

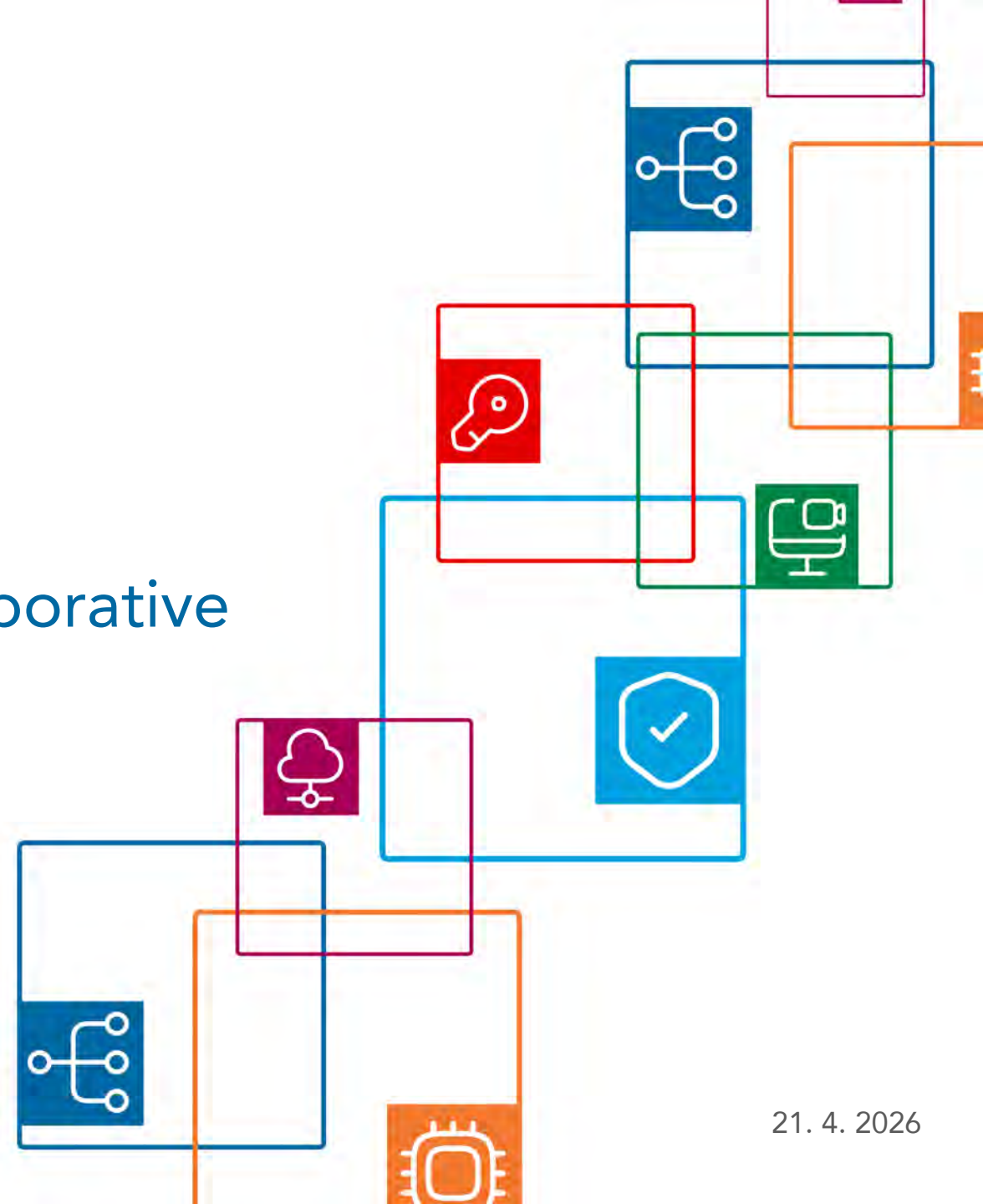
MetaCentrum NGI

For scientific computations, collaborative research and its support services

Jiří Vorel

Mendel University in Brno

vorel@cesnet.cz meta@cesnet.cz



■ CESNET is

- An association of Czech universities and the Academy of Sciences that operates a high-speed national e-infrastructure dedicated to science, research, and education
- Available to the academic and research community in the Czech Republic (CESNET members)
- Part of the e-INFRA CZ e-infrastructure

<https://www.cesnet.cz/>

<https://www.e-infra.cz/>

Network



CESNET – an academic computer network with a range of ICT services.



Computing



MetaCentrum – processing big data and demanding tasks.



Data storage



Tools for backing up, archiving and sharing user data.



Security



Robust cybersecurity monitoring and enforcement.



Multimedia



Services for remote study and work, for individuals and teams.



Identity



Secure login to CESNET & a portfolio of connected services.



- CESNET offers (for individuals)

<https://www.cesnet.cz/en/services>

- NGI MetaCentrum for complex calculations and scientific data processing

<https://www.metacentrum.cz/en/>

- Data storage for storing scientific data <https://docs.du.cesnet.cz/en/docs/introduction/introduction>

- OwnCloud service for data synchronisation and sharing

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

- FileSender for temporary data exchange <https://du.cesnet.cz/en/navody/filesender/start>

- Zoom platform for web conferences <https://vidcon.cesnet.cz/cs/app/ac/zoomterms>



Experience and excellence in leading tech solutions

WE ARE CESNET WE UNITE SCIENCE

We deliver advanced ICT services for science, research, and education. As pioneers of the first academic networks nearly 30 years ago, we maintain them to this day, ensure secure access, and provide robust environments for data storage, high-performance computing, and team collaboration. Our members include public universities and the Academy of Sciences of the Czech Republic.

[About CESNET](#)

We push boundaries

We explore new frontiers in information and communication technologies, transforming our research into practical, advanced services.

Our services

Network



Computing



Data storage



Security



Multimedia



Identity



Individual services



Services are directly accessible to all students, researchers, academics, and university staff.

MetaCentrum



FileSender



ownCloud



Meetings



Useful links



Current backbone load



Speedtest



Looking Glass

■ e-INFRA CZ

- Large research infrastructure
- E-infrastructure for research and development in the Czech Republic
- Provides capacities and resources for the transmission, storage and processing of scientific data
- Supercomputing, grid and cloud computing, secure high-capacity distributed data storage, software tools
- Consortium of CESNET + CERIT-SC + IT4Innovations



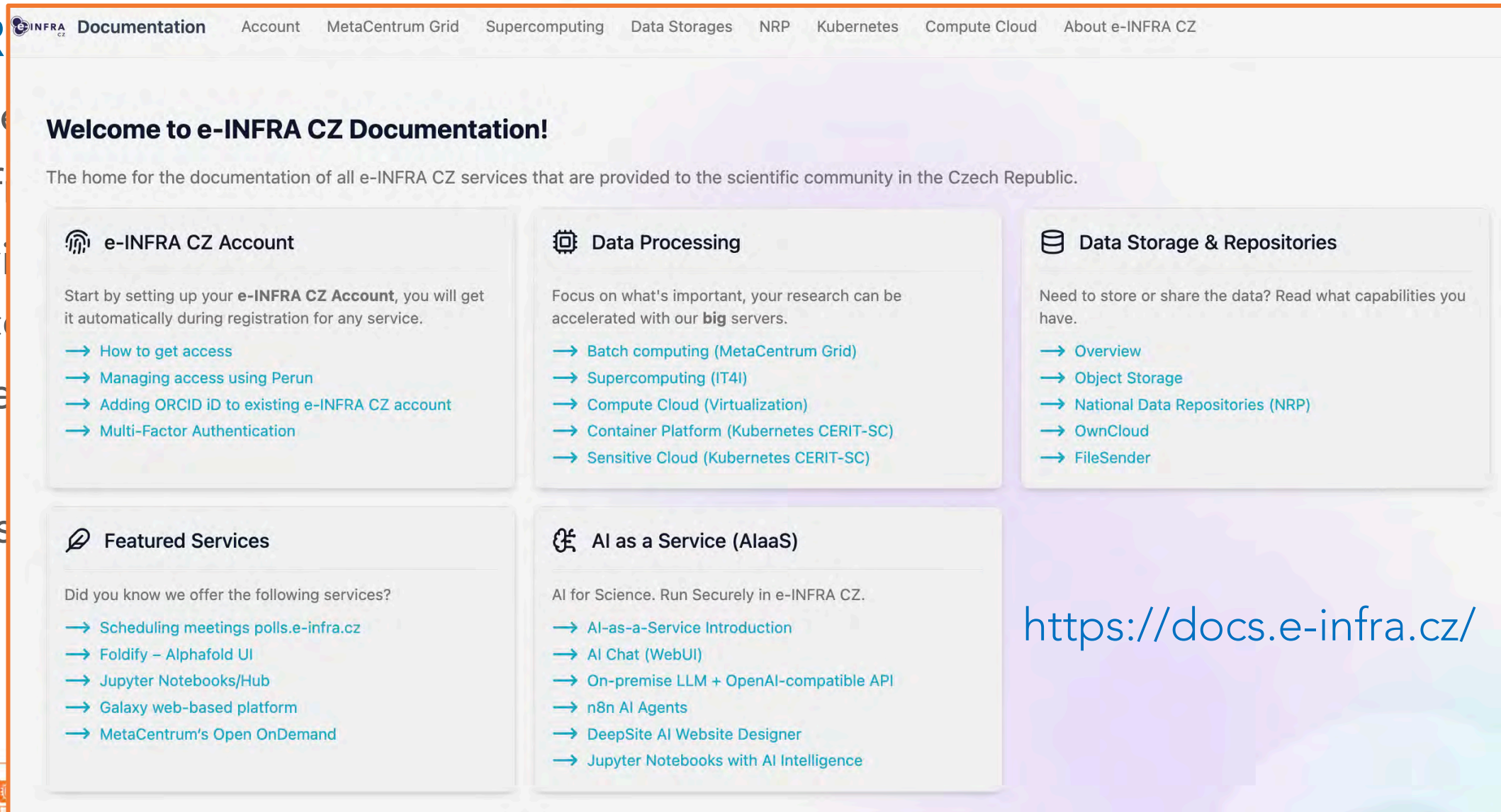


A complete overview of e-INFRA CZ services

e-INFRA CZ

■ e-INFRA CZ

- Large
- E-inf
- Provi
- proc
- Super
- data
- Cons



The screenshot shows the e-INFRA CZ Documentation website. The navigation bar includes: Documentation, Account, MetaCentrum Grid, Supercomputing, Data Storages, NRP, Kubernetes, Compute Cloud, and About e-INFRA CZ. The main content area features a welcome message and several service categories:

- Welcome to e-INFRA CZ Documentation!**
The home for the documentation of all e-INFRA CZ services that are provided to the scientific community in the Czech Republic.
- e-INFRA CZ Account**
Start by setting up your **e-INFRA CZ Account**, you will get it automatically during registration for any service.
 - [How to get access](#)
 - [Managing access using Perun](#)
 - [Adding ORCID iD to existing e-INFRA CZ account](#)
 - [Multi-Factor Authentication](#)
- Data Processing**
Focus on what's important, your research can be accelerated with our **big** servers.
 - [Batch computing \(MetaCentrum Grid\)](#)
 - [Supercomputing \(IT4I\)](#)
 - [Compute Cloud \(Virtualization\)](#)
 - [Container Platform \(Kubernetes CERIT-SC\)](#)
 - [Sensitive Cloud \(Kubernetes CERIT-SC\)](#)
- Data Storage & Repositories**
Need to store or share the data? Read what capabilities you have.
 - [Overview](#)
 - [Object Storage](#)
 - [National Data Repositories \(NRP\)](#)
 - [OwnCloud](#)
 - [FileSender](#)
- Featured Services**
Did you know we offer the following services?
 - [Scheduling meetings polls.e-infra.cz](#)
 - [Foldify – Alphafold UI](#)
 - [Jupyter Notebooks/Hub](#)
 - [Galaxy web-based platform](#)
 - [MetaCentrum's Open OnDemand](#)
- AI as a Service (AlaaS)**
AI for Science. Run Securely in e-INFRA CZ.
 - [AI-as-a-Service Introduction](#)
 - [AI Chat \(WebUI\)](#)
 - [On-premise LLM + OpenAI-compatible API](#)
 - [n8n AI Agents](#)
 - [DeepSite AI Website Designer](#)
 - [Jupyter Notebooks with AI Intelligence](#)

<https://docs.e-infra.cz/>

MetaCentrum in a nutshell

■ MetaCentrum is

- A national grid infrastructure (NGI)
- The activity of the CESNET association
- Part of the e-INFRA CZ e-infrastructure
- 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)
- Secured and trustful service

<https://www.cesnet.cz/>

<https://www.metacentrum.cz/>

<https://www.e-infra.cz/>

<https://docs.metacentrum.cz/>



■ MetaCentrum is

- A national grid infrastructure (NGI)
- The activity of the CESNET association
- Part of the e-INFRA CZ e-infrastructure
- A provider of computational resources, application software (both commercial and free/open source) and data storage

<https://www.cesnet.cz/>

<https://www.metacentrum.cz/>

<https://www.e-infra.cz/>

<https://docs.metacentrum.cz/>



Acknowledgement formula for the MetaCentrum infrastructure

Computational resources were provided by the e-INFRA CZ project (ID:90254), supported by the Ministry of Education, Youth and Sports of the Czech Republic.

Acknowledgement formula for ELIXIR CZ resources

Computational resources were provided by the ELIXIR-CZ project (ID:90255), part of the international ELIXIR infrastructure.

■ MetaCentrum offers

- Access without the grant competitions
- The possibility to apply for membership at any time
- Access to all resources without submitted projects (with one exception)
- Immediate access to hardware resources and licences (once an application has been approved)
- Grid (shared) usage principle (privileged access for cluster owners)
- CPU/GPU resources, CLI access, GUI applications, Kubernetes and cloud services, etc.
- Various application software (commercial, free and open source)
- Sharing data within a group

<https://www.cesnet.cz/>

<https://www.metacentrum.cz/>

<https://www.e-infra.cz/>

<https://docs.metacentrum.cz/>



MetaCentrum in a nutshell

■ MetaCentrum offers

- Access without the grant competitions
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- CPU/GPU resources, CLI access, services, etc.
- Various application software (compilers, etc.)
- Sharing data within a group

<https://www.cesnet.cz/>

<https://www.metacentrum.cz/>

<https://www.e-infra.cz/>

<https://docs.metacentrum.cz/>



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)
- Providing extreme amounts of resources to individual tasks
- 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

<https://www.cesnet.cz/>

<https://www.metacentrum.cz/>

<https://www.e-infra.cz/>

<https://docs.metacentrum.cz/>

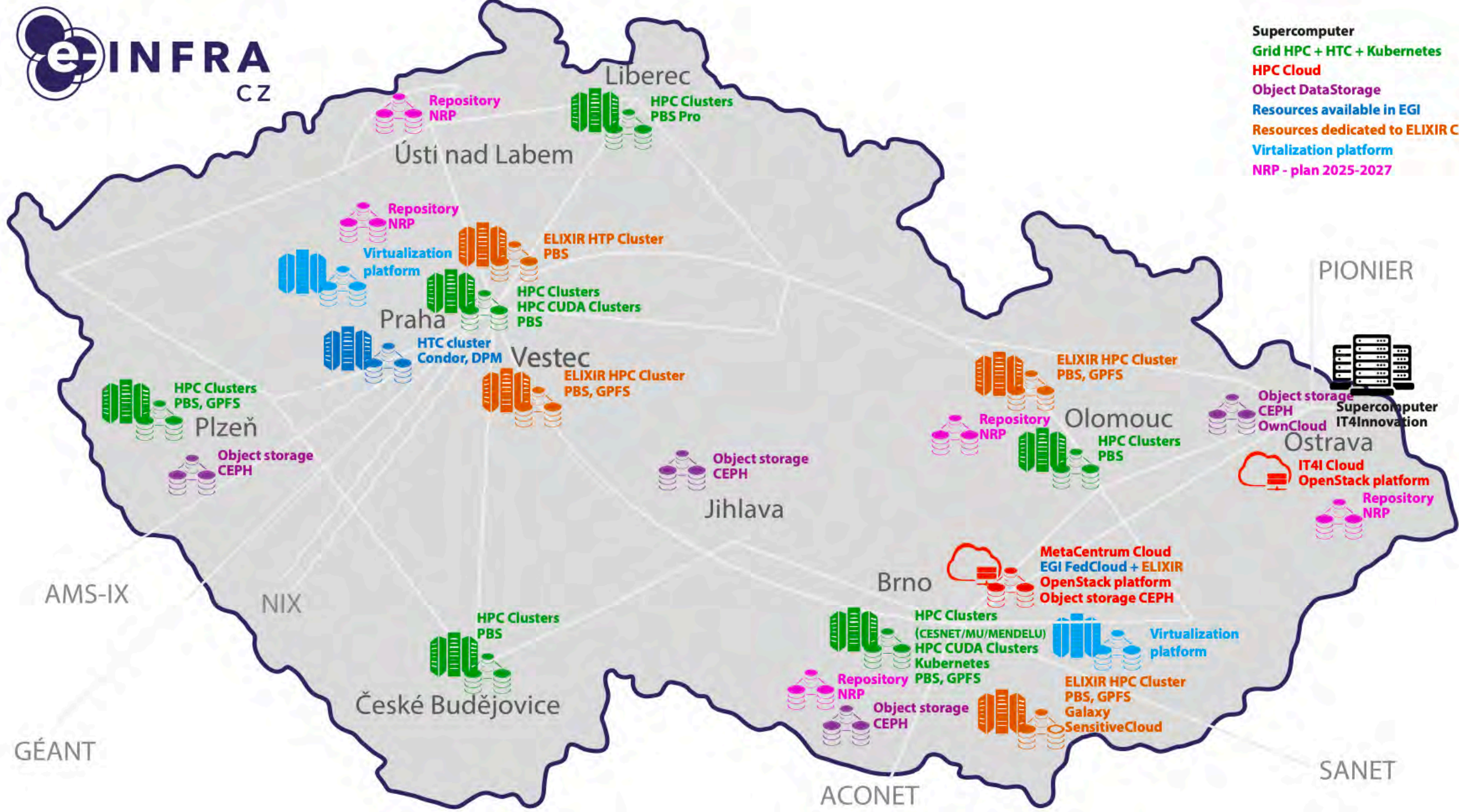
<https://du.cesnet.cz/>

cesnet
datacare
■■■■■

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



- Supercomputer
- Grid HPC + HTC + Kubernetes
- HPC Cloud
- Object DataStorage
- Resources available in EGI
- Resources dedicated to ELIXIR CZ
- Virtualization platform
- NRP - plan 2025-2027

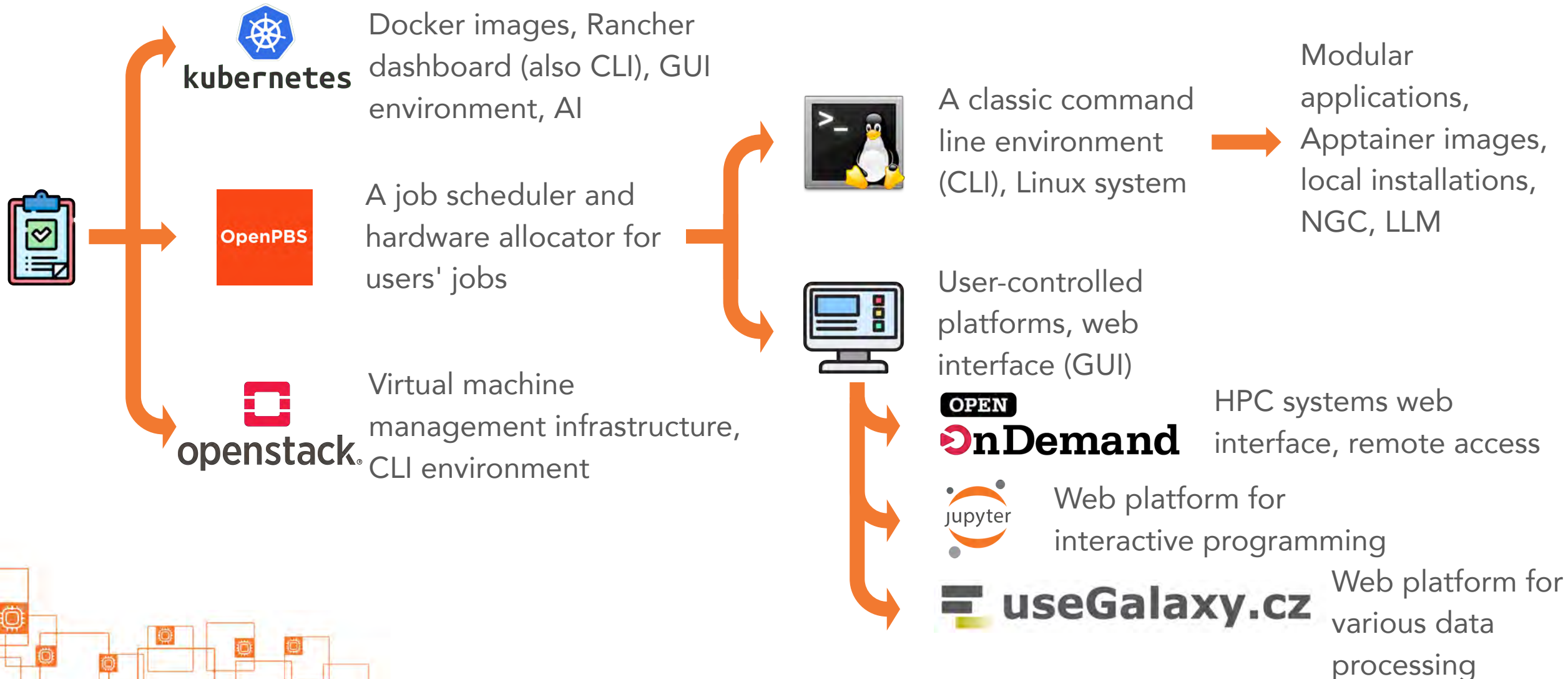


A close-up, high-angle shot of the One Ring from J.R.R. Tolkien's Middle-earth. The ring is positioned diagonally, showing its inner and outer surfaces. It is inscribed with the Elvish word 'Eärendil' in the Tengwar script. The ring is set against a background of a golden, textured fabric, possibly silk or a similar material, which has a subtle, repeating pattern. The lighting is warm and dramatic, highlighting the metallic sheen of the ring and the intricate details of the script. The overall mood is one of ancient power and mystery.

ONE APPLICATION TO RULE THEM ALL

One application to rule them all

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

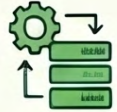


MetaCentrum in Numbers 2025



registered users

4 621



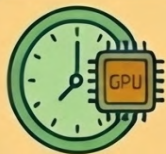
PBS (meta-pbs)



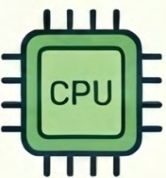
7.6 mil.
jobs



25 392
CPU years



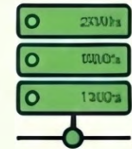
283
GPU years



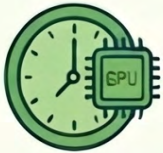
39 988
CPU cores /
332 GPU



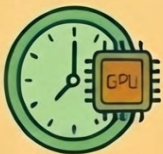
OPENSTACK



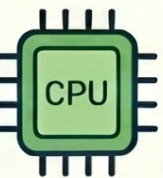
80.7 thous.
VM



10 586
CPU years



59
GPU years



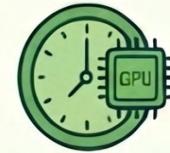
9 670
CPU cores /
84 GPU



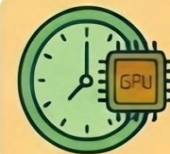
KUBERNETES



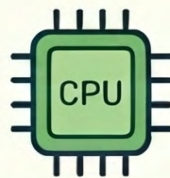
6.4 mil.
pods



1 760
CPU years



43
GPU years

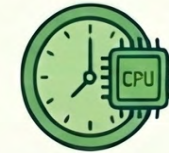


3 008
CPU cores /
47 GPU

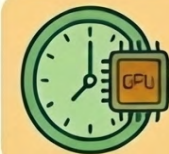


SENSITIVE CLOUD

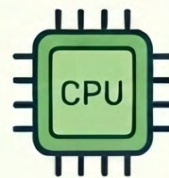
37.8 thous.
pods



657
CPU years

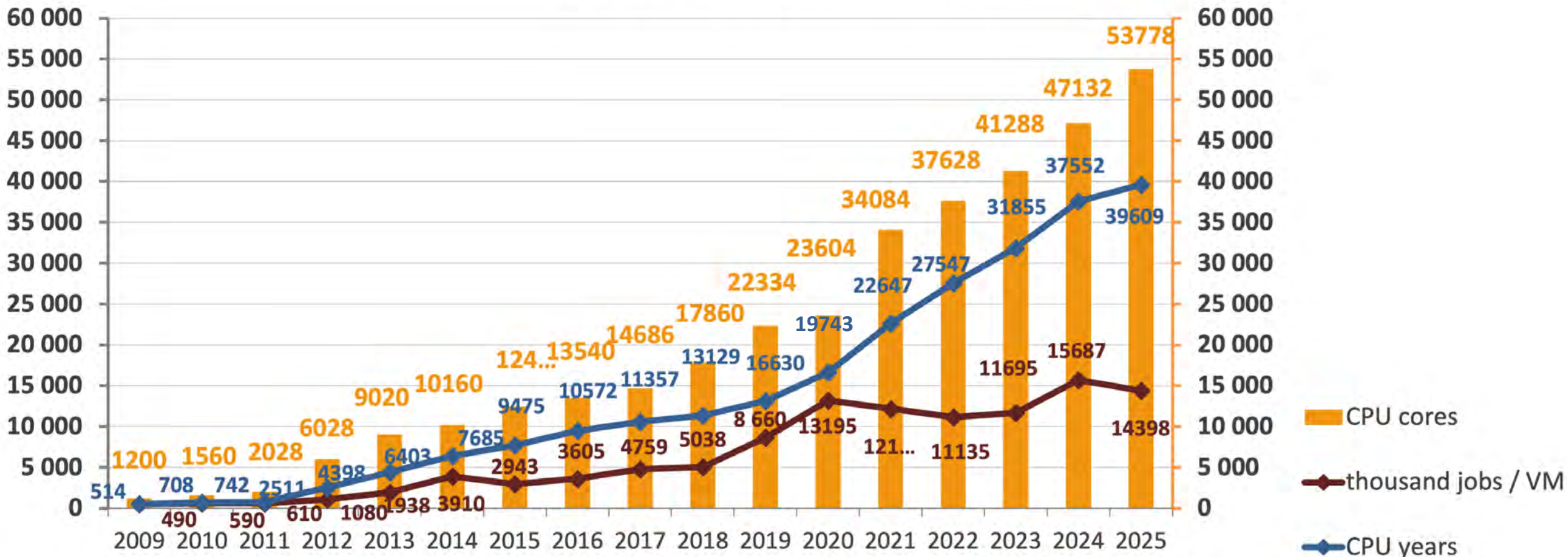


35
GPU years



1 112
CPU cores /
40 GPU

Number of CPUs, executed jobs and corresponding CPU years (PBS, Cloud, K8s, Sensitive Cloud)

