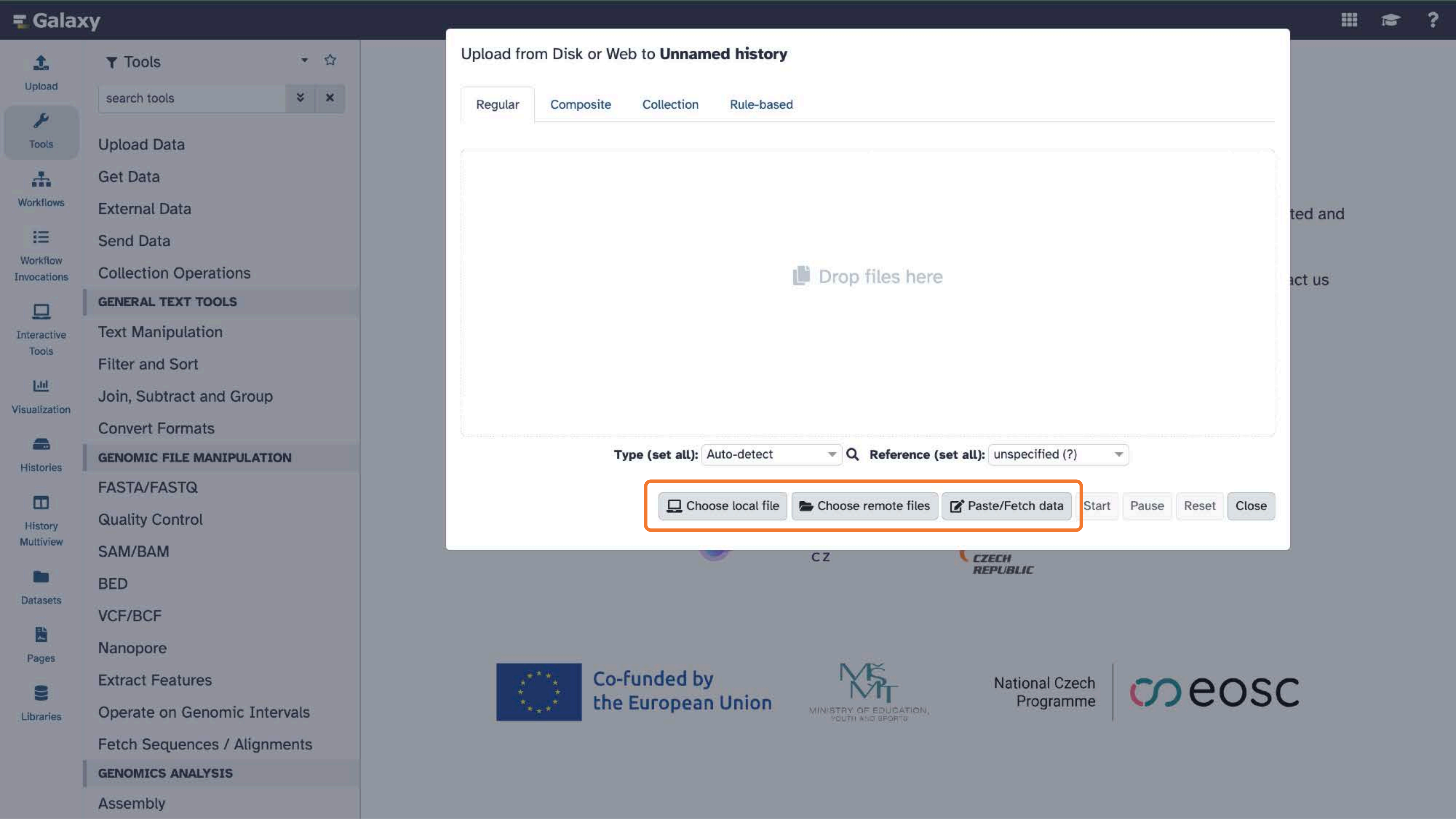


Upload from Disk or Web to **Unnamed history**

Drop files here

Type (set all): Auto-detect

Reference (set all): unspecified (?)

Upload from Disk or Web to **Unnamed history**

You added 1 file(s) to the queue. Add more files or click 'Start' to proceed.

New File 115 b Auto-detect unspecified (?) 0%

Download data from the web by entering URLs (one per line) or directly paste content.

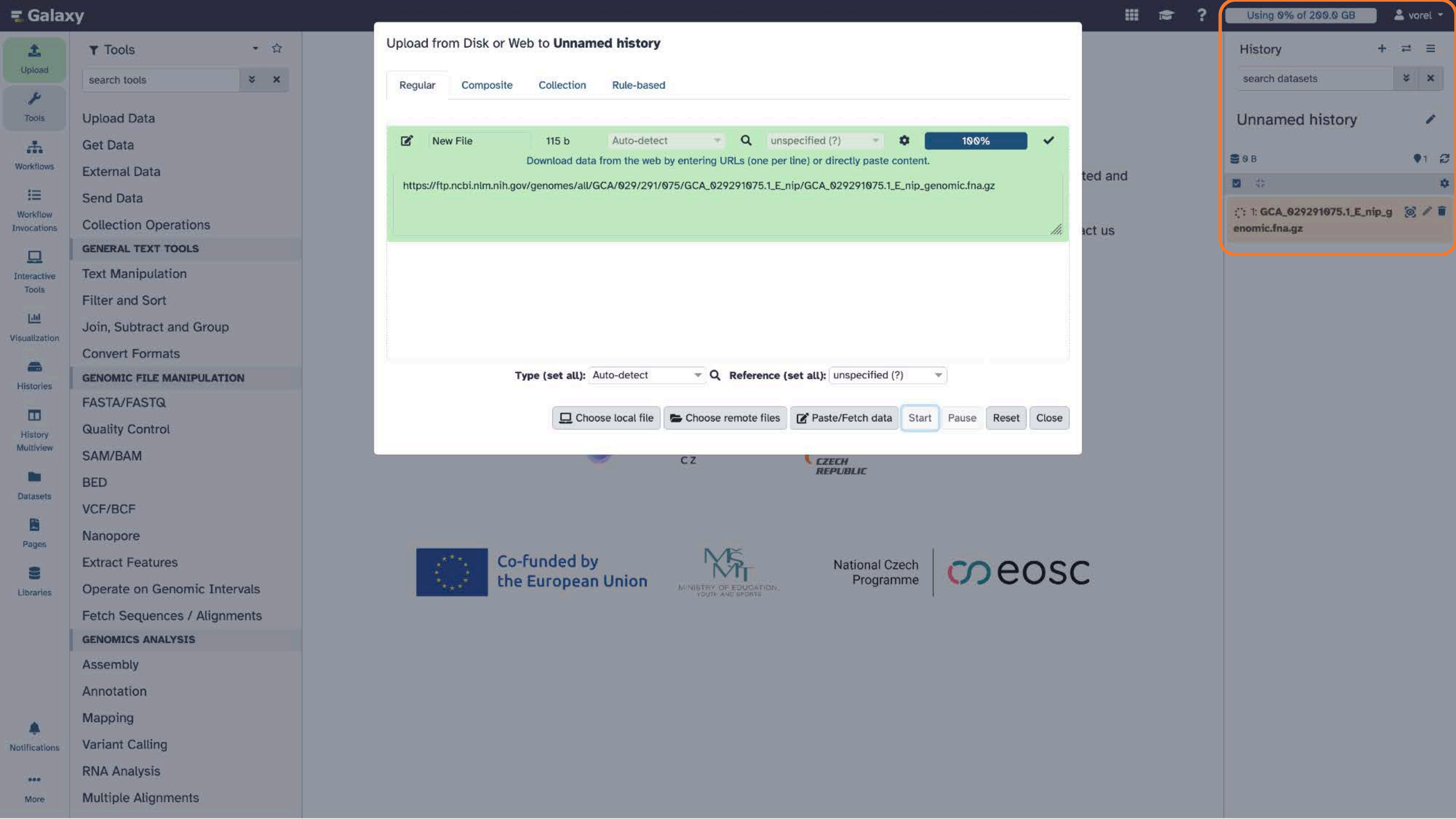
```
https://ftp.ncbi.nlm.nih.gov/genomes/all/GCA/029/291/075/GCA_029291075.1_E_nip/GCA_029291075.1_E_nip_genomic.fna.gz
```

Type (set all): Auto-detect **Reference (set all):** unspecified (?)

Unnamed history

This history is empty.

You can load your own data or get data from an external source.



Upload from Disk or Web to **Unnamed history**

New File | 115 b | Auto-detect | unspecified (?) | 100%

Download data from the web by entering URLs (one per line) or directly paste content.

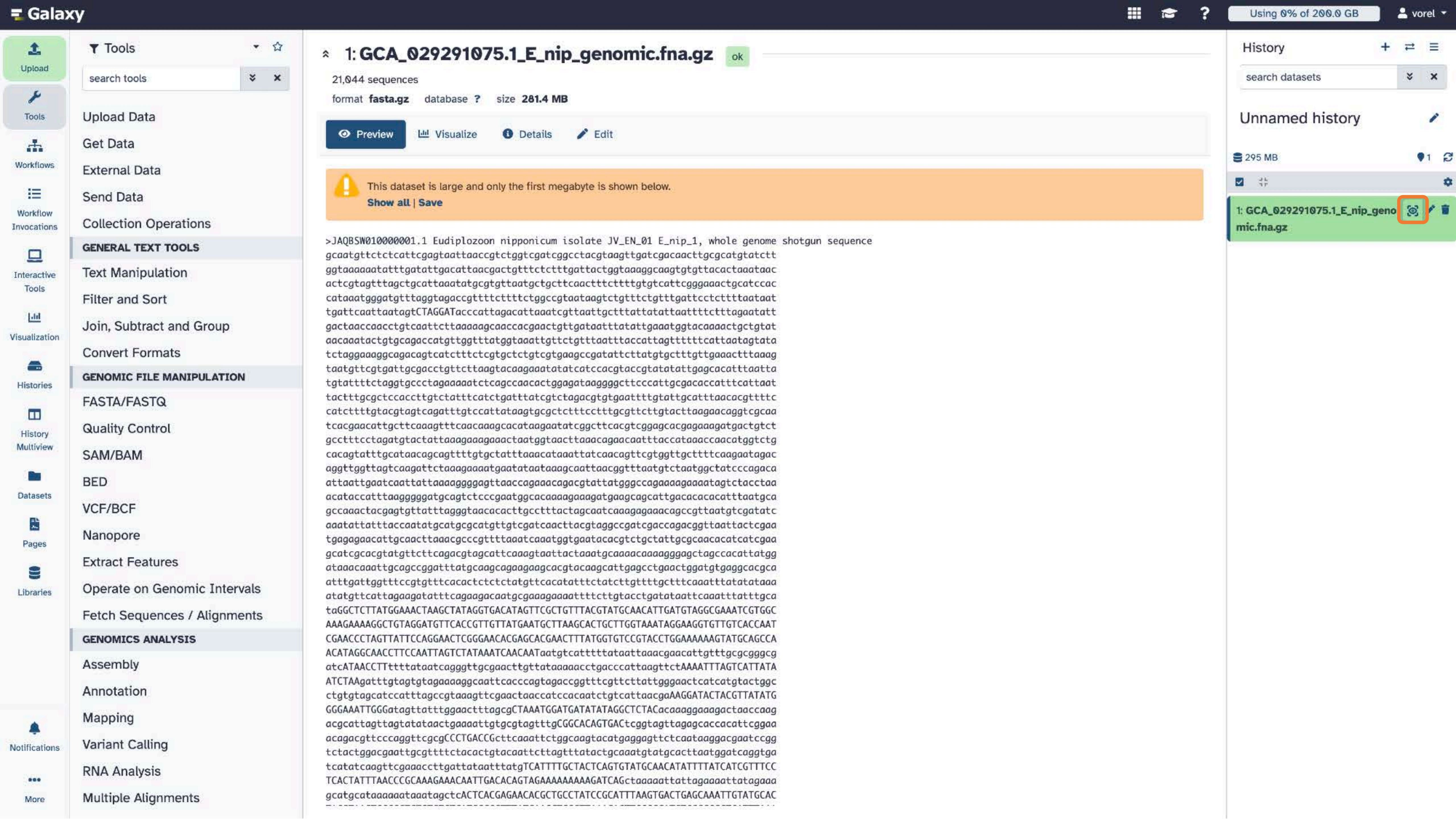
https://ftp.ncbi.nlm.nih.gov/genomes/all/GCA/029/291/075/GCA_029291075.1_E_nip/GCA_029291075.1_E_nip_genomic.fna.gz

Type (set all): Auto-detect **Reference (set all):** unspecified (?)

Unnamed history

0 B 1

1: GCA_029291075.1_E_nip_genomic.fna.gz



1: GCA_029291075.1_E_nip_genomic.fna.gz ok

21,044 sequences

format **fasta.gz** database ? size **281.4 MB**

This dataset is large and only the first megabyte is shown below.
Show all | **Save**

```
>JAQBSW010000001.1 Eudiplozoon nipponicum isolate JV_EN_01 E_nip_1, whole genome shotgun sequence
gcaatgttctctcattcgagtaattaaccgtctggtcgatcggcctacgtaagttgatcgacaacttgcgcatgtatctt
ggtaaaaaatatttgatattgacattaacgactgtttctctttgattactggtaaaggcaagtgtgttacactaaataac
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gactaaccaacctgtcaattcttaaaaagcaaccacgaactgttgataatttatattgaaatggtacaaaactgctgtat
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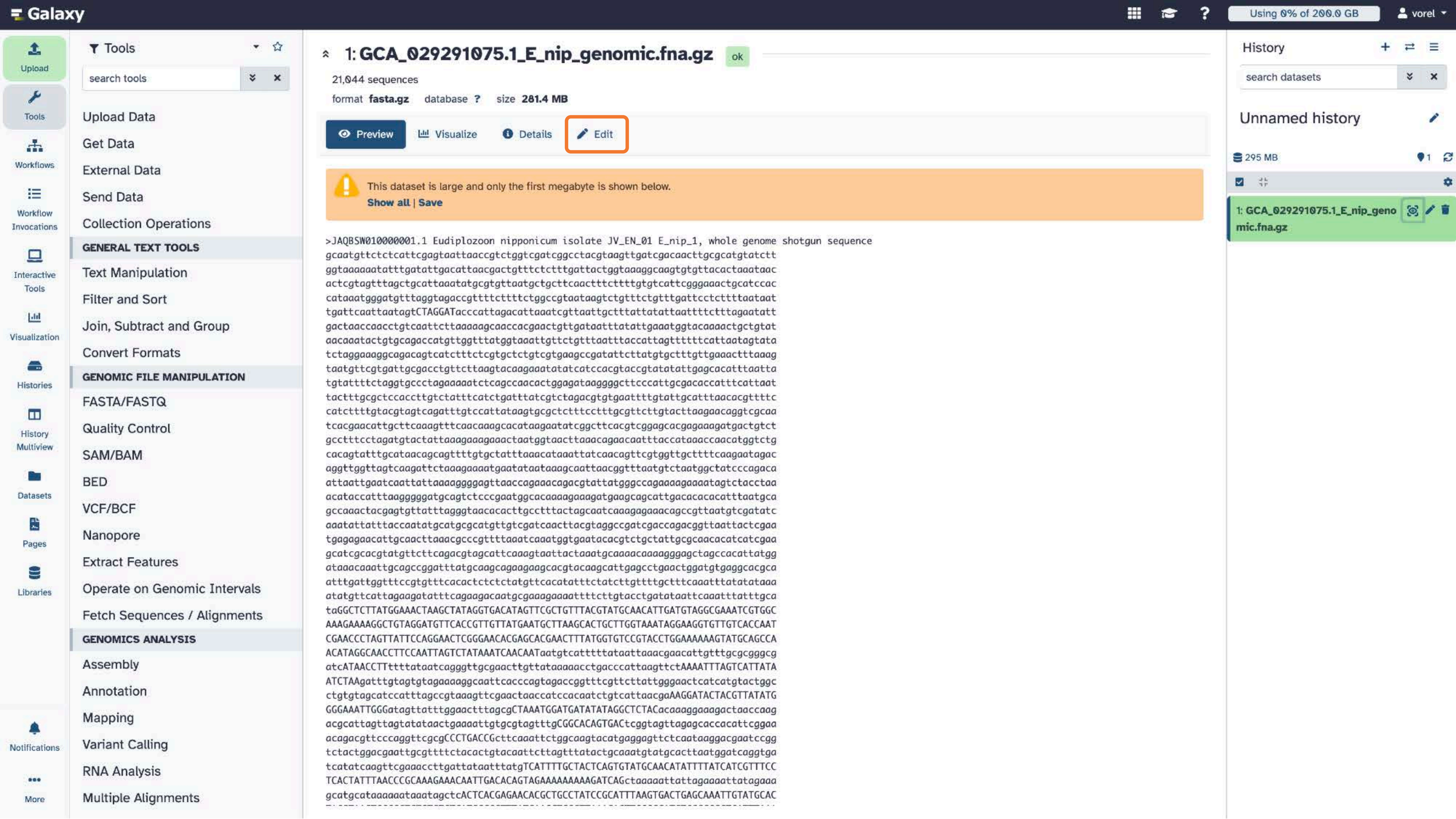
```