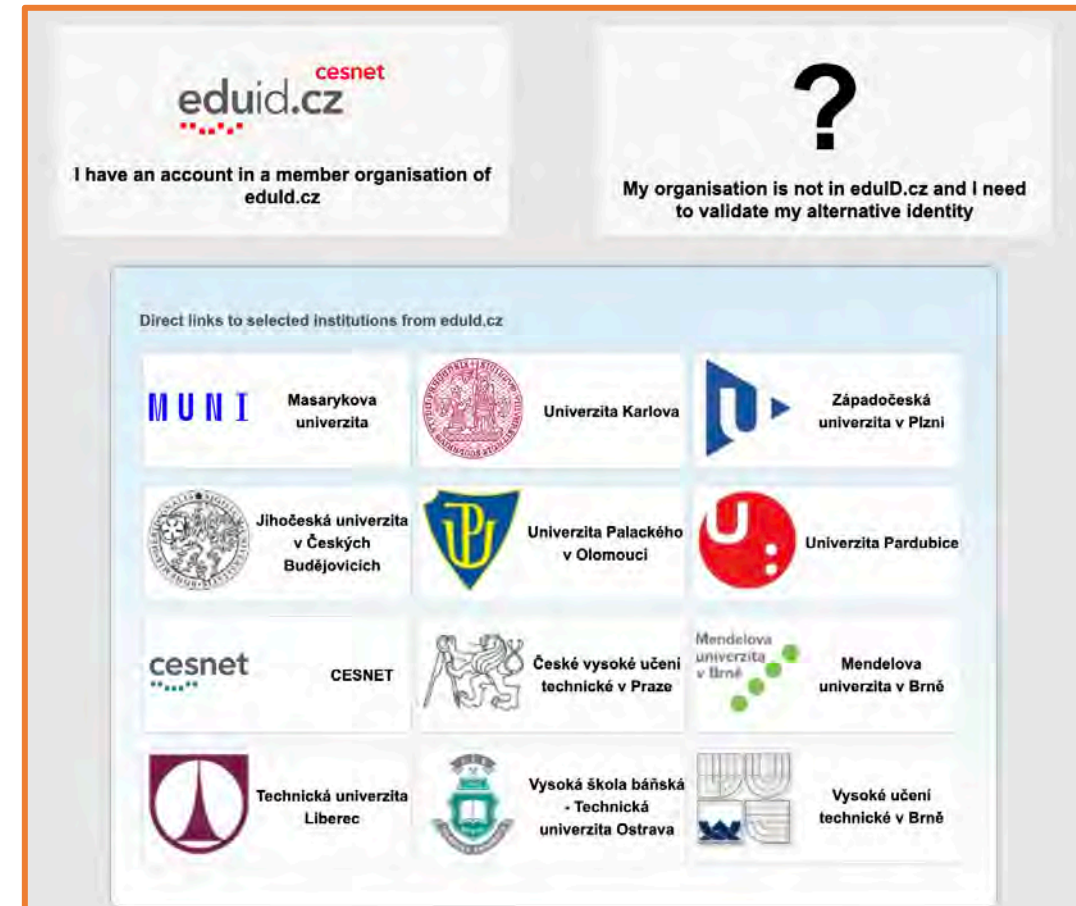


<https://docs.metacentrum.cz/en/docs/access/account>

<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 are valid until 2 February of the following year
- Accounts are renewed in January
- Immediate access to hardware resources
- Partner access by prior arrangement



http
http



Most new applications are approved within one or two working days

Submitting an application



Choose your home institution

... manual approval

Log in through the institution (i.e. local name and password) from the eduID federation

- Accounts are valid until 2 February of the following year
- Accounts are renewed in January
- Immediate access to hardware resources
- Partner access by prior arrangement

The screenshot shows the eduID.cz login interface. At the top left is the eduID.cz logo with the text "I have an account in a member organisation of eduID.cz". To its right is a question mark icon with the text "My organisation is not in eduID.cz and I need to validate my alternative identity". Below these are "Direct links to selected institutions from eduID.cz". A grid of 12 institution logos is displayed, including 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, and Vysoké učení technické v Brně. The Mendelova univerzita v Brně logo is highlighted with an orange border.

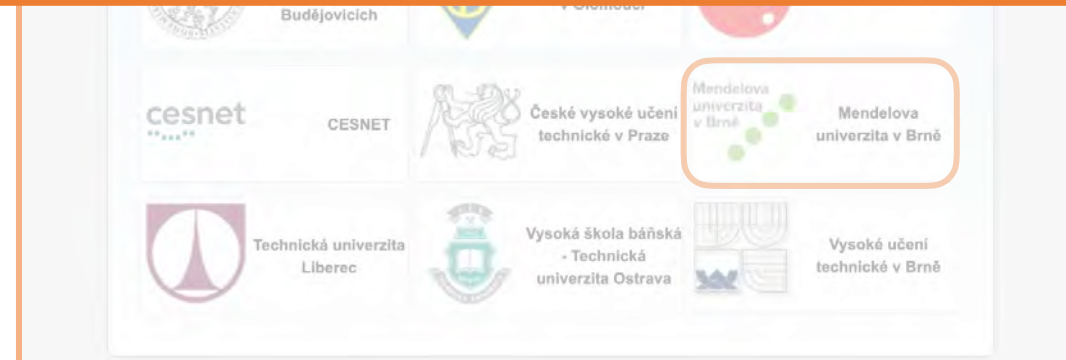
http
http



Choose your home institution

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 are valid until 2 February of the following year
- Accounts are renewed in January
- Immediate access to hardware resources
- Partner access by prior arrangement

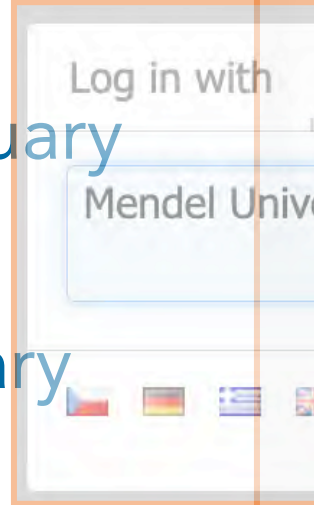


http
http



Use local credentials (local username and password)

- Anytime during the year, manual approval
- Log in through the institution (i.e. local name, eduID federation)
- Accounts are valid until 2 February of the following year
- Accounts are renewed in January
- Immediate access to hardware resources
- Partner access by prior arrangement



MENDELU

Shibboleth

Přihlásit se k e-Infrastruktura CESNET

Uživatelské jméno (login)

Heslo

Nepamatovat přihlášení

Smazat předešlé povolení k uvolnění Vašich informací k této službě.

Přihlášení

cesnet

E-infrastruktura CESNET je komplexní sada informatických nástrojů použitelných pro řešení problémů z celé řady oborů.



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, acknowledgements 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!

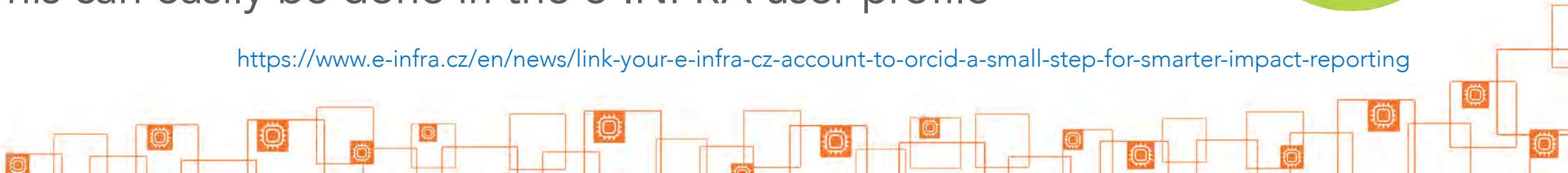
Link your account to ORCID

■ Link your e-INFRA CZ account to ORCID

- The future of national computing and storage services depends on demonstrating that researchers are truly using them
- Currently, much of the valuable research output of e-INFRA CZ/MetaCentrum users is 'invisible' to our funders
- We are developing a new automated system that will harvest users' publications
- Users only need to link their ORCID iD and use the correct acknowledgement in their publications.
- This can easily be done in the e-INFRA user profile

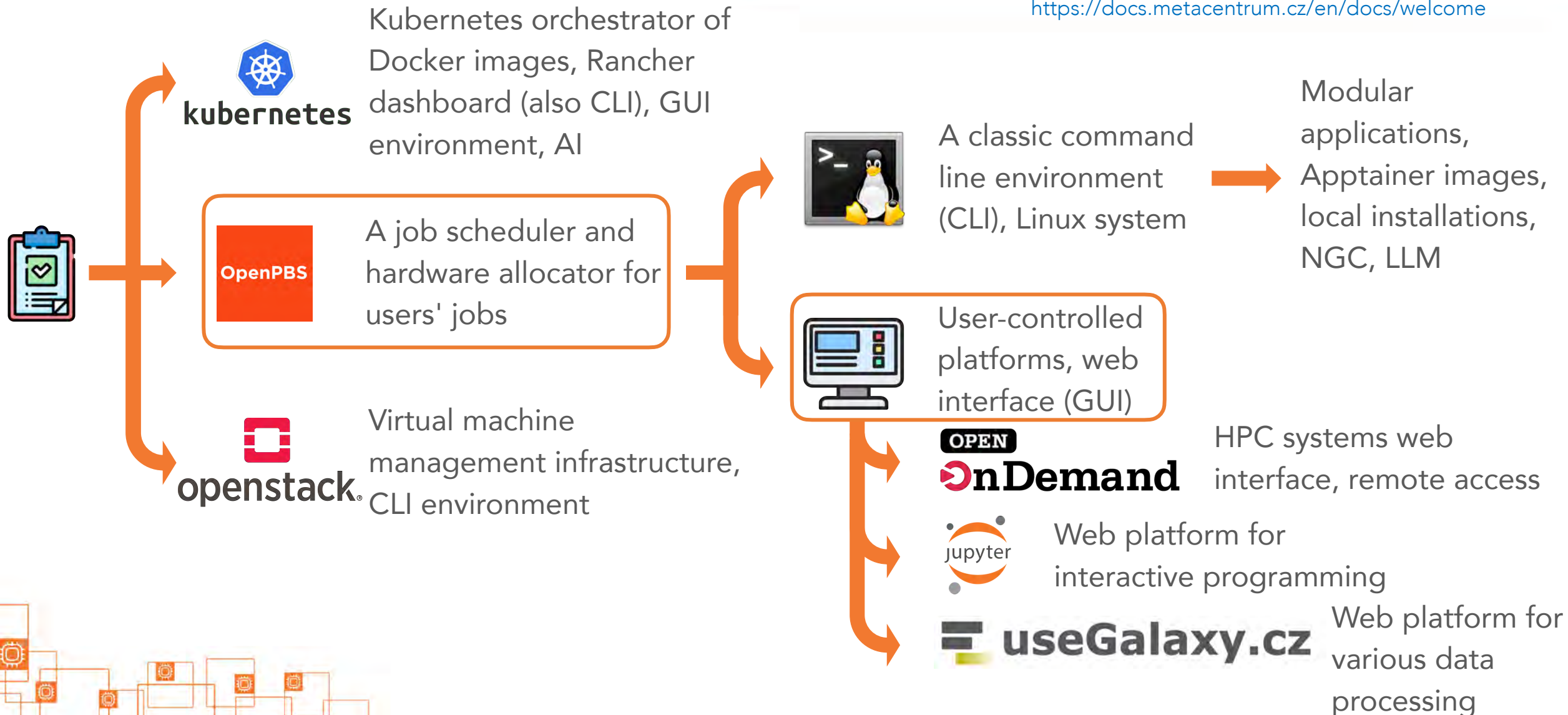


<https://www.e-infra.cz/en/news/link-your-e-infra-cz-account-to-orcid-a-small-step-for-smarter-impact-reporting>



How to use it

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



- Grid computing (OpenPBS scheduler)
 - Centrally managed HTC/HPC clusters
 - Classic command line environment (CLI)
 - GUI platforms
 - The 'most powerful' environment
 - Long batch jobs (days/weeks)
 - Interactive jobs
 - Parallel and multi-node computing
 - GPU acceleration (NVIDIA H100)

```

cesnet
[BOOKWORM]vorel@skirit:~$

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 interactive analysis software for NGS and microarray data. More information at https://docs.metacentrum.cz/en/docs/related/chipster.

[BOOKWORM]vorel@skirit:~$

```



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

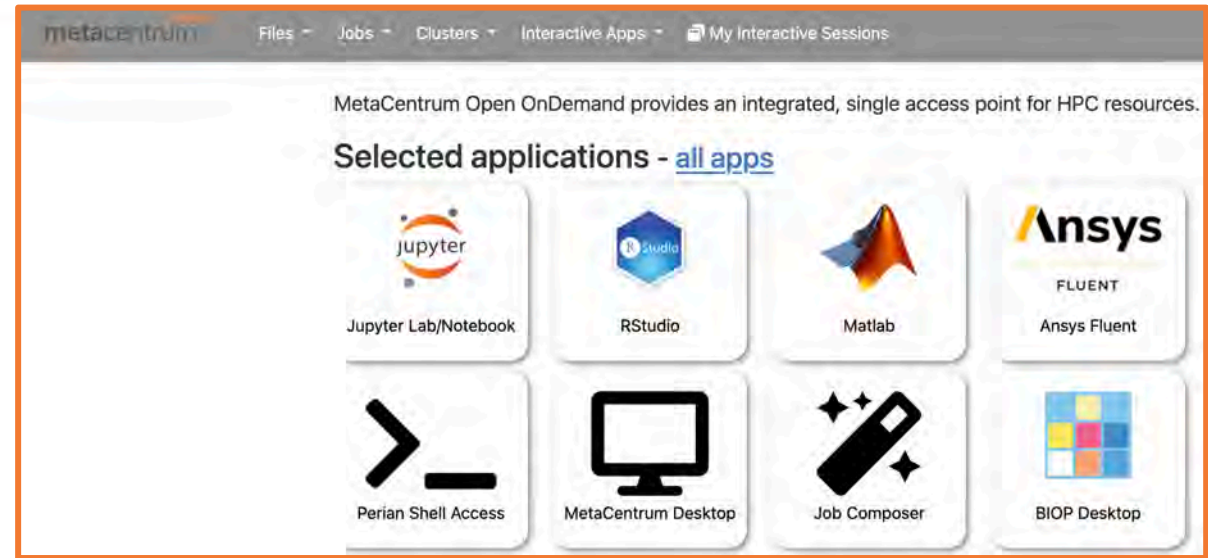


■ Open OnDemand



<https://ondemand.metacentrum.cz/>

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

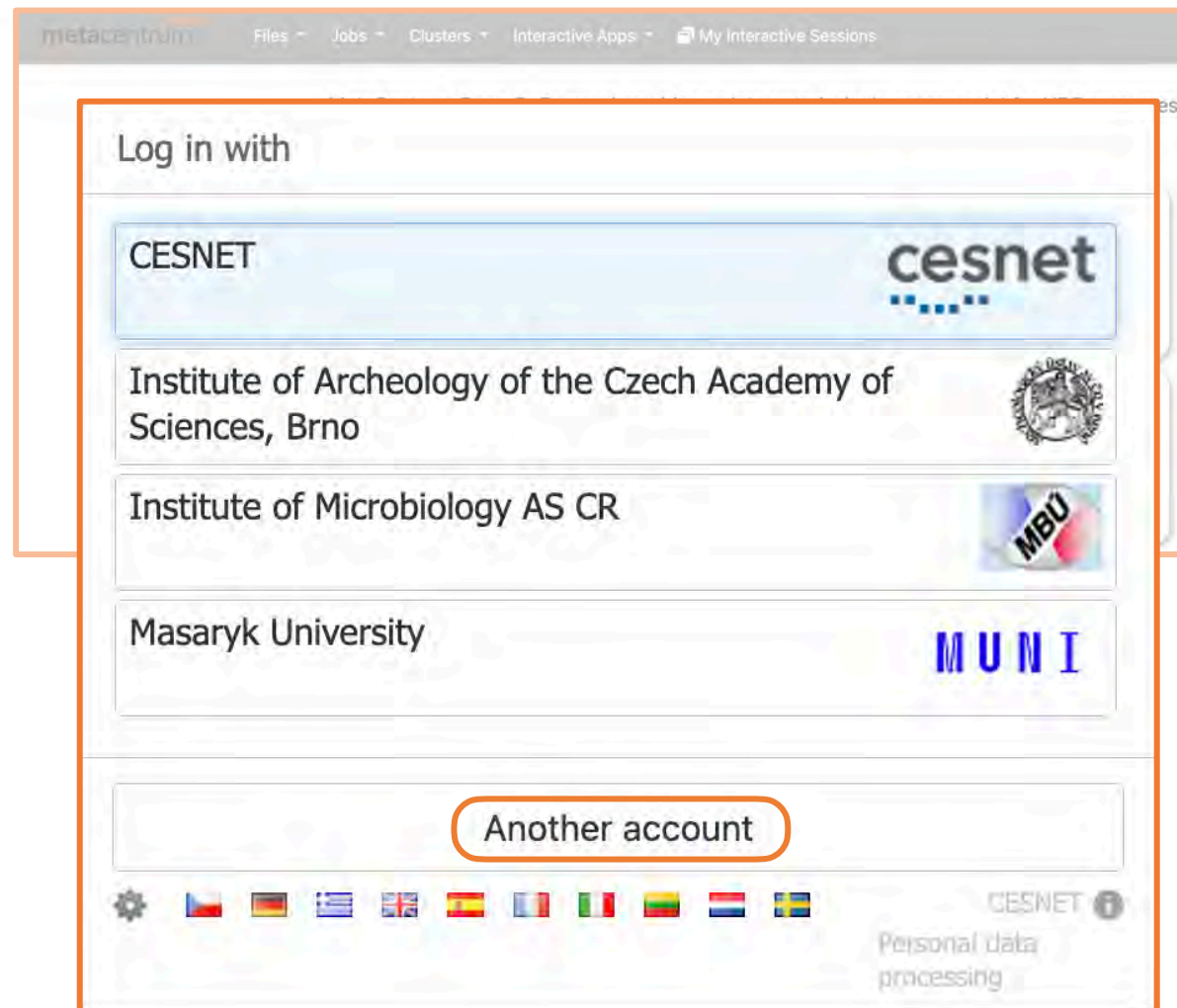


■ Open OnDemand



<https://ondemand.metacentrum.cz/>

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





MetaCentrum users can also log in using the 'e-INFRA CZ password' option with their MetaCentrum username and password

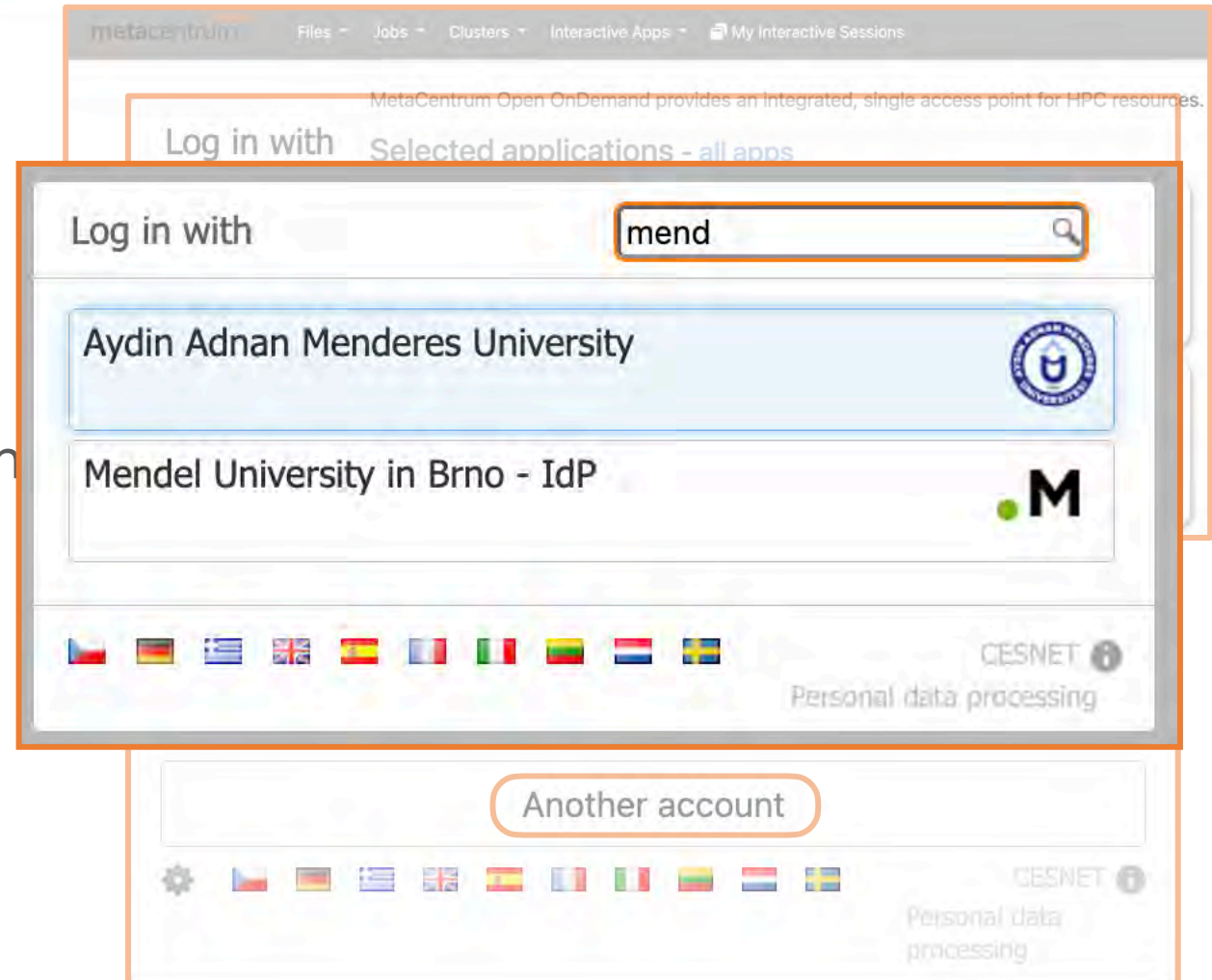
Open OnDemand

■ Open OnDemand



<https://ondemand.metacentrum.cz/>

- Web application on top of OpenPBS scheduler
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MetaCentrum users can also log in using the 'e-INFRA CZ password' option with their MetaCentrum username and password

Open OnDemand

■ Open OnDemand



<https://ondemand.metacentrum.cz/>

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

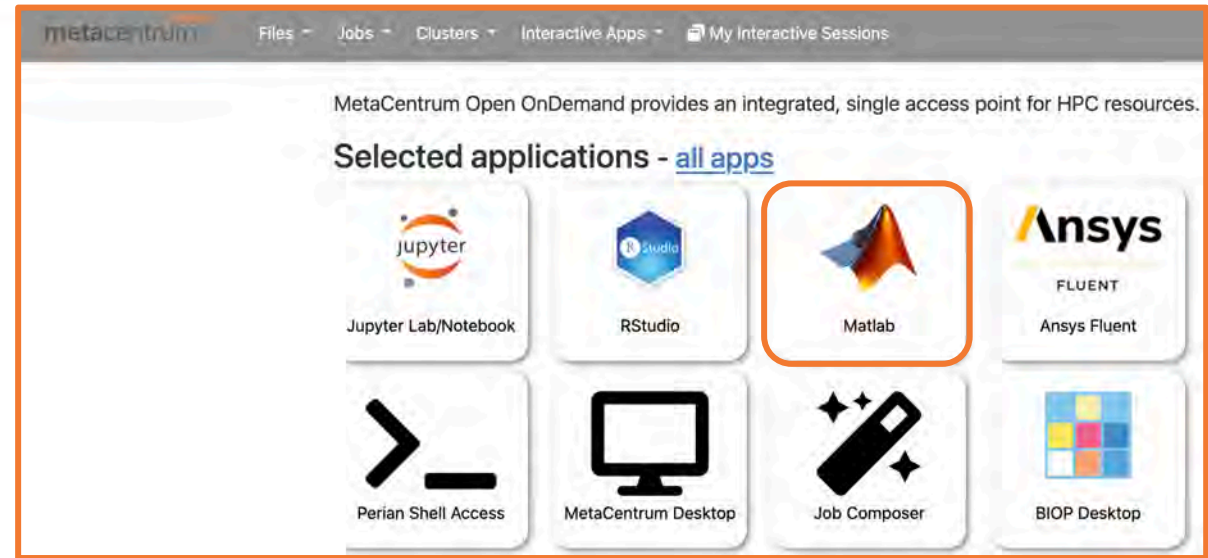


■ Open OnDemand



<https://ondemand.metacentrum.cz/>

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



<https://docs.metacentrum.cz/en/docs/software/sw-list/matlab>





MATLAB, the language of engineers and scientists, is a programming and numeric computation environment for algorithm development, data analysis, and visualisation

Open OnDemand

■ Open OnDemand



<https://ondemand.metacentrum.cz/>

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

The screenshot shows the Open OnDemand web interface for configuring a Matlab session. The left sidebar lists various interactive apps, with 'Matlab' selected. The main content area shows the configuration for the Matlab app, including a description and several adjustable parameters:

- Number of hours:** 5
- Number of CPUs on single node:** 4
- Memory (GB):** 4
- GPUs:** 0
- Scratch local (GB):** 10

A blue 'Launch' button is visible at the bottom of the configuration area. A note at the bottom states: '* The Matlab session data for this session can be accessed under the [data root directory](#).'



Open OnDemand

■ Open OnDemand



https

- W
- C
- R

The screenshot displays the Open OnDemand web interface. At the top, a green notification bar states "Session was successfully created." Below this, the breadcrumb navigation shows "Home / My Interactive Sessions". The main content area is divided into two columns. The left column, titled "Interactive Apps", lists several options: "Kubernetes on OpenStack (KOST) (beta)", "OpenStack VM (beta)", "Ansys/Ensignt", and "RStudio Server". The right column displays details for a "Matlab" session. The session name is "Matlab (17158555.pbs-m1.metacentrum.cz)" with a status of "Starting", "1 node", and "4 cores". It was created on "2026-02-04 11:36:14 CET" with a "Session ID" of "803f66c0-0228-4b47-93ed-a5fbae0841dc". A "Delete" button is visible. A message below the session details reads: "Your session is currently starting... Please be patient as this process can take a few minutes." At the bottom of the interface, there are configuration options for "VMD Desktop" (set to "Servers"), "Scratch local (GB)" (set to "10"), and a "Launch" button. A note at the bottom states: "* The Matlab session data for this session can be accessed under the [data root directory](#)."



■ Open OnDemand



The screenshot displays the Open OnDemand web interface. At the top, a green notification bar states "Session was successfully created." Below this, the breadcrumb navigation shows "Home / My Interactive Sessions". On the left, a sidebar titled "Interactive Apps" lists various applications: "Kubernetes on OpenStack (KOST) (beta)", "OpenStack VM (beta)", "Ansys/Ensignt", "Ansys/Fluent", "Ansys/Workbench", "BIOP Desktop", and "CLCgenomicsWB". The main content area features a card for a "Matlab" session. The card header includes the session name "Matlab (17158555.pbs-m1.metacentrum.cz)", resource allocation "1 node | 4 cores", and status "Running". A red "Delete" button is located in the top right of the card. Below the header, the card provides session details: "Host: galdor20.metacentrum.cz", "Created at: 2026-02-04 11:36:14 CET", "Time Remaining: 4 hours and 58 minutes", and "Session ID: 803f66c0-0228-4b47-93ed-a5fbae0841dc". At the bottom of the card, there are two sliders: "Compression" (0 (low) to 9 (high)) and "Image Quality" (0 (low) to 9 (high)). A blue "Launch Matlab" button is positioned at the bottom left, and a "View Only (Share-able Link)" button is at the bottom right.

The ribbon menu is organized into several categories:

- FILE:** New Script, New Live Script, New, Open, Find Files, Go to File, Import Data, Save Workspace.
- VARIABLE:** Clean Data, Open Variable, Clear Workspace.
- CODE:** Run and Time, Clear Commands.
- SIMULINK:** Simulink.
- ENVIRONMENT:** Layout, Set Path, Add-Ons, Settings.
- RESOURCES:** Help, Request Support, Feedback, Learn MATLAB.

File navigation path: / > auto > brno11-elixir > home > vorel >

The interface is split into two main sections:

- Files:** A file browser showing the current directory structure. The path is / > auto > brno11-elixir > home > vorel >. The file list includes:
 - .icewm
 - NikoK_Klimno_genome
 - NikoK_Ktang_genome
 - NikoR_metabarcoding
- Command Window:** A large empty area for entering MATLAB commands.

Search

No items match your search.

FAVORITES

- Curve Fitter
- Optimization
- PID Tuner
- System Identification
- Wireless Waveform...
- Wireless Channel ...
- Signal Analyzer
- Instrument Control
- SimBiology Model ...
- SimBiology Model ...
- MATLAB Coder
- Standalone Applicatio...

MATLAB

- Class Diagram ...
- Code Analyzer
- Code Compatibil...
- Data Cleaner
- Dependency Analyzer
- Experiment Manager
- Hardware Manager
- Profiler
- Test Browser

MACHINE LEARNING AND DEEP LEARNING

- Classification Learner
- Deep Network ...
- Deep Network ...
- Neural Net Clustering
- Neural Net Fitting
- Neural Net Pattern ...
- Neural Net Time Series
- Regression Learner
- Reinforce... Learning...

MATH, STATISTICS AND OPTIMIZATION

- Curve Fitter
- Distribution Fitter
- Optimization
- PDE Modeler

CONTROL SYSTEM DESIGN AND ANALYSIS

- Control System ...
- Control System ...
- Diagnostic Feature ...
- Fuzzy Logic Designer
- Health Indicator ...
- Linear System ...
- MPC Designer
- Model Reducer
- Neuro-Fuzzy Designer
- PID Tuner
- System Identification

SIMSCAPE

- Battery Builder
- Flexible Body Mod...
- Graph Data Extractor

RF AND MIXED-SIGNAL

- Antenna Array ...
- Antenna Designer
- Matching Network ...
- Mixed-Signal Analyzer
- PCB Antenna Designer
- Parallel Link Designer
- RF Budget Analyzer
- SerDes Designer
- Serial Link Designer
- Signal Integrity ...
- Transmission Line ...

ROBOTICS AND AUTONOMOUS SYSTEMS

- Flight Log
- Inverse
- ROS 2
- ROS Data
- SLAM Map
- UAV

HOME PLOTS APPS

Design App Get More Apps Install App Curve

FILE

/ > auto > brn011-elixir > h

Files

Name

- .icewm
- NikoK_Klimno_genome
- NikoK_Ktang_genome
- NikoR_metabarcoding

Workspace

Name	Value	Size	C

Curve Fitter

CURVE FITTER

Open Save Duplicate
 FILE

Select Data Exclusion Rules Validation Data
 DATA

Polynomial Exponent... Logarith... Fourier
 FIT TYPE

Update Fit Fit
 Auto Manual
 FIT

Residuals Plot Contour Plot
 Fit Plot Prediction Bounds None
 VISUALIZATION

Colormap Export
 PREFERENCES EXPORT

untitled fit 1

Select data to fit curves or surfaces.

Fit Options

Polynomial

Degree

Robust

Center and scale

Advanced Options

[Read about fit options](#)

Results

Fit Name: untitled fit 1

Table of Fits

Fit State	Fit name	Data	Fit type	R-square	SSE	DFE	Adj R-sq	RMSE	# Coeff	Validation D
	untitled fit 1		poly1							

HOME PLOTS APPS EDITOR PUBLISH VIEW

New Open Save Compare Print Go To Find Bookmark Refactor Analyze Run Section Run and Advance Run Step Stop

FILE NAVIGATE CODE ANALYZE SECTION RUN

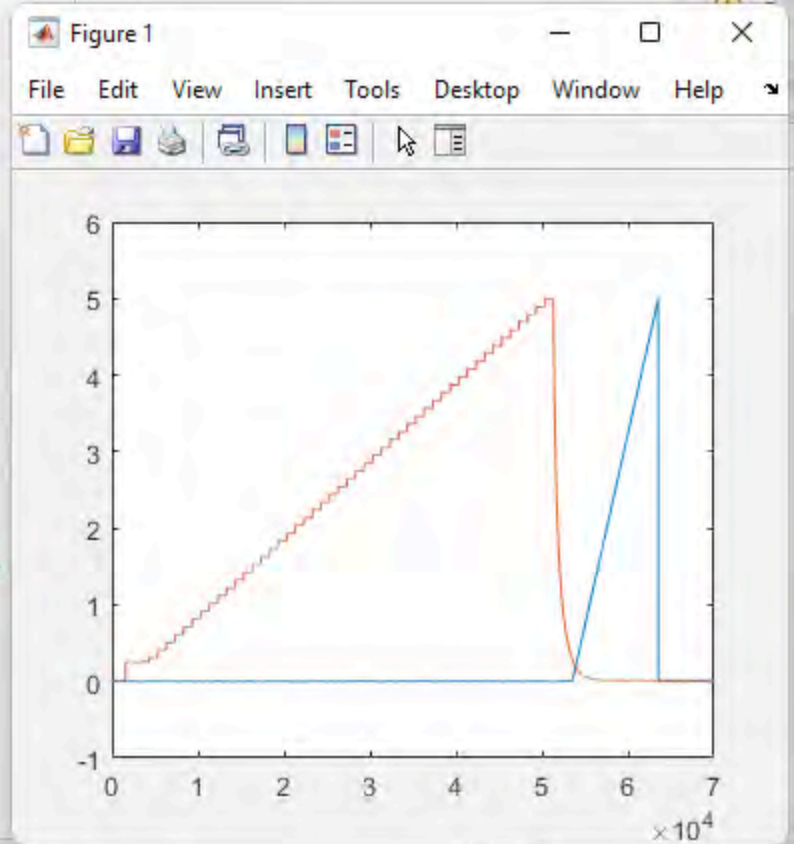
C:\Users\{user}\AppData\Roaming\MathWorks\MATLAB Add-Ons\Collections\Digilent Toolbox

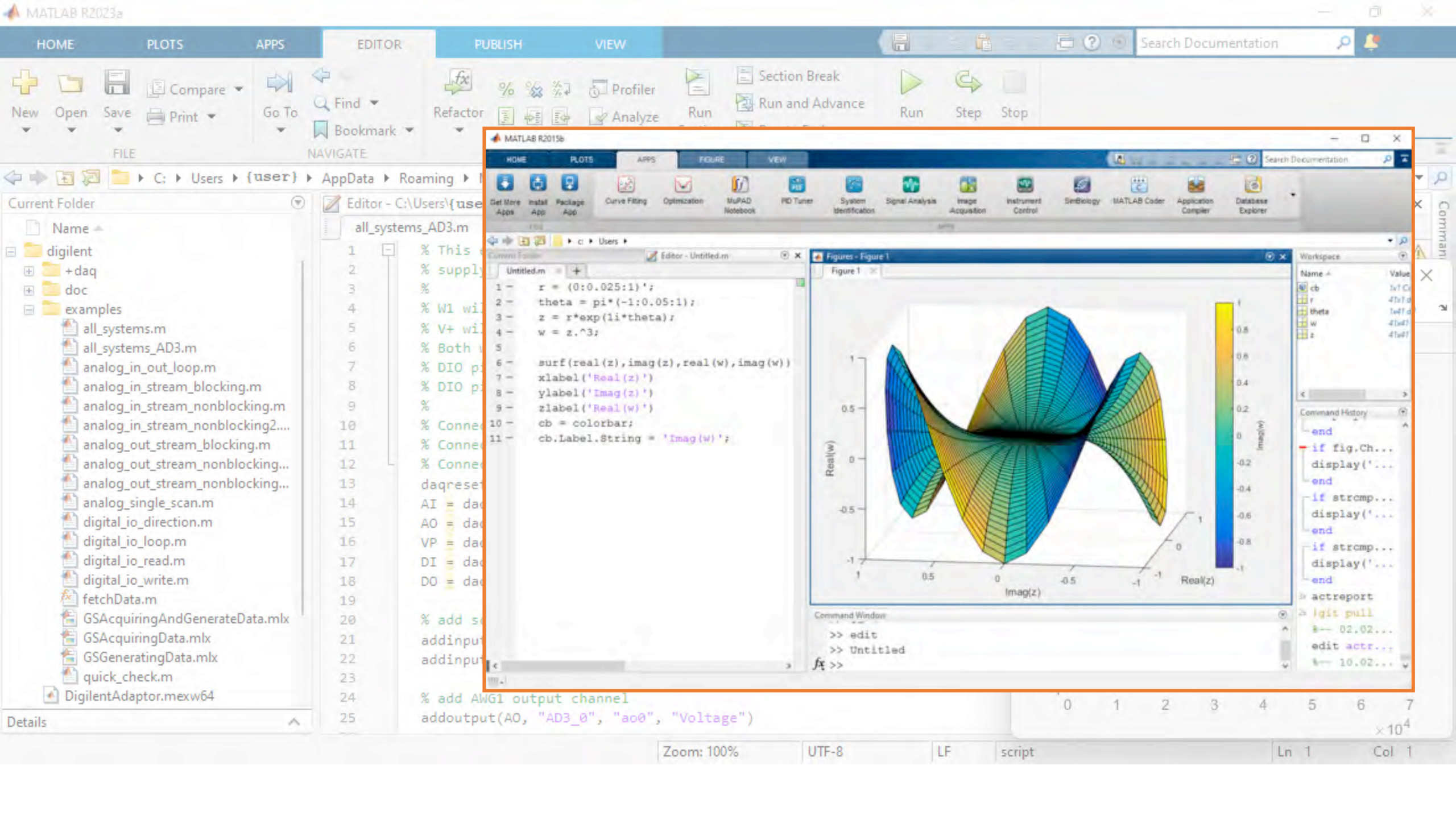
Current Folder

- digilent
 - +daq
 - doc
 - examples
 - all_systems.m
 - all_systems_AD3.m
 - analog_in_out_loop.m
 - analog_in_stream_blocking.m
 - analog_in_stream_nonblocking.m
 - analog_in_stream_nonblocking2...
 - analog_out_stream_blocking.m
 - analog_out_stream_nonblocking...
 - analog_out_stream_nonblocking...
 - analog_single_scan.m
 - digital_io_direction.m
 - digital_io_loop.m
 - digital_io_read.m
 - digital_io_write.m
 - fetchData.m
 - GSAcquiringAndGenerateData.mlx
 - GSAcquiringData.mlx
 - GSGeneratingData.mlx
 - quick_check.m
 - DigilentAdaptor.mexw64

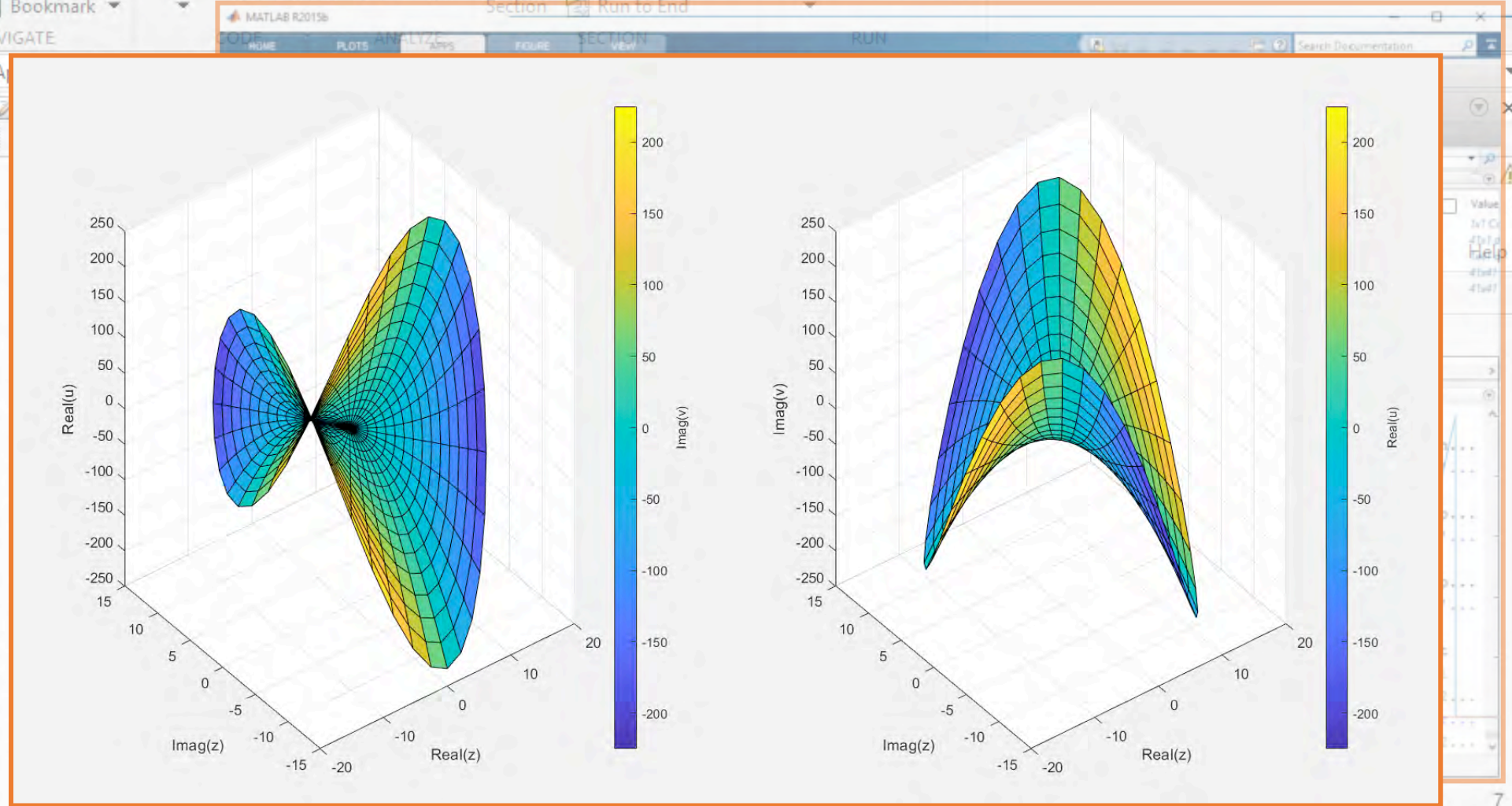
```

1 % This example uses the two scope channels, one AWG channel, one power
2 % supply channel and all digital channels on the AD3
3 %
4 % W1 will generate a ramp from 0 to 5V for 1 second at 1KHz
5 % V+ will generate a ramp from 0 to 5V for 5 seconds at 10Hz
6 % Both will be acquired at 10KHz by scope channels 1 and 2
7 % DIO pins 0-7 will be used to output primes less than 128
8 % DIO pins 8-15 will acquire the primes generated by DIO0-7
9 %
10 % Connect W1 to 1+ and GND to 1-
11 % Connect V+ to 2+ and GND to 2-
12 % Connect DIO0 to DIO8, DIO1 to DIO9 ... DIO7 to DIO15
13 daqreset;
14 AI = daq("digilent") % DAQ session for the scope channels
15 AO = daq("digilent") % DAQ session for the AWG channel
16 VP = daq("digilent") % DAQ session for the V+ power supply
17 DI = daq("digilent") % DAQ session for the DIO channels used as input
18 DO = daq("digilent") % DAQ session for the DIO channels used as output
19
20 % add scope input channels
21 addinput(AI, "AD3_0", "ai0", "Voltage")
22 addinput(AI, "AD3_0", "ai1", "Voltage")
23
24 % add AWG1 output channel
25 addoutput(AO, "AD3_0", "ao0", "Voltage")
    
```

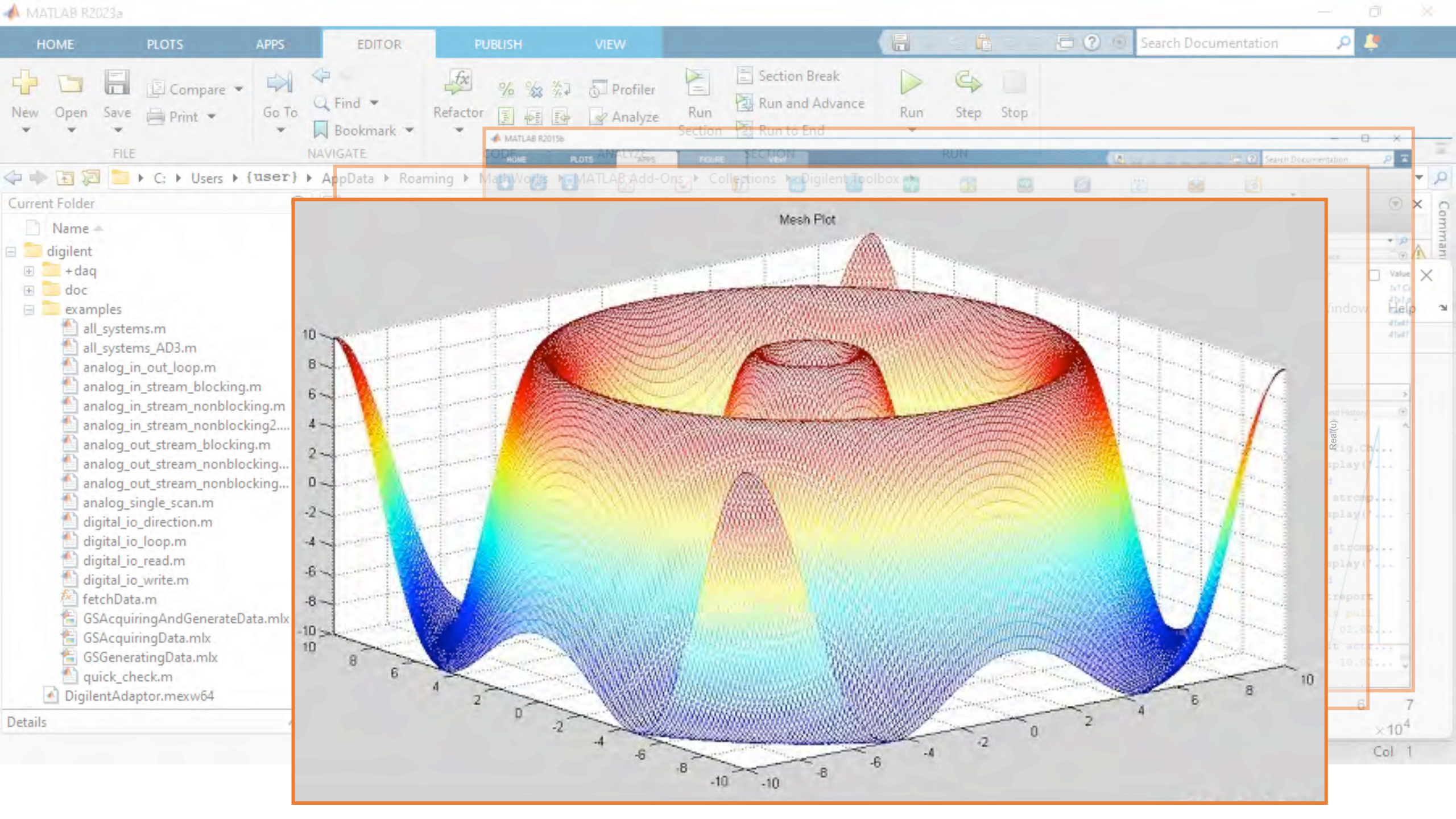




- Current Folder
- Name
 - digilent
 - +daq
 - doc
 - examples
 - all_systems.m
 - all_systems_AD3.m
 - analog_in_out_loop.m
 - analog_in_stream_blocking.m
 - analog_in_stream_nonblocking.m
 - analog_in_stream_nonblocking2...
 - analog_out_stream_blocking.m
 - analog_out_stream_nonblocking...
 - analog_out_stream_nonblocking...
 - analog_single_scan.m
 - digital_io_direction.m
 - digital_io_loop.m
 - digital_io_read.m
 - digital_io_write.m
 - fetchData.m
 - GSAcquiringAndGenerateData.mlx
 - GSAcquiringData.mlx
 - GSGeneratingData.mlx
 - quick_check.m
 - DigilentAdaptor.mexw64



```
addoutput(AO, "AD3_0", "ao0", "Voltage")
```



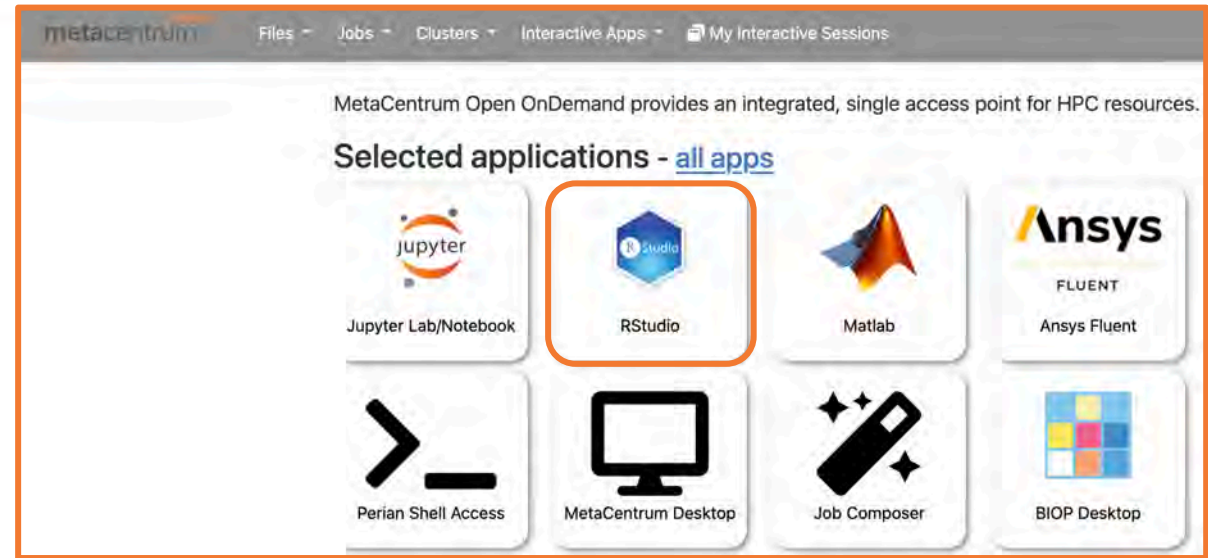
Open OnDemand

■ Open OnDemand



<https://ondemand.metacentrum.cz/>

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



<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 applications

Home / My Interactive Sessions / RStudio Server

Interactive Apps

- Cloud
 - Kubernetes on OpenStack (KOST) (beta)
 - OpenStack VM (beta)
- Desktops
 - Ansys/Ensignt
 - Ansys/Fluent
 - Ansys/Workbench
 - BIOP Desktop
 - CLCgenomicsWB
 - MZMINE
 - Matlab
 - MetaCentrum Desktop
 - QuPath
 - VMD Desktop
- Servers
 - Julia Pluto.jl
 - Jupyter - Evo2 (beta)
 - Jupyter Notebook/Lab
 - Matlab webapp (beta)
 - 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

Launch

* The RStudio Server session data for this session can be accessed under the [data root directory](#).

■ Open OnDemand



<https://ondemand.metacentrum.cz/>

- Web application on top of OpenPBS scheduler

Scratch local (GB)

RStudio-geospatial-4.2.2

RStudio-geospatial-4.3.0

RStudio-geospatial-4.4.1

✓ RStudio-geospatial-4.5.1

Single-cell-R-training

RStudio working directory location:

/storage/brno2

Launch

Session data for this session can be accessed under the [data](#)

RStudio Image version

RStudio-geospatial-4.5.1

RStudio working directory location:

✓ /storage/brno2

/storage/plzen1

/storage/praha1

/storage/brno12-cerit

[root directory.](#)

10

RStudio Image version

RStudio-geospatial-4.5.1

RStudio working directory location:

/storage/brno2

Launch

* The RStudio Server session data for this session can be accessed under the [data](#) root directory.

matlab webapp (beta)

RStudio Server

■ Open OnDemand



<https://ondemand.metacentrum.cz/>

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

A screenshot of the Open OnDemand web interface showing the configuration for the RStudio Server application. The page is titled "RStudio Server" and includes a navigation breadcrumb: "Home / My Interactive Sessions / RStudio Server". On the left, a sidebar lists various interactive applications under categories like "Cloud", "Desktops", and "Servers". The "RStudio Server" application is selected and highlighted in blue. The main content area shows configuration options for the RStudio Server, including "Number of hours" (set to 2), "Number of CPUs on single node" (set to 2), "Memory (GB)" (set to 10), "GPUs" (set to 0), "Scratch local (GB)" (set to 10), "RStudio Image version" (set to RStudio-geospatial-4.5.1), and "RStudio working directory location" (set to /storage/brno2). A prominent blue "Launch" button is located at the bottom of the configuration area. A note at the bottom states: "* The RStudio Server session data for this session can be accessed under the [data root directory](#)."/>

Home / My Interactive Sessions / RStudio Server

Interactive Apps

Cloud

- Kubernetes on OpenStack (KOST) (beta)
- OpenStack VM (beta)

Desktops

- Ansys/Ensignt
- Ansys/Fluent
- Ansys/Workbench
- BIOP Desktop
- CLCgenomicsWB
- MZMINE
- Matlab
- MetaCentrum Desktop
- QuPath
- VMD Desktop

Servers

- Julia Pluto.jl
- Jupyter - Evo2 (beta)
- Jupyter Notebook/Lab
- Matlab webapp (beta)
- 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

Launch

* The RStudio Server session data for this session can be accessed under the [data root directory](#).

■ Open OnDemand

<https://ondemand.metacentrum.cz>

- Web application
- OpenPBS scheduler
- Running (not

Session was successfully created.