1: GCA_029291075.1_E_nip_genomic.fna.gz ok

21,044 sequences

format **fasta.gz** database **?** size **281.4 MB**

This dataset is large and only the first megabyte is shown below.
Show all | **Save**

```
>JAQBSW010000001.1 Eudiplozoon nipponicum isolate JV_EN_01 E_nip_1, whole genome shotgun sequence
gcaatgttctctcattcgagtaattaaccgtctggtcgatcggcctacgtaagttgatcgacaacttgcgcatgtatctt
ggtaaaaaatatttgatattgacattaacgactgtttctctttgattactggtaaaggcaagtgtgttacactaaataac
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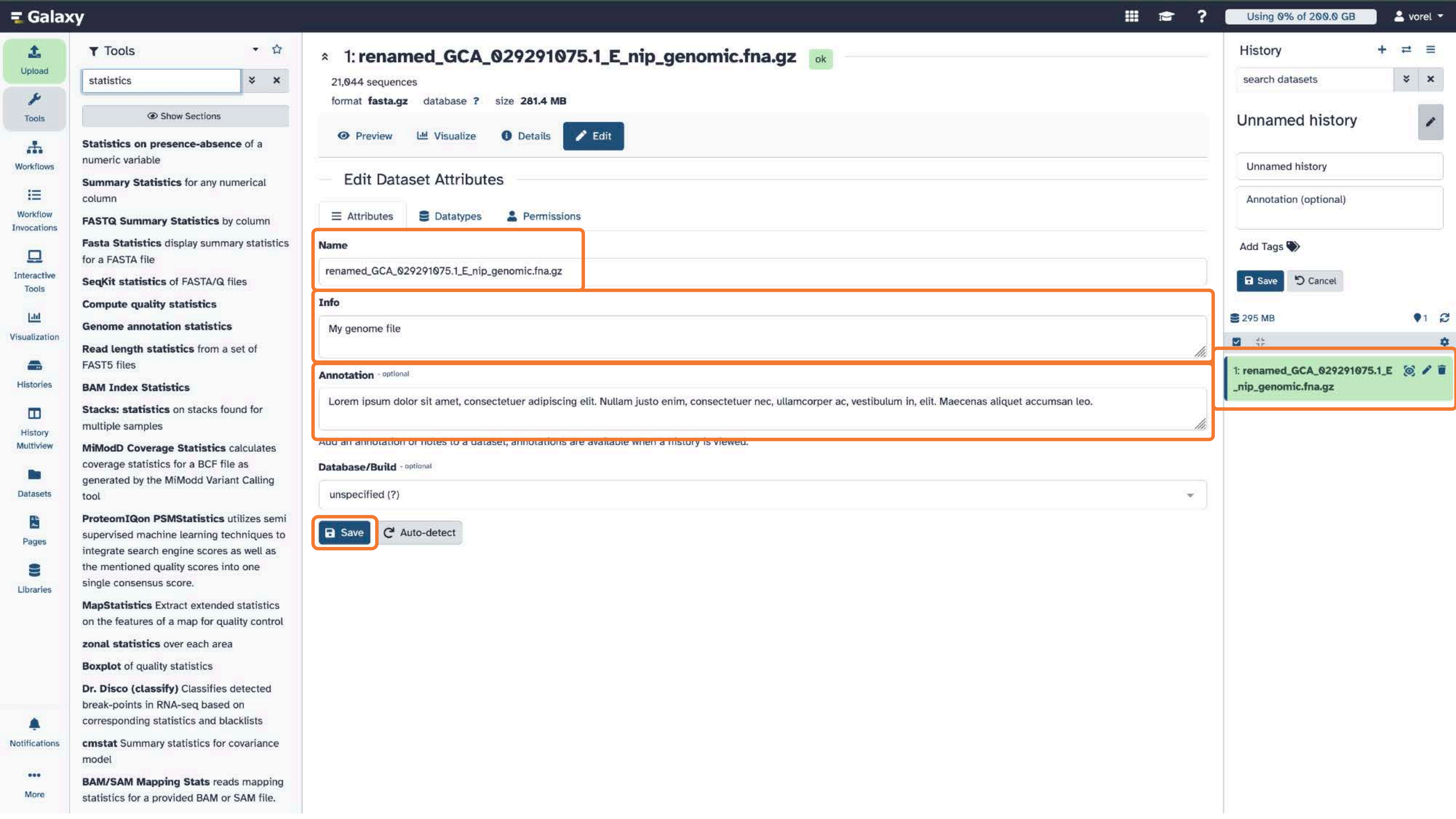


statistics

Statistics on presence-absence of a numeric variable

Summary Statistics for any numerical column

FASTQ Summary Statistics by column

Fasta Statistics display summary statistics for a FASTA file

SeqKit statistics of FASTA/Q files

Compute quality statistics

Genome annotation statistics

Read length statistics from a set of FAST5 files

BAM Index Statistics

Stacks: statistics on stacks found for multiple samples

MiModD Coverage Statistics calculates coverage statistics for a BCF file as generated by the MiModd Variant Calling tool

ProteomIQon PSMStatistics utilizes semi supervised machine learning techniques to integrate search engine scores as well as the mentioned quality scores into one single consensus score.

MapStatistics Extract extended statistics on the features of a map for quality control

zonal statistics over each area

Boxplot of quality statistics

Dr. Disco (classify) Classifies detected break-points in RNA-seq based on corresponding statistics and blacklists

cmstat Summary statistics for covariance model

BAM/SAM Mapping Stats reads mapping statistics for a provided BAM or SAM file.

1: renamed_GCA_029291075.1_E_nip_genomic.fna.gz ok

21,044 sequences

format **fasta.gz** database **?** size **281.4 MB**

Edit Dataset Attributes

Name

renamed_GCA_029291075.1_E_nip_genomic.fna.gz

Info

My genome file

Annotation - optional

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Nullam justo enim, consectetuer nec, ullamcorper ac, vestibulum in, elit. Maecenas aliquet accumsan leo.

Add an annotation or notes to a dataset; annotations are available when a history is viewed.

Database/Build - optional

unspecified (?)

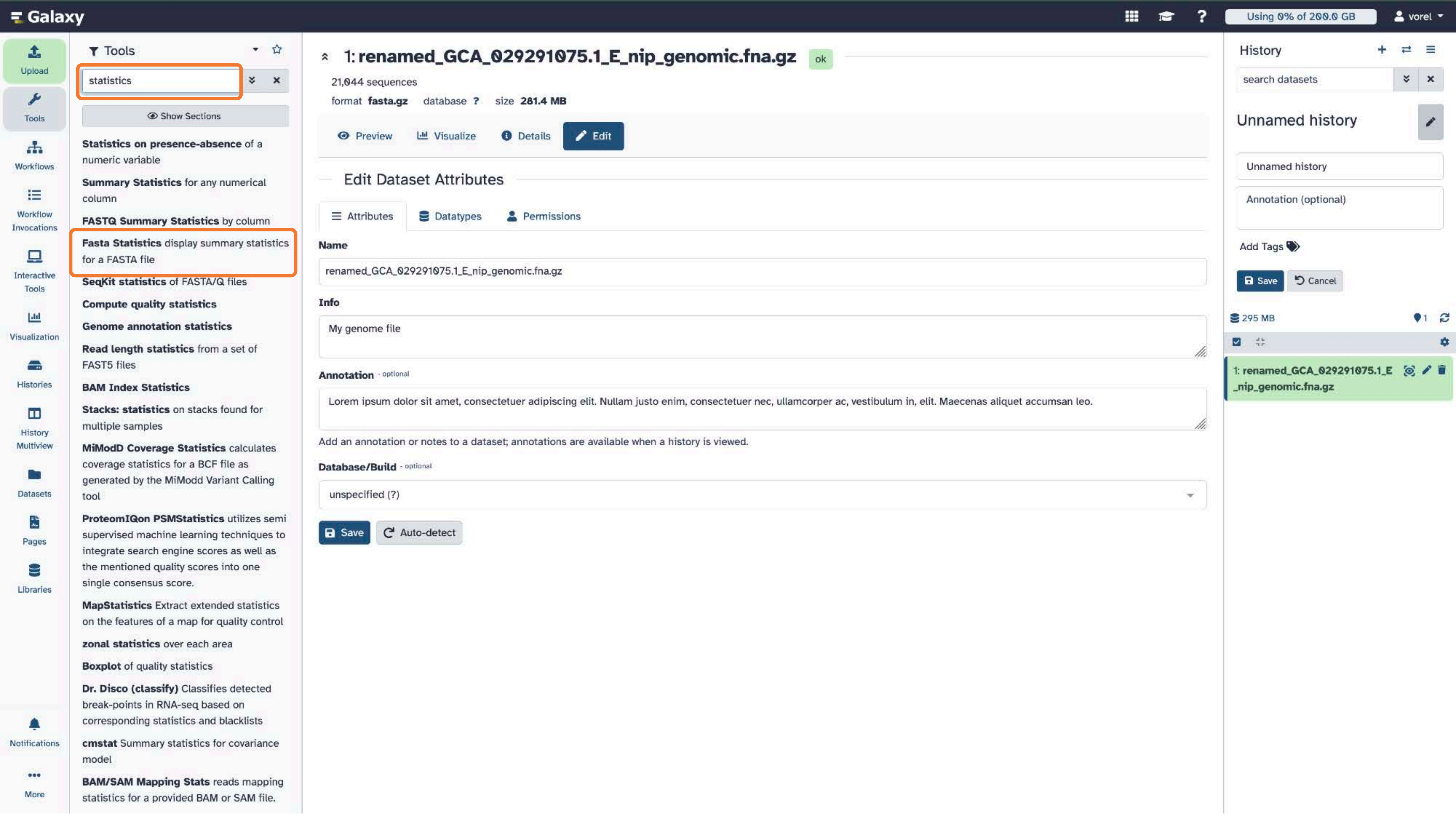
Save

Unnamed history

Unnamed history

Annotation (optional)

1: renamed_GCA_029291075.1_E_nip_genomic.fna.gz



Tools

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Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Nullam justo enim, consectetuer nec, ullamcorper ac, vestibulum in, elit. Maecenas aliquet accumsan leo.

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Database/Build - optional

unspecified (?)

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Annotation (optional)

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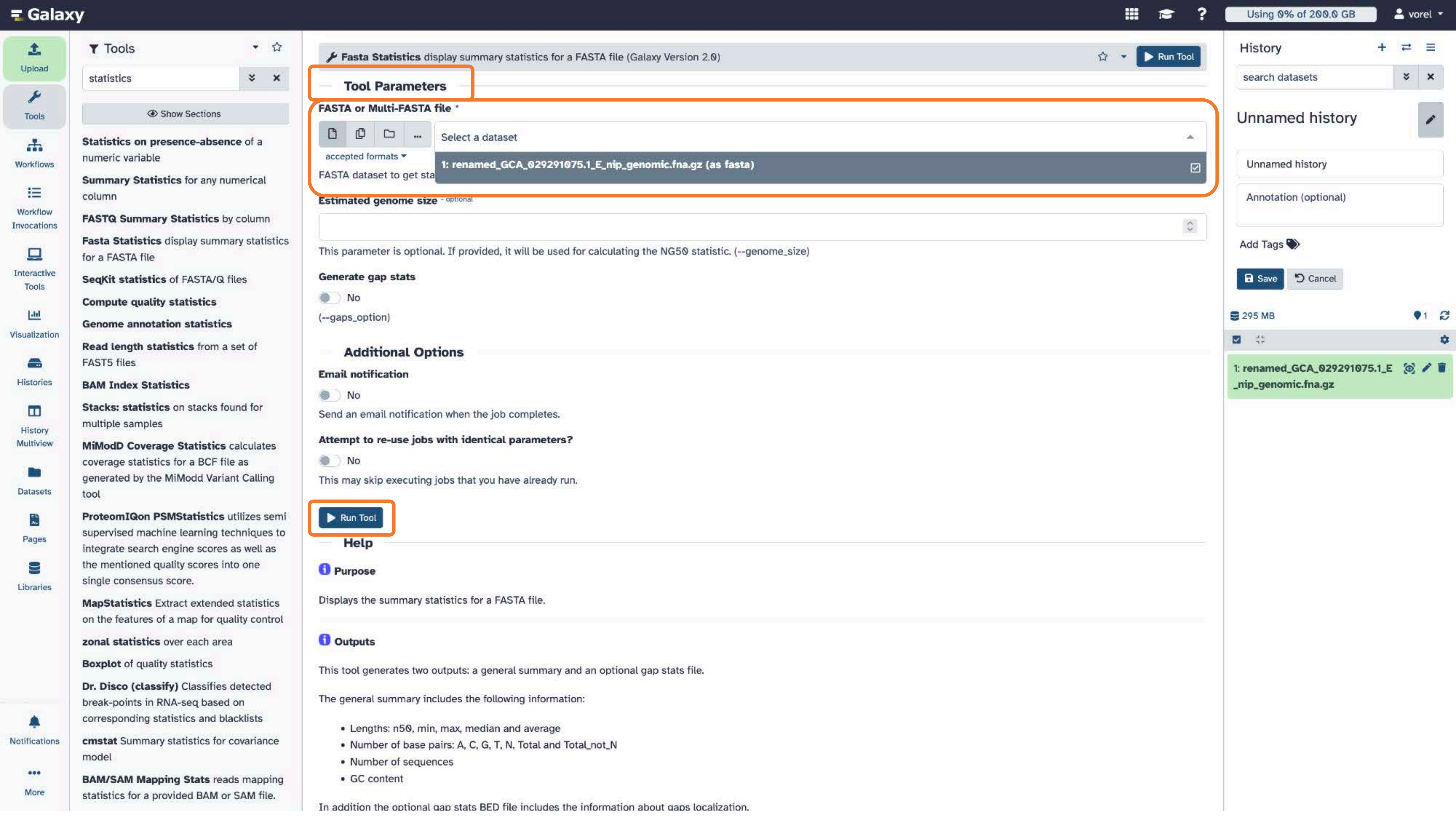

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MapStatistics Extract extended statistics on the features of a map for quality control

zonal statistics over each area

Boxplot of quality statistics

Dr. Disco (classify) Classifies detected break-points in RNA-seq based on corresponding statistics and blacklists

cmstat Summary statistics for covariance model

BAM/SAM Mapping Stats reads mapping statistics for a provided BAM or SAM file.

Fasta Statistics display summary statistics for a FASTA file (Galaxy Version 2.0)

Tool Parameters

FASTA or Multi-FASTA file *

1: renamed_GCA_029291075.1_E_nip_genomic.fna.gz (as fasta)

FASTA dataset to get sta

Estimated genome size - optional

This parameter is optional. If provided, it will be used for calculating the NG50 statistic. (--genome_size)

Generate gap stats

No

(--gaps_option)

Additional Options

Email notification

No

Send an email notification when the job completes.

Attempt to re-use jobs with identical parameters?

No

This may skip executing jobs that you have already run.

Help

Purpose

Displays the summary statistics for a FASTA file.

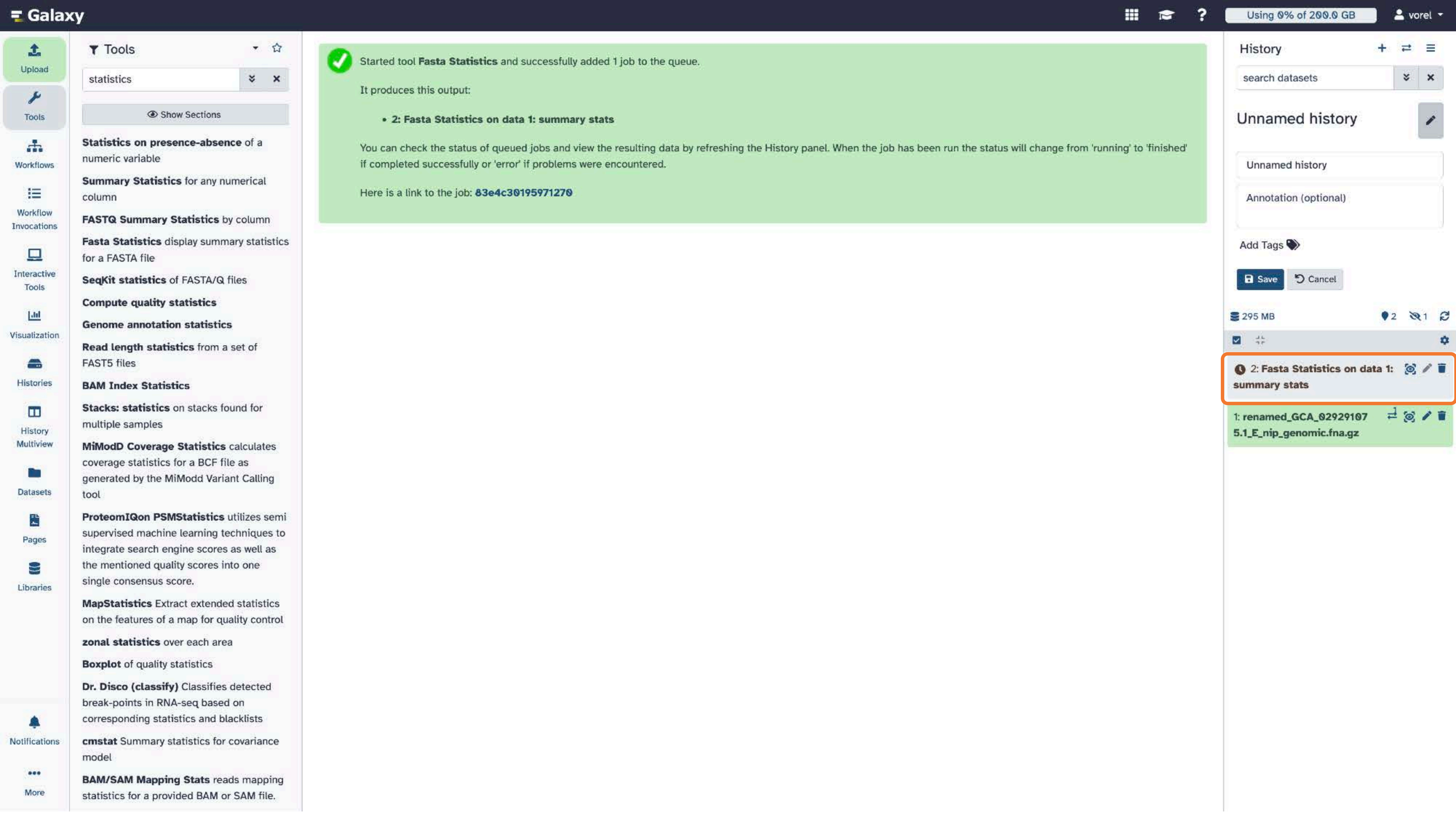
Outputs

This tool generates two outputs: a general summary and an optional gap stats file.

The general summary includes the following information:

- Lengths: n50, min, max, median and average
- Number of base pairs: A, C, G, T, N, Total and Total_not_N
- Number of sequences
- GC content

In addition the optional gap stats BED file includes the information about gaps localization.



Started tool **Fasta Statistics** and successfully added 1 job to the queue.

It produces this output:

- **2: Fasta Statistics on data 1: summary stats**

You can check the status of queued jobs and view the resulting data by refreshing the History panel. When the job has been run the status will change from 'running' to 'finished' if completed successfully or 'error' if problems were encountered.

Here is a link to the job: **83e4c30195971270**

Statistics on presence-absence of a numeric variable

Summary Statistics for any numerical column

FASTQ Summary Statistics by column

Fasta Statistics display summary statistics for a FASTA file

SeqKit statistics of FASTA/Q files

Compute quality statistics

Genome annotation statistics

Read length statistics from a set of FAST5 files

BAM Index Statistics

Stacks: statistics on stacks found for multiple samples

MiModD Coverage Statistics calculates coverage statistics for a BCF file as generated by the MiModd Variant Calling tool