Home / My Interactive Sessions

Interactive Apps

Cloud

- Kubernetes on OpenStack (KOST) (beta)
- OpenStack VM (beta)

Desktops

- Ansys/Ensignt
- Ansys/Fluent
- Ansys/Workbench

RStudio Server (19079987.pbs-m1.metacentrum.cz)

1 node | 2 cores | Running

Host: tarkil16.grid.cesnet.cz

Created at: 2026-04-15 16:41:20 CEST

Time Remaining: 1 hour and 59 minutes

Session ID: feeacd78-2c6a-422f-a09a-92164d94a35c

Ⓜ Connect to RStudio Server

ⓧ Delete

App List

- MZMINE
- Matlab
- MetaCentrum Desktop
- QuPath
- VMD Desktop
- Servers
 - Julia Pluto.jl
 - Jupyter - Evo2 (beta)
 - Jupyter Notebook/Lab
 - Matlab webapp (beta)
 - RStudio Server**

Scratch local (GB): 10

RStudio Image version: RStudio-geospatial-4.5.1

RStudio working directory location: /storage/brno2

Launch

* The RStudio Server session data for this session can be accessed under the [data root directory](#).

```
File Edit Code View Plots Session Build Debug Profile Tools Help
Go to file/function Addins
Console Terminal Background Jobs
R 4.5.1 /auto/brno2/home/vorel/
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.
>
```

vorel Project: (None)

Environment History Connections Tutorial

Import Dataset 187 MiB

R Global Environment

Environment is empty

Files Plots Packages Help Viewer Presentation

Home Find in Topic

R Resources

- [Learning R Online](#)
- [CRAN Task Views](#)
- [R on StackOverflow](#)
- [Getting Help with R](#)

Manuals

- [An Introduction to R](#)
- [Writing R Extensions](#)
- [R Data Import/Export](#)

Reference

- [Packages](#)

Miscellaneous Material

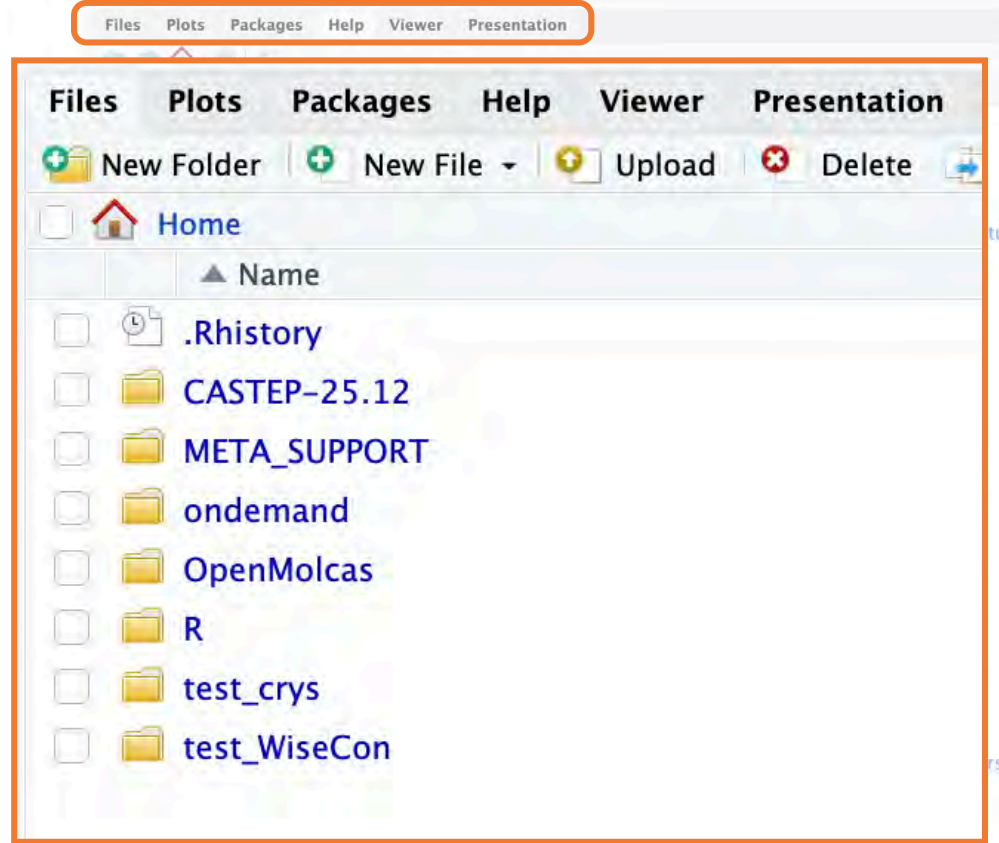
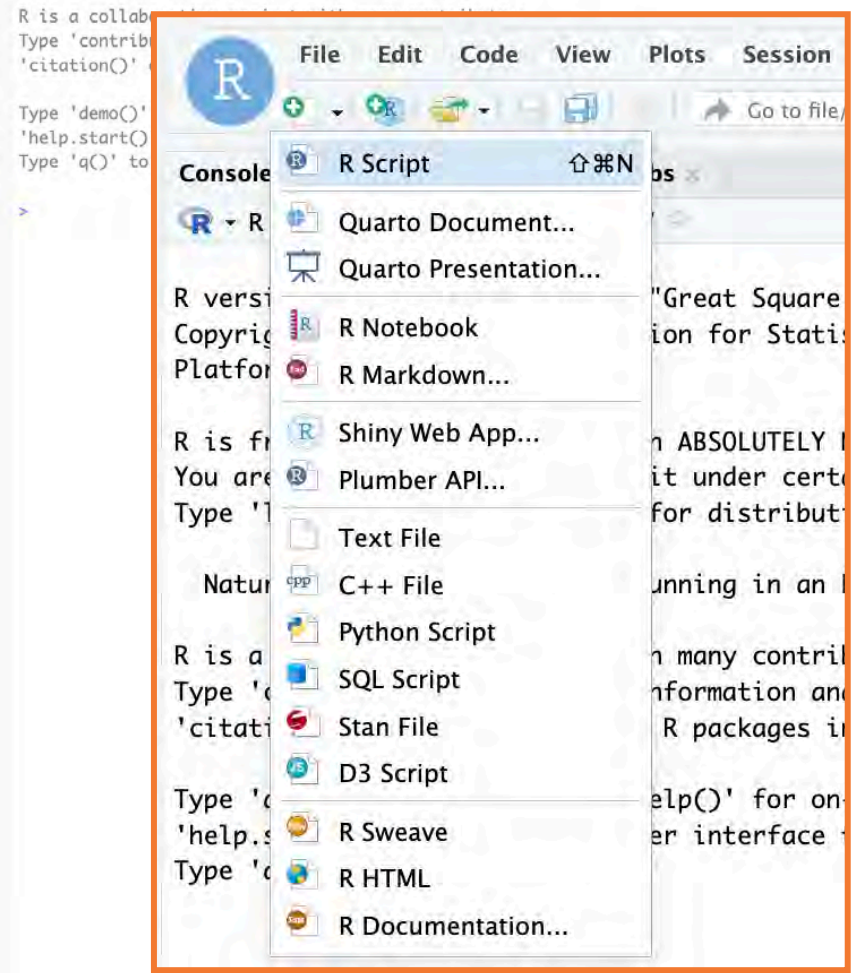
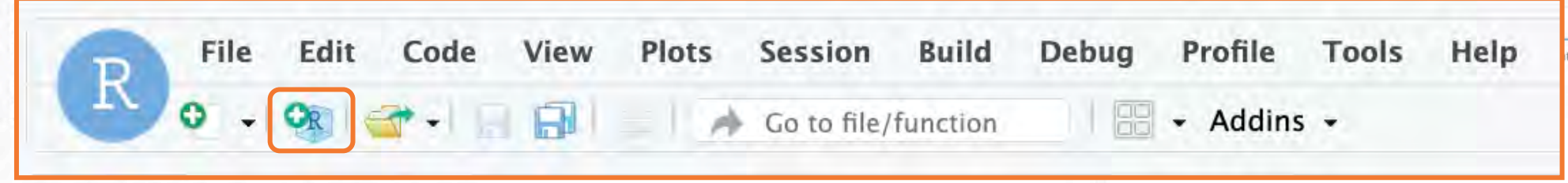
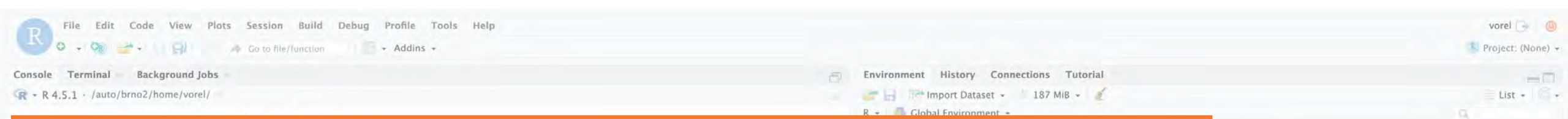
About R	Authors	Resources
License	FAQ	Thanks
NEWS	User Manuals	Technical papers

RStudio

- [Posit Support](#)
- [Posit Community Forum for the RStudio IDE](#)
- [Posit Cheat Sheets](#)
- [RStudio Packages](#)
- [Posit Products](#)

- [The R Language Definition](#)
- [R Installation and Administration](#)
- [R Internals](#)

- [Search Engine & Keywords](#)



R 4.5.1 · /auto/brno2/home/vorel/

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

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 '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.

```
> getwd()
[1] "/auto/brno2/home/vorel"
> version
```

```
platform      x86_64-pc-linux-gnu
arch          x86_64
os            linux-gnu
system        x86_64, linux-gnu
status
major         4
minor         5.1
year          2025
month         06
day           13
svn rev       88306
language      R
version.string R version 4.5.1 (2025-06-13)
nickname      Great Square Root
```

```
> installed.packages()
```

	Package	LibPath	Version	Priority
abind	"abind"	"/usr/local/lib/R/site-library"	"1.4-8"	NA
ade4	"ade4"	"/usr/local/lib/R/site-library"	"1.7-23"	NA
adegenet	"adegenet"	"/usr/local/lib/R/site-library"	"2.1.11"	NA
ape	"ape"	"/usr/local/lib/R/site-library"	"5.8-1"	NA
arrow	"arrow"	"/usr/local/lib/R/site-library"	"22.0.0"	NA
askpass	"askpass"	"/usr/local/lib/R/site-library"	"1.2.1"	NA
assertthat	"assertthat"	"/usr/local/lib/R/site-library"	"0.2.1"	NA
backports	"backports"	"/usr/local/lib/R/site-library"	"1.5.0"	NA
base64enc	"base64enc"	"/usr/local/lib/R/site-library"	"0.1-3"	NA
BH	"BH"	"/usr/local/lib/R/site-library"	"1.87.0-1"	NA
BiocManager	"BiocManager"	"/usr/local/lib/R/site-library"	"1.30.26"	NA
BiocVersion	"BiocVersion"	"/usr/local/lib/R/site-library"	"3.22.0"	NA
bit	"bit"	"/usr/local/lib/R/site-library"	"4.6.0"	NA
bit64	"bit64"	"/usr/local/lib/R/site-library"	"4.6.0-1"	NA
blob	"blob"	"/usr/local/lib/R/site-library"	"1.2.4"	NA
blogdown	"blogdown"	"/usr/local/lib/R/site-library"	"1.22"	NA
bookdown	"bookdown"	"/usr/local/lib/R/site-library"	"0.45"	NA
brew	"brew"	"/usr/local/lib/R/site-library"	"1.0-10"	NA
brio	"brio"	"/usr/local/lib/R/site-library"	"1.1.5"	NA
broom	"broom"	"/usr/local/lib/R/site-library"	"1.0.10"	NA
bslib	"bslib"	"/usr/local/lib/R/site-library"	"0.9.0"	NA
cachem	"cachem"	"/usr/local/lib/R/site-library"	"1.1.0"	NA
callr	"callr"	"/usr/local/lib/R/site-library"	"3.7.6"	NA
cellranger	"cellranger"	"/usr/local/lib/R/site-library"	"1.1.0"	NA
CFtime	"CFtime"	"/usr/local/lib/R/site-library"	"1.7.1"	NA
classInt	"classInt"	"/usr/local/lib/R/site-library"	"0.4-11"	NA
cli	"cli"	"/usr/local/lib/R/site-library"	"3.6.5"	NA
clipr	"clipr"	"/usr/local/lib/R/site-library"	"0.8.0"	NA
coda	"coda"	"/usr/local/lib/R/site-library"	"0.19-4.1"	NA
colorspace	"colorspace"	"/usr/local/lib/R/site-library"	"2.1-2"	NA
cols4all	"cols4all"	"/usr/local/lib/R/site-library"	"0.10"	NA
commonmark	"commonmark"	"/usr/local/lib/R/site-library"	"2.0.0"	NA
conflicted	"conflicted"	"/usr/local/lib/R/site-library"	"1.2.0"	NA
covr	"covr"	"/usr/local/lib/R/site-library"	"3.6.4"	NA
cpp11	"cpp11"	"/usr/local/lib/R/site-library"	"0.5.2"	NA
crayon	"crayon"	"/usr/local/lib/R/site-library"	"1.5.3"	NA

```
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  
  
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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.  
  
>
```

Environment is empty

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		

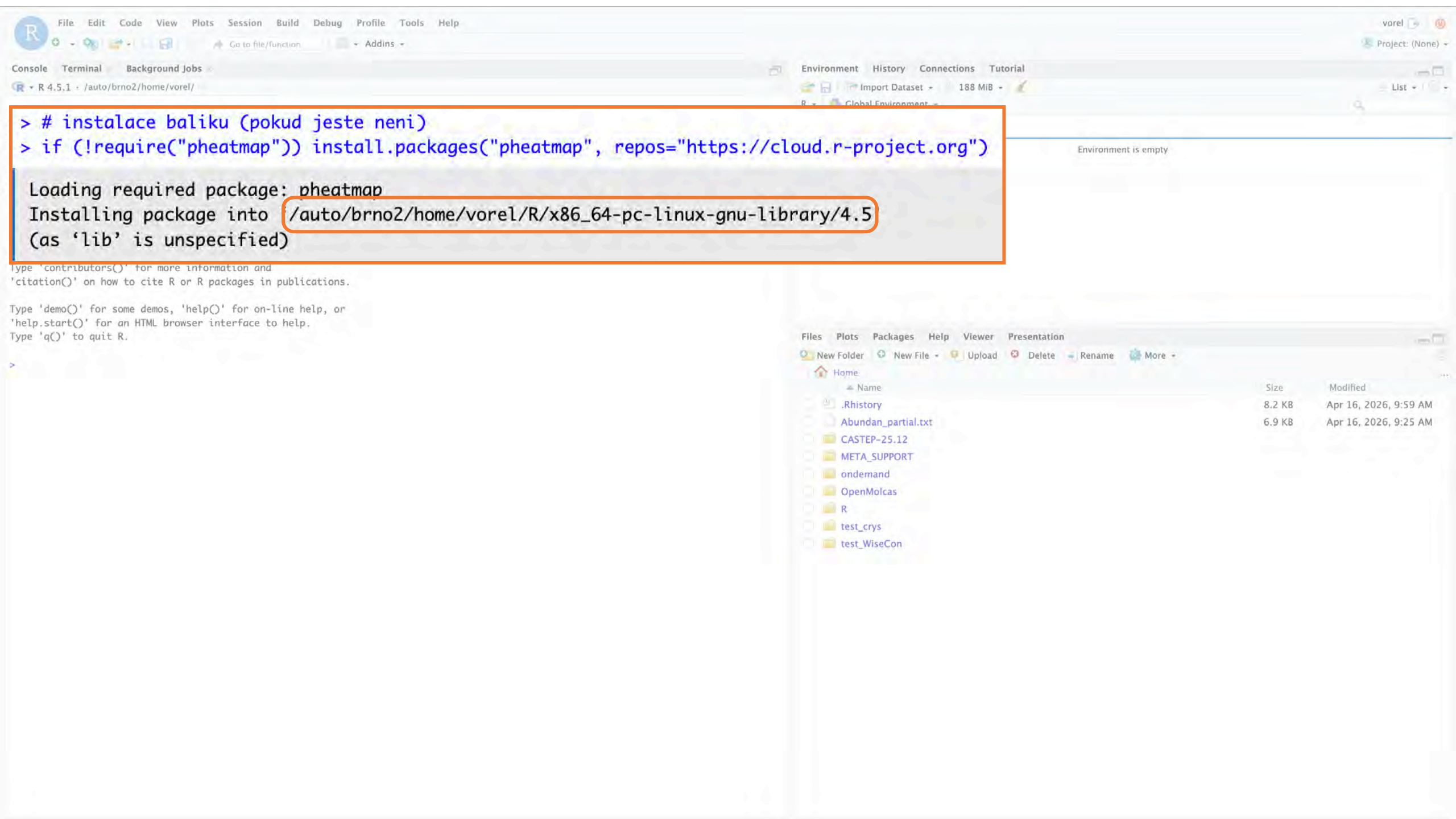
R version 4.5.1 (2025-06-13) -- "Great Square Root"

```
> 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

26, 9:59 AM
26, 9:25 AM



```

> 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"
+ )

```

<https://cloud.r-project.org>)

x-gnu-library/4.5

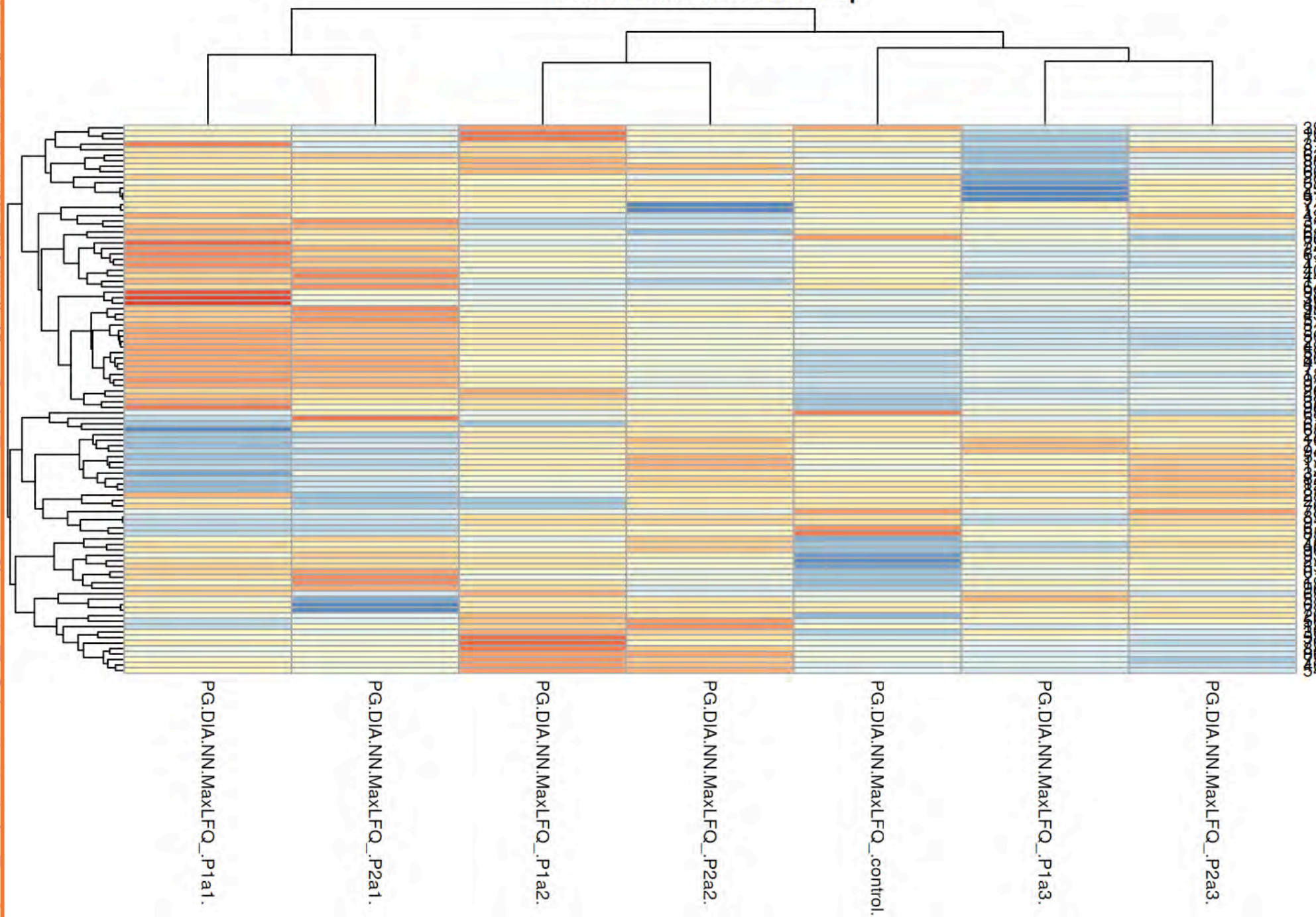
Files Plots Packages Help Viewer Presentation

New Folder New File Upload Delete Rename More

Home

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		

Protein abundance heatmap



vorel
Project: (None)
List

Modified
Apr 16, 2026, 9:59 AM
Apr 16, 2026, 9:25 AM

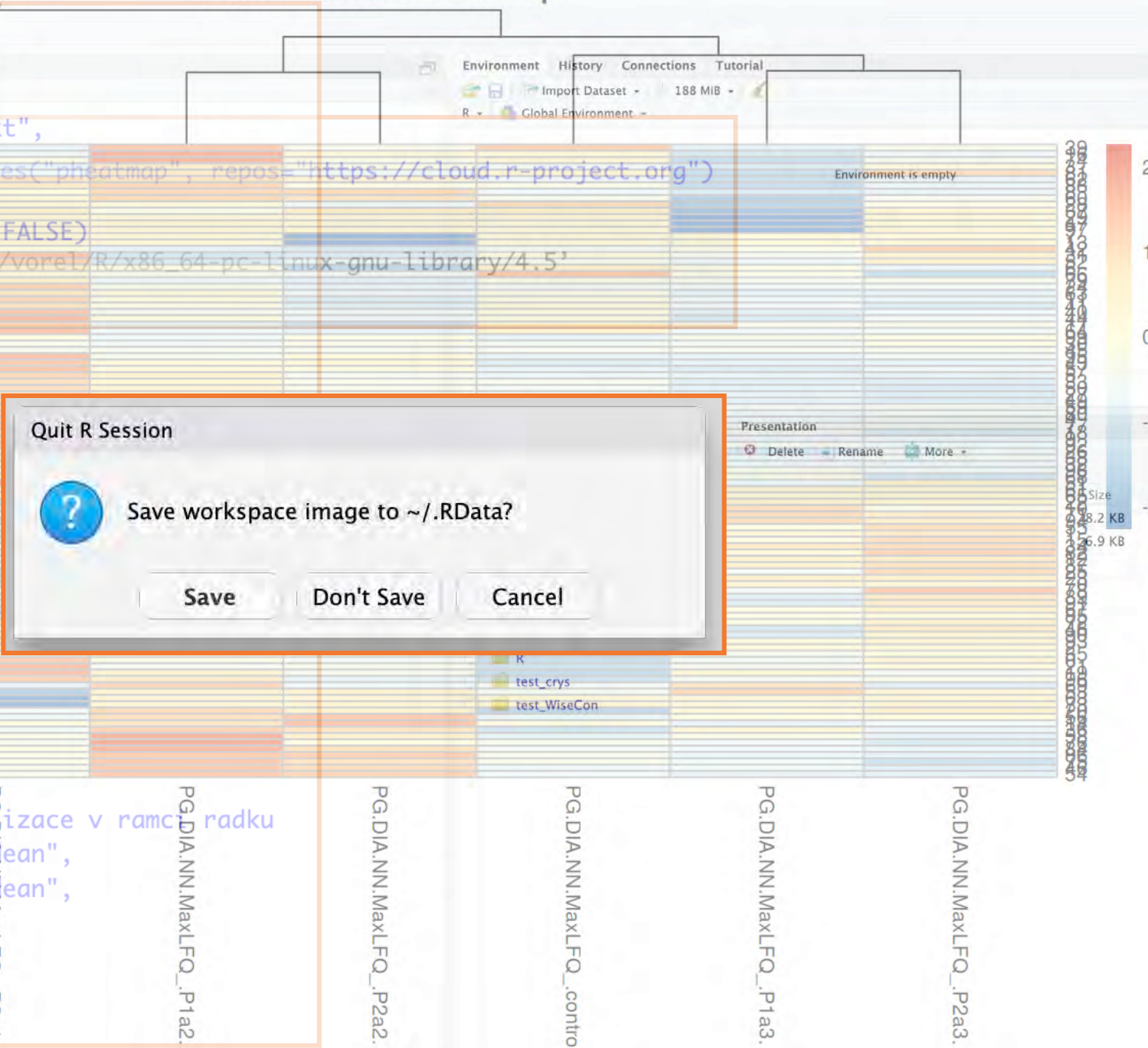
```
File Edit Co  
> library  
Console Terminal B  
R 4.4.1  
> # nacte  
> data$PG  
R version 4.4.1 (2025-05-16)  
Copyright (C) 2025 The R Foundation for Statistical Computing  
Platform: x86_64-pc-linux-gnu  
R is free software and you are welcome to redistribute it under certain  
conditions. See the file LICENSE for details.  
Loading required namespace: 'R6'  
Installing shared libraries: OK  
> # nasta  
Type 'compilers()' for a list of available compilers.  
> data$PG  
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.  
> # prev  
> data[]  
+ as.  
+ })  
> # log t  
> data_lo  
> # vykre  
> pheatma  
+ dat  
+ sca  
+ clu  
+ clu  
+ clu  
+ fon  
+ mai  
+ )
```

Protein abundance heatmap