ProteomIQon PSMStatistics utilizes semi supervised machine learning techniques to integrate search engine scores as well as the mentioned quality scores into one single consensus score.

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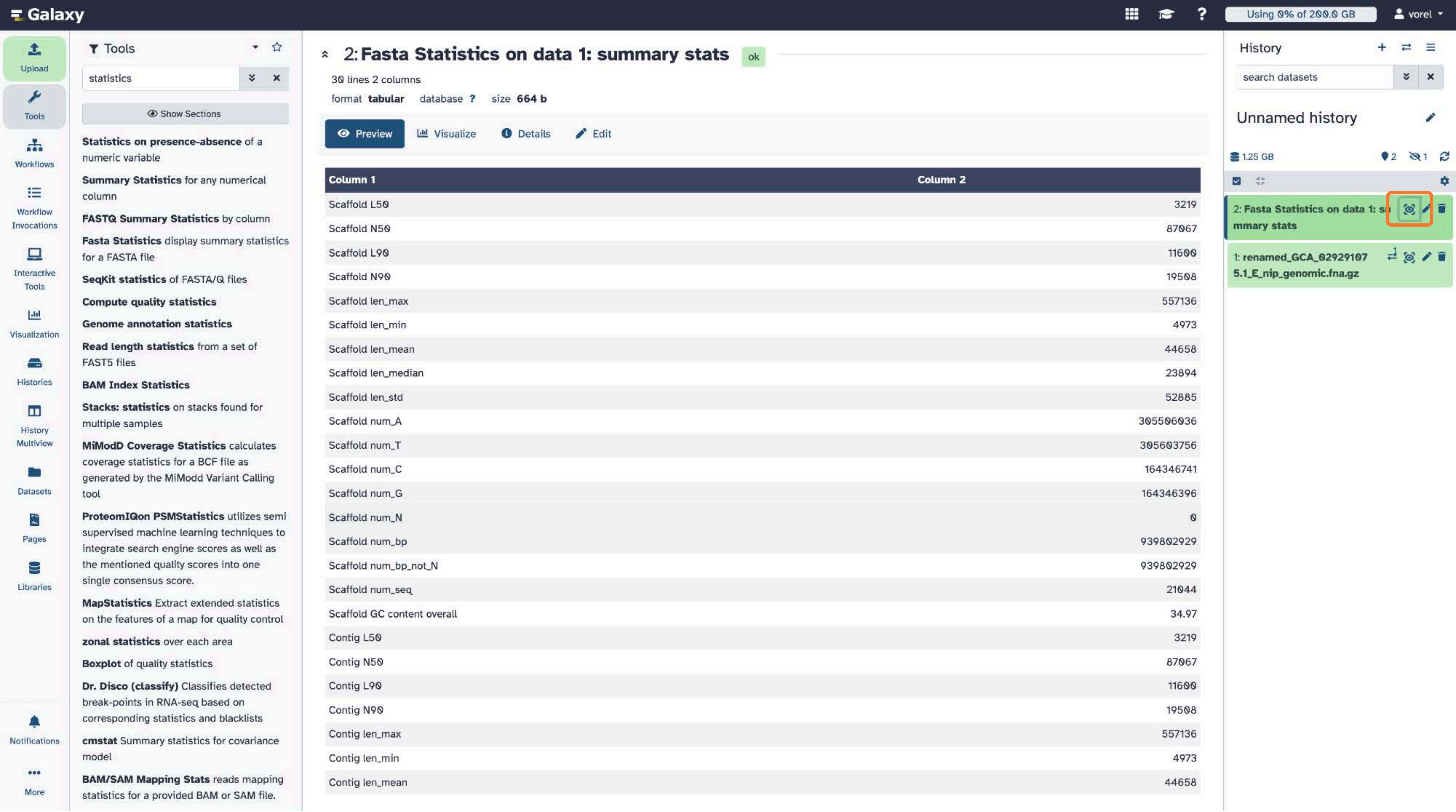
1: **renamed_GCA_029291075.1_E_nip_genomic.fna.gz**



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SeqKit statistics of FASTA/Q files

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cmstat Summary statistics for covariance model

BAM/SAM Mapping Stats reads mapping statistics for a provided BAM or SAM file.

2: Fasta Statistics on data 1: summary stats ok

30 lines 2 columns

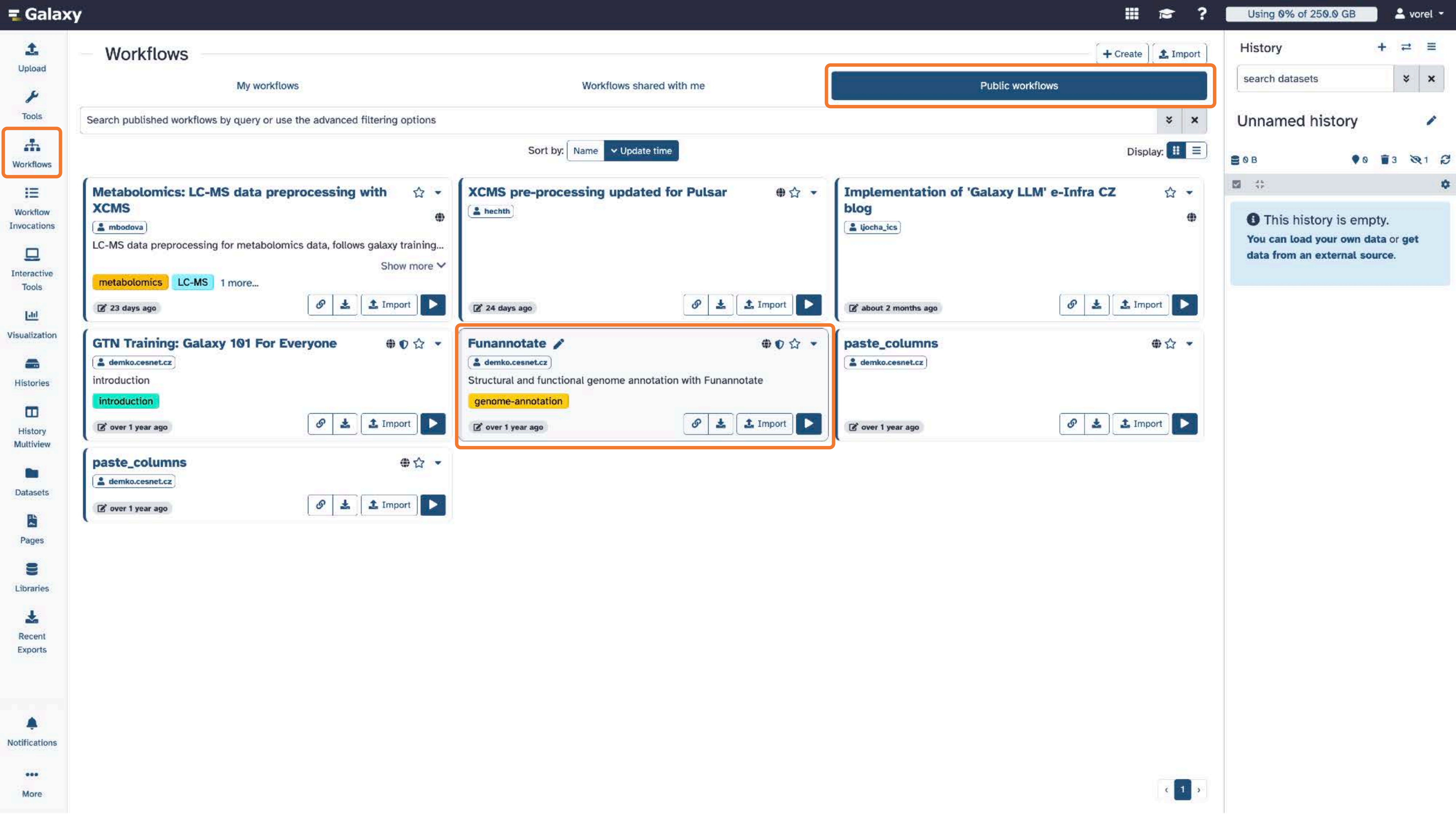
format **tabular** database **?** size **664 b**

Column 1	Column 2
Scaffold L50	3219
Scaffold N50	87067
Scaffold L90	11600
Scaffold N90	19508
Scaffold len_max	557136
Scaffold len_min	4973
Scaffold len_mean	44658
Scaffold len_median	23894
Scaffold len_std	52885
Scaffold num_A	305506036
Scaffold num_T	305603756
Scaffold num_C	164346741
Scaffold num_G	164346396
Scaffold num_N	0
Scaffold num_bp	939802929
Scaffold num_bp_not_N	939802929
Scaffold num_seq	21044
Scaffold GC content overall	34.97
Contig L50	3219
Contig N50	87067
Contig L90	11600
Contig N90	19508
Contig len_max	557136
Contig len_min	4973
Contig len_mean	44658

Unnamed history

2: Fasta Statistics on data 1: summary stats

1: renamed_GCA_029291075.1_E_nip_genomic.fna.gz



Metadata: LC-MS data preprocessing with XCMS
mbodova
LC-MS data preprocessing for metabolomics data, follows galaxy training...
metabolomics LC-MS
23 days ago

XCMS pre-processing updated for Pulsar
hechth
24 days ago

Implementation of 'Galaxy LLM' e-Infra CZ blog
ljocha_ics
about 2 months ago

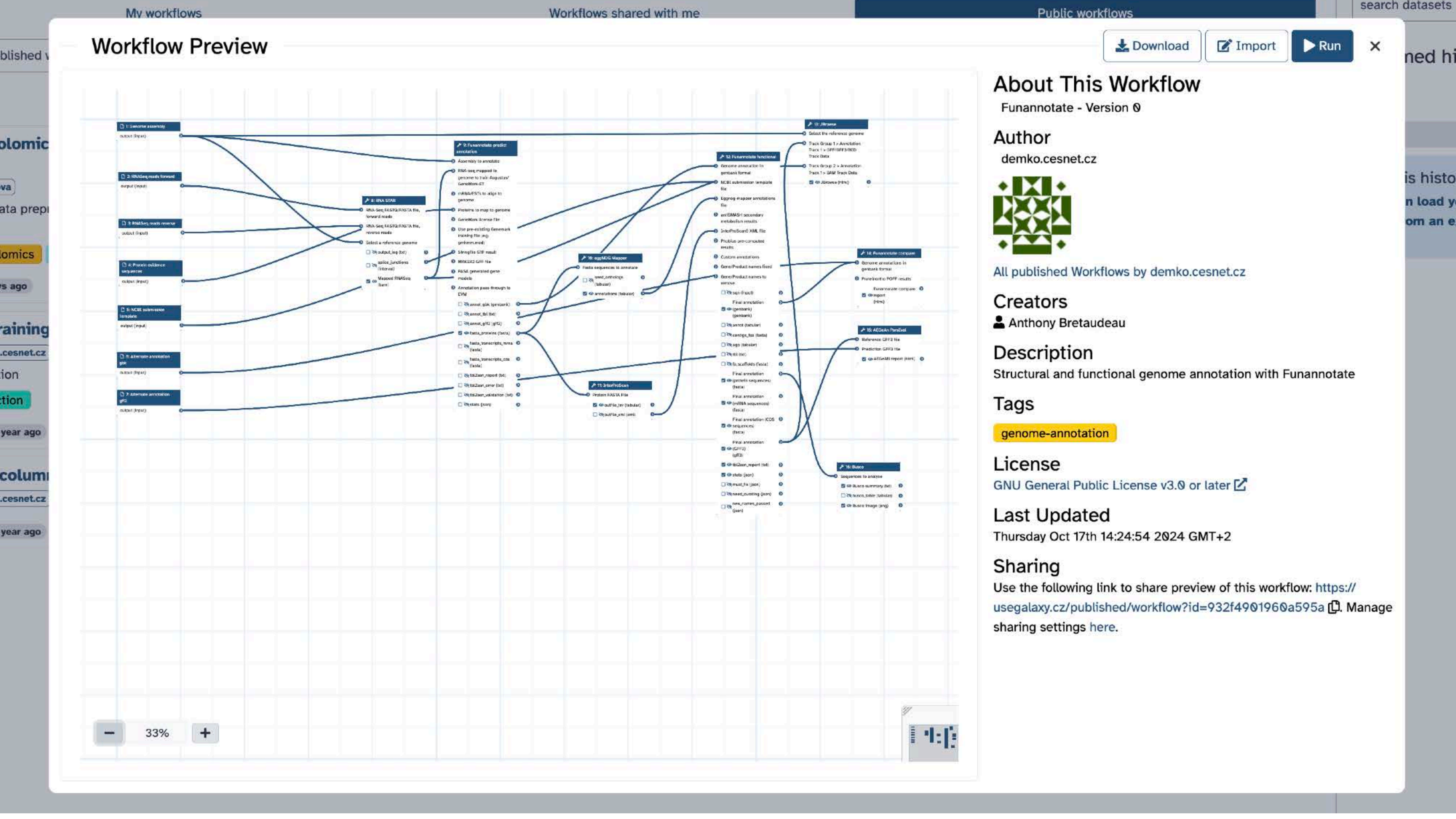
GTN Training: Galaxy 101 For Everyone
demko.cesnet.cz
introduction
introduction
over 1 year ago

Funannotate
demko.cesnet.cz
Structural and functional genome annotation with Funannotate
genome-annotation
over 1 year ago

paste_columns
demko.cesnet.cz
over 1 year ago

paste_columns
demko.cesnet.cz
over 1 year ago

This history is empty.
You can load your own data or get data from an external source.



Workflow Preview

About This Workflow

Funannotate - Version 0

Author

demko.cesnet.cz

All published Workflows by demko.cesnet.cz

Creators

Anthony Bretaudeau

Description

Structural and functional genome annotation with Funannotate

Tags

genome-annotation

License

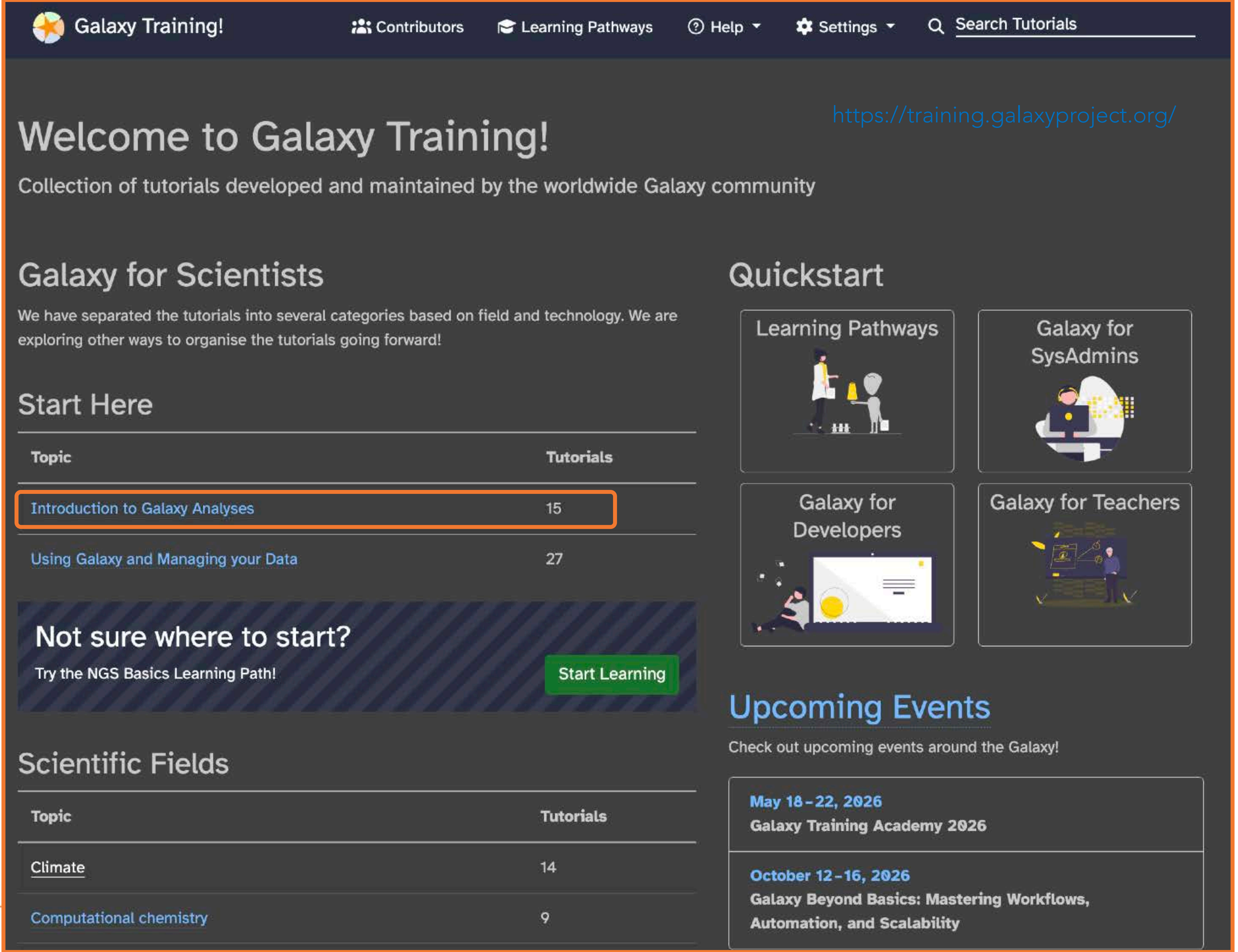
GNU General Public License v3.0 or later

Last Updated

Thursday Oct 17th 14:24:54 2024 GMT+2

Sharing

Use the following link to share preview of this workflow: https://usegalaxy.cz/published/workflow?id=932f4901960a595a. Manage sharing settings here.



https://training.galaxyproject.org/

Welcome to Galaxy Training!

Collection of tutorials developed and maintained by the worldwide Galaxy community

Galaxy for Scientists

We have separated the tutorials into several categories based on field and technology. We are exploring other ways to organise the tutorials going forward!

Start Here

Topic	Tutorials
Introduction to Galaxy Analyses	15
Using Galaxy and Managing your Data	27

Not sure where to start?

Try the NGS Basics Learning Path!

Scientific Fields

Topic	Tutorials
Climate	14
Computational chemistry	9

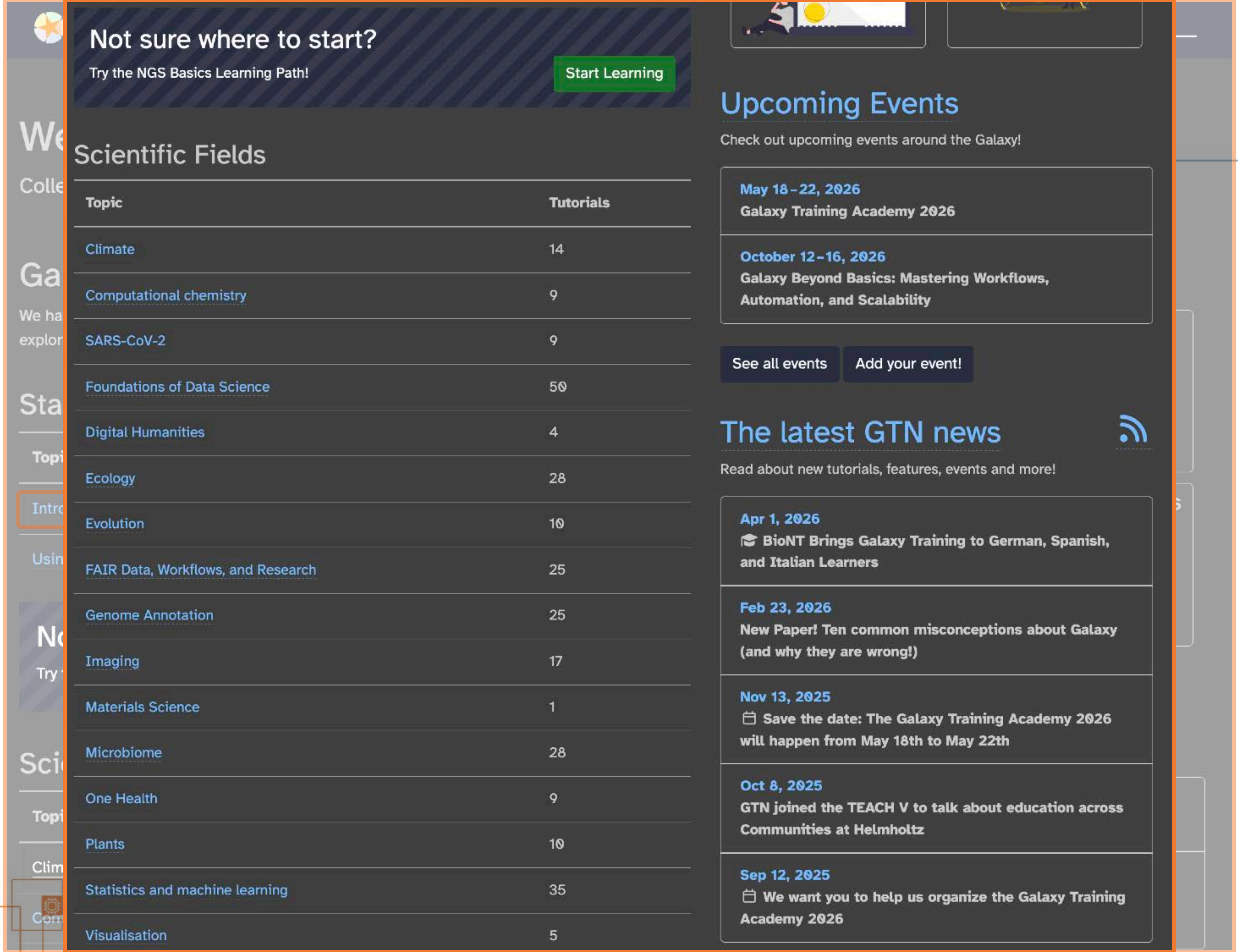
Quickstart

Upcoming Events

Check out upcoming events around the Galaxy!

May 18 – 22, 2026
Galaxy Training Academy 2026

October 12 – 16, 2026
Galaxy Beyond Basics: Mastering Workflows, Automation, and Scalability



Not sure where to start?

Try the NGS Basics Learning Path!

Scientific Fields

Topic	Tutorials
Climate	14
Computational chemistry	9
SARS-CoV-2	9
Foundations of Data Science	50
Digital Humanities	4
Ecology	28
Evolution	10
FAIR Data, Workflows, and Research	25
Genome Annotation	25
Imaging	17
Materials Science	1
Microbiome	28
One Health	9
Plants	10
Statistics and machine learning	35
Visualisation	5

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The latest GTN news

Read about new tutorials, features, events and more!

Apr 1, 2026
🎓 **BioNT Brings Galaxy Training to German, Spanish, and Italian Learners**

Feb 23, 2026
New Paper! Ten common misconceptions about Galaxy (and why they are wrong!)

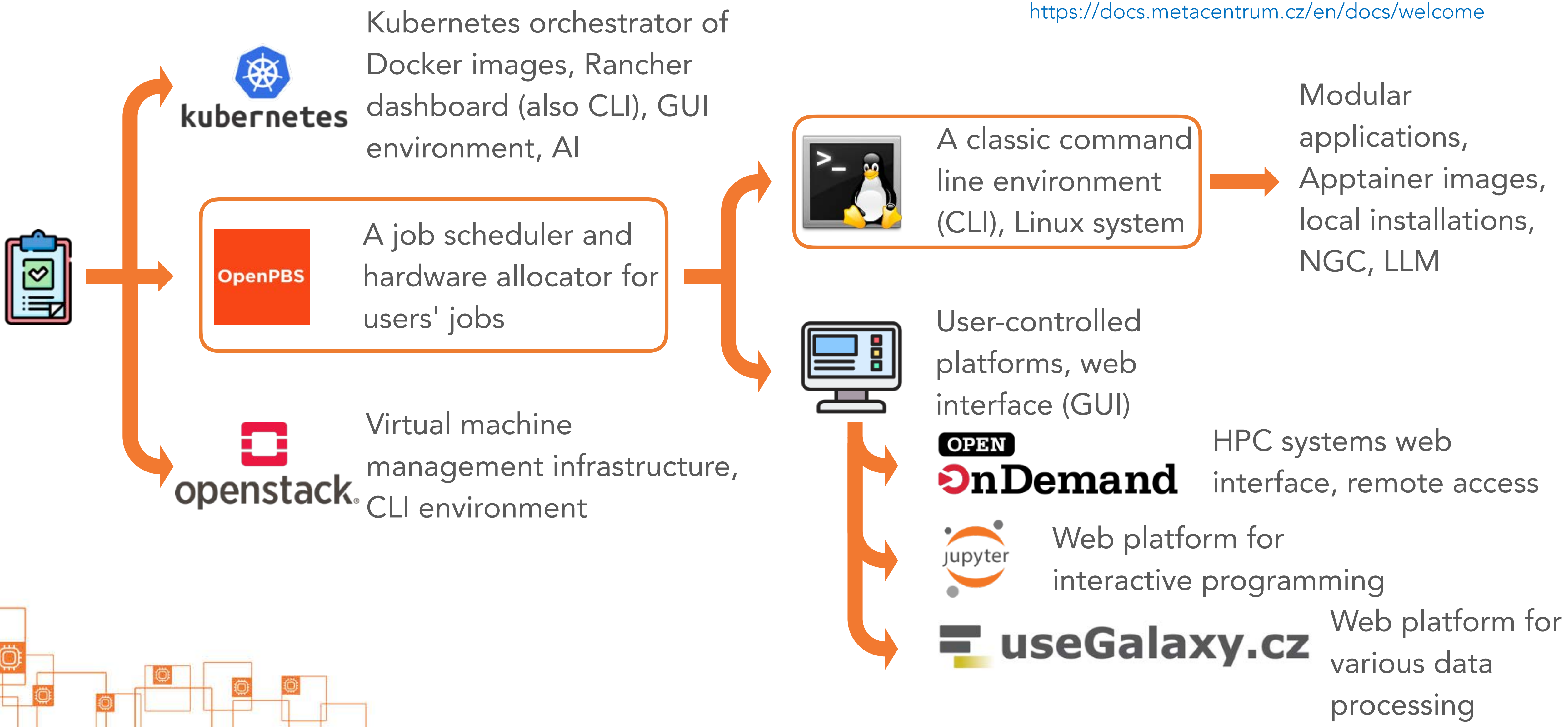
Nov 13, 2025
📅 **Save the date: The Galaxy Training Academy 2026 will happen from May 18th to May 22th**

Oct 8, 2025
GTN joined the TEACH V to talk about education across Communities at Helmholtz

Sep 12, 2025
📅 **We want you to help us organize the Galaxy Training Academy 2026**

How to use it

https://docs.metacentrum.cz/en/docs/welcome



kubernetes

Kubernetes orchestrator of Docker images, Rancher dashboard (also CLI), GUI environment, AI

OpenPBS

A job scheduler and hardware allocator for users' jobs

openstack

Virtual machine management infrastructure, CLI environment

A classic command line environment (CLI), Linux system

Modular applications, Apptainer images, local installations, NGC, LLM

User-controlled platforms, web interface (GUI)

OPEN OnDemand

HPC systems web interface, remote access

jupyter

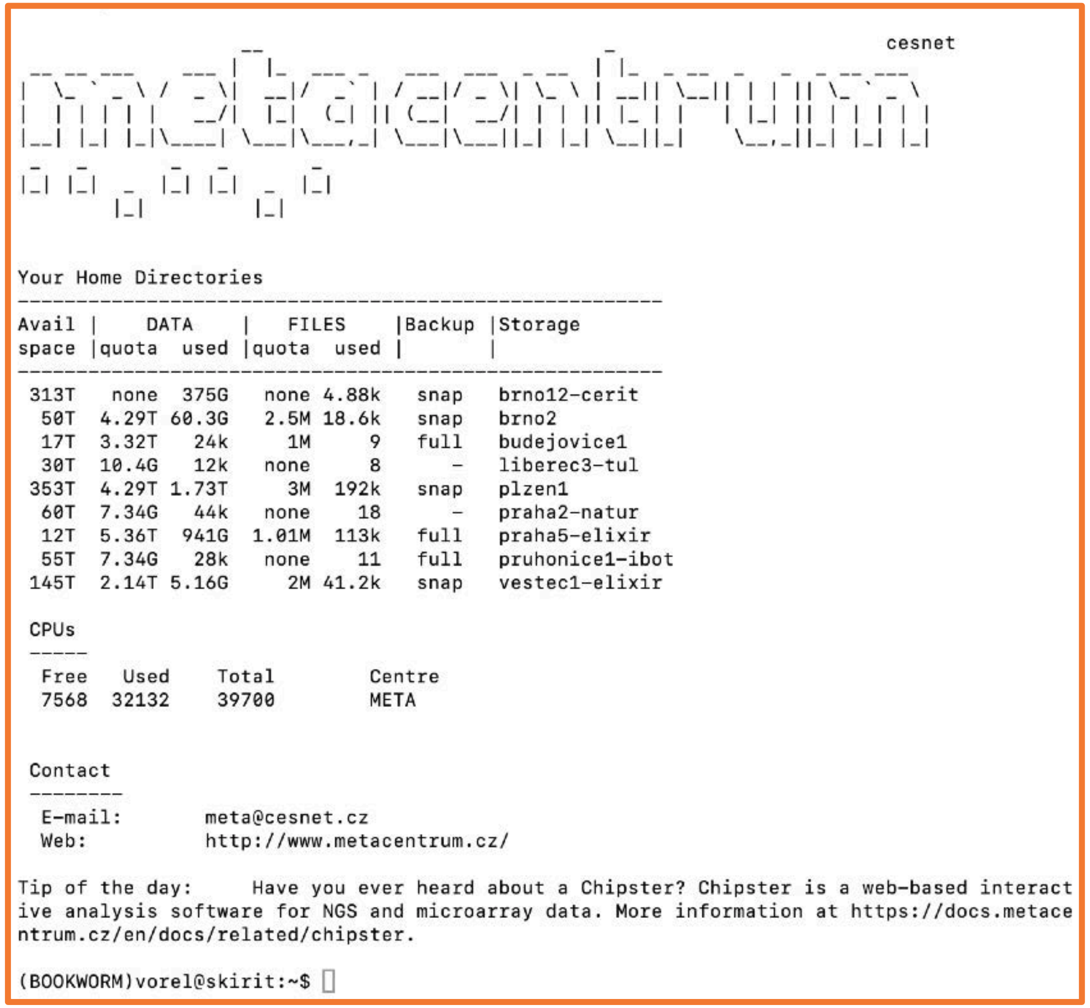
Web platform for interactive programming

useGalaxy.cz

Web platform for various data processing

Grid computing (CLI)

- Grid computing (OpenPBS scheduler)
  - Maximum flexibility
  - Long batch jobs (days/weeks)
  - Interactive jobs
  - Parallel and multi-node computing
  - GPU acceleration (NVIDIA H100, 96 GB)