```
> library(pheatmap)
> # nacteni dat
> data <- read.delim("Abundan.partial.txt",
+ list.as.factor(dk1.GEMMUS+parent)
+ 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(asub(",", ".", x))
+ })
> # log transformace (bezpecna pro nuly)
> data_log <- log10(data + 1)
> # vykresleni heatmapy
> pheatmap(
+   data_log,
+   scale = "row",
+   clustering_distance_rows = "euclidean",
+   clustering_distance_cols = "euclidean",
+   clustering_method = "complete",
+   fontsize = 8,
+   main = "Protein abundance heatmap",
+ )
```

Quit R Session

Save workspace image to ~/.RData?



vorel

Project: (None)

Environment History Connections Tutorial

Environment: 188 MIB

R - Global Environment

Environment is empty

Presentation: Delete Rename More

Size: 8.2 KB, 6.9 KB

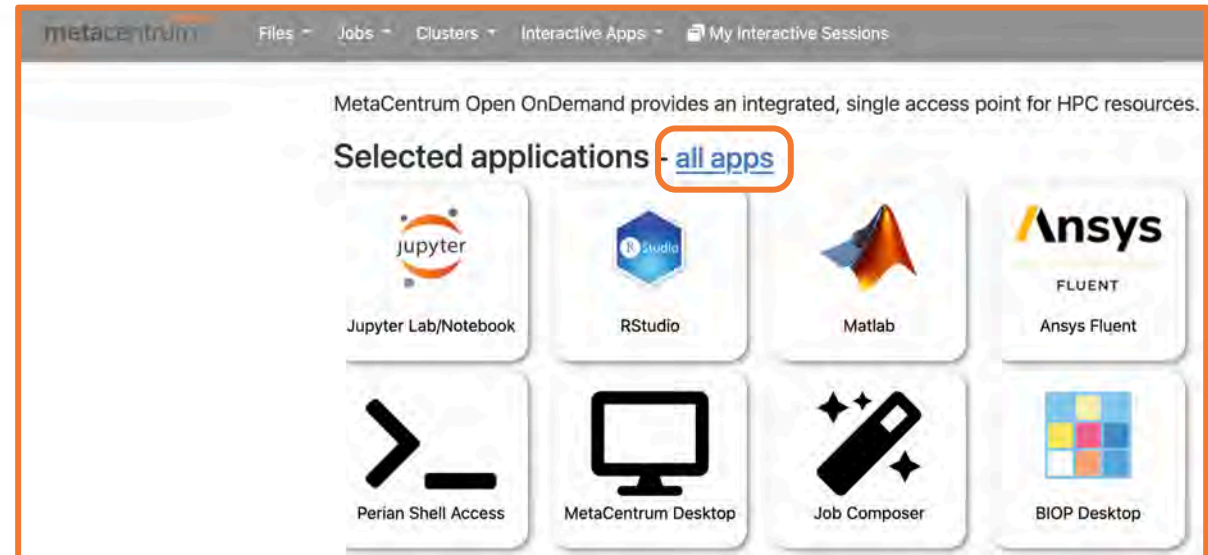
Modified: Apr 16, 2026, 9:59 AM, Apr 16, 2026, 9:25 AM

■ Open OnDemand



<https://ondemand.metacentrum.cz/>

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





ANSYS is engineering simulation software that integrates the physics of structural, fluid and electromagnetic systems to model real-world behaviour

Open OnDemand

The screenshot shows the Open OnDemand web interface. The top navigation bar includes 'metacentrum', 'Files', 'Jobs', 'Clusters', 'Interactive Apps', 'My Interactive Sessions', and 'Help'. The main content area shows a search for 'ansys' with 3 results. The results are listed in a table with columns for Name, Category, and Sub Category. The 'Ansys/Fluent' entry is highlighted with an orange box.

Name	Category	Sub Category
Ansys/Enight	Interactive Apps	Desktops
Ansys/Fluent	Interactive Apps	Desktops
Ansys/Workbench	Interactive Apps	Desktops

Showing 1 to 3 of 3 entries (filtered from 24 total entries)

<https://docs.metacentrum.cz/en/docs/software/sw-list/ansys>



metacentrum **Open OnDemand** Files Jobs Clusters

https://ondemand.metacentrum.cz

Home / All Apps

Show 10 entries

Name
Ansys/Ensign
Ansys/Fluent
Ansys/Workbench

Showing 1 to 3 of 10 entries

- Web application
- OpenPBS scheduler
- Running (noto)

Home / My Interactive Sessions / Ansys/Fluent

Interactive Apps

Cloud

- Kubernetes on OpenStack (KOST) (beta)
- OpenStack VM (beta)

Desktops

- Ansys/Ensign
- Ansys/Fluent**
- Ansys/Workbench
- BIOP Desktop
- CLCgenomicsWB
- MZMINE
- Matlab
- MetaCentrum Desktop
- QuPath
- VMD Desktop

Servers

- Julia Pluto.jl

Ansys/Fluent

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)

Launch

* The Ansys/Fluent session data for this session can be accessed under the [data root directory](#).



Ansys/Fluent (19140872.pbs-m1.metacentrum.cz)

1 node | 2 cores | Running

Host: adan48.grid.cesnet.cz

Delete

Created at: 2026-04-17 12:26:25 CEST

Time Remaining: 59 minutes

Session ID: 67a55148-ef8a-48fd-ae52-06296c1a86e6

Compression

0 (low) to 9 (high)

Image Quality

0 (low) to 9 (high)

Launch Ansys/Fluent

View Only (Share-able Link)

- Web application
- OpenPBS scheduler
- Running (not only)

Show 10 entries

Name

Ansys/Ensign

Ansys/Fluent

Ansys/Workbench

Showing 1 to 3 of 3 entries

MZMINE

Matlab

MetaCentrum Desktop

QuPath

VMD Desktop

Servers

Julia Pluto.jl

CPUS

0

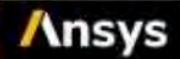
Scratch local (GB) <https://docs.metacentrum.cz/en/docs/software/sw-list/ansys>

0

Launch

* The Ansys/Fluent session data for this session can be accessed under the [data root directory](#).

Fluent Launcher 2024 R2

Fluent Launcher 

Home | General Options | Parallel Settings | Scheduler | Environment

Meshing

Solution

Materials Processing

Capability Level: Premium

Read

Recent Files

Dimension: 2D 3D

Solver Options: Double Precision Native GPU Solver

Parallel (Local Machine): Solver Processes: 1

Working Directory: /storage/praha1/home/vorel

Show Beta Launcher Options

Start **Reset** **Cancel** **Help**

Open OnDemand

Files Jobs Cl...

https://ondemand.metacent...

Home / A...

Show 10 ter...

Name

- Ansys Ansys/En...
- Ansys Ansys/Fl...
- Ansys Ansys/W...

Showing 1 to 3

- Web application
- OpenPBS sche...
- Running (not...



Mesh

Display... Info Units... Check... Quality... Transform... Make Polyhedra... Scale... Append... Replace Mesh... Replace Zone... Delete... Deactivate... Activate... Combine... Separate... Adjacency... Mesh... Overset... Dynamic Mesh... Gap Model... Turbo Models... Turbo Create... Turbo Performance... Spectral Content... Turbo Workflow... Turbo Topology... Periodic Instancing... Adapt Surface

Outline View

Case View

Filter Text

Setup

General

Materials

Solution

Results

Surfaces

Graphics

Plots

Dashboard

Animations

Reports

Parameters & Customization

Simulation Reports

Task Page

General

Mesh

Scale...

Check

Report Quality

Display...

Units...

Solver

Type

 Pressure-Based Density-Based

Velocity Formulation

 Absolute Relative

Time

 Steady Transient Gravity

User Window 1

Ansys
2024 R2

0 selected all




Console

Warning:

'glxinfo' is not found (graphics capability check failed), hardware acceleration will be disabled
 In the absence of hardware-accelerated drivers, the performance of all graphics operations will be severely affected. Make sure you have a supported graphics card, latest graphics driver, and a supported remote visualization tool with direct server-side rendering enabled. If you feel your system meets these requirements, try forcing the accelerated driver by using the command line flag (-driver <name>) or setting the HOOPS_PICTURE environment variable. Refer to the documentation for more details.

Posting ANSYS Product Improvement Program startup data
 Done.

> |

File	Domain	Physics	User-Defined	Solution
Read		ing		Support
Write				
Parametric Project				
Import		ABAQUS		Input File...
Export		CFX		Filbin File...
Export to CFD-Post...		CGNS		ODB File...
Table File Manager...		EnSight...		
Solution Files...		GAMBIT...		
Interpolate...		HYPERMESH ASCII...		
FSI Mapping		Mechanical APDL		
Save Picture...		NASTRAN		
Data File Quantities...		PLOT3D Grid...		
Batch Options...		Tecplot...		

Select File

Look in:

- Comp...
- vorel
 - /auto/vestec1-elixir/home/vorel
 - /auto/vestec1-elixir/home
 - /auto/vestec1-elixir
 - /auto
 - /
 - Computer

Recent Places

- /auto/vestec1-elixir/home/vorel

ABAQUS File:

Files of type: ABAQUS Input Files (*.inp*)

Filter String:

OK Cancel Filter

Console
Warning:
'glxinfo' is not f
In the absence of
supported graphics
you feel your syst
setting the HOOPS_

Posting ANSYS Prod
Done.

> |

Display

Views... Headlight Lighting

Options... Gouraud

Camera...

Graphics

Lights... Compose...

Colormap... Annotate...

Mouse

Left: mouse-rotate Probe: short description

Middle: mouse-zoom Fluent Defaults

Right: mouse-probe Workbench Defaults

Outline View

Filter Text

- Setup
 - General
 - Models
 - Materials
 - Cell Zone Conditions
 - Boundary Conditions
 - Mesh Interfaces
 - Dynamic Mesh
 - Reference Values
 - Reference Frames
 - Named Expressions
- Solution
 - Methods
 - Controls
 - Report Definitions
 - Monitors
 - Cell Registers
 - Initialization
 - Calculation Activities
 - Run Calculation
- Results
 - Surfaces
 - Graphics
 - Mesh
 - Contours
 - contour-2
 - contour-1
 - Vectors
 - Pathlines
 - Particle Tracks
 - Plots
 - Scene
 - Animations
 - Reports
- Parameters & Customization

Task Page

Run Calculation

Check Case... Update Dynamic Mesh...

Pseudo Transient Settings

Fluid Time Scale

Time Step Method: Automatic Time Scale Factor: 1

Length Scale Method: Conservative Verbosity: 0

Parameters

Number of Iterations: 420 Reporting Interval: 1

Profile Update Interval: 1

Solution Processing

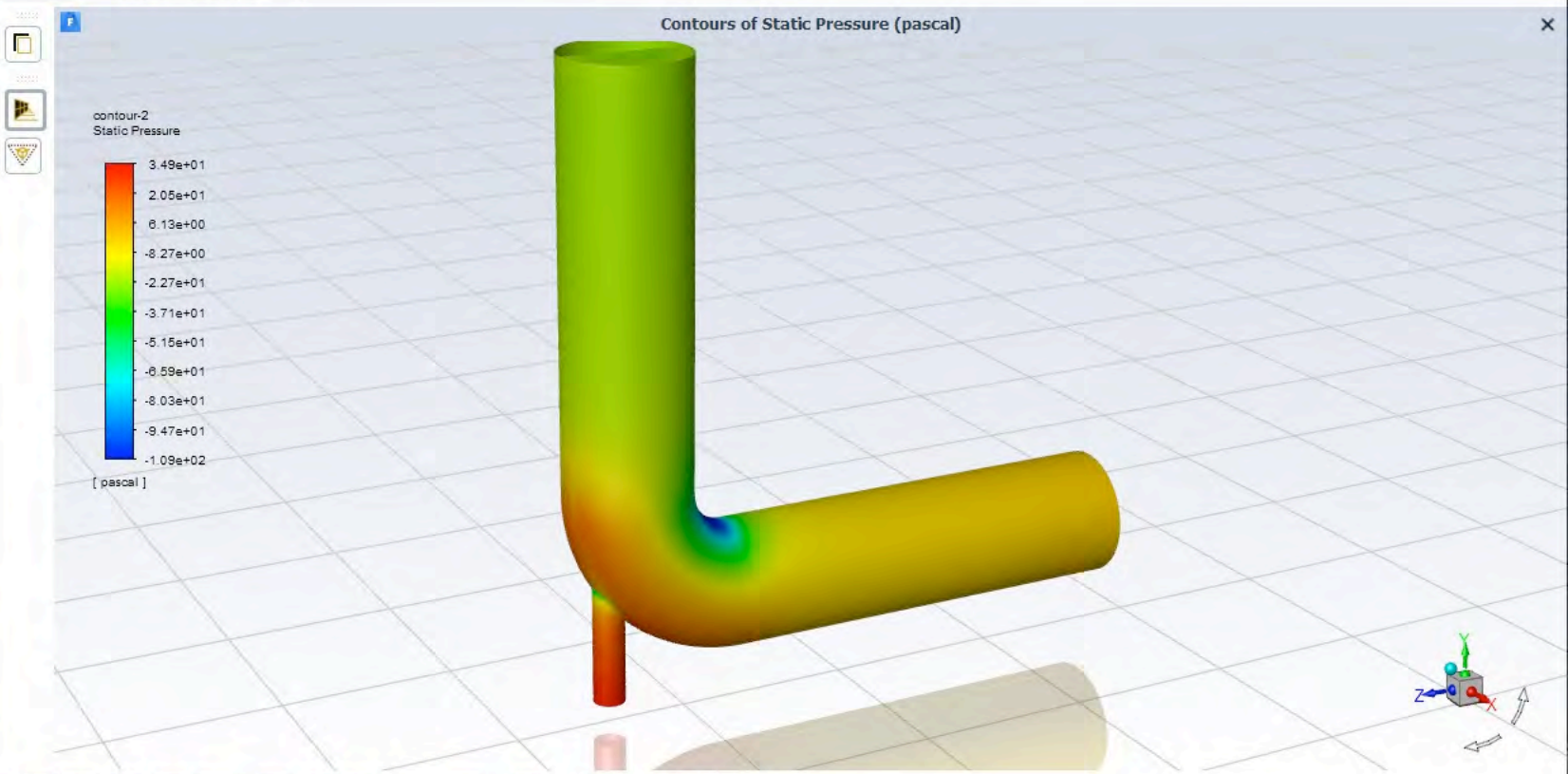
Statistics

Data Sampling for Steady Statistics

Data File Quantities...

Solution Advancement

Calculate



Console

Done.

Feature already enabled.

Reading "\ | gunzip -c \"D:\YOUTUBE\1. CFD.NINJA\ANSYS STUDENT\3. Fluent\Elbow\elbow3d_files\dp0\FLU\Fluent\SYS-1-00093.dat.gz\" \"\"...

Parallel variables...

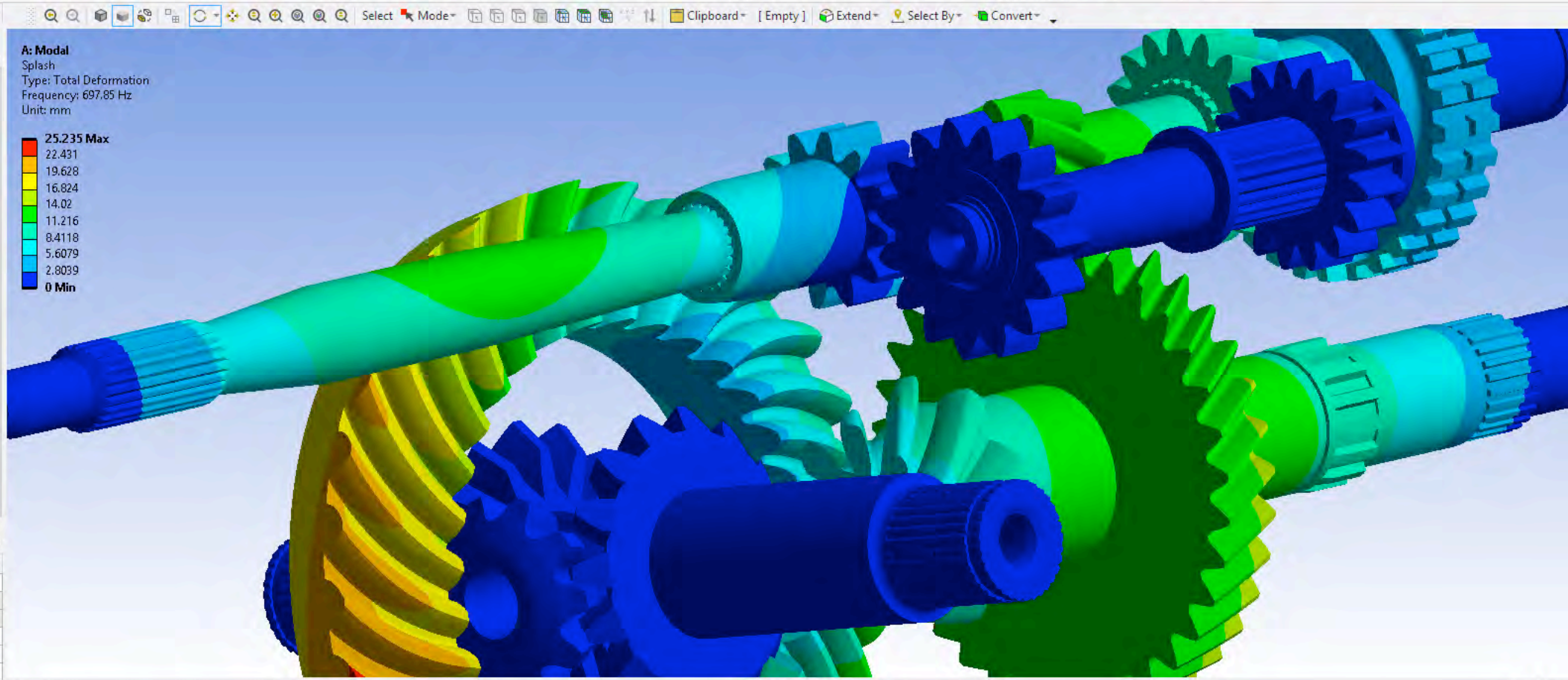
Done.

Outline

Name Search Outline

Project

- Model (A4)
 - Geometry
 - Materials
 - Coordinate Systems
 - Connections
 - Mesh
 - Named Selections
 - Modal (A5)
 - Pre-Stress (None)
 - Analysis Settings
 - Fixed Support
 - Fixed Support 2
 - Fixed Support 3
 - Fixed Support 4
 - Fixed Support 5
 - Fixed Support 6
 - Fixed Support 7
 - Solution (A6)
 - Solution Information
 - Total Deformation
 - Total Deformation 2
 - Total Deformation 3
 - Total Deformation 4
 - Splash
 - Total Deformation 6
 - Total Deformation 7
 - Total Deformation 8
 - Total Deformation 9
 - Total Deformation 10
 - Total Deformation 11
 - Total Deformation 12



Details of "Splash"

Scope

Scoping Method: Geometry Selection
 Geometry: All Bodies

Definition

Type: Total Deformation
 Mode: 5
 Identifier:
 Suppressed: No

Results

Minimum: 0. mm
 Maximum: 25.235 mm
 Minimum Occurs On: Shaft.Solid
 Maximum Occurs On: Ring Gear.3\Solid1

Information



Tabular Data

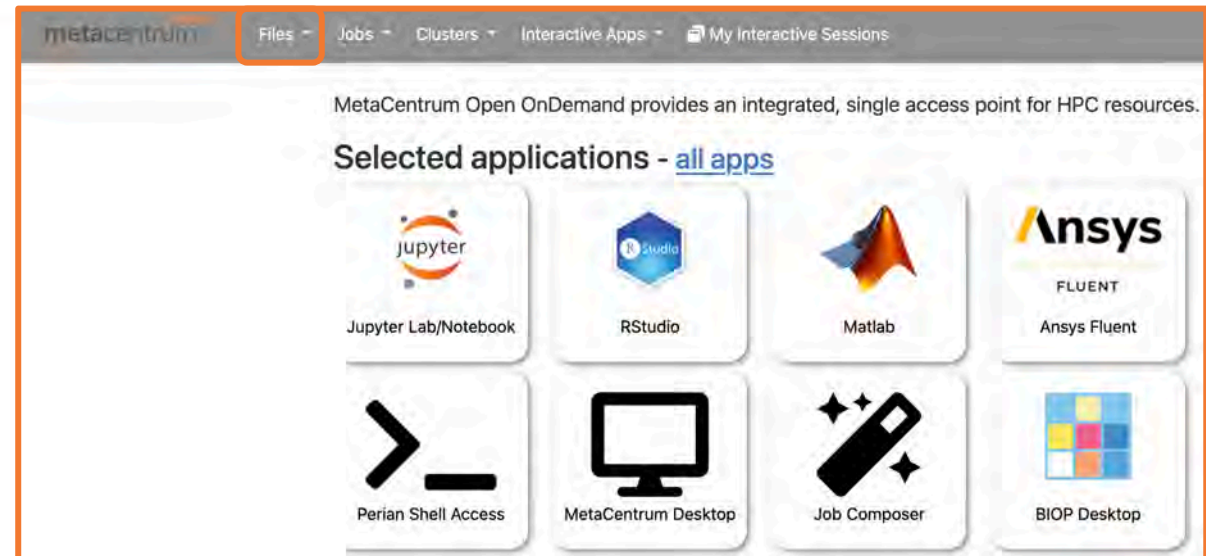
Mode	Frequency [Hz]
1	184.09
2	387.12
3	395.05
4	688.41
5	697.85
6	703.87
7	917.9
8	1064.
9	1137.
10	1188.3
11	1303.4
12	1542.4

■ Open OnDemand



<https://ondemand.metacentrum.cz/>

- Web application on top of OpenPBS scheduler
- Running (not only) GUI applications
- Browsing storages (tab 'Files')



Open OnDemand

■ Open OnDemand

<https://ondemand.metacentrum.cz>

- Web application
- OpenPBS scheduler
- Running (not on demand)
- Browsing storage

The screenshot displays the Open OnDemand web interface. The top navigation bar includes 'metacentrum', 'Files', 'Jobs', 'Clusters', 'Interactive Apps', and 'My Interactive Sessions'. A file browser is open, showing a list of home directories under the 'Home Directory' section. The 'cesnet_s3' and 'projects' entries are highlighted with orange boxes. To the right, there is a section titled 'all apps' with several application tiles: 'Matlab', 'Ansys FLUENT Ansys Fluent', 'Job Composer', and 'BIOP Desktop'. A 'desktop' tile is partially visible on the left. The interface is designed to provide a single access point for HPC resources.

[Open in Terminal](#) [Refresh](#) [New File](#) [New Directory](#) [Upload](#) [Download](#) [Copy/Move](#) [Delete](#)

Home Directory

- brno2
- brno12
- praha5-elixir
- brno11-elixir
- brno14-ceitec
- brno3-cerit
- budejovice1
- liberec3
- plzen1
- plzen4-ntis
- praha1
- praha2-natur
- praha5-elixir
- praha6-fzu
- pruhonice1-ibot
- projects
- projects2
- projects-du-praha
- cesnet_s3

cesnet_s3: / [Change directory](#) [Copy path](#)

Show Owner/Mode Show Dotfiles Filter: Showing 1 rows - 0 rows selected

<input type="checkbox"/>	Type ▲	Name	Size	Modified at
<input type="checkbox"/>	Folder	meta-archive	-	20. 8. 2024 17:59:00


Open in Terminal Refresh New File New Directory Upload Download Copy/Move Delete

- Home Directory
- brno2
- brno12
- praha5-elixir
- brno11-elixir
- brno14-ceitec
- brno3-cerit
- budejovice1
- liberec3
- plzen1
- plzen4-ntis
- praha1
- praha2-natur
- praha5-elixir
- praha6-fzu
- pruhonice1-ibot
- projects

cesnet_s3: / meta-archive / Change directory Copy path

Show Owner/Mode Show Dotfiles Filter: Showing 12 rows - 0 rows selected

Type	Name	Size	Modified at
Folder	03_E_nip_genom	-	17. 4. 2026 10:19:50
Folder	03_E_nip_trans	-	17. 4. 2026 10:19:50
Folder	04_Viremie_AV_Kapr_Karas	-	17. 4. 2026 10:19:50
Folder	04_Viremie_AV_Plotice_Cejn	-	17. 4. 2026 10:19:50
Folder	05_Nikol_Kmentova	-	17. 4. 2026 10:19:50
Folder	06_Kasa_mansoni_hepatica_vejce	-	17. 4. 2026 10:19:50
Folder	07_Haem_cont_metylacDNA	-	17. 4. 2026 10:19:50
Folder	08_JI_hetero_trans	-	17. 4. 2026 10:19:50
File	01_Echo.tar.gz	662.80 GB	9. 10. 2022 15:21:53
File	02_TomasPakosta.tar.gz	3.56 GB	14. 11. 2020 18:46:42
File	02_TomasPakosta_posledni_vymysl.zip	13.46 GB	19. 3. 2025 14:40:50
File	022.tar.gz	473.75 GB	11. 12. 2023 19:47:56

 OnDemand is suboptimal for S3 operations. Consider using a third-party FTP client instead.

Open in Terminal Refresh New File New Directory Upload Download Copy/Move Delete

- Home Directory
- brno2
- brno12
- praha5-elixir
- brno11-elixir
- brno14-ceitec
- brno3-cerit
- budejovice1
- liberec3
- plzen1
- plzen4-ntis
- praha1
- praha2-natur
- praha5-elixir
- praha6-fzu
- pruhonice1-ibot
- projects

cesnet_s3: / meta-archive / Change

Type	Name
Folder	03_E_nip_genom
Folder	03_E_nip_trans
Folder	04_Viremie_AV
Folder	04_Viremie_AV
Folder	05_Niko_Kment
Folder	06_Kasa_manso
Folder	07_Haem_cont_r
Folder	08_JI_hetero_tra
File	01_Echo.tar.gz
File	02_TomasPakost
File	02_TomasPakost
File	Kapentagyrus_Ju...

Drop files here, [browse files](#) or [browse folders](#)

Empty directories will be included in the upload only when a directory upload is initiated via drag and drop. This is because the File and Directory Entries API is available only on a drop event, not during an input change event.

Powered by Uppy

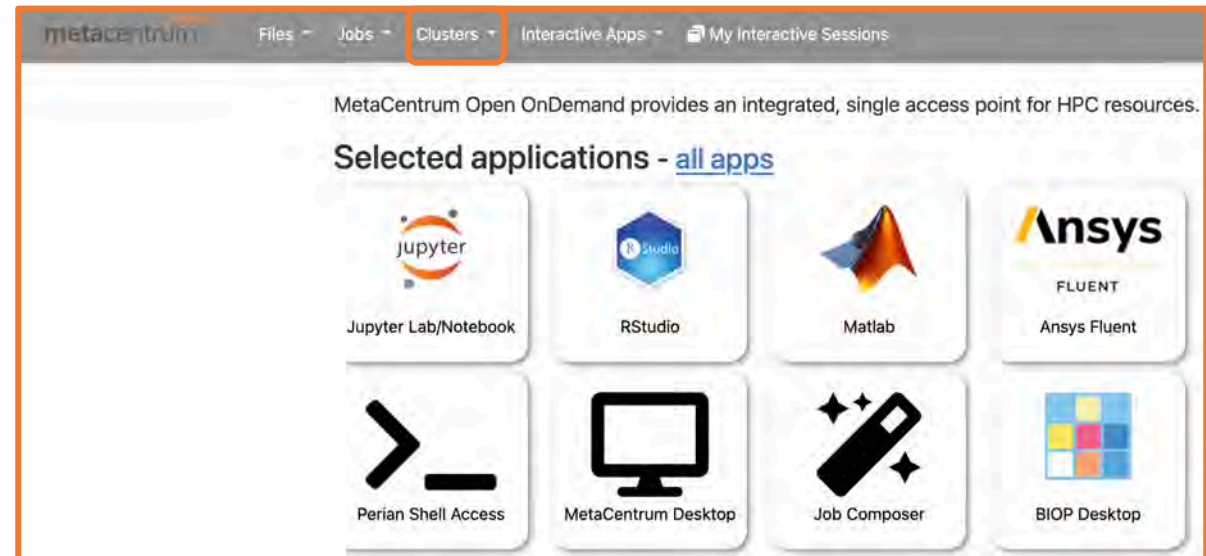
 Upload data from the local computer

■ Open OnDemand



<https://ondemand.metacentrum.cz/>

- Web application on top of OpenPBS scheduler
- Running (not only) GUI applications
- Browsing storages (tab 'Files')
- Command line (tab 'Clusters')



■ Open OnDemand

<https://ondemand.metacentrum.cz/>

- Web application or OpenPBS scheduler
- Running (not only)
- Browsing storages
- Command line (tab)





Your Home Directories

Avail space	DATA quota	DATA used	FILES quota	FILES used	Backup	Storage
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:

Job ID	Username	Queue	Jobname	SessID	NDS	TSK	Req'd Memory	Req'd Time	Elap S	Time
19137135.pbs-m1.met*	vorel	interac*	STDIN	387033	1	1	400mb	18:00	R	00:00

(BOOKWORM)vorel@zenith:~\$

Themes: Cobalt2

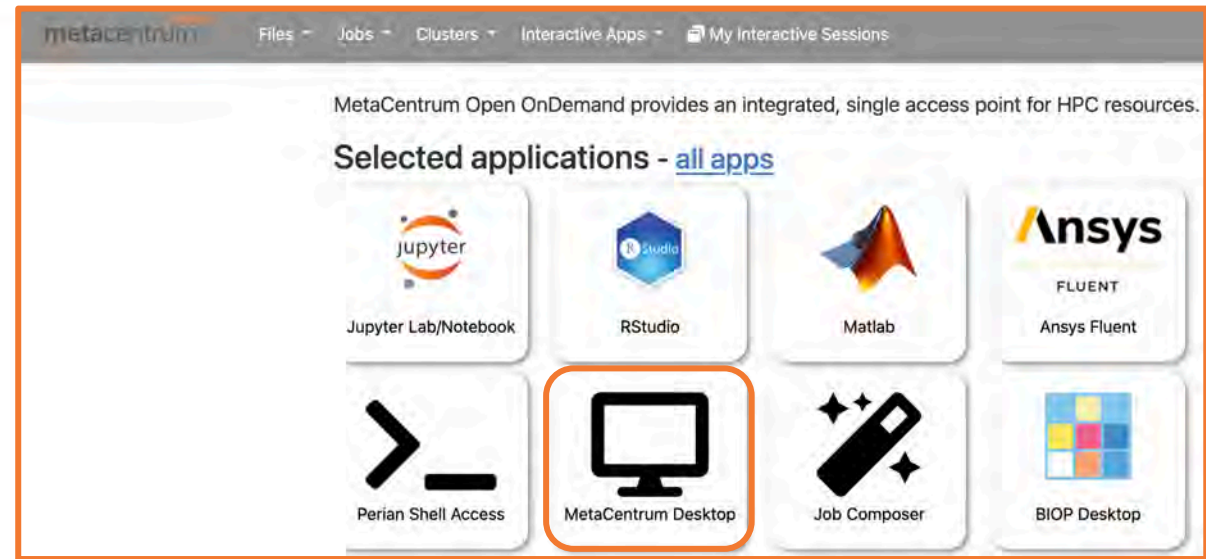
- Default
- Bright
 - CLRS
 - Github
 - Solarized Light
 - Tomorrow
- Dark
 - Cobalt2**
 - idleToes
 - Monokai Remastered
 - Pastel Dark
 - Red Alert
 - Tomorrow Night Blue
 - Tomorrow Night Bright
 - Tomorrow Night Eighties
 - Tomorrow Night

■ Open OnDemand



<https://ondemand.metacentrum.cz/>

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



■ Open OnDemand



<https://ondemand.metacentrum.cz/>

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

The screenshot shows the Open OnDemand web interface. The breadcrumb navigation at the top reads "Home / My Interactive Sessions / MetaCentrum Desktop". On the left, a sidebar lists various interactive applications under categories: "Interactive Apps", "Cloud" (Kubernetes on OpenStack (KOST) (beta), OpenStack VM (beta)), "Desktops" (Ansys/Enlight, Ansys/Fluent, Ansys/Workbench, BIOP Desktop, CLCgenomicsWB, MZMINE, Matlab), "MetaCentrum Desktop" (highlighted), QuPath, VMD Desktop, "Servers" (Julia Pluto.jl, Jupyter - Evo2 (beta), Jupyter Notebook/Lab, Matlab webapp (beta), RStudio Server). The main content area is titled "MetaCentrum Desktop" and contains a description: "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." Below this are configuration fields: "Number of hours" (2), "Number of CPUs on single node" (1), "Memory (GB)" (10), "GPUs" (0), and "Scratch local (GB)" (0). A blue "Launch" button is at the bottom, highlighted with an orange border. A note at the bottom states: "* The MetaCentrum Desktop session data for this session can be accessed under the [data root directory](#)."

■ Open OnDemand

<https://ondemand.metacentrum.cz>

- Web application
- OpenPBS scheduler
- Running (not on demand)
- Browsing storage
- Command line (tab 'Clusters')
- Launch a virtual desktop (MetaCentrum Desktop app)

The screenshot displays the Open OnDemand interface for a specific session. At the top, the breadcrumb navigation shows 'Home / My Interactive Sessions / MetaCentrum Desktop'. The session title is 'MetaCentrum Desktop (19144708.pbs-m1.metacentrum.cz)', with status indicators for '1 node', '1 core', and 'Running'. A 'Delete' button is visible in the top right. Below the title, the host is 'galdor20.metacentrum.cz', the creation time is '2026-04-17 15:01:21 CEST', and the time remaining is '1 hour and 59 minutes'. The session ID is '6ec1a410-d8da-4e60-a8eb-dd0e255a4c00'. Two sliders are present: 'Compression' (0 to 9, low to high) and 'Image Quality' (0 to 9, low to high). A blue 'Launch MetaCentrum Desktop' button is highlighted with an orange border. To the right is a 'View Only (Share-able Link)' button. Below the main session card, a sidebar lists other applications: 'VMD Desktop', 'Jupyter - Evo2 (beta)', 'Jupyter Notebook/Lab', 'Matlab webapp (beta)', and 'RStudio Server'. A 'Launch' button is highlighted with an orange border. A note at the bottom right states: 'The MetaCentrum Desktop session data for this session can be accessed under the [data root directory](#).'





Geneious is a comprehensive, user-friendly bioinformatics software for molecular biology and DNA, RNA and protein sequence analysis



xterm

- Mathematics
- Genomics
 - CLCbio Genomics Workbench 9.5.3
 - Geneious 7.1.5**
 - SNP and AFLP Package for Phylogenetic analysis
- Medicine
- Geoscience
- Visualisation
- Technical and material simulations
- Utilities
 - Tablet
 - FingerPrinted Contigs
 - UEA sRNA Workbench
- Programs
- Settings
- Logout

1 2 3 4

geneious^g R7

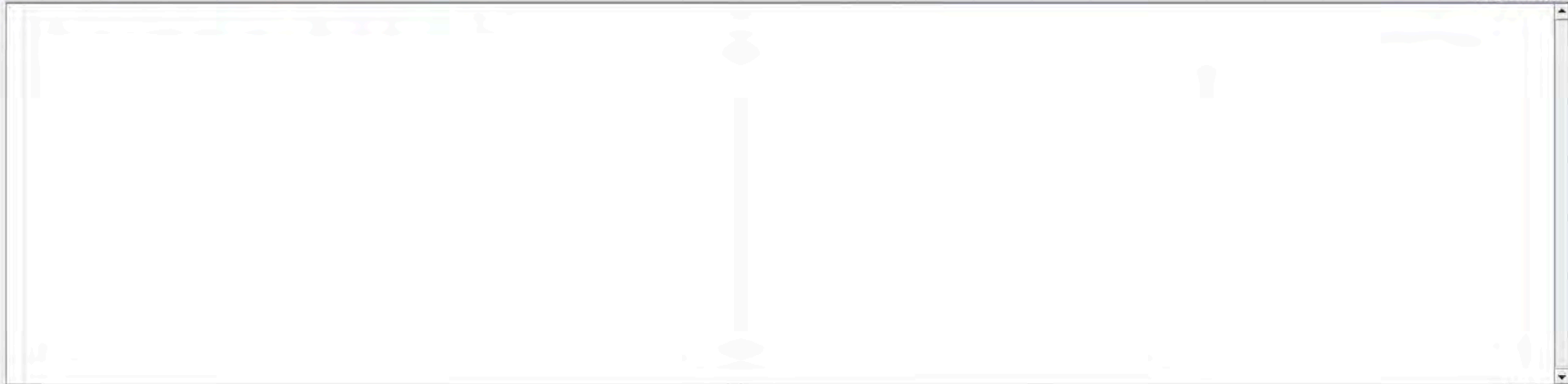
Starting plugin: Workflows

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Geneious is a registered trademark of Biomatters Ltd. Applicable in all regions.



Unfortunately, our latest version is 7.1.5 (2014)

- Sources
- Local (0)
 - Sample Documents (623)
 - Deleted Items (0)
 - Shared Databases
 - Operations
 - NCBI
 - Gene
 - Genome
 - Nucleotide
 - PopSet
 - Protein
 - PubMed
 - SNP
 - Structure
 - Taxonomy
 - UniProt



✖ Hide

**Customized shortcut keys**

Tip #3

Go to the *Keyboard* tab in *Tools / Preferences* to change any of the shortcut keys in Geneious. You can even create new shortcuts for your favourite operations.

Previous Tip

Next Tip

File Edit View Tools Sequence Annotate & Predict Help

- New Folder...
- Rename Folder...
- Set Folder Color...
- Move Folder...
- Delete Document/Folder Delete
- Erase Document/Folder Permanently... Shift+Delete
- Restore from Deleted Items
- Erase All Deleted Items...
- Save Ctrl+S
- Save As... Ctrl+Shift+S
- Download Document(s) Ctrl+W
- Cancel Download(s) Ctrl+Shift+W
- Back Up Data...
- Restore Backup...
- Import Ctrl+H
- Export
- Print Ctrl+P
- Save As Image File Ctrl+Alt+S
- Exit

Assemble Tree Primers Cloning Back Up Support Help

Q Tiger Search

0 of 0 selected

- From File... Ctrl+H
- From Clipboard Import documents into Genelous from files on your computer.
- Sample Documents
- Vector NTI Database
- Preferences...



Customized shortcut keys

Tip #3

Go to the *Keyboard* tab in *Tools / Preferences* to change any of the shortcut keys in Genelous. You can even create new shortcuts for your favourite operations.

[Previous Tip](#)[Next Tip](#)

Using 70 / 399996 MB memory

- Sources
- Local (0)
- Sample Documents (623)
- Deleted Items (0)
- Shared Databases
- Operations
- NCBI
 - Gene
 - Genome
 - Nucleotide
 - PopSet
 - Protein
 - PubMed
 - SNP
 - Structure
 - Taxonomy
 - UniProt

Choose Files to Import

Look In: Sample Importable Files

- /
- storage
- brno2
- home
- vorel
- .geneious7.1.data
- Sample Importable Files

File Name:

Files of Type: All Files

Import Cancel

Go to the *Keyboard* tab in *Tools / Preferences* to change any of the shortcut keys in Geneious. You can even create new shortcuts for your favourite operations.

Previous Tip Next Tip

- Sources
- Local (0)
 - Sample Documents (623)
 - Deleted Items (0)
 - Shared Databases
 - Operations
 - NCBI
 - Gene
 - Genome
 - Nucleotide
 - PopSet
 - Protein
 - PubMed
 - SNP
 - Structure
 - Taxonomy
 - UniProt

Choose Files to Import

Look In: Sample Importable Files

- /
 - storage
 - brno2
 - home
 - vorel
 - .geneious7.1.data
 - Sample Importable Files
- sampleTree.tree

File Name:

Files of Type: All Files

Import Cancel

Go to the *Keyboard* tab in *Tools / Preferences* to change any of the shortcut keys in Geneious. You can even create new shortcuts for your favourite operations.

Previous Tip Next Tip

- Sources
- Local (0)
- Sample Documents (623)
- Deleted Items (0)
- Shared Databases
- Operations
- NCBI
 - Gene
 - Genome
 - Nucleotide
 - PopSet
 - Protein
 - PubMed
 - SNP
 - Structure
 - Taxonomy
- UniProt

Choose Files to Import

Look in: vorel

- CASTEP-25.1.2
- META_SUPPORT
- ondemand
- OpenMolcas
- R
- test_crys
- test_WiseCon
- Abundan_partial.bt
- E_nip_transcriptome_nucl_final_80.fsa**

File Name: E_nip_transcriptome_nucl_final_80.fsa

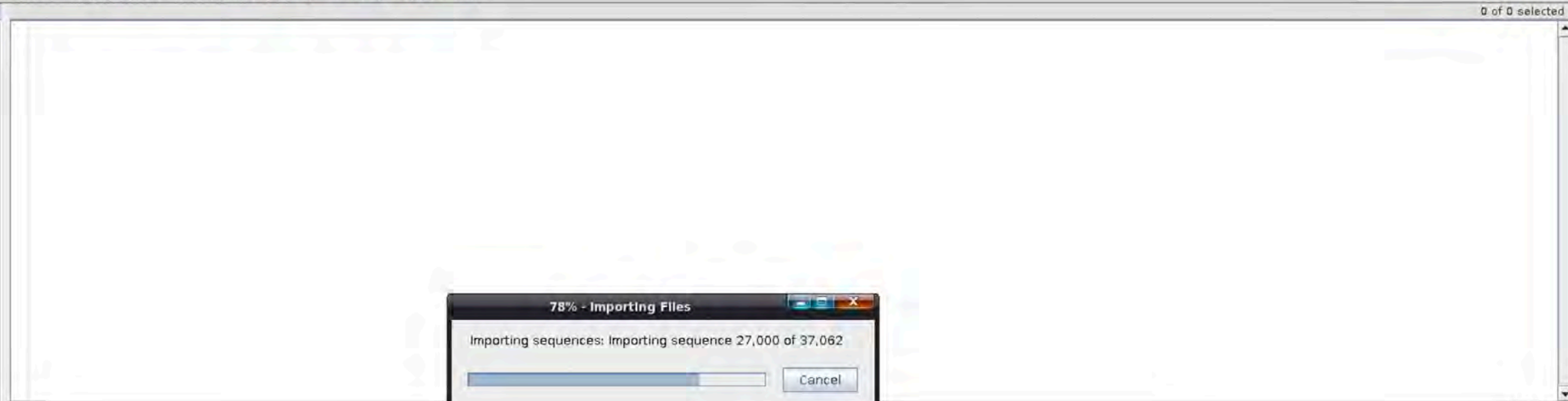
Files of Type: All Files

Import Cancel

Go to the **Keyboard** tab in **Tools / Preferences** to change any of the shortcut keys in Geneious. You can even create new shortcuts for your favourite operations.

Previous Tip Next Tip

- Sources
- Local (0)
- Sample Documents (623)
- Deleted Items (0)
- Shared Databases
- Operations
- NCBI
 - Gene
 - Genome
 - Nucleotide
 - PopSet
 - Protein
 - PubMed
 - SNP
 - Structure
 - Taxonomy
 - UniProt



78% - Importing Files

Importing sequences: Importing sequence 27,000 of 37,062

Cancel

Customized shortcut keys
Tip #3

Go to the *Keyboard* tab in *Tools / Preferences* to change any of the shortcut keys in Geneious. You can even create new shortcuts for your favourite operations.

Previous Tip Next Tip

Sources

- Local (0)
 - Sample Documents (624)
 - Deleted Items (0)
- Shared Databases
- Operations
- NCBI
 - Gene
 - Genome
 - Nucleotide
 - PopSet
 - Protein
 - PubMed
 - SNP
 - Structure
 - Taxonomy
 - UniProt

Name	Description
E_nip_transcriptome_...	

# Sequenc...	Min Seque...	Max Seque...	Path (Impo...	Filename (I...
37,062	90	15,822	/storage/br...	E_nip_trans...

Sequence View Lengths Graph Text View Info

37,062 nucleotide sequences

E_nip_trans_62433_m.388819