```
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| | | | | |  __/ || (_| | (_|  __/ | | | |_| |  | |_| | | | | | |
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 _   _        _   _        _
|_| |_|  _   |_| |_|  _   |_|
        |_|            |_|


Your Home Directories
-------------------------------------------------------------------
Avail |     DATA      |     FILES     |Backup |Storage
space |quota   used  |quota   used  |       |
-------------------------------------------------------------------
 313T    none   375G    none 4.88k    snap    brno12-cerit
  50T   4.29T  60.3G    2.5M 18.6k    snap    brno2
  17T   3.32T    24k      1M     9    full    budejovice1
  30T   10.4G    12k    none     8       -    liberec3-tul
 353T   4.29T  1.73T      3M  192k    snap    plzen1
  60T   7.34G    44k    none    18       -    praha2-natur
  12T   5.36T   941G   1.01M  113k    full    praha5-elixir
  55T   7.34G    28k    none    11    full    pruhonice1-ibot
 145T   2.14T  5.16G      2M 41.2k    snap    vestec1-elixir

 CPUs
 -----
  Free   Used     Total         Centre
  7568  32132     39700         META


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

Tip of the day:     Have you ever heard about a Chipster? Chipster is a web-based interact
ive analysis software for NGS and microarray data. More information at https://docs.metace
ntrum.cz/en/docs/related/chipster.

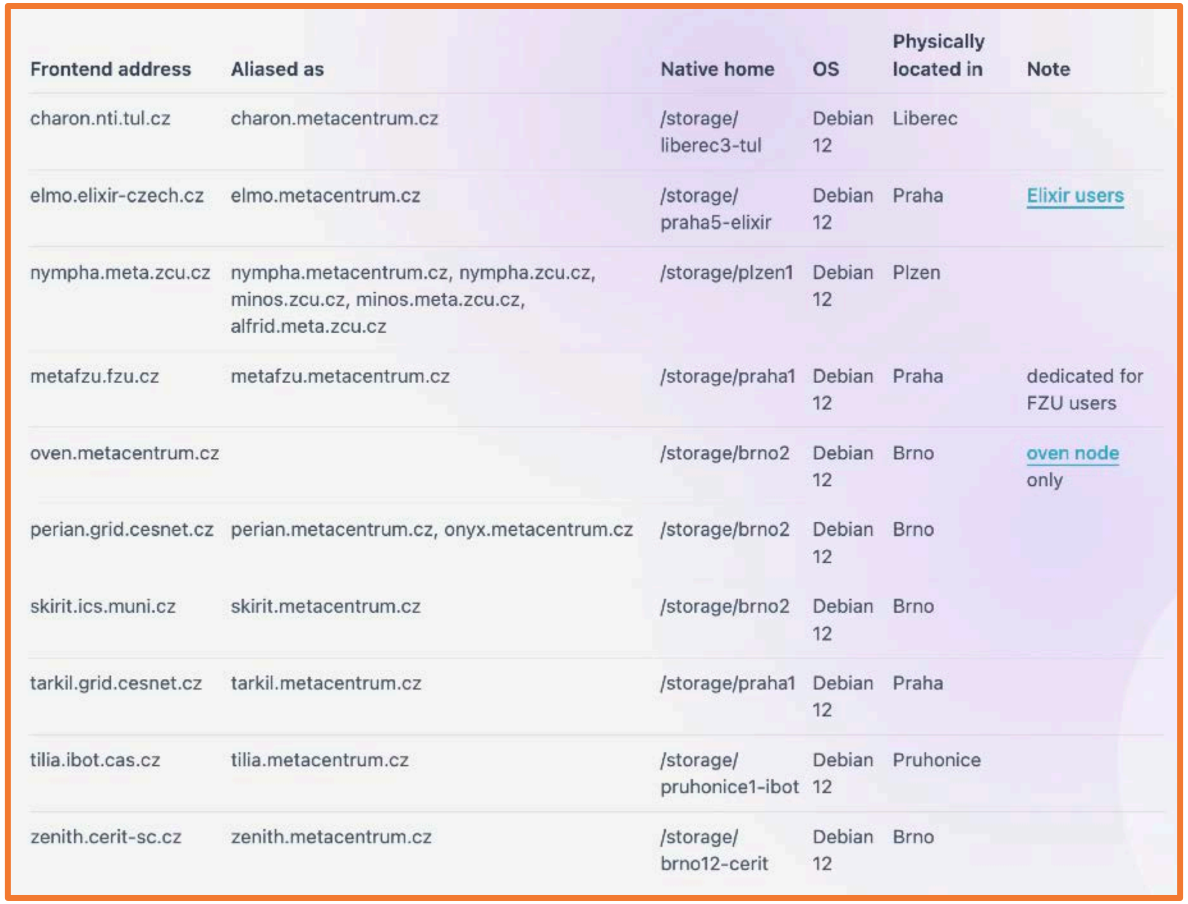
(BOOKWORM)vorel@skirit:~$ ▯
```

https://docs.metacentrum.cz/en/docs/welcome

Frontend servers (login nodes)

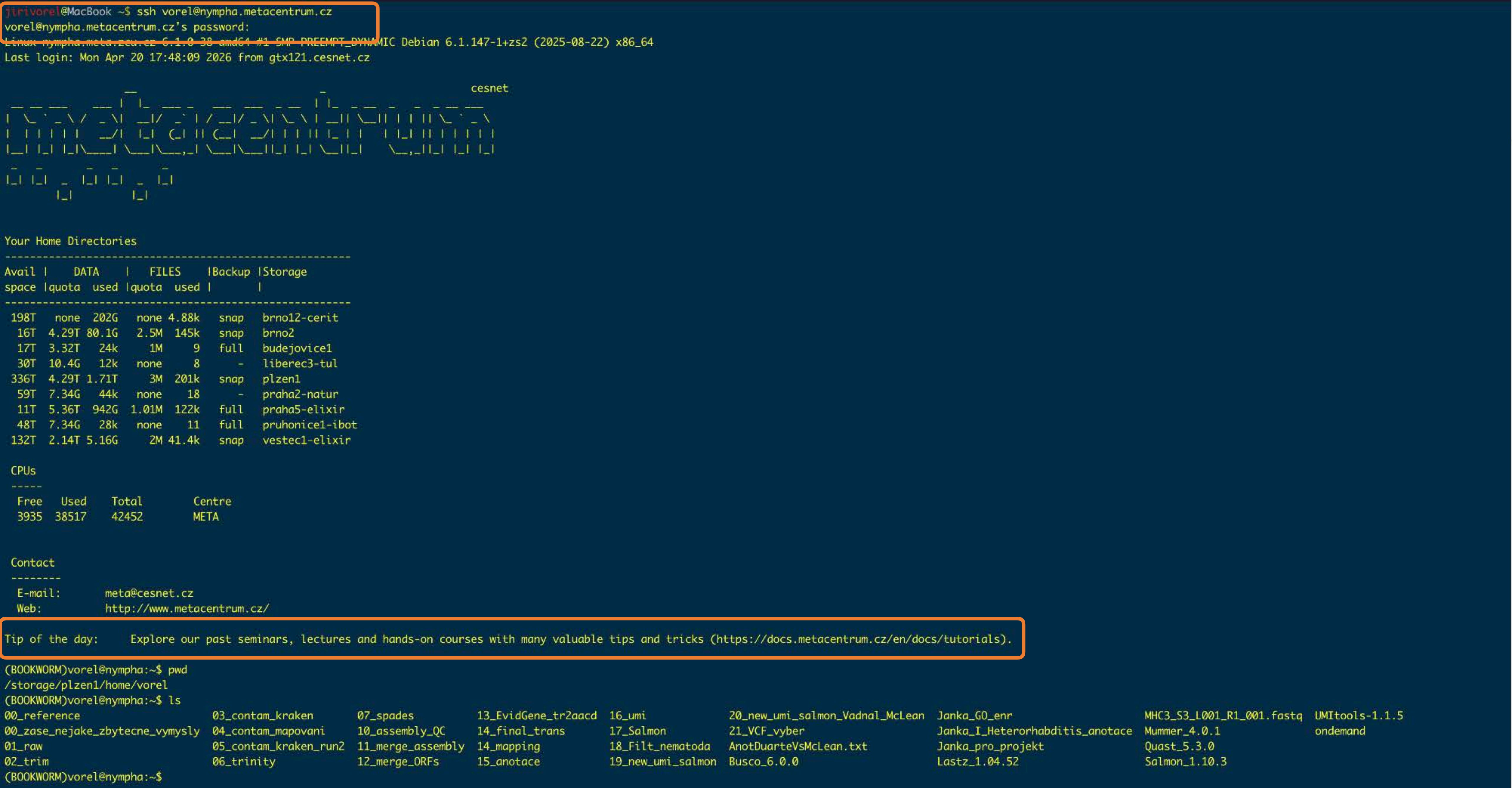
https://docs.metacentrum.cz/en/docs/computing/infrastructure/frontends

- Primary access point
- SSH access via password (creating a Kerberos ticket)
  - SSH key authentication is not supported



Frontend address	Aliased as	Native home	OS	Physically located in	Note
charon.nti.tul.cz	charon.metacentrum.cz	/storage/liberec3-tul	Debian 12	Liberec	
elmo.elixir-czech.cz	elmo.metacentrum.cz	/storage/praha5-elixir	Debian 12	Praha	Elixir users
nympha.meta.zcu.cz	nympha.metacentrum.cz, nympha.zcu.cz, minos.zcu.cz, minos.meta.zcu.cz, alfrid.meta.zcu.cz	/storage/plzen1	Debian 12	Plzen	
metafzu.fzu.cz	metafzu.metacentrum.cz	/storage/praha1	Debian 12	Praha	dedicated for FZU users
oven.metacentrum.cz		/storage/brno2	Debian 12	Brno	oven node only
perian.grid.cesnet.cz	perian.metacentrum.cz, onyx.metacentrum.cz	/storage/brno2	Debian 12	Brno	
skirit.ics.muni.cz	skirit.metacentrum.cz	/storage/brno2	Debian 12	Brno	
tarkil.grid.cesnet.cz	tarkil.metacentrum.cz	/storage/praha1	Debian 12	Praha	
tilia.ibot.cas.cz	tilia.metacentrum.cz	/storage/pruhonice1-ibot	Debian 12	Pruhonice	
zenith.cerit-sc.cz	zenith.metacentrum.cz	/storage/brno12-cerit	Debian 12	Brno	

Geographically separated servers mean better distribution of users and load, which makes the servers more stable and provides an alternative during an outage



```
jirivorel@MacBook ~$ ssh vorel@nympha.metacentrum.cz
vorel@nympha.metacentrum.cz's password:
Linux nympha.meta.zcu.cz 6.1.0-38-amd64 #1 SMP PREEMPT_DYNAMIC Debian 6.1.147-1+zs2 (2025-08-22) x86_64
Last login: Mon Apr 20 17:48:09 2026 from gtx121.cesnet.cz

                    __                        _                       cesnet
 __ __ ___     ___ |  |_  ___ _   ___  ___  _ __  | |_  _ __ _   _  _ __ ___
|  \_ ` _ \ /  _ \|  __|/  _` | /  __|/  _ \| \_ \ |  __|| \__|| | | || \_ ` _ \
|  | | | | |   __/|  |_|  (_| || (__ |  __/| | | ||  |_ | |   | |_| || | | | | |
|__| |_| |_|\____| \___|\___,_| \___|\___||_| |_| \__||_|    \__,_||_| |_| |_|
 _   _      _   _     _
|_| |_|  _  |_| |_|  _  |_|
        |_|          |_|



Your Home Directories
-------------------------------------------------------
Avail |    DATA     |   FILES    |Backup |Storage
space |quota  used |quota  used |       |
-------------------------------------------------------
 198T   none  202G   none 4.88k   snap   brno12-cerit
  16T  4.29T 80.1G   2.5M  145k   snap   brno2
  17T  3.32T   24k     1M     9   full   budejovice1
  30T  10.4G   12k   none     8      -   liberec3-tul
 336T  4.29T 1.71T     3M  201k   snap   plzen1
  59T  7.34G   44k   none    18      -   praha2-natur
  11T  5.36T  942G  1.01M  122k   full   praha5-elixir
  48T  7.34G   28k   none    11   full   pruhonice1-ibot
 132T  2.14T 5.16G     2M 41.4k   snap   vestec1-elixir

 CPUs
 -----
  Free   Used    Total        Centre
  3935  38517    42452        META


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

Tip of the day:     Explore our past seminars, lectures and hands-on courses with many valuable tips and tricks (https://docs.metacentrum.cz/en/docs/tutorials).
(BOOKWORM)vorel@nympha:~$ pwd
/storage/plzen1/home/vorel
(BOOKWORM)vorel@nympha:~$ ls
00_reference                     03_contam_kraken       07_spades          13_EvidGene_tr2aacd  16_umi             20_new_umi_salmon_Vadnal_McLean  Janka_GO_enr                     MHC3_S3_L001_R1_001.fastq  UMItools-1.1.5
00_zase_nejake_zbytecne_vymysly  04_contam_mapovani     10_assembly_QC     14_final_trans       17_Salmon          21_VCF_vyber                     Janka_I_Heterorhabditis_anotace  Mummer_4.0.1               ondemand
01_raw                           05_contam_kraken_run2  11_merge_assembly  14_mapping           18_Filt_nematoda   AnotDuarteVsMcLean.txt           Janka_pro_projekt                Quast_5.3.0
02_trim                          06_trinity             12_merge_ORFs      15_anotace           19_new_umi_salmon  Busco_6.0.0                      Lastz_1.04.52                    Salmon_1.10.3
(BOOKWORM)vorel@nympha:~$
```

Disk storage arrays

- Several geographically separated disk arrays (storages) are available

https://docs.metacentrum.cz/en/docs/computing/infrastructure/mount-storages

- Designed for so-called live data

https://docs.metacentrum.cz/en/docs/data/storage-department

  - Backups of valuable primary data and results preferably to S3/NRP object storage

https://docs.du.cesnet.cz/en/docs/object-storage-s3/s3-service

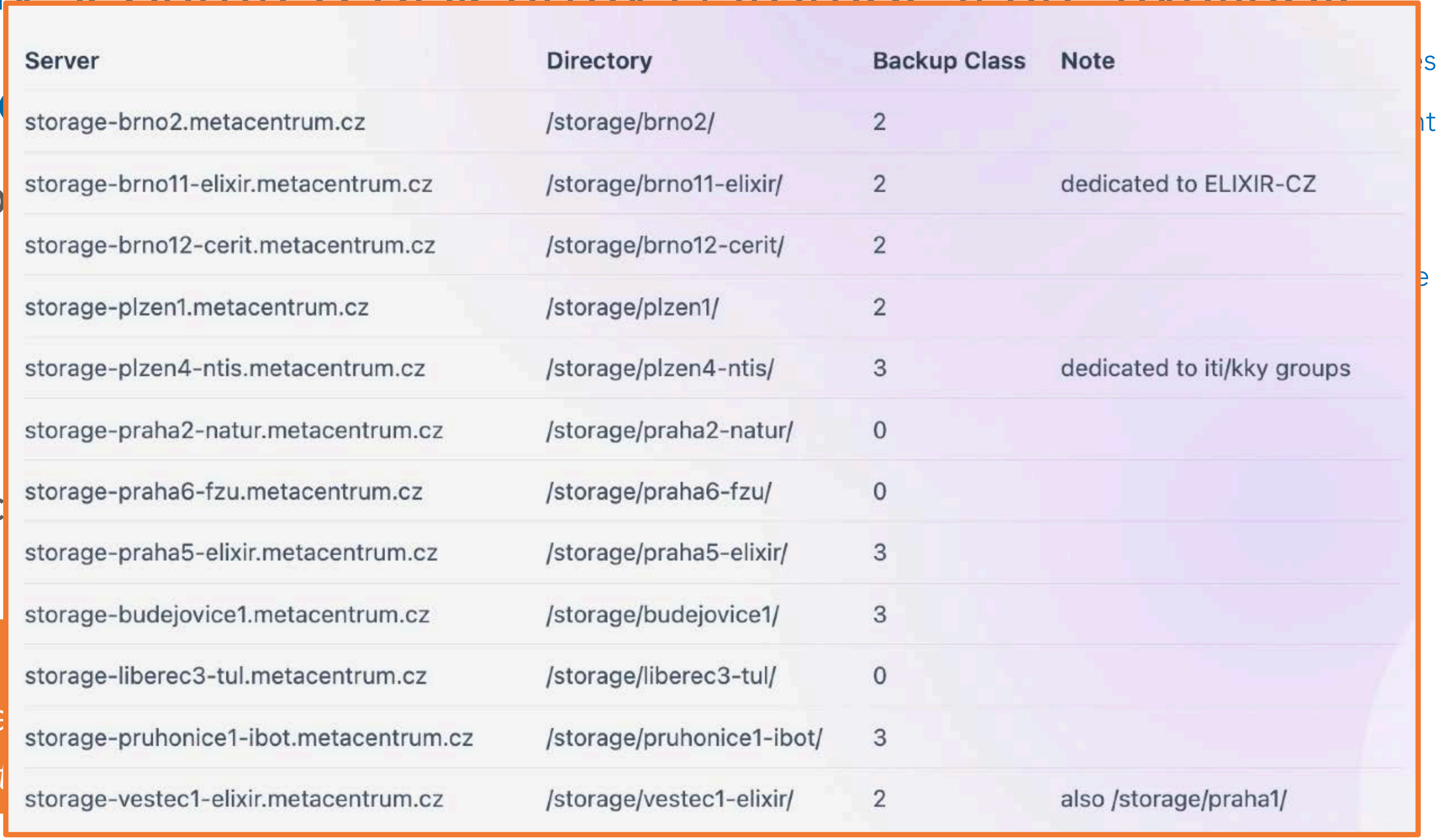
    - Available to all users
    - *s3cmd/s5cmd* commands are available for manipulating data on S3 storage
    - Need to request the creation of an S3 bucket ('folder') and create a configuration file

> ☝ *By default, a user's home directories have permissions set to 755 (= other users can read it). To increase privacy, permissions can be set to 700 on /storage/city/home/$USER.*

Disk storage arrays

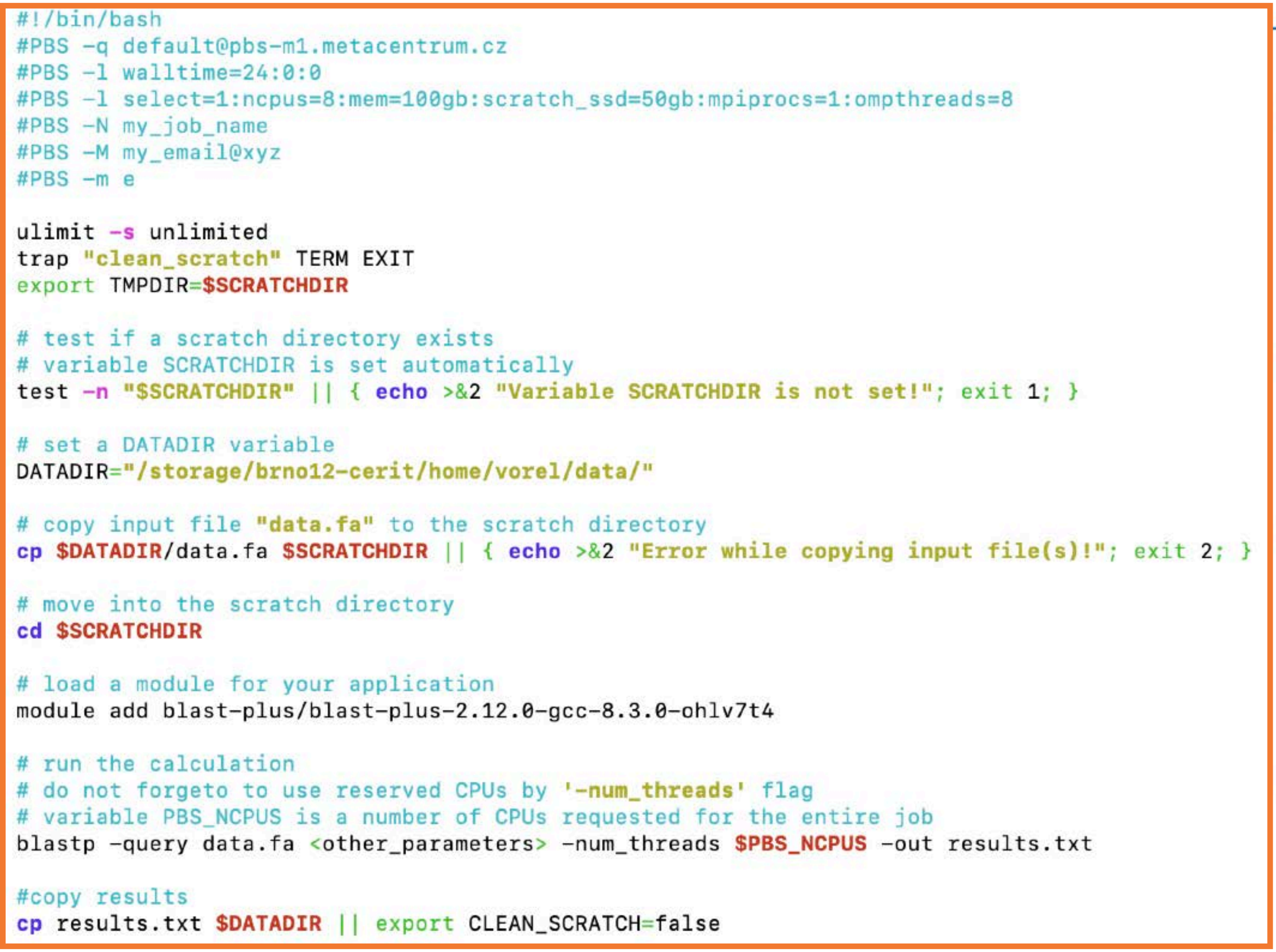
- Several geographically separated disk arrays (storages) are available
- Designed for so-callec
  - Backups of valuable p
    storage
    - Available to all users
    - *s3cmd/s5cmd* comma
    - Need to request the c

By default,
755 (= othe
can be set t



Server	Directory	Backup Class	Note
storage-brno2.metacentrum.cz	/storage/brno2/	2	
storage-brno11-elixir.metacentrum.cz	/storage/brno11-elixir/	2	dedicated to ELIXIR-CZ
storage-brno12-cerit.metacentrum.cz	/storage/brno12-cerit/	2	
storage-plzen1.metacentrum.cz	/storage/plzen1/	2	
storage-plzen4-ntis.metacentrum.cz	/storage/plzen4-ntis/	3	dedicated to iti/kky groups
storage-praha2-natur.metacentrum.cz	/storage/praha2-natur/	0	
storage-praha6-fzu.metacentrum.cz	/storage/praha6-fzu/	0	
storage-praha5-elixir.metacentrum.cz	/storage/praha5-elixir/	3	
storage-budejovice1.metacentrum.cz	/storage/budejovice1/	3	
storage-liberec3-tul.metacentrum.cz	/storage/liberec3-tul/	0	
storage-pruhonice1-ibot.metacentrum.cz	/storage/pruhonice1-ibot/	3	
storage-vestec1-elixir.metacentrum.cz	/storage/vestec1-elixir/	2	also /storage/praha1/

Batch job script example



```
#!/bin/bash
#PBS -q default@pbs-m1.metacentrum.cz
#PBS -l walltime=24:0:0
#PBS -l select=1:ncpus=8:mem=100gb:scratch_ssd=50gb:mpiprocs=1:ompthreads=8
#PBS -N my_job_name
#PBS -M my_email@xyz
#PBS -m e

ulimit -s unlimited
trap "clean_scratch" TERM EXIT
export TMPDIR=$SCRATCHDIR

# test if a scratch directory exists
# variable SCRATCHDIR is set automatically
test -n "$SCRATCHDIR" || { echo >&2 "Variable SCRATCHDIR is not set!"; exit 1; }

# set a DATADIR variable
DATADIR="/storage/brno12-cerit/home/vorel/data/"

# copy input file "data.fa" to the scratch directory
cp $DATADIR/data.fa $SCRATCHDIR || { echo >&2 "Error while copying input file(s)!"; exit 2; }

# move into the scratch directory
cd $SCRATCHDIR

# load a module for your application
module add blast-plus/blast-plus-2.12.0-gcc-8.3.0-ohlv7t4

# run the calculation
# do not forgeto to use reserved CPUs by '-num_threads' flag
# variable PBS_NCPUS is a number of CPUs requested for the entire job
blastp -query data.fa <other_parameters> -num_threads $PBS_NCPUS -out results.txt

#copy results
cp results.txt $DATADIR || export CLEAN_SCRATCH=false
```

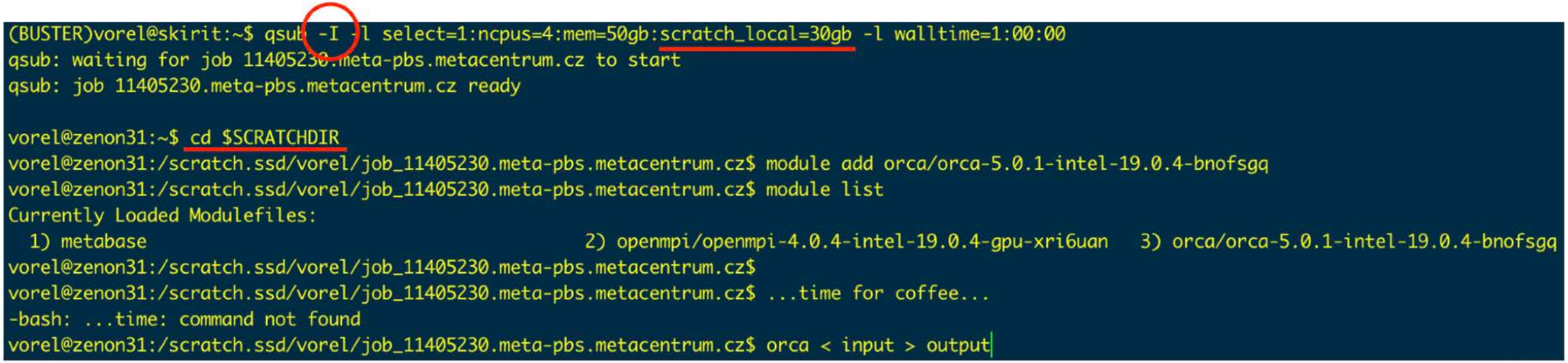
- Define HW resources (`-l`), queue (`-q`), and walltime (`-l`), set the job name (`-N`) and email alert (`-m`)
- You can define as many variables as you want
- Available modules can be listed by command `module ava *key_word*` on any frontend
- The scratch directory will be cleaned automatically

https://docs.metacentrum.cz/en/docs/computing/run-basic-job#batch-job

Interactive job

- The opposite of batch jobs (waiting for the user's input...)
- Best choice for test calculations (which should not be run directly on frontends)
- An interactive job is requested by the qsub command with the -I (uppercase "i") option

https://docs.metacentrum.cz/en/docs/computing/run-basic-job#interactive-job



```
(BUSTER)vorel@skirit:~$ qsub -I -l select=1:ncpus=4:mem=50gb:scratch_local=30gb -l walltime=1:00:00
qsub: waiting for job 11405230.meta-pbs.metacentrum.cz to start
qsub: job 11405230.meta-pbs.metacentrum.cz ready

vorel@zenon31:~$ cd $SCRATCHDIR
vorel@zenon31:/scratch.ssd/vorel/job_11405230.meta-pbs.metacentrum.cz$ module add orca/orca-5.0.1-intel-19.0.4-bnofsgq
vorel@zenon31:/scratch.ssd/vorel/job_11405230.meta-pbs.metacentrum.cz$ module list
Currently Loaded Modulefiles:
  1) metabase                                         2) openmpi/openmpi-4.0.4-intel-19.0.4-gpu-xri6uan   3) orca/orca-5.0.1-intel-19.0.4-bnofsgq
vorel@zenon31:/scratch.ssd/vorel/job_11405230.meta-pbs.metacentrum.cz$
vorel@zenon31:/scratch.ssd/vorel/job_11405230.meta-pbs.metacentrum.cz$ ...time for coffee...
-bash: ...time: command not found
vorel@zenon31:/scratch.ssd/vorel/job_11405230.meta-pbs.metacentrum.cz$ orca < input > output
```

GPU acceleration

- **GPU acceleration for significant speedup of calculations**
- ~140 nodes, ~500 GPU cards (GTX 1080Ti - H100 100GB)
- Requires application with GPU support
- Maximum eight GPU cards on a single node, typically two or four
- Special DGX cluster with eight Nvidia H100 80GB GPU cards
  - Grant competition
- Specific parameters
  - `gpu_mem` (minimum amount of memory on the card)
  - `gpu_cap` (a minimal version of GPU architecture)
  - `cuda_version` (version of CUDA installed on the node)

https://docs.metacentrum.cz/en/docs/computing/gpu-comput/gpu-job

GPU acceleration

```
#!/bin/bash
#PBS -N run1_dorado_mod
#PBS -l select=1:ncpus=4:ngpus=1:mem=30gb:scratch_ssd=250gb:gpu_mem=20gb:gpu_cap=compute_80
#PBS -l walltime=8:0:0

cd $SCRATCHDIR

scp storage-brno12-cerit.metacentrum.cz:~/Metylace_hemonch/RUN_1_IRE/02_run1_IRE_reads.pod5 $SCRATCHDIR
scp -r storage-brno12-cerit.metacentrum.cz:~/Metylace_hemonch/SOFT/dorado_0.9.1/models/dna_r9.4.1_e8_sup@v3.3* $SCRATCHDIR
cp /storage/brno12-cerit/home/vorel/Metylace_hemonch/Haemonch_refer/haemonchus_contortus.PRJEB506.WBPS19.genomic.fa $SCRATCHDIR

export PATH=/storage/brno12-cerit/home/vorel/Metylace_hemonch/SOFT/dorado_0.9.1/bin/:$PATH
export LD_LIBRARY_PATH=/storage/brno12-cerit/home/vorel/Metylace_hemonch/SOFT/dorado_0.9.1/lin/:$LD_LIBRARY_PATH
module add minimap2/2.22