```

1      10      20      30      40      50
|      |      |      |      |
ATGAAGCTAAGCATAGGACAACATCGATTTGGGTGACCATTTGGATACA
ACTTATGACGGTTGGTGAGCAAAATTTAATAACGCCGACTAGAGGAGAAG
GCAAAAATGCTTCGCATGGTGCAACATCTGGAGATGGGTTCGAACAAAT
GACACAAATATTATTTCAAGTCATTAATAGGTTTAAAGTTGATACAAACAA
TTTTTTACAAAACGCAATGAAGCTCAGCAGAGAACAACGTCGTATGATGG
AAATTTATAAAAAAAGCTATATAA
    
```

E_nip_trans_15128_m.116119

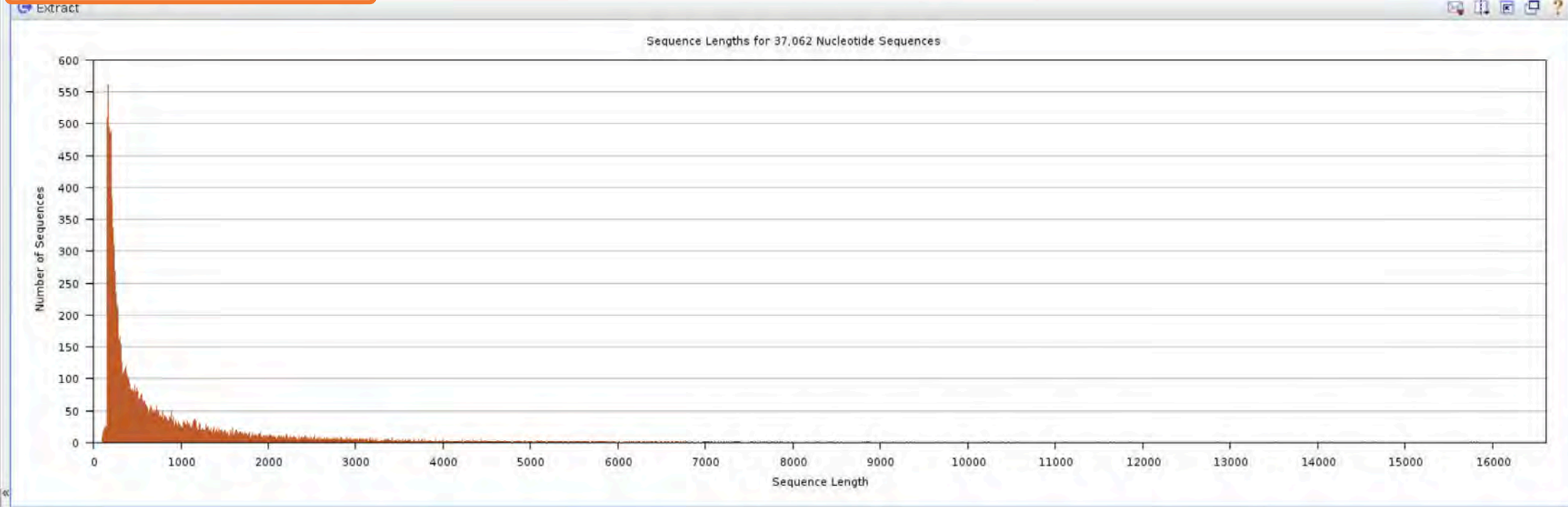
```

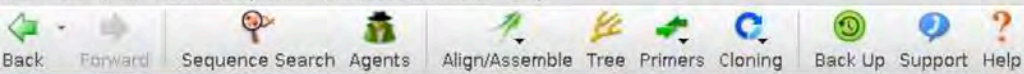
1      10      20      30      40      50
|      |      |      |      |
GGAAGTCTTTGCTTCCTTTACGGATTTCTTTTTCCGACAGAAATGATCA
TATCTCAAATCCTCATTATTTTACAAGGAGCGGGTCGTAGGAAGGTTG
TTCTTCTAATTATTGATGGCCTTCGCCGCTGATCGATTTTATCGGATGAT
ATGCTGCAACACTGGCCGAATCTTAAAGTTATATAGATGAAGGAATGGT
TGACTGTTCAACCTGTCGATTAAGAGCGCCAACAGTTACACTGCCACGTT
TAAAAGCGATTGTTCTGGTGGTGTGCCGCAATTTGTGGATTTTATATAT
AATCTTAAATGCAAAAGAAGTTAAGAAGACAATTTTATCCGAAGATTGAA
    
```

- Sources
- Local (0)
- Sample Documents (624)
- Deleted Items (0)
- Shared Databases
- Operations
- NCBI
 - Gene
 - Genome
 - Nucleotide
 - PopSet
 - Protein
 - PubMed
 - SNP
 - Structure
 - Taxonomy
- UniProt

Name	Description	# Sequenc...	Min Seque...	Max Seque...	Path (Impo...	Filename (I...
E_nip_transcriptome_...		37,062	90	15,822	/storage/br...	E_nip_trans...

Sequence View Lengths Graph Text View Info





Sources

- Local (0)
 - Sample Documents (624)
 - Deleted Items (0)
- Shared Databases
 - NCBI
 - Gene
 - Genome
 - Nucleotide
 - PopSet
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 - SNP
 - Structure
 - Taxonomy
 - UniProt

Name	Description	# Sequenc...	Min Seque...	Max Seque...	Path (Imp...
E_nip_transcriptome_nucl_final_80	-	37,062	90	15,822	/storage/...

Sequence View Lengths Graph Text View Info

Extract R.C. Translate Add/Edit Annotation Allow Editing Annotate & Predict Save

1. E_nip_tran... ATGAAGCTAAGCATAGGACAACATCGATTTGGGTGACCAATTTGGATACAACCTTATGACGGTGGTGAGCAAAATTTAAACGGGGACTAGAGG
 2. E_nip_tran... GGAAGTCTTTGCTTCCTTTACGGATTTCTTTTCCGACAGAAATGATCATATCTCAAATCCTCATTATTTTACAAAGGAGCGGGTCGTAGGGAA
 3. E_nip_tran... ATGCGTTATCGTTTTAAAGTTATCTTTCCATCTCGGTTAATTCCTAGTCTTTTCAAAGGCAATCGTAAAGTCCGATTTTCTGCTTCACTTTG
 4. E_nip_tran... TTGAACGATGTAGATGCTTTCTTTACAATGTTAGAAACCGGAGAAAATTTATTTTTCAGAAAGGAGAGTTGTGCCAGTTGCCAGGAGTATACTG
 5. E_nip_tran... ATGCTCAGATGTTTACAGAGCCTTGGATACACAGAGCTTCTCAAATCGAGTCTTTTGGCAGGCACTCTCAAACATCCACATTTTACAGTCCAT
 6. E_nip_tran... TTTATGACGCGCAATGAAACTAAGCTTGTCTACCAATTAACAAGAGAGTTAGCGCAAAATAAATCTGCCACTGAAACCCTGTTTGTAGATGAAGA
 7. E_nip_tran... ATGGGTTTTGTTTTACTGCTGTGCTGATATACAGTGTCAATATGAATACAAGCAATTCATTTTTTACTGCATCTTTACTTGTACATTTGTTCT
 8. E_nip_tran... ATGGAAGGTCGTCGACTAGCACTGCGCGTCCACGGCCGACGCAAAATGTTACGAAAACGTTTTATTTGATGCTCAAATGACAGTGTGCGAGGG
 9. E_nip_tran... GAAAATCGATGTGCGCACCAATCTACGAATGAGACTTTCAGCTCTTGTAAATTAATACTAATAAATACTGTTTATTTGTTCAATAAAACCAAA
 10. E_nip_tra... ATGTTTTGGACTTTTAAACGTCGAACGCTTACTTTTAAATTTGCTAATTTCTTGGCCAGATAAAAAGCAGTCTTTTTCAGAAATGCCAACATTA
 11. E_nip_tra... ATGGCGAAGTATCAATCTAAATGTCAATACGTGTTTCTTCATCAATGCTCGGCGGTGCTACATTTTCTGATTTATTTTTCGATATTGTTGACGGGTTG
 12. E_nip_tra... AATCGTCAAGCAATGGACTCCATCGGTCGAGCTACCTCCGGTCCGCAACTTTTTCGATCTCACATTTACATAGAAGATCTATCACTGCATC
 13. E_nip_tra... GAGCGTTTGAATTCAGTACCTTTGCAATAGGATACAGGACCCCTACTACAAATTCGAACCAATTAATTTTACGAGAAAACCTATTATTGAACTTT
 14. E_nip_tra... ATGGTCTACCACTTGACAGCATACCGTAGTAGAAGTGAAGTGTCTTAAAGCCTTGGTGGACGATCTGGCGACCGAACAGCCCTGGCGAATTTGAA
 15. E_nip_tra... ATGTACGATTGTTTATCCCGTATATACTGCCCTTGGTATCGCATTGTTGATGTTTCAATTTTGTCTCCCTGGTAAAAACACAACGTGTGTGGAT
 16. E_nip_tra... ATGATATGTTTTATTTTACATTTCAATCTATTTTTAGAAATTTTATTCATGTCATCAATTTAAATGGGTTACATTTTGTATTTGTGCATCGGCA
 17. E_nip_tra... ATGATATTTACGTTTTATAGAAAATTTCCCAAAATTTGCTCCCAATTTGTCAACATTTGTTCCCTCTGTTTACAAAATGTTTTGTTCTTGTCA
 18. E_nip_tra... GGCCGAGACGAGCATAAAACAAAAGAAAAGAAAGGAGCGTGGACAAGAGGCAATTTCTGAGAAAAGCTAGCAAATCCACCCTTGGACTAGTGACCC
 19. E_nip_tra... CACAACAATCCCTCTTAAACAGCAGAGGATCAAGAAATTTGAGTCAAACCCGGTGAATAAATACTATCATCACCAAAAGCAACTTACAA
 20. E_nip_tra... ATGTCGCCCAATATTGCTCTACGATTTGGCATAAGCGGTATCAACACGCATTTTCGACTTCACTAATAATTTAGTGGTGTCTATGTTTACTTTT
 21. E_nip_tra... ATGATAAATATGCCTTTAGCAAAACATTTCCCTTTCTGTGAATCATTATTTATCTTTACTGACTTTGTAACATGCACATTTATGTCACACAA
 22. E_nip_tra... ATGCAAAATGAGGTTTTATACAACAAATTTGTTCAATTTATTTCTCCGTTTCATCTCTACTGTTCTAGTGCATCCTTTTTATGGCGTGTTTAG
 23. E_nip_tra... ATGTTGTACCATAAAGTTTGGTACTGCAAAAATTTTGGCTAATCTCAATTTGAGTTTGTCTTTTACTGTTTTCATCACATTTAAATTTTACAA
 24. E_nip_tra... ATGAGGCAACGTTTACGCAAGTGCAGACAACGTTTCTCCTGCTAGATATGATGGTAATGAAATTTACTTTTGGACACTAATCTTTTCTCATCAC
 25. E_nip_tra... AATGGTAGGATATTTTGTGCTGGATATCATGGCTTTCCGAAACACAACGCAACTCCCATAGTACTGAGGAAATTTTGTGTTAAAAGAGGCTTAA
 26. E_nip_tra... ATGTTTTGTTTTTACGACTCATTTACGGTCAATGGAATGAACTCCAACGTTCCACGCCAAATTTATGATAAAGTTCAGTCTTTTCTTTCT
 27. E_nip_tra... ATGGTATCTGACATAGTTCTTTTTCGAGACGGCTGTGGAACAATGGGAAATTTTCCCTGCTATTAATCGTAATCGGTTGCCATTTAACGTTAT
 28. E_nip tra... GGGGAGAAAAGATGACAAAAGCACCGAGTCGGAGCCTTGTCTTCAAGATAAAAACACTCTATTTTGTGCTATGAACATATTAATCGCTCAAAAGG

100%

General

Colors: ACGT- Edit

Graphs

Annotations

Complement

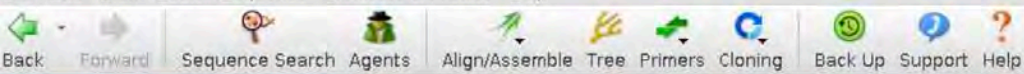
Translation

Wrap

Show Names

Show

Show sequence numbers



Sources

- Local (0)
 - Sample Documents (624)
 - Deleted Items (0)
- Shared Databases
 - NCBI
 - Gene
 - Genome
 - Nucleotide
 - PopSet
 - Protein
 - PubMed
 - SNP
 - Structure
 - Taxonomy
 - UniProt

Name	Description	# Sequenc...	Min Sequ...	Max Sequ...	Path (Imp...
E_nip_transcriptome_nucl_final_80		37,062	90	15,822	/storage/...

Sequence View Lengths Graph Text View Info

Extract R.C. Translate Add Annotation Allow Editing Annotate & Predict Save