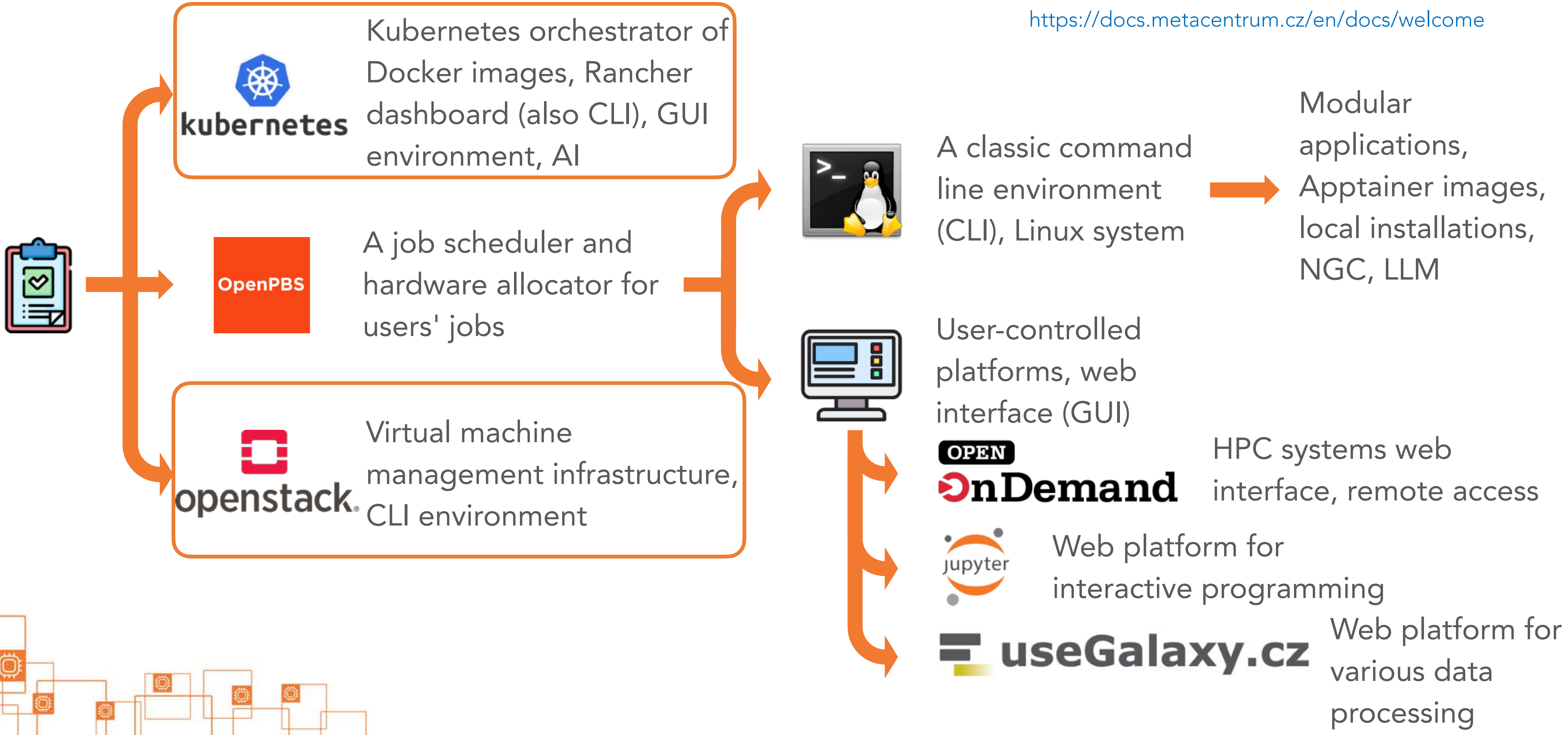
dorado basecaller dna_r9.4.1_e8_sup@v3.3 ./02_run1_IRE_reads.pod5 -v -x cuda:all --min-qscore 5 --trim all \
--reference haemonchus_contortus.PRJEB506.WBPS19.genomic.fa --modified-bases 5mCG_5hmCG > 03_dorado_run1_IRE.bam
```

- gpu_cap (a minimal version of GPU architecture)
- cuda_version (version of CUDA installed on the node)

https://docs.metacentrum.cz/en/docs/computing/gpu-comput/gpu-job

How to use it

https://docs.metacentrum.cz/en/docs/welcome



kubernetes – Kubernetes orchestrator of Docker images, Rancher dashboard (also CLI), GUI environment, AI

OpenPBS – A job scheduler and hardware allocator for users' jobs

openstack – Virtual machine management infrastructure, CLI environment

A classic command line environment (CLI), Linux system → Modular applications, Apptainer images, local installations, NGC, LLM

User-controlled platforms, web interface (GUI)

- **OPEN OnDemand** – HPC systems web interface, remote access
- **jupyter** – Web platform for interactive programming
- **useGalaxy.cz** – Web platform for various data processing

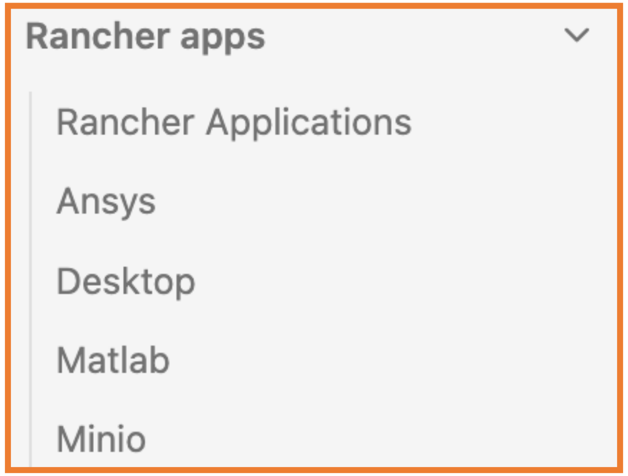
Kubernetes Container Platform

- Kubernetes

https://docs.cerit.io/en/docs/platform/overview

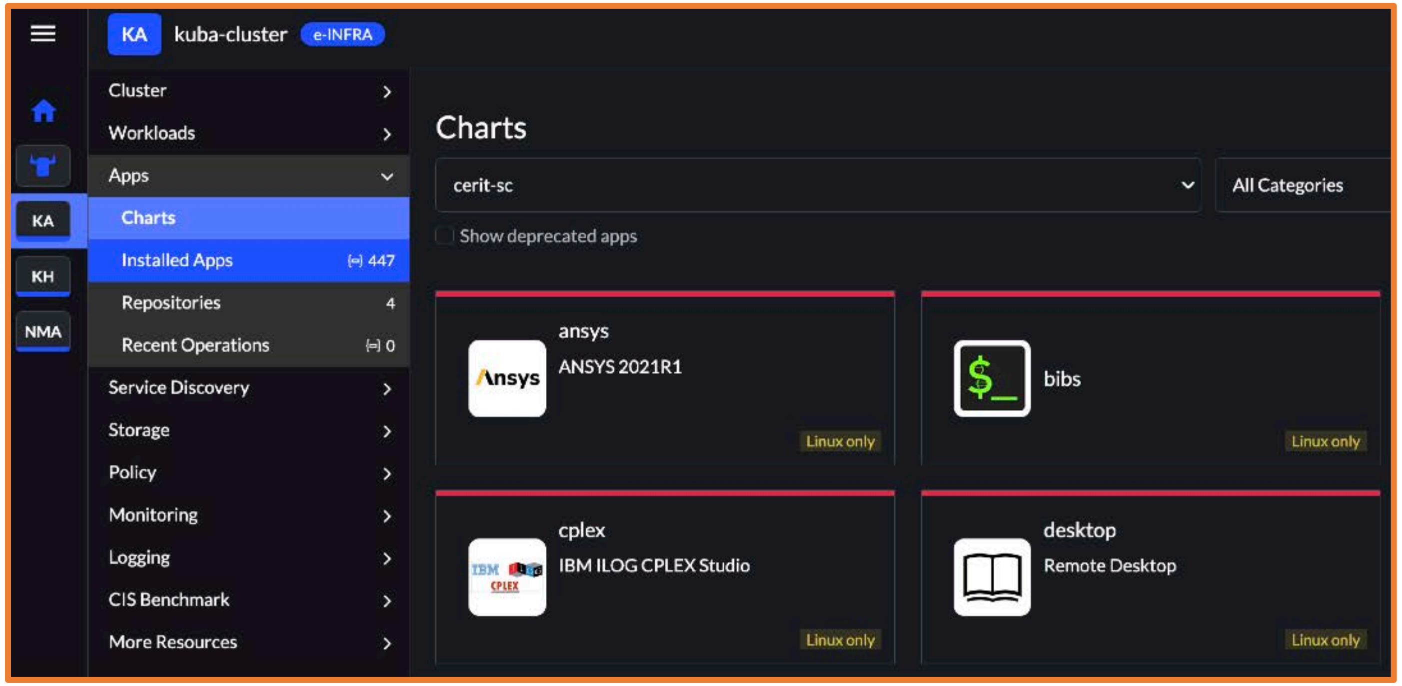
  - Open-source container orchestration engine that automates the deployment, scaling and management of containerised applications
  - A Docker image is an essential part of container infrastructure. It contains an application and all its necessary components, such as libraries and other files

https://docs.cerit.io/en/docs/news



Rancher apps

- Rancher Applications
- Ansys
- Desktop
- Matlab
- Minio



Kubernetes Container Platform

- Kubernetes
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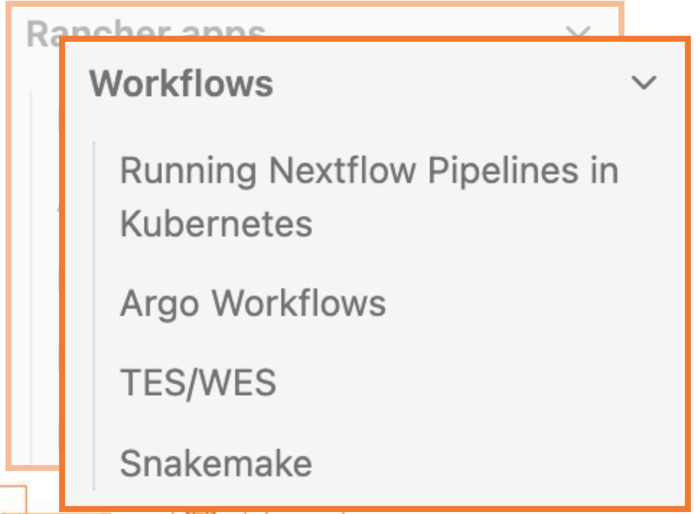
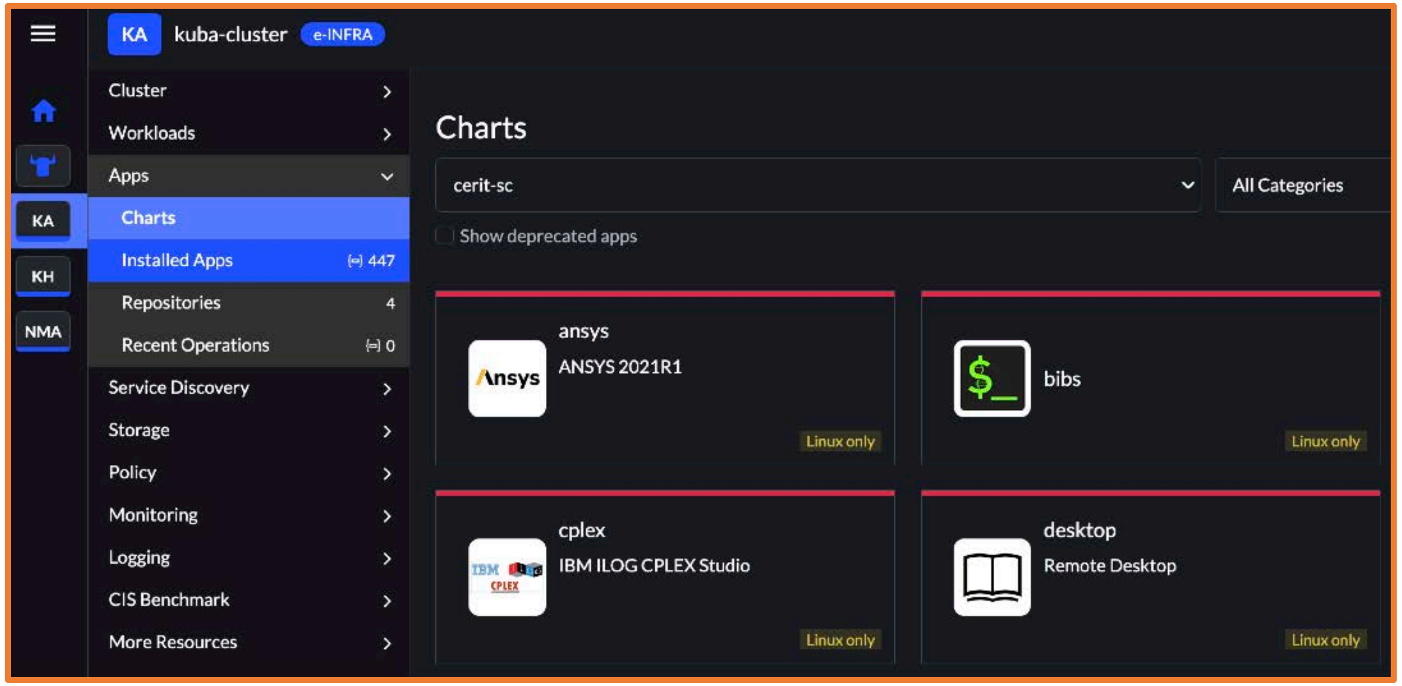
  - A Docker image is an essential part of container infrastructure. It contains an application and all its necessary components, such as libraries and other files

https://docs.cerit.io/en/docs/platform/overview

https://docs.cerit.io/en/docs/news



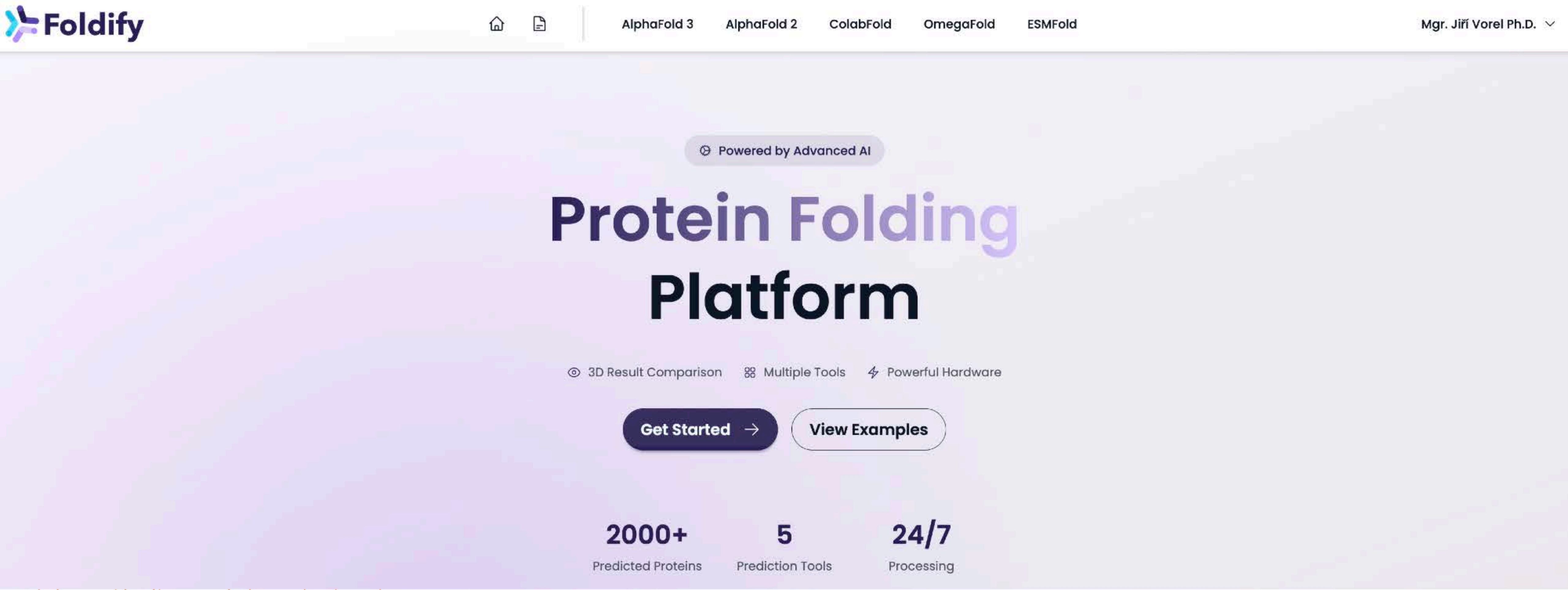


Foldify

It can also run as a batch job in the MetaCentrum grid infrastructure

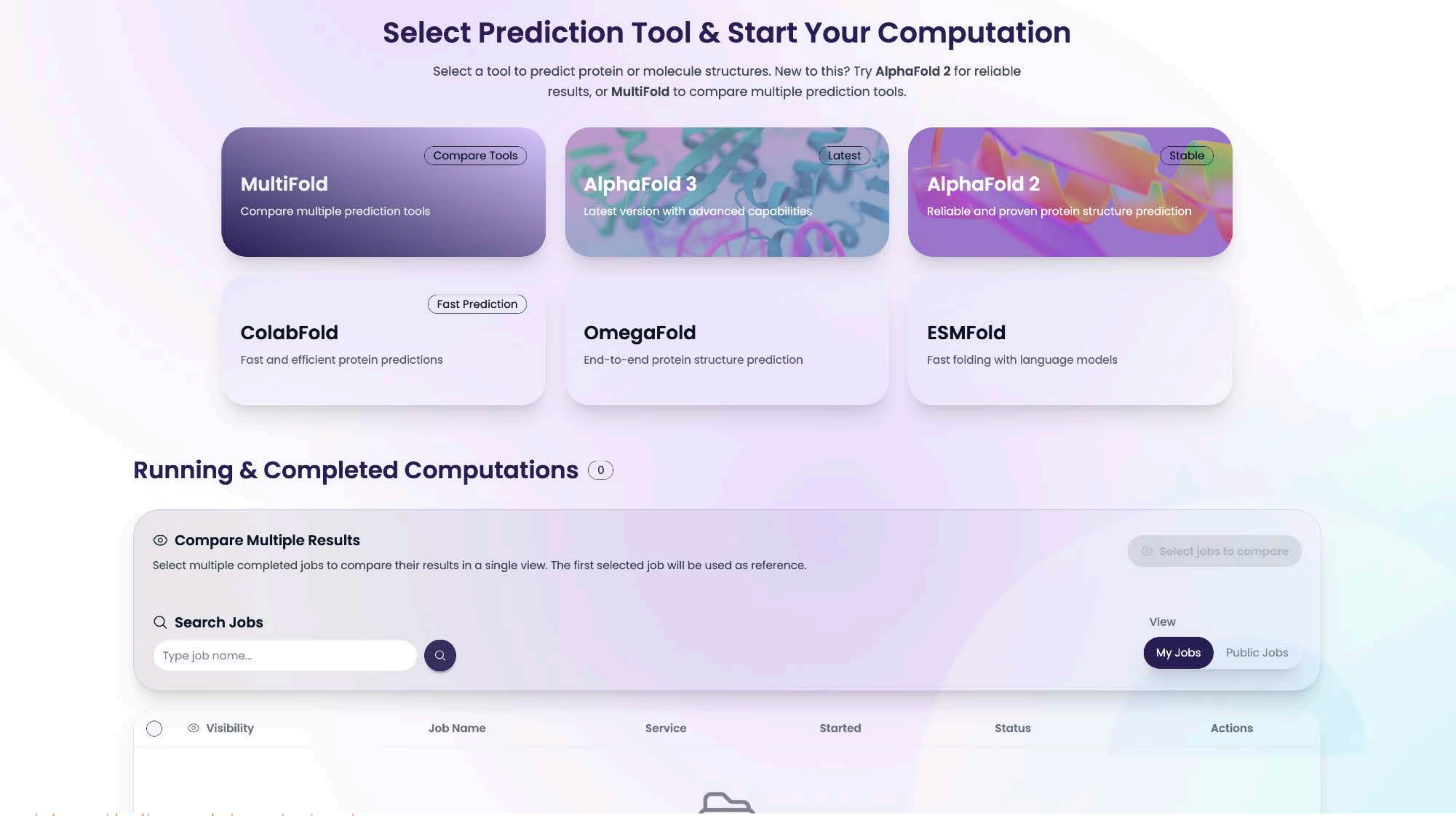
https://docs.cerit.io/en/docs/web-apps/foldify

- Foldify
  - A web application based on the Alphafold tools



Protein Folding Platform

2000+	5	24/7
Predicted Proteins	Prediction Tools	Processing



Select Prediction Tool & Start Your Computation

Select a tool to predict protein or molecule structures. New to this? Try **AlphaFold 2** for reliable results, or **MultiFold** to compare multiple prediction tools.

MultiFold
Compare multiple prediction tools

AlphaFold 3
Latest version with advanced capabilities

AlphaFold 2
Reliable and proven protein structure prediction

ColabFold
Fast and efficient protein predictions

OmegaFold
End-to-end protein structure prediction

ESMFold
Fast folding with language models

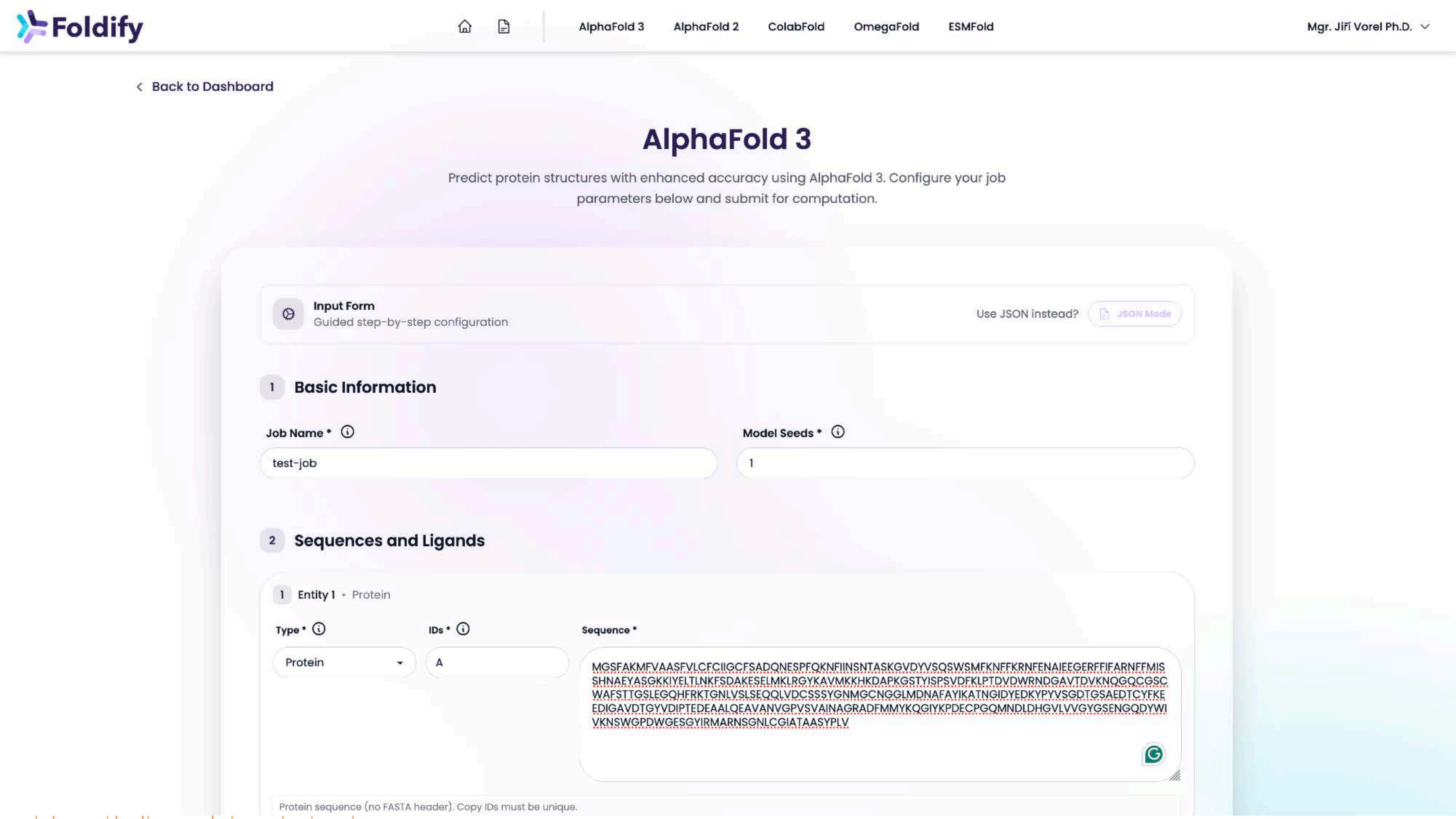
Running & Completed Computations (0)

Compare Multiple Results

Select multiple completed jobs to compare their results in a single view. The first selected job will be used as reference.

Search Jobs

○	Visibility	Job Name	Service	Started	Status	Actions



AlphaFold 3

Predict protein structures with enhanced accuracy using AlphaFold 3. Configure your job parameters below and submit for computation.

Input Form
Guided step-by-step configuration

Use JSON instead?

1 Basic Information

Job Name *: test-job

Model Seeds *: 1

2 Sequences and Ligands

1 Entity 1 • Protein

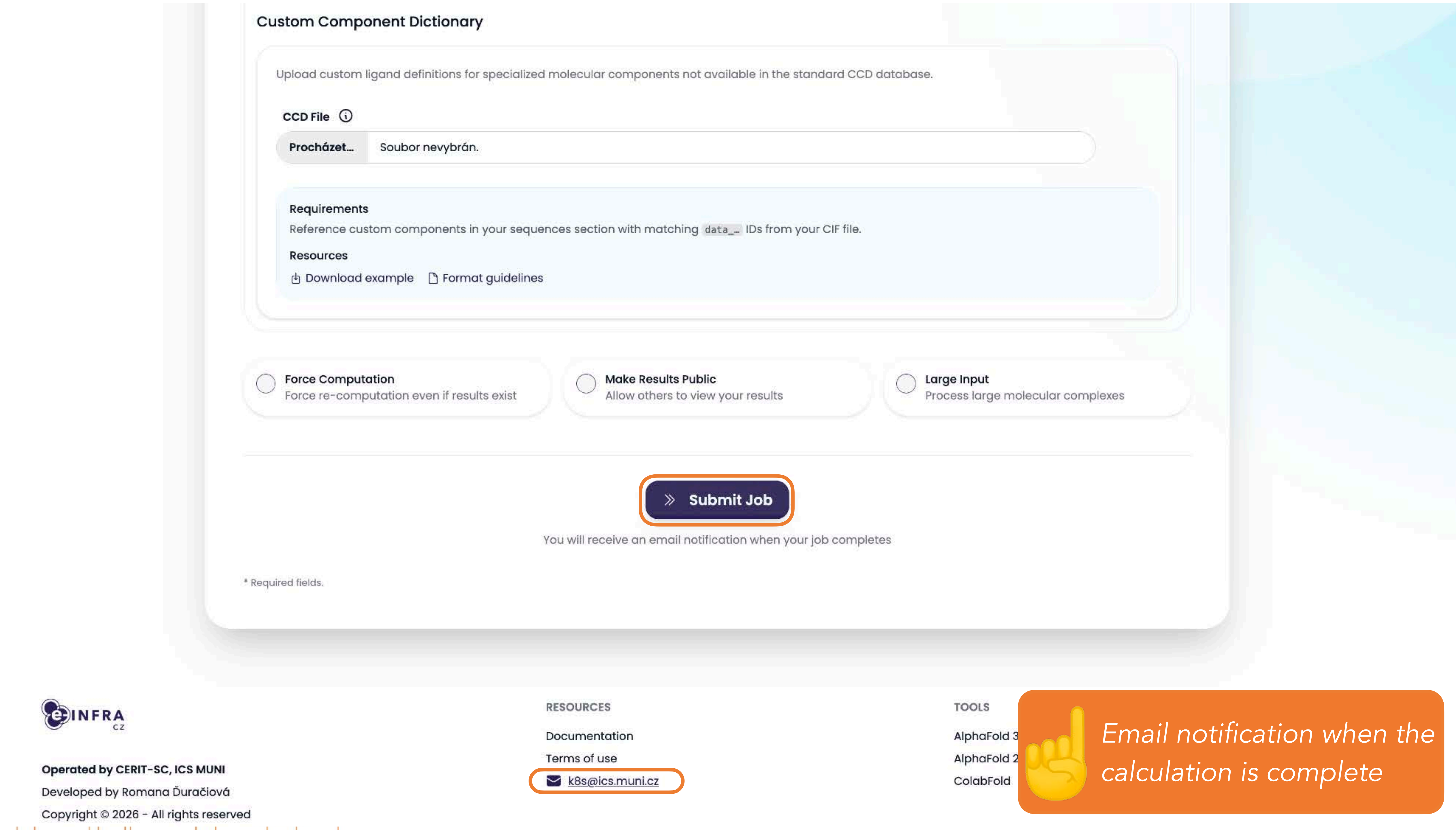
Type *: Protein

IDs *: A

Sequence *:

MGSFAKMFVAASFVLCFCIIGCFSADQNESPFQKNFIINSNTASKGVDYVSQSWSMFKNFFKRNFENAIEEGERFFIFARNFFMISSHNAEYASGKKIYELTLNKFSDAKESELMKLRGYKAVMKKHKDAPKGSTYISPSVDFKLPTDVDWRNDGAVTDVKNQGQCGSCWAFSTTGSLEGQHFRKTGNLVSLSEQQLVDCSSSYGNMGCNGGLMDNAFAYIKATNGIDYEDKYPYVSGDTGSAEDTCYFKEEDIGAVDTGYVDIPTEDEAALQEAVANVGPVSVAINAGRADFMMYKQGIYKPDECPGQMNDLDHGVLVVGYGSENGQDYWIVKNSWGPDWGESGYIRMARNSGNLCGIATAASYPLV

Protein sequence (no FASTA header). Copy IDs must be unique.



Custom Component Dictionary

Upload custom ligand definitions for specialized molecular components not available in the standard CCD database.

CCD File ⓘ

Requirements

Reference custom components in your sequences section with matching `data_…` IDs from your CIF file.

Resources

○ **Force Computation** Force re-computation even if results exist

○ **Make Results Public** Allow others to view your results

○ **Large Input** Process large molecular complexes

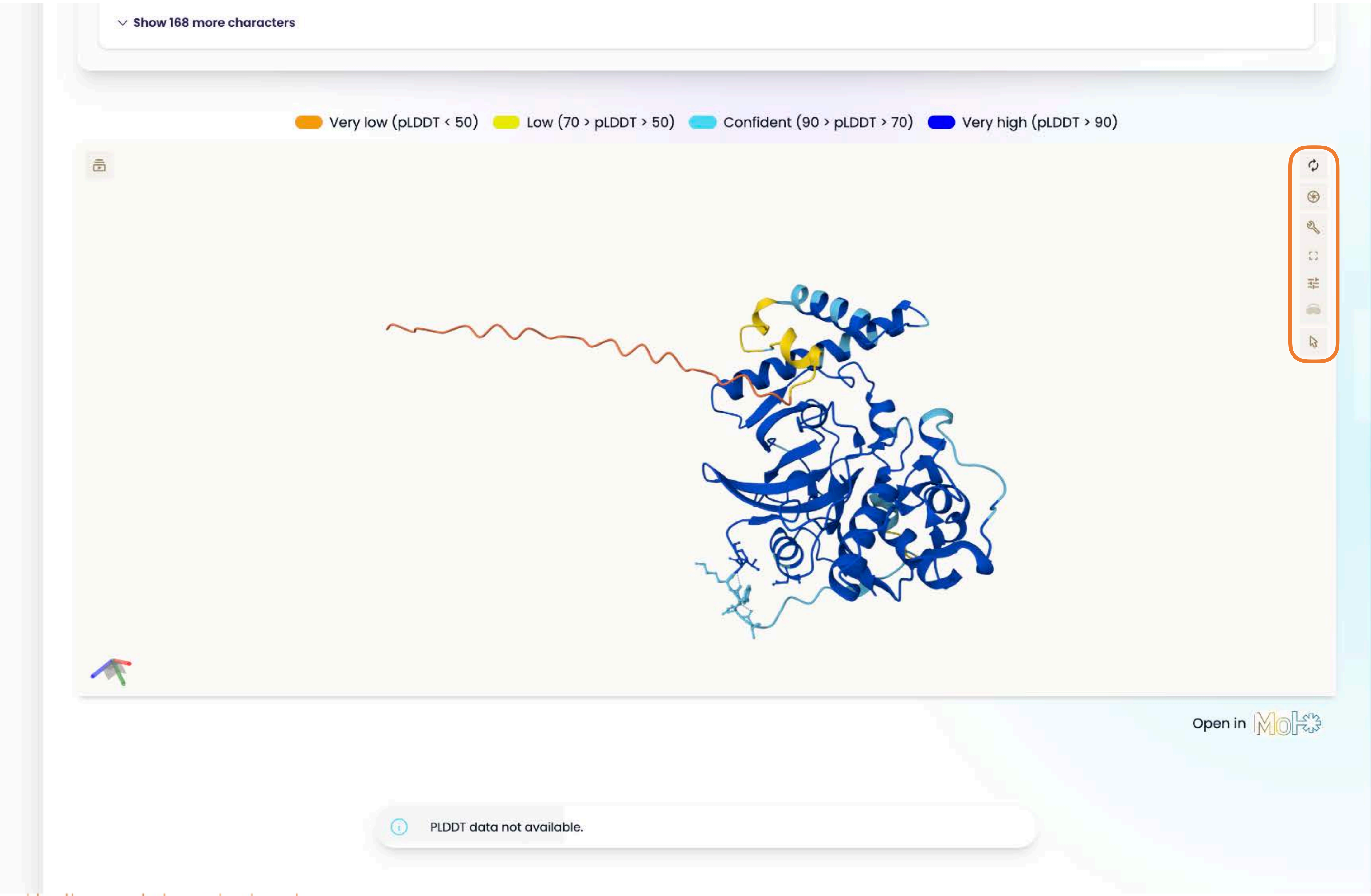
You will receive an email notification when your job completes

* Required fields.

Operated by CERIT-SC, ICS MUNI

Developed by Romana Ďuračiová

Email notification when the calculation is complete



Show 168 more characters

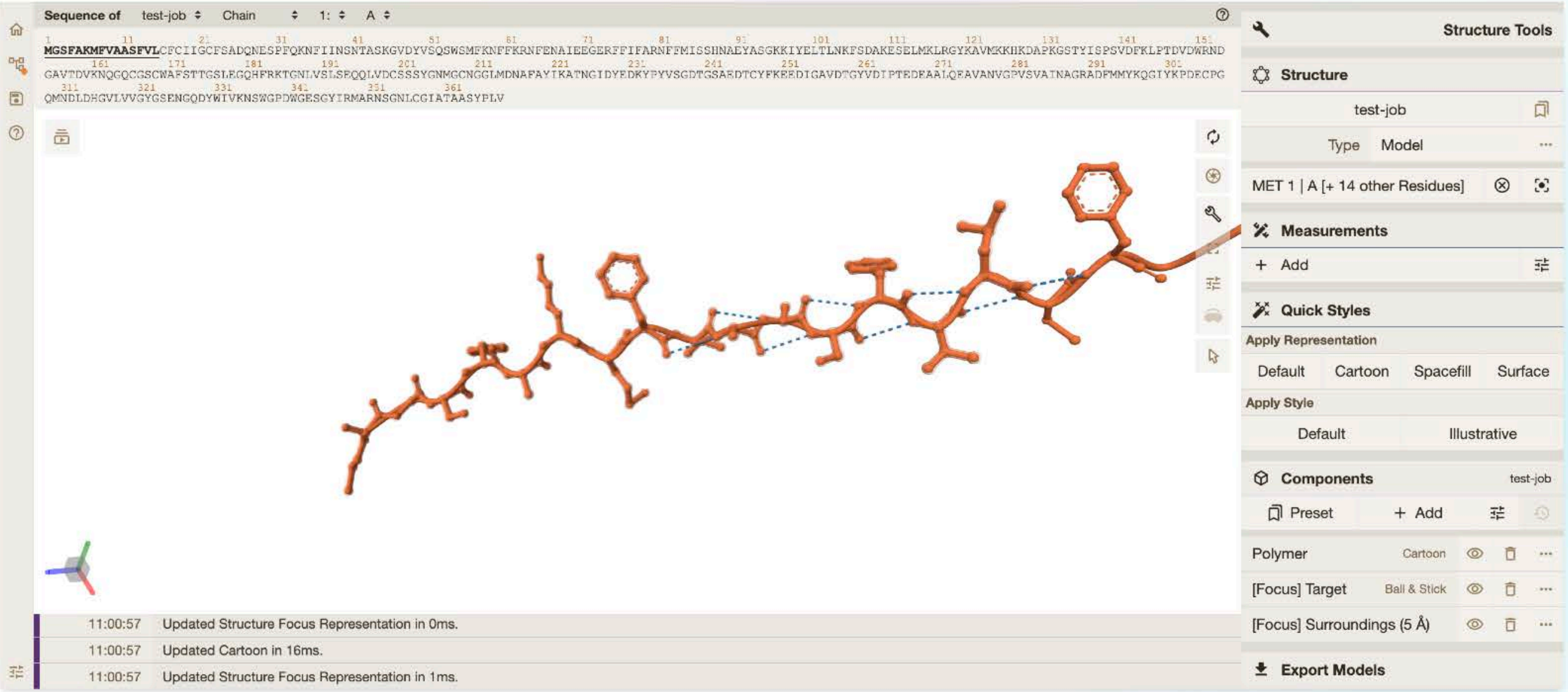
🟧 Very low (pLDDT < 50) 🟨 Low (70 > pLDDT > 50) 🟦 Confident (90 > pLDDT > 70) 🟦 Very high (pLDDT > 90)

PLDDT data not available.