```

1. E_nip_trans_62433_m.388819 ATAGGACAACATCGATTTGGGGTGACCATTGGATACAACCTATGACGGTTGGTGAGCAAAATTTAATAACGGCGGACTAGAGG
2. E_nip_trans_15128_m.116119 TTCCITTTACGGATTTCTTTTTCCGACAGAAATGATCATATCTCAAATCCTCATATTTTACACAAGGAGCGGGTCTAGGGAA
3. E_nip_trans_15129_m.116134 TTTAAAGTTATCTTTCCATCTCGGTAAATTCCTAGTCTTTGCAAAAAGGCAATCTGTAAAGGTGCATTTTCTGCTTCACTTTG
4. E_nip_trans_62435_m.388825 GATGCTTTCTCTTATACAATGTTAGAAACCGGAGAAAATTTATTTTCAGAAAGGAGAGTTGTGCCAGTTGCCAGGAGTATACTG
5. E_nip_trans_62436_m.388830 TTACAGAGCCTTGGATACACAGAGCTTCTCAAATCAGTGTCTTTTCCAGGCACTCTCAAACATCCACATTTTACAGTCCAT
6. E_nip_trans_62437_m.388836 ATTGAAACTAAGCTTGTCTACCAATTTAAACAAAGAGTTAGCGCAAAATAAATCTGCCACTGAAACCCTGTTTGTAGATGAAGA
7. E_nip_trans_62438_m.388838 TTACTGCTGTGCTCGATACAGTGTCAATTAAGAATCAAGCAATTCATTTTTTACTGCATCTTTACTTGTACATTTGTTCT
8. E_nip_trans_58176_m.369436 CGACTAGCACTGCGCGTCCACGGCCGACGCAAAATGTTACGAAAACGTTTTTATTCGATGCTCAAATGACAGTGTGCGAGGG
9. E_nip_trans_58178_m.369439 GCGCACCATCTACGAATGAGACTTCAAGCTCTTGTAAATTAATCTAAATACTGTTTATTTGCTTCAATAAAACCAAAATTT
10. E_nip_trans_25560_m.179161 TTTAAACGTGCAACTGCTTACTTTAATTAATTCGTAATTTCTGGCCAGATAAAAGCAGTCTTTTCAGAAATGCCAACATTAAT
11. E_nip_trans_66120_m.404978 CAATCTAAATGTCAATACGTGTTTTCTCATCAATGCTCGGCGGTGCTACATTTTCTGATTTATTTGCGATATTGTTGACGGGTTG
12. E_nip_trans_25563_m.179177 AATGGACTCCAATCGGTCGAGCTACCTCCGGTCCGCCAACTTTTTCGATCTCACATTCACATAGAAGATCTATCACTGCATG
13. E_nip_trans_25564_m.179179 TTCAGTACCTTTTGAATACAGTACAGCCCTACTACAAATCGAACCAATTAATTTTACGAGAAAACCTATTATTGAATTTT
14. E_nip_trans_72870_m.485524 TTGCAGCATACCGTAGTAGAAGTGAAGTGTCTTAAAAGCCTTGGACGATCTGGCGACCGAACAGCCCTGGCGAATTTGTAAT
15. E_nip_trans_25565_m.179181 TTTATCCCCTATATACTGCCCTTTGGTATCGCATTGTTGATGTTTCAATTTTGTCTCCCTGGTAAAAACACAACGTGTGTTGGAT
16. E_nip_trans_25566_m.179185 TTTTTACATTCATCTATTTTTAGAAATTTTATTCATGTCCATCAATAAAAAGGTTTACATTTTGTATTTTGTGCACTGGGCA
17. E_nip_trans_72872_m.485542 TTTTTATAGAAAAATCCCCAAAATTTGCTCCCAATTTGTCAACATTTGTTCCCTCTGTTTACAAAATGTTTTGTTCTTGTCCAGT
18. E_nip_trans_25567_m.179186 CATAAACAAAAAGAAAAAGAAAGGAGCGTGGACAAGAGGCAATTTCTGAGAAAAGCTAGCAAATCCACCCTGACTAGTGACCC
19. E_nip_trans_72873_m.485545 CCTAAAAACGCACAGGAGTACAAAGAAATGAGTCAAAACCCTGGTAAAAACATAAAATCTATCATCACCAAAAAAGCAACTTACA
20. E_nip_trans_66127_m.405379 ATTGCTCTACGTATTTGGCATAAGCCGTATCAACACGCATTTTCGACATTTCACTAATAATTTAGTGGTCTATGTTACTTTT
21. E_nip_trans_25569_m.179191 CCTTTAGCAAAACATTTCCCTTTCTTGTGAATCATTATTTATCTTTACTGACTTTGTAACATGCACATTAATGTCACACAA
22. E_nip_trans_45290_m.316723 TTTTATTAACAACAAATTTGTTCAATCTATATTTCTCCGTTTCACTCTCTACTGCTTCTAGTGCATCCTTTTTTAGGGGTGTTTAG
23. E_nip_trans_45292_m.316746 AGTTTCGGTACTGCAAAAATTTTGGCTAATCTAATTTGAGTTTGTCTTTTACTGTCAGCTTTTATCAATTAATAATTTTACAA
24. E_nip_trans_45293_m.316748 CTTAGCCAGTGCAGACAACGTTTCTCCTCTAGATATGATGGTAATGAAATTTACTTTTGGACACTAACTTTTTCTCATCAQ
25. E_nip_trans_33510_m.237751 TTTTTGTCGGATATCATGGCTTTCGGAAAGCAACGCAACTCCCATAGTCTGAGGAAATTTGTTTAAAAGAGGGCTTTAAC
26. E_nip_trans_72877_m.485566 TTTACGACTCATTTTACGGTCATGGAAGTCAACTCCAACGTTCCACGCCAAATTTATGATAAAGTTTCAAGTCTTTTCTTT
27. E_nip_trans_45294_m.316753 ATAGTTCTTTTTCGAGACGGCTGTGGAACAATGGGAAATTTTCTTCTGCTATTAATGTAATCGGTTGCCATTAACGTTAT
28. E_nip_trans_33511_m.237761 GACAAAAGCACCGAGTCCGAGCCCTTGTCTTCAAGATAAAAACACTCTATTTTGTGCTATGAACATATTAATCGCTGCAAAAGG
  
```

100%

General

Colors: ACGT- Edit

Graphs

Annotations

Complement

Translation

Wrap

Show Names

Show [Description]

Show sequence numbers

Sources

- Local (0)
 - Sample Documents (624)
 - Deleted Items (2)
- Shared Databases
 - NCBI
 - Gene
 - Genome
 - Nucleotide
 - PopSet
 - Protein
 - PubMed
 - SNP
 - Structure
 - Taxonomy
 - UniProt

Name	Description	# Sequenc...	Min Seque...	Max Seque...	Path (Imp...
E_nip_transcriptome_nucl_final_80		37,062	90	15,822	/storage/...

Sequence View Lengths Graph Text View Info

Extract R.C. Translate Add Annotation

1 10 20 70 80 90

1. E_nip_tran... ATGAAGCTAAGCATAGGACAACA
 2. E_nip_tran... GGAAGTCTTTGCTTCCTTACGG
 3. E_nip_tran... ATGCGTTATCGTTTTAAAGTTA
 4. E_nip_tran... TTGAACGATGTAGATGCTTCTC
 5. E_nip_tran... ATGCTCAGATGTTACAGAGCCT
 6. E_nip_tran... TTTATGACAGCCATTGAAACTAA
 7. E_nip_tran... ATGGGTTTTGTTTTACTGCTGTG
 8. E_nip_tran... ATGGAAGGTCGTGACTAGCACT
 9. E_nip_tran... GAAAATCGATGTGCGCACCATCT
 10. E_nip_tra... ATGTTTTGGACTTTTTAAACGTGGA
 11. E_nip_tra... ATGGCGAAGTATCAATCTAAATG
 12. E_nip_tra... AATCGTCACGACAATGGACTCCA
 13. E_nip_tra... GAGCGTTTGAAATTCAGTACCTT
 14. E_nip_tra... ATGGTCTACCAC TTGCAGCATACC
 15. E_nip_tra... ATGTACGATTGTTTTACCCGTATA
 16. E_nip_tra... ATGATATGTTTTATACATTTCTAT
 17. E_nip_tra... ATGATATTTACGTTTTATAGAAAA
 18. E_nip_tra... GGCCGAGACGAGCATAAACAAAA
 19. E_nip_tra... CACAACAA TCCCTCTAAAAACGC
 20. E_nip_tra... ATGTCCGCCAATATTGCTCTACG
 21. E_nip_tra... ATGATAAAATAGCCTTTAGCAAAA
 22. E_nip_tra... ATGCAAAATGAGGTTTTATACAAC
 23. E_nip_tra... ATGTGTACCATAAGTTCCGTACTG
 24. E_nip_tra... ATGAGGCAACGTTAGCCAAGTCA
 25. E_nip_tra... AATGGTAGGATATTTTTGTCGGAT
 26. E_nip_tra... ATGTTTTGTTTTATTTACGACTCA
 27. E_nip_tra... ATGGTATCTGACATAGTTTCTTCC
 28. E_nip_tra... GGGGAGAAAGATGACAAAAGCACC

Translate

Translate selected region (273 bases)
 Translate entire sequences

Extraction name: E_nip_trans_62433_m.388819_translation

Genetic code: Standard

Translation frame: 1

Treat first codon as start of coding region

Modify sequence names to indicate that they represent a translation

OK Cancel

100%

General

Colors: ACGT- Edit

Graphs

Annotations

Complement

Translation

Wrap

Show Names

Show

Show sequence numbers

- Sources
- Local (0)
- Sample Documents (625)
- Deleted Items (2)
- Shared Databases
- Operations
- NCBI
 - Gene
 - Genome
 - Nucleotide
 - PopSet
 - Protein
 - PubMed
 - SNP
 - Structure
 - Taxonomy
 - UniProt

Name	Description	Sequence ...	# Sequenc...	Min Seque...	Max Sequ...
E_nip_trans_62433_m.388819 translation-		90	-	-	-
E_nip_transcriptome_nucl_final_80		-	37,062	90	15,822

Extract B.C. Translate Add/Edit Annotation Allow Editing Annotate & Predict Save

100%

General

Colors: ARND- Edit

Graphs Options >

Annotations Options >

Wrap

Show Name

Show Description

1 10 20 30 40 50 60 70 80 90

MKLSIGQHRFWVTIWIQLMTVGEQNLITRIRGEGKNASHGATSIGDGFQIDTNIISVINRFKVDTNNFLQAMKLSREQRRMMEIYKTI

- Sources
- Local (0)
 - Sample Documents (626)
 - Deleted Items (2)
 - Shared Databases
 - Operations
 - NCBI
 - Gene
 - Genome
 - Nucleotide
 - PopSet
 - Protein
 - PubMed
 - SNP
 - Structure
 - Taxonomy
 - UniProt

Name	Description	Sequence ...	# Sequenc...	Min Seque...	Max Sequ...
<input checked="" type="checkbox"/>	E_nip_trans_15128_m.116119 translation -	1,147	-	-	-
<input checked="" type="checkbox"/>	E_nip_trans_62433_m.388819 translation -	90	-	-	-
<input checked="" type="checkbox"/>	E_nip_transcriptome_nucl_final_80	-	37,062	90	15,822

Sequence View | Dotplot (Self) | Text View | Info

Extract | R.C. | Translate | Add/Edit Annotation | Allow Editing | Annotate & Predict | Save

```

1      10     20     30     40     50     60     70     80     90    100
GSLCFLYGLFSDRNDHISNPHYFHKERVVGVKVVLLIIDGLRADSILSDDMLQHWPNLKS YIDEGMVD CSTCRLKAPT VTL PRLKAIVSGRVPQFVDFIYNLNA
110    120    130    140    150    160    170    180    190    200
KEVKEDNFIRRLKNDNWNISFGDDTIWIKMFPNTFNFADGTTSFVVNDFYEVDSNVSRNIQPI MTKPSEWEFMILHYLGLDHIHIGHIEGPKGSSMNTKIREMDTV
210    220    230    240    250    260    270    280    290    300
IGKIIINNFKALYFEEDWMLIVTGDHGMSDNNGHGGSSHG ETVTPLL YISPKFKHLTSEARSACGDASWFRLLNVASDQSDI ASTVGLLTGVGIPSSSLGVL RH
320    330    340    350    360    370    380    390    400    410
QVVLAMWFDQASRLHQIANLLEHFAHLIGCLPQNNNSKDG SFVHLDLECASKLTTKMEVGVLNKRLRS IFEVLKQCSMEANETT VLRKACL DALSSNYLFEER
420    430    440    450    460    470    480    490    500    510
YYELMDIARRMQDRGLTDAGEPNLILMLFGAALLIVLAVLAWWSLIRLLSNEGSTLLGAKACKGDKQMRNSDPHYGHLDLAYFLNAAILTPRLVNLITVCAVI
520    530    540    550    560    570    580    590    600    610
ALGLHAFSLASSSYVEEHQFWYHSCITCCLLFLVLVNYQNSGEQSEMGRGSSSEAACSRNDNEGSYTS CSNQAPINIKRKYSNKEILPIIRQDFSVSANYDDF
620    630    640    650    660    670    680    690    700    710
ADGSHALGV SCTSEHGHVDGIKLLKDDVNNL GDRSSIQMDSMPFDCGLFNTKSSKKNNF EFGFLGMSTAKFMRLRQSRVLP IICVLMVDRFLLRKL FATGD AWI
720    730    740    750    760    770    780    790    800    810
HLPDISDWLNSPEHSDYLWFAQIFSWAGLIVWRVYAVFRQQLSTKTYTKSAFQLWSAVASIVLVAATQLMYRHNSEVLASHKGSANWILF TARLAYLA IILIDL
820    830    840    850    860    870    880    890    900    910
LVLGTWWYMSRDRRANRYSDINQPTLWSEVVLAE RNPP LAQAIGLLACLGRPAVTL LVLWCVL VKEALIGRLLQLEAAITVASTNNSARSTNL DYVGGSKRK
920    930    940    950    960    970    980    990    1,000    1,010
ISRGEFETDNSFELKNNVF SHKSVYFRDQARGWGARRIRLLFCTAVLYWAE GWITTYFQQGNSHSFSTLDVSAGYVGVSEYSP IINGILLGVYTFAGPLFWYS AF
1,020    1,030    1,040    1,050    1,060    1,070    1,080    1,090    1,100    1,110
ILRFAPPHHSRSLRYAVADKDDNAKYFDLCNEVEEVNAQRVATGIYFSRIFLGLLVLPAAVFFCVC AFLRYHLFVWTVFAPRLLYL VVFHAIFVVPFYCFCSFI
1,120    1,130    1,140    1,147
TVY
    
```

100%

General

Colors: ARND- Edit

Graphs Options >

Annotations Options >

Wrap

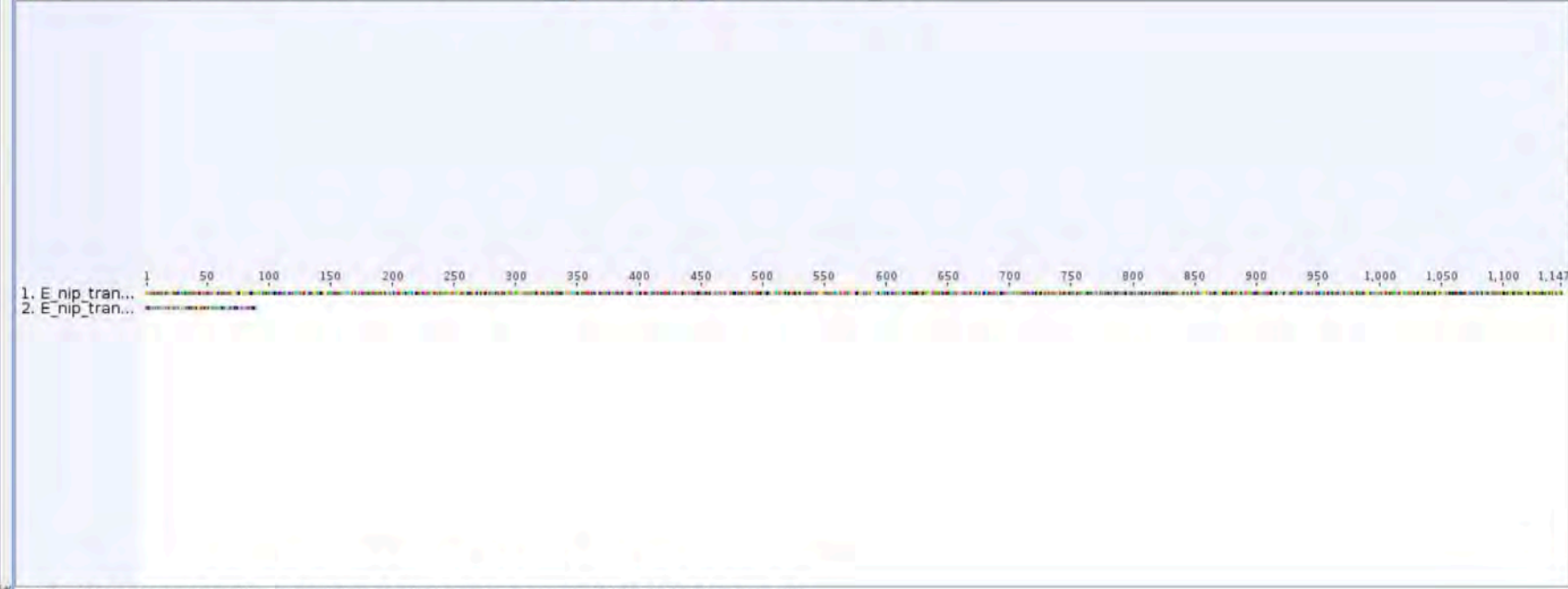
Show Name

Show

Sources

- Local (0)
- Sample Documents (626)
 - Deleted Items (3)
- Shared Databases
- Operations
- NCBI
 - Gene
 - Genome
 - Nucleotide
 - PopSet
 - Protein
 - PubMed
 - SNP
 - Structure
 - Taxonomy
 - UniProt

Description	Sequence ...	# Sequenc...	Min Seque...	Max Seq...
Align a small number of similar length sequences such as genes	1,147	-	-	-
Map to Reference...	90	-	-	-
De Novo Assemble...	-	37,062	90	15,822
Align Whole Genomes...	-	-	-	-
Map Primers...	-	-	-	-



81%

General

Colors: ARND- Edit

Graphs Options >

Annotations Options >

Wrap

Show Names

Show [unclear] >

Show sequence numbers

Sources

- Local (0)
- Sample Documents (626)
 - Deleted Items (3)
- Shared Databases
- Operations
- NCBI
 - Gene
 - Genome
 - Nucleotide
 - PopSet
 - Protein
 - PubMed
 - SNP
 - Structure
 - Taxonomy
 - UniProt

Name	Description	Sequence ...	# Sequenc...	Min Seque...	Max Sequ...
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/> E_nip_trans_15128_m.116110_translation	1,147	-	-	-
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/> E_nip_trans_62433_m.3	90	-	-	-
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/> E_nip_transcriptome_nu	-	37,062	90	15,822

Alignment

Geneious Alignment
 MUSCLE Alignment
 ClustalW Alignment
 Realign Region
 Translation Align

Consensus Align:

Maximum number of iterations:

Use custom MUSCLE executable: Change...

Maximum number of trees to build:

Sequence Order: Group sequences by similarity Preserve sequence order

Optimization: Diagonal Anchor

Keep tree from: Iteration 1 Iteration 2

Profile score: Sum of pairs

Distance measure: Iteration 1: Subsequent:

Clustering method: Iteration 1 & 2: Subsequent:

Tree Rooting method: Iteration 1 & 2: Subsequent:

Sequence weighting scheme: Iteration 1 & 2: Subsequent:

Terminal gaps: Objective score:

Anchor spacing: Gap open score:

Diagonals: Min length: Margin:

Minimum column anchor scores: Min best: Min smoothed:

Hydrophobicity: Multiplier: Window size:

Maximum Memory (MB):

Extra Options:

Sequence View Dotplot

Extract R.C

1. E_nip_tran...
2. E_nip_tran...

8%

General

Colors: ARND- Edit

Graphs Options >

Annotations Options >

Wrap

Show Names

Show

Show sequence numbers

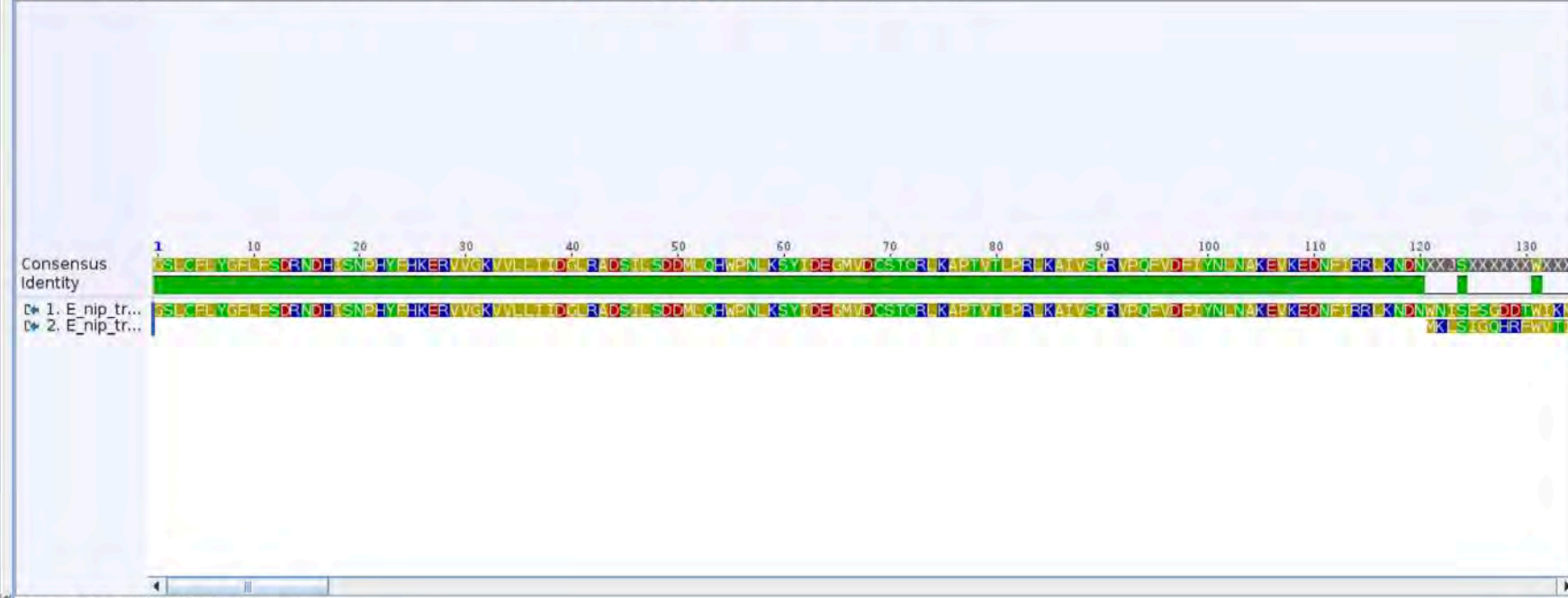
Sources

- Local (0)
- Sample Documents (627)
- Deleted Items (3)
- Shared Databases
- Operations
- NCBI
 - Gene
 - Genome
 - Nucleotide
 - PopSet
 - Protein
 - PubMed
 - SNP
 - Structure
 - Taxonomy
 - UniProt

Name	Description	Sequence ...	# Sequenc...	Min Seque...	Max Sequ...
<input checked="" type="checkbox"/>	E_nip_trans_15128_m.116119 translation -	1,147	-	-	-
<input checked="" type="checkbox"/>	E_nip_trans_62433_m.388819 translation -	90	-	-	-
<input checked="" type="checkbox"/>	E_nip_transcriptome_nucl_final_80	-	37,062	90	15,822
<input checked="" type="checkbox"/>	Protein alignment	Alignment of 2 sequences: E_nip_trans_15128_m.116119 translation, E_nip_trans_62433_m.388819 translation	1,147	2	90

Alignment View | Dotplot | Distances | Text View | Info

Extract | R.C. | Translate | Add/Edit Annotation | Allow Editing | Annotate & Predict | Save



71%

General

Colors: ARND- Polarity Edit

Graphs Options >

Annotations

Consensus

Highlighting Options >

Wrap

Show Names

Show [font style]

Show sequence numbers



All GUI applications can be launched using MetaCentrum Desktop