```
MGSFAKMFVAASFVLCFCIIGCFSADQNESPFQKNFIINSNTASKGVDYVSQSWSMFKNFFKRNFENAIEEGERFFIFARNFFMISSHNAEYASGKKIYELTLNKFSDAKESELMKLRGYKAVMKKHKDAPKGSTYISPSVDFKLPTDVDWRNDGAVTDVK
NQGQCGSCWAFSTTGSLEGQHFRKTGNLVSLSEQQLVDC...
```

Show 168 more characters

🟧 Very low (pLDDT < 50) 🟨 Low (70 > pLDDT > 50) 🟦 Confident (90 > pLDDT > 70) 🟦 Very high (pLDDT > 90)



```
1         11        21        31        41        51        61        71        81        91        101       111       121       131       141       151
MGSFAKMFVAASFVLCFCIIGCFSADQNESPFQKNFIINSNTASKGVDYVSQSWSMFKNFFKRNFENAIEEGERFFIFARNFFMISSHNAEYASGKKIYELTLNKFSDAKESELMKLRGYKAVMKKHKDAPKGSTYISPSVDFKLPTDVDWRND
         161       171       181       191       201       211       221       231       241       251       261       271       281       291       301
GAVTDVKNQGQCGSCWAFSTTGSLEGQHFRKTGNLVSLSEQQLVDCSSSYGNMGCNGGLMDNAFAYIKATNGIDYEDKYPYVSGDTGSAEDTCYFKEEDIGAVDTGYVDIPTEDEAALQEAVANVGPVSVAINAGRADFMMYKQGIYKPDECPG
   311       321       331       341       351       361
QMNDLDHGVLVVGYGSENGQDYWIVKNSWGPDWGESGYIRMARNSGNLCGIATAASYPLV
```

```
11:00:57  Updated Structure Focus Representation in 0ms.
11:00:57  Updated Cartoon in 16ms.
11:00:57  Updated Structure Focus Representation in 1ms.
```

Open in Mol*

Related services

- Compute cloud

  https://docs.platforms.cloud.e-infra.cz/en/docs
  - Runs on OpenStack (allows users to create and manage their own cloud computing resources)
  - 17 computational clusters with 8,968 cores, 96 GPU cards, and 178 TB RAM
  - Virtual machines (CLI) are accessed using SSH keys
- Sensitive cloud

  https://docs.cerit.io/en/docs/sensitivecloud/account
  - Provides a secure computing and storage environment for sensitive data processing and research, operated by CERIT-SC (part of e-INFRA CZ)
  - Follows security standards such as ISO 27000, C5, ISO 15189, and ECRIN
  - Relies on container technology via Kubernetes, MFA required

CESNET S3 storage

- CESNET S3 service

  https://docs.du.cesnet.cz/en/docs/object-storage-s3/s3-service

  - Provided by the CESNET Data Storage Department
  - Long-term and secure storage for valuable scientific data (archive, backup)
  - Users must be registered and have generated keys (credentials) to configure any S3 client

    https://access.du.cesnet.cz/
  - S3 storage can be accessed via the command line or a GUI client (for Windows, Linux, Mac, OnDemand)
  - All scenarios are described step-by-step in the documentation
  - Any archived/backed up data should be free of unnecessary clutter and compressed appropriately
  - Data is organised into buckets (main directories)

CESNET S3 storage

CESNET S3 service

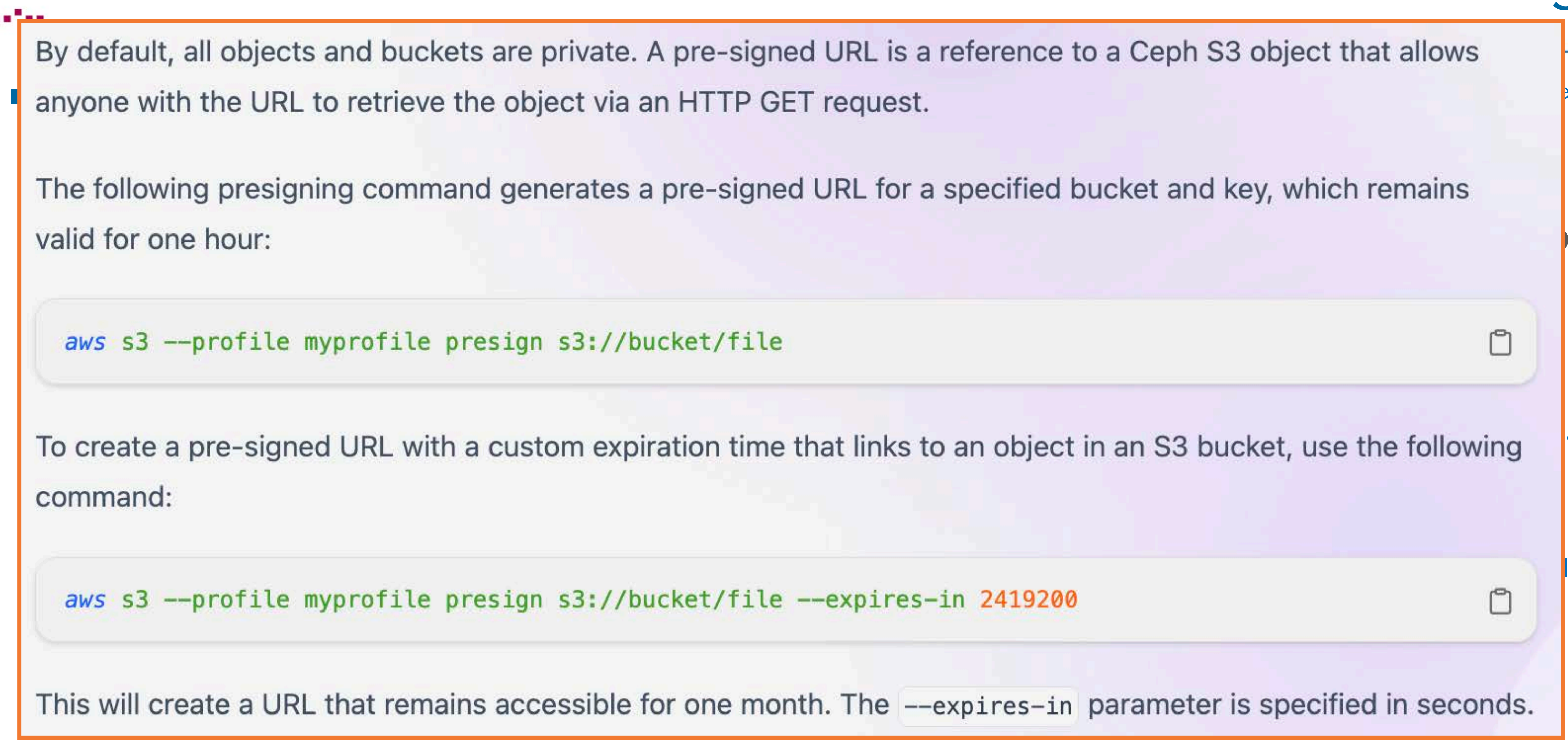
https://docs.du.cesnet.cz/en/docs/object-storage-s3/s3-service

- Personal space has a quota of 2 TB (increasable)
- Personal accounts do not support sharing between users and/or groups (by default, all objects and buckets are private)
- Data (buckets) can be shared via the manually generated temporary URLs

  https://docs.du.cesnet.cz/en/docs/object-storage-s3/s3-features#sharing-an-s3-object-using-presigned-url
- Or by setting up bucket policies for sharing

  https://docs.du.cesnet.cz/en/docs/object-storage-s3/s3-features#set-up-bucket-policies-for-sharing-aws-cli-s3-plugin

CESNET S3 storage



By default, all objects and buckets are private. A pre-signed URL is a reference to a Ceph S3 object that allows anyone with the URL to retrieve the object via an HTTP GET request.

The following presigning command generates a pre-signed URL for a specified bucket and key, which remains valid for one hour:

```
aws s3 --profile myprofile presign s3://bucket/file
```

To create a pre-signed URL with a custom expiration time that links to an object in an S3 bucket, use the following command:

```
aws s3 --profile myprofile presign s3://bucket/file --expires-in 2419200
```

This will create a URL that remains accessible for one month. The `--expires-in` parameter is specified in seconds.

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y

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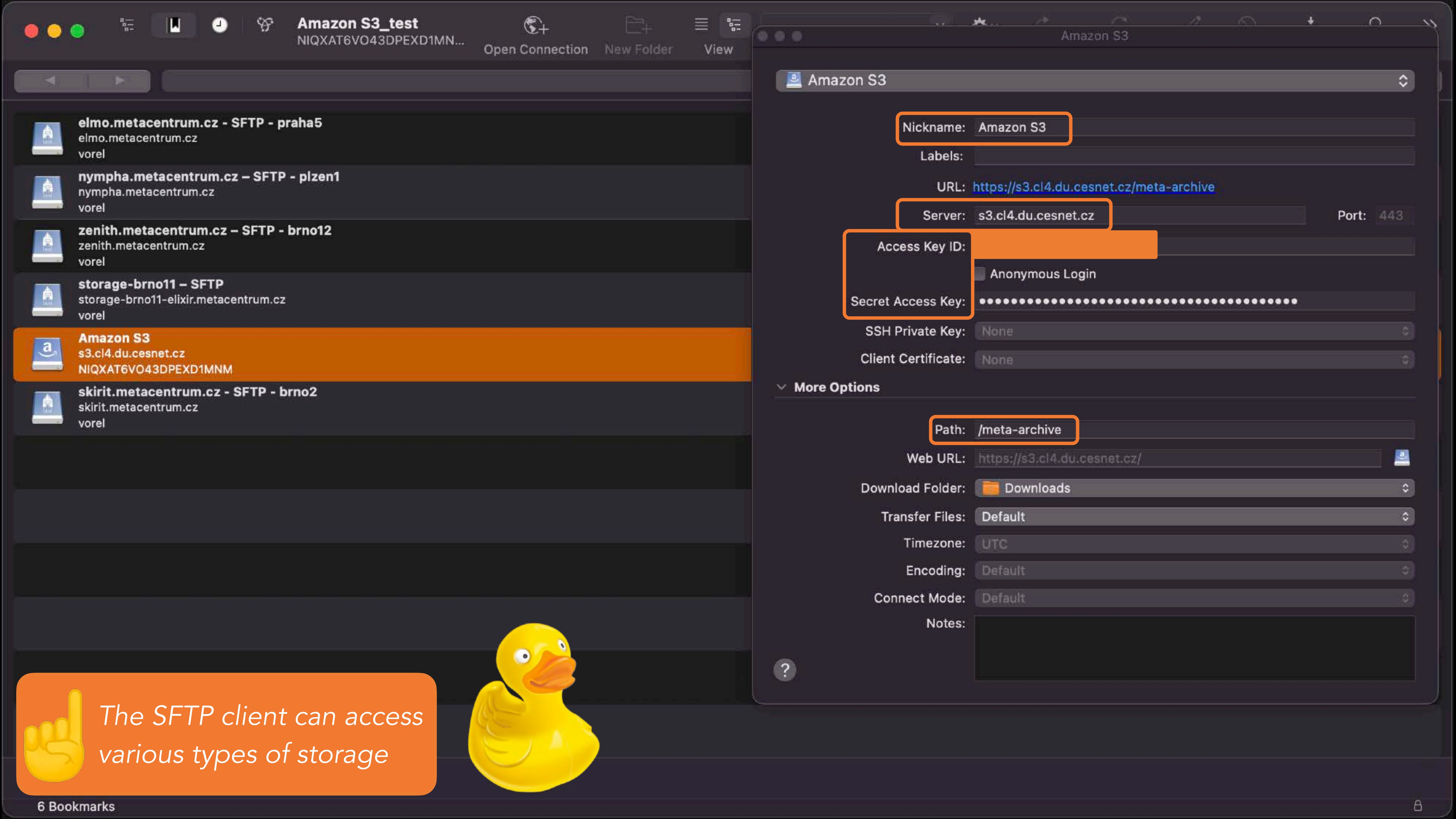


elmo.metacentrum.cz - SFTP - praha5
elmo.metacentrum.cz
vorel

nympha.metacentrum.cz – SFTP - plzen1
nympha.metacentrum.cz
vorel

zenith.metacentrum.cz – SFTP - brno12
zenith.metacentrum.cz
vorel

storage-brno11 – SFTP
storage-brno11-elixir.metacentrum.cz
vorel

Amazon S3
s3.cl4.du.cesnet.cz
NIQXAT6VO43DPEXD1MNM

skirit.metacentrum.cz - SFTP - brno2
skirit.metacentrum.cz
vorel

6 Bookmarks

Amazon S3

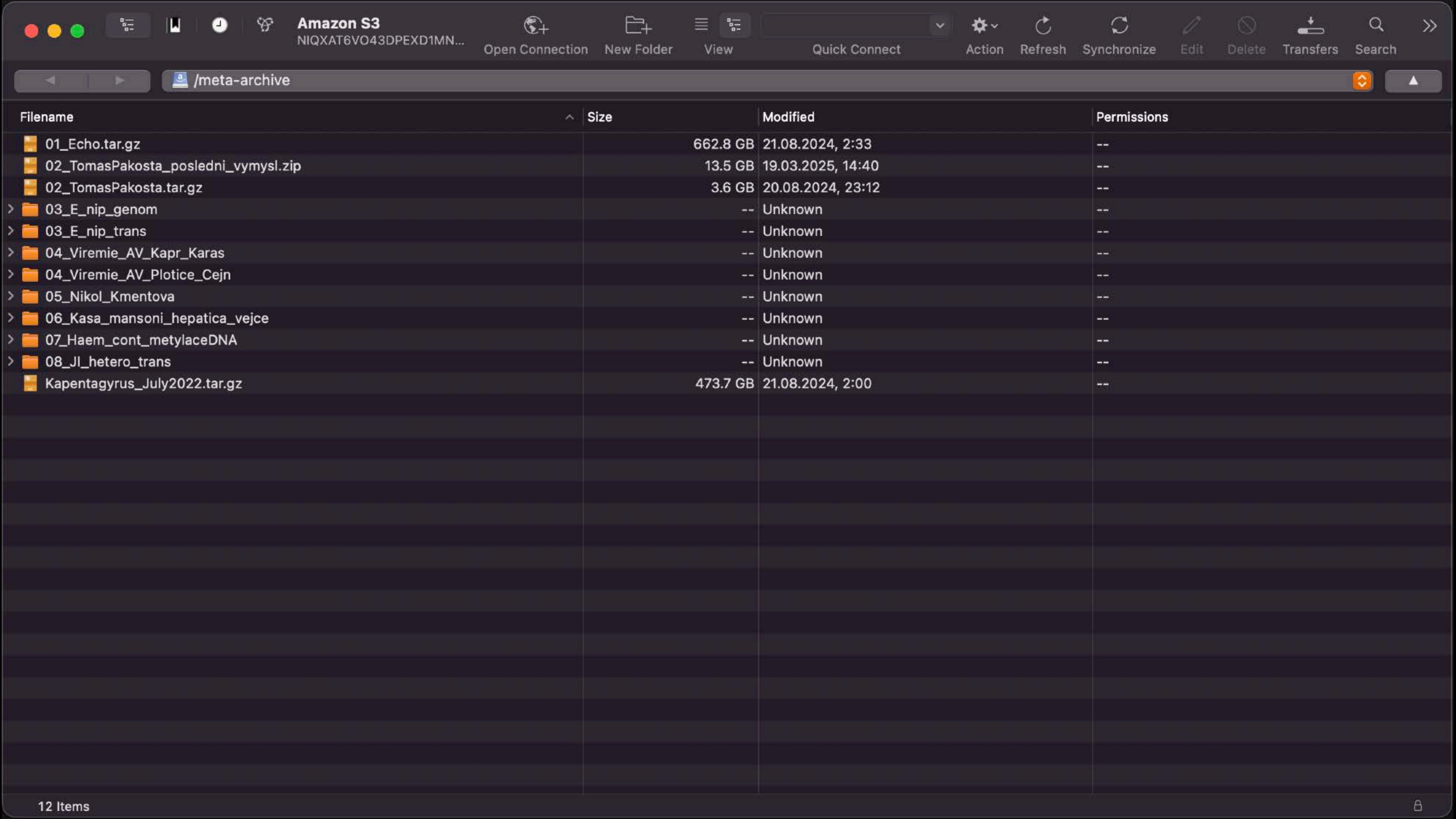
Amazon S3

Nickname: Amazon S3
Labels:
URL: https://s3.cl4.du.cesnet.cz/meta-archive
Server: s3.cl4.du.cesnet.cz
Port: 443
Access Key ID: [redacted]
☐ Anonymous Login
Secret Access Key: ••
SSH Private Key: None
Client Certificate: None

More Options

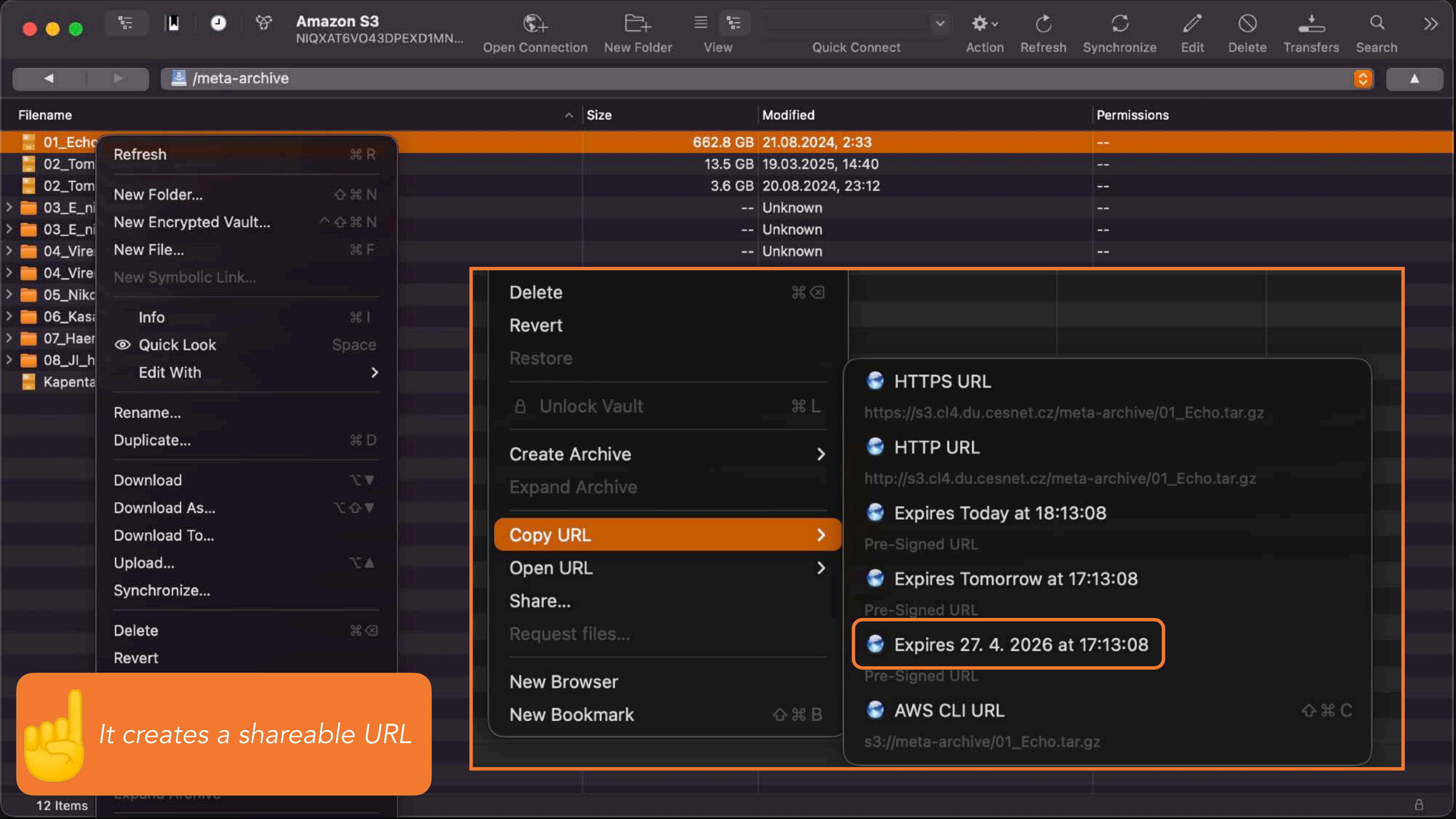
Path: /meta-archive
Web URL: https://s3.cl4.du.cesnet.cz/
Download Folder: Downloads
Transfer Files: Default
Timezone: UTC
Encoding: Default
Connect Mode: Default
Notes:

☝️ *The SFTP client can access various types of storage*



Filename	Size	Modified	Permissions
01_Echo.tar.gz	662.8 GB	21.08.2024, 2:33	--
02_TomasPakosta_posledni_vymysl.zip	13.5 GB	19.03.2025, 14:40	--
02_TomasPakosta.tar.gz	3.6 GB	20.08.2024, 23:12	--
03_E_nip_genom	--	Unknown	--
03_E_nip_trans	--	Unknown	--
04_Viremie_AV_Kapr_Karas	--	Unknown	--
04_Viremie_AV_Plotice_Cejn	--	Unknown	--
05_Nikol_Kmentova	--	Unknown	--
06_Kasa_mansoni_hepatica_vejce	--	Unknown	--
07_Haem_cont_metylaceDNA	--	Unknown	--
08_JI_hetero_trans	--	Unknown	--
Kapentagyrus_July2022.tar.gz	473.7 GB	21.08.2024, 2:00	--

12 Items

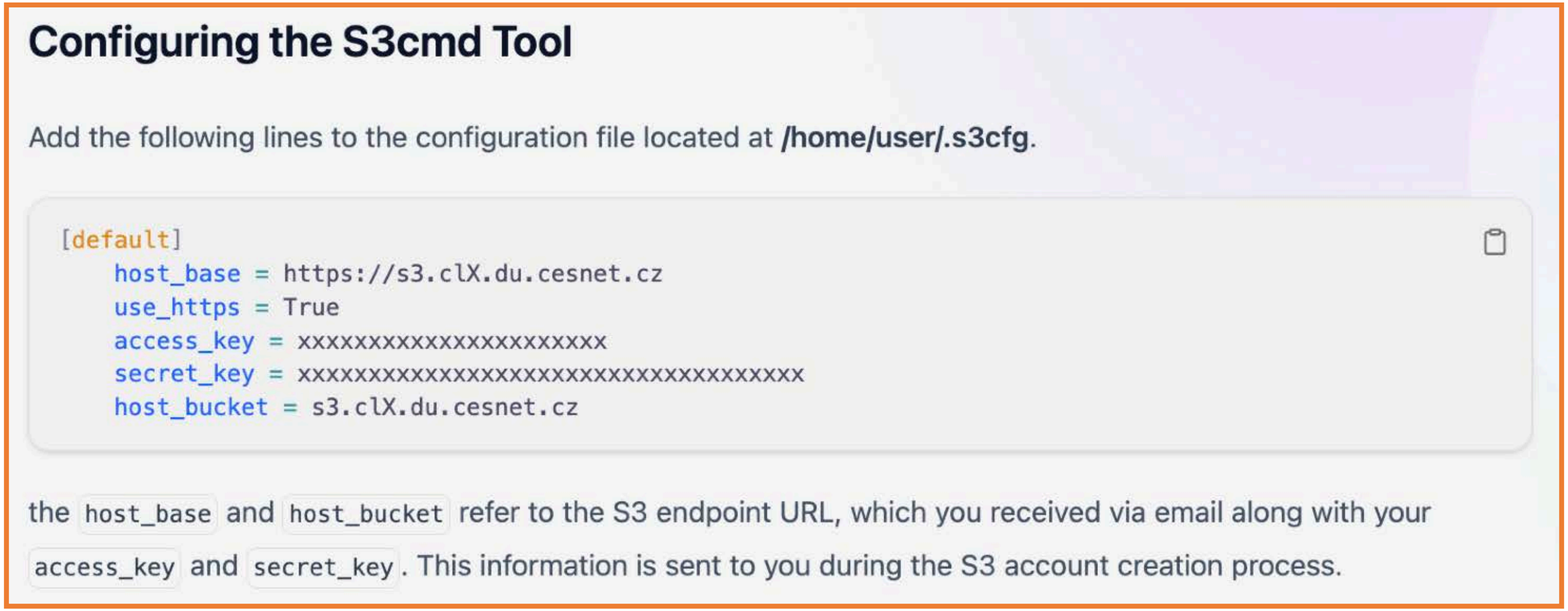


It creates a shareable URL

CESNET S3 storage

https://docs.du.cesnet.cz/en/docs/object-storage-s3/s3-service

- CESNET S3 service
  - S3 storage can be accessed from the MetaCentrum disk storages via CLI
  - For example *s3cmd*, *s5cmd* (faster version of *s3cmd*) or *aws* tools
  - Tools need to be configured with access keys



Configuring the S3cmd Tool

Add the following lines to the configuration file located at **/home/user/.s3cfg**.

```
[default]
    host_base = https://s3.clX.du.cesnet.cz
    use_https = True
    access_key = xxxxxxxxxxxxxxxxxxxxxx
    secret_key = xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
    host_bucket = s3.clX.du.cesnet.cz
```

the `host_base` and `host_bucket` refer to the S3 endpoint URL, which you received via email along with your `access_key` and `secret_key`. This information is sent to you during the S3 account creation process.

Related services

- FileSender
  - Web service for sending files
  - A download link is sent to the recipient and the file is stored for a maximum of one month before being automatically deleted
  - Connection with MetaCentrum is possible

https://du.cesnet.cz/en/navody/filesender/start

- OwnCloud
  - Cloud storage with 100 GB of space per user (increasable)
  - Clients are available for all OS (Windows, Linux, OS X, iOS, Android)
  - Automatic data synchronisation between multiple devices

https://du.cesnet.cz/en/navody/owncloud/start

Access is granted without the need for further registration

Conclusions

https://www.cesnet.cz/ https://www.metacentrum.cz/

https://www.e-infra.cz/ https://docs.metacentrum.cz/

- Free and immediately accessible, no grant proposals
- All we ask: acknowledge e-INFRA CZ (ID:90254) in your publications
- For everyone, no programming skills required
- Scales with your needs, from a small interactive session to large and long-term parallel jobs
- Hundreds of tools included, ready to use
- Dedicated user support and step-by-step documentation