```
xterm
(BOOKMORM)vorel@galdor19:~$ pwd
/storage/brno2/home/vorel
(BOOKMORM)vorel@galdor19:~$ ls
Hbundan_partial.txt  CASTEP-25.12  IGV_Linux_2.19.7_WithJava.zip  META_SUPPORT  OpenMolcas  R  igv  ondemand  test_WiseCon  test_crys
(BOOKMORM)vorel@galdor19:~$
(BOOKMORM)vorel@galdor19:~$ unzip -q IGV_Linux_2.19.7_WithJava.zip
(BOOKMORM)vorel@galdor19:~$
(BOOKMORM)vorel@galdor19:~$ ls
Hbundan_partial.txt  CASTEP-25.12  IGV_Linux_2.19.7  IGV_Linux_2.19.7_WithJava.zip  META_SUPPORT  OpenMolcas  R  igv  ondemand  test_WiseCon  test_crys
(BOOKMORM)vorel@galdor19:~$
(BOOKMORM)vorel@galdor19:~$ bash IGV_Linux_2.19.7/igv.sh
echo Using bundled JDK.
openjdk version "21.0.4" 2024-07-16 LTS
OpenJDK Runtime Environment Temurin-21.0.4+7 (build 21.0.4+7-LTS)
OpenJDK 64-Bit Server VM Temurin-21.0.4+7 (build 21.0.4+7-LTS, mixed mode, sharing)
█
```



Human (GRCh38/hg38)

All

Go



1

2

3

4

5

6

7

8

9

10

11

12

13

14

15

16

17

18

19

20

21

22

X

Y

Click on a chromosome number to jump to that chromosome, or click and drag to zoom in.

Refseq Select

[0 - 127]

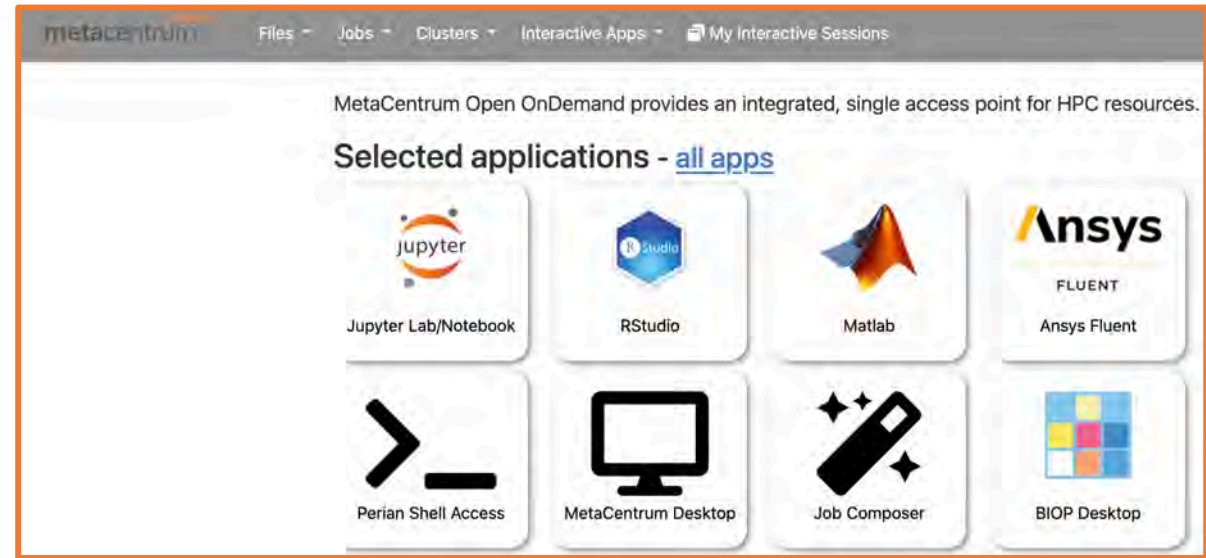


■ Open OnDemand



<https://ondemand.metacentrum.cz/>

- Web application on top of OpenPBS scheduler
- Running (not only) GUI applications
- Browsing storages (tab 'Files')
- Command line (tab 'Clusters')
- Launch a virtual desktop (MetaCentrum Desktop app)
- Running virtual machines (OpenStack) and Docker images (Kubernetes on OpenStack), tab 'Interactive Apps'

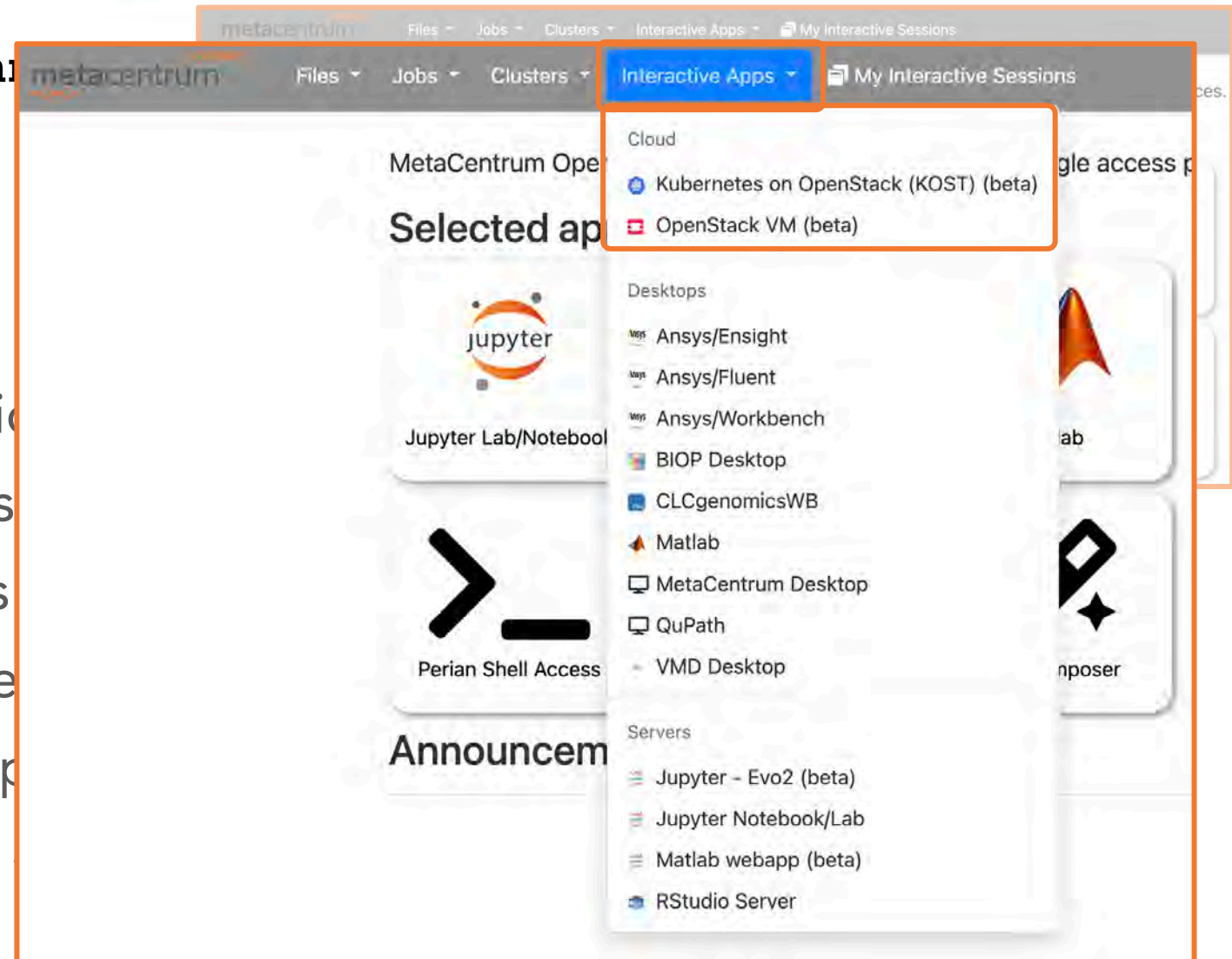


■ Open OnDemand



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- Browsing storages (tab 'Files')
- Command line (tab 'Clusters')
- Launch a virtual desktop (MetaCentrum Desktop)
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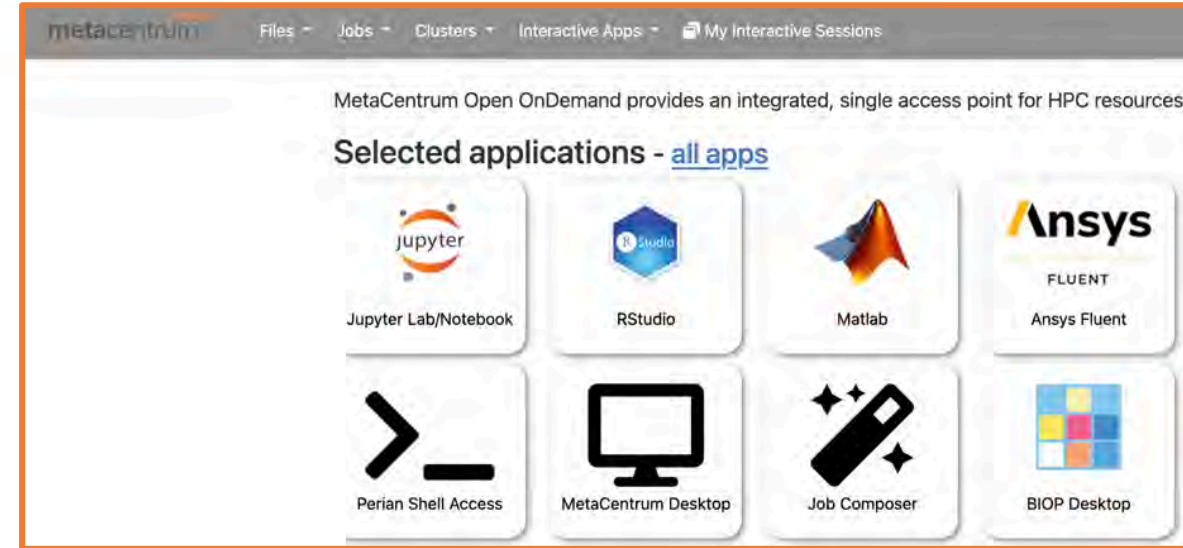


Jupyter Notebook in Open OnDemand

■ 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)



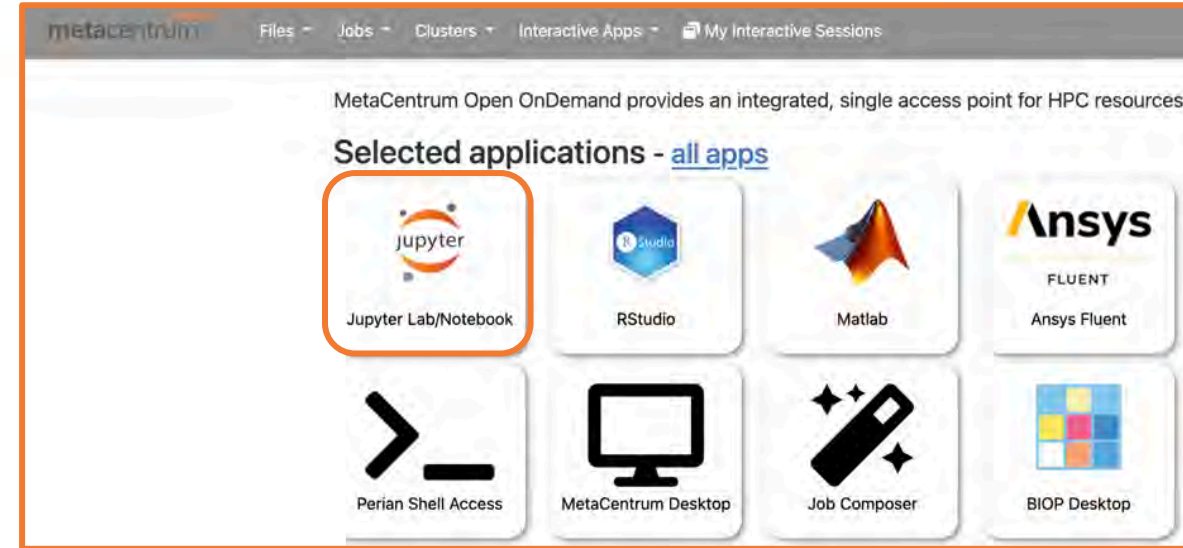
<https://docs.cerit.io/en/docs/web-apps/jupyterhub>

Jupyter Notebook in Open OnDemand

■ Jupyter Notebook

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

Jupyter Notebook

<https://ondemand.metacentrum.cz/>



Jupyter

- 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, etc.)
- Embeds plots, widgets, and equations
- Promotes reproducible, shareable workflows
- Also accessible in the Kubernetes ecosystem

A screenshot of a cloud service portal interface for configuring a Jupyter Notebook/Lab. The interface is divided into two main sections: a left sidebar with a list of applications and a main configuration area on the right. The sidebar lists various applications under categories like 'Cloud', 'Desktops', and 'Servers'. 'Jupyter Notebook/Lab' is selected and highlighted in blue. The main configuration area is titled 'Jupyter Notebook/Lab' and contains several settings: 'Mode' (radio buttons for 'Jupyter Notebook' and 'Jupyter Lab'), 'Number of hours' (input field with '1'), 'Number of CPUs on single node' (input field with '1'), 'Memory (GB)' (input field with '5'), 'GPUs' (input field with '0'), 'Scratch local (GB)' (input field with '5'), 'Jupyter Image' (dropdown menu showing 'Metacentrum/debian11.sif'), 'Full path of custom singularity image with Jupyter notebook' (empty text field), 'PBS Queue' (dropdown menu showing 'interactive'), and 'Jupyter working directory location:' (dropdown menu showing '/storage/brno2'). A large blue 'Launch' button is at the bottom right.

Session was successfully created. [Close]

Home / My Interactive Sessions

Interactive Apps

Cloud

Kubernetes on OpenStack (KOST) (beta)

OpenStack VM (beta)

Desktops

Ansys/Ensignt

Ansys/Fluent

Ansys/Workbench

Jupyter Notebook/Lab (18240652.pbs-m1.metacentrum.cz) 1 node | 1 core | Running

Host: tarkil16.grid.cesnet.cz [Delete]

Created at: 2026-03-20 15:33:47 CET

Time Remaining: 59 minutes

Session ID: 2b8b5f4a-7b31-4bcf-b61c-bbd32245560a

[Connect to Jupyter]

Jupyter Notebook

https://ondema

Web-based mixing

Excellent analysis

- 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)

Jupyter Notebook/Lab

Matlab webapp (beta)

RStudio Server

Jupyter Image

Metacentrum/debian11.sif

Full path of custom singularity image with Jupyter notebook

PBS Queue

interactive

Jupyter working directory location:

/storage/brno2

<https://docs.cerit.ac.uk/en/docs/web-apps/jupyterhub>

Launch



Select items to perform actions on them.

Upload

New ▾


 0 ▾  /

Name ↓

Last Modified

File size

  CASTEP-25.12

před 2 měsíci

  META_SUPPORT

před 5 měsíci

  ondemand

před 2 lety

  OpenMolcas

před 9 měsíci

  test_crys

před 2 lety

  Untitled.ipynb

před hodinou

4.98 kB




Select items to perform actions on them.

Upload

New ▾

 0 ▾ /

Name ▾

  CASTEP-25.12  META_SUPPORT  ondemand  OpenMolcas  test_crys  Untitled.ipynb

Notebook:

Python 3 (ipykernel)

SMLv2

Other:

Text File

Folder

Terminal

predefined

před hodinou

4.98 kB





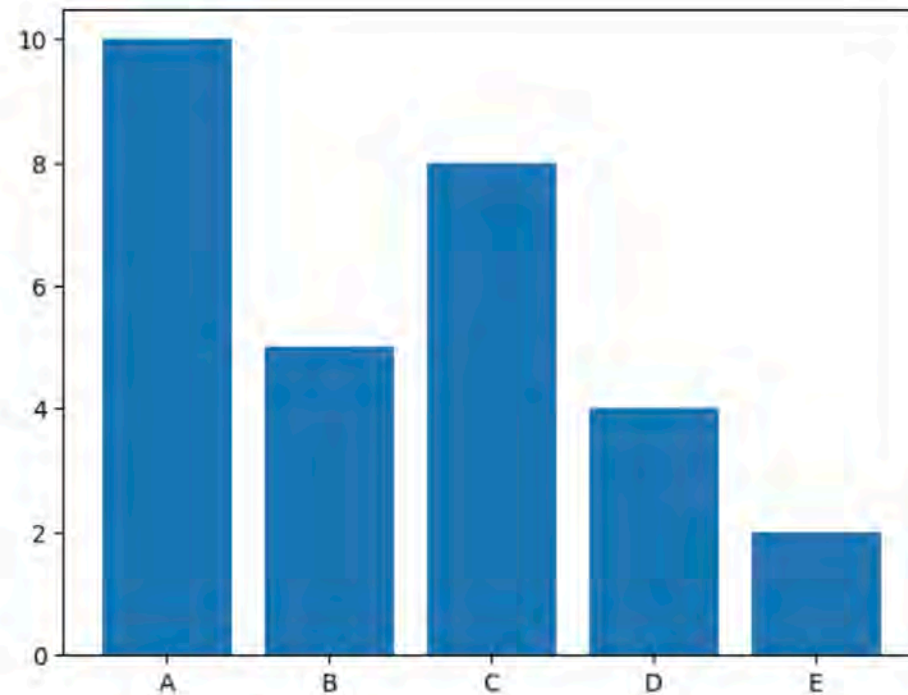
```
[1]: import os
current_working_directory = os.getcwd()
print(current_working_directory)

/autob/brno2/home/vorel
```

```
[2]: pip install matplotlib --quiet

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

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



Notebook Intelligence 

{"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.

Ask Notebook Intelligence...

exaple1.ipynb @  

Launcher

exaple1.ipynb

age_data.csv

        Code   git   

```
[3]: 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

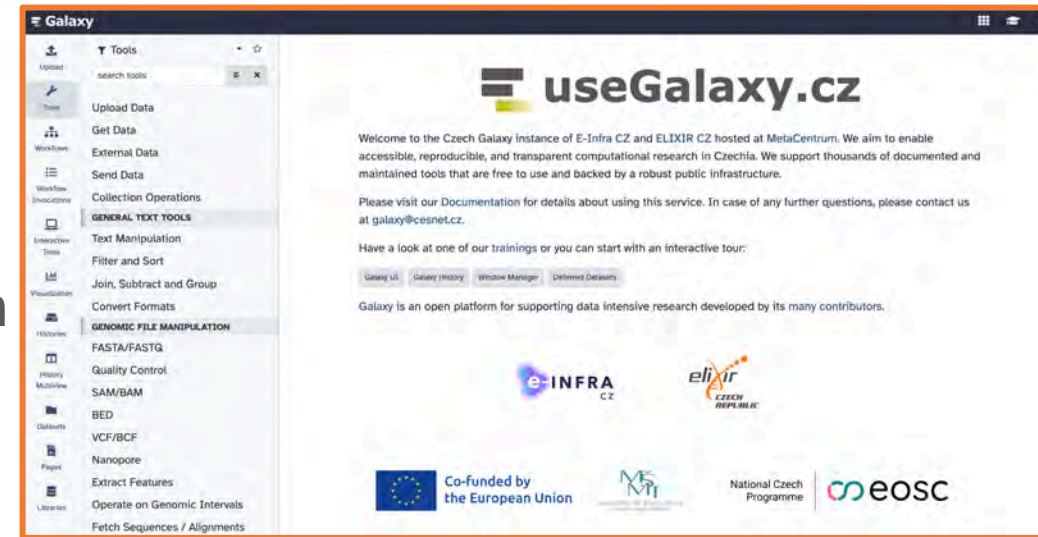
[]:

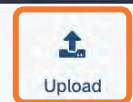
      

■ Galaxy useGalaxy.cz

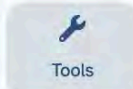
<https://usegalaxy.cz/>

- 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





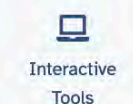
Upload



Tools



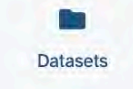
Workflows

Workflow
InvocationsInteractive
Tools

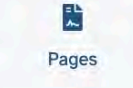
Visualization



Histories

History
Multiview

Datasets



Pages



Libraries

Tools

search tools

Upload Data

Get Data

External Data

Send Data

Collection Operations

GENERAL TEXT TOOLS

Text Manipulation

Filter and Sort

Join, Subtract and Group

Convert Formats

GENOMIC FILE MANIPULATION

FASTA/FASTQ

Quality Control

SAM/BAM

BED

VCF/BCF

Nanopore

Extract Features

Operate on Genomic Intervals

Fetch Sequences / Alignments

GENOMICS ANALYSIS

Assembly



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 UI

Galaxy History

Window Manager

Deferred Datasets

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



Co-funded by
the European Union



National Czech
Programme





Upload



Tools



Workflows

Workflow
InvocationsInteractive
Tools

Visualization



Histories

History
Multiview

Datasets



Pages



Libraries

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GENOMIC FILE MANIPULATION

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GENOMICS ANALYSIS

Assembly

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

Regular

Composite

Collection




Rule-based

 Drop files here

Type (set all): Auto-detect



Reference (set all): unspecified (?)

 Choose local file Choose remote files Paste/Fetch data

Start

Pause

Reset

Close

Co-funded by
the European UnionMINISTRY OF EDUCATION,
YOUTH AND SPORTSNational Czech
Programme

Upload

Tools

Workflows

Workflow Invocations

Interactive Tools

Visualization

Histories

History Multiview

Datasets

Pages

Libraries

Tools

Upload Data

Get Data

External Data

Send Data

Collection Operations

GENERAL TEXT TOOLS

Text Manipulation

Filter and Sort

Join, Subtract and Group

Convert Formats

GENOMIC FILE MANIPULATION

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GENOMICS ANALYSIS

Assembly

Upload from

search

Regular

Label	Details
FTP Directory	Galaxy User's FTP Directory
InvenioRDM TESTING	Testing instance of Invenio, content is NOT preserved and DOIs created in this instance are not real.
Zenodo TESTING	Testing instance of Zenodo, content is NOT preserved and DOIs created in this instance are not real.
Zenodo	Zenodo is a general-purpose open-access repository. For each submission, a DOI is created, making items easily citeable.

Create a new remote file source

+ Create new

Cancel Select



Co-funded by the European Union



National Czech Programme



Upload

Tools

Upload Data

Get Data

External Data

Send Data

Collection Operations

GENERAL TEXT TOOLS

Text Manipulation

Filter and Sort

Join, Subtract and Group

Convert Formats

GENOMIC FILE MANIPULATION

FASTA/FASTQ

Quality Control

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BED

VCF/BCF

Nanopore

Extract Features

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GENOMICS ANALYSIS

Assembly

Annotation

Mapping

Variant Calling

RNA Analysis

Multiple Alignments

Upload from Disk or Web to Unnamed history

Regular Composite Collection Rule-based

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 (?)

Choose local file Choose remote files Paste/Fetch data **Start** Pause Reset Close

Using 0% of 200.0 GB vorel

History

search datasets

Unnamed history

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



Co-funded by
the European Union



National Czech
Programme

eosc

- Upload
- Tools
 - search tools
- Upload Data
- Get Data
- External Data
- Send Data
- Collection Operations
- GENERAL TEXT TOOLS
 - Text Manipulation
 - Filter and Sort
 - Join, Subtract and Group
 - Convert Formats
- GENOMIC FILE MANIPULATION
 - FASTA/FASTQ
 - Quality Control
 - SAM/BAM
 - BED
 - VCF/BCF
 - Nanopore
 - Extract Features
 - Operate on Genomic Intervals
 - Fetch Sequences / Alignments
- GENOMICS ANALYSIS
 - Assembly
 - Annotation
 - Mapping
 - Variant Calling
 - RNA Analysis
 - Multiple Alignments
- Workflows
- Workflow Invocations
- Interactive Tools
- Visualization
- Histories
- History Multiview
- Datasets
- Pages
- Libraries
- Notifications
- More

Upload from Disk or Web to Unnamed history

Regular Composite Collection Rule-based

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 (?)

Choose local file Choose remote files Paste/Fetch data Start Pause Reset Close

Using 0% of 200.0 GB vorel

History + = ≡

search datasets

Unnamed history

0 B

1: GCA_029291075.1_E_nip_g enomic.fna.gz



Upload

Tools

Upload Data

Get Data

External Data

Send Data

Collection Operations

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Multiple Alignments

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

Regular Composite Collection Rule-based

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 (?)

Choose local file Choose remote files Paste/Fetch data Start Pause Reset **Close**

History

search datasets

Unnamed history

295 MB

1: GCA_029291075.1_E_nip_genomic.fna.gz



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Tools

Upload

Tools

Workflows

Workflow Invocations

Interactive Tools

Visualization

Histories

History Multiview

Datasets

Pages

Libraries

Notifications

More

Tools

search tools

Upload Data

Get Data

External Data

Send Data

Collection Operations

GENERAL TEXT TOOLS

Text Manipulation

Filter and Sort

Join, Subtract and Group

Convert Formats

GENOMIC FILE MANIPULATION

FASTA/FASTQ

Quality Control

SAM/BAM

BED

VCF/BCF

Nanopore

Extract Features

Operate on Genomic Intervals

Fetch Sequences / Alignments

GENOMICS ANALYSIS

Assembly

Annotation

Mapping

Variant Calling

RNA Analysis

Multiple Alignments

1: **GCA_029291075.1_E_nip_genomic.fna.gz** ok

21,044 sequences
format **fasta.gz** database ? size **281.4 MB**

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```
>JAQBSW01000001.1 Eudiplozoon nipponicum isolate JV_EN_01 E_nip_1, whole genome shotgun sequence
gcaatgttctctcattcgagtaattaaccgtctggctgatccgctacgtaagttgatcgacaacttgcgatgtatcct
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tgattcaatataatagctAGGATaccattagacattaaatcgtaaatgtctttatataataatcttttagaatt
gactaaccaactgtcaattcttaaaagcaaccgcaactgtgataattatattgaaatggtaaaaaactgctgtat
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tactttgctcctccttctattctatctgatttatcgtctagacgtggaatttggattgcatttaacacgttttct
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cacagtttgcataacagcagtttggctatttaaacataaattatcaacagttcgtggttctttcaagaatagac
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```

History

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Unnamed history

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Tools

Upload

Tools

Workflows

Workflow Invocations

Interactive Tools

Visualization

Histories

History Multiview

Datasets

Pages

Libraries

Notifications

More

Tools

search tools

Upload Data

Get Data

External Data

Send Data

Collection Operations

GENERAL TEXT TOOLS

Text Manipulation

Filter and Sort

Join, Subtract and Group

Convert Formats

GENOMIC FILE MANIPULATION

FASTA/FASTQ

Quality Control

SAM/BAM

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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**

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Details

Edit



This dataset is large and only the first megabyte is shown below.

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>JAQBSW01000001.1 Eudiplozoon nipponicum isolate JV_EN_01 E_nip_1, whole genome shotgun sequence

```

gcaatgttctctcattcgagtaattaaccgtctggctgatcggcctacgtaagttgatcgacaacttgcgatgtatcct
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gcatgcataaaaaataaattagctcACTCACGAGAACACGCTGCTATCCGATTTAAGTGACTGAGCAAATTTGATGCAC

```

History

search datasets

Unnamed history

295 MB

1: GCA_029291075.1_E_nip_geno

mic.fna.gz

- Upload
- Tools
- Workflows
- Workflow Invocations
- Interactive Tools
- Visualization
- Histories
- History Multiview
- Datasets
- Pages
- Libraries
- Notifications
- More

Tools

statistics

Show Sections

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

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zonal statistics over each area

Boxplot of quality statistics

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1: renamed_GCA_029291075.1_E_nip_genomic.fna.gz ok

21,044 sequences
format **fasta.gz** database ? size **281.4 MB**

Preview Visualize Details Edit

Edit Dataset Attributes

Attributes Datatypes Permissions

Name
renamed_GCA_029291075.1_E_nip_genomic.fna.gz

Info
My genome file

Annotation - optional
Lorem ipsum dolor sit amet, consectetur adipiscing elit. Nullam justo enim, consectetur 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 Auto-detect

History

search datasets

Unnamed history

Unnamed history

Annotation (optional)

Add Tags

Save Cancel

295 MB

1: renamed_GCA_029291075.1_E_nip_genomic.fna.gz

- Upload
- Tools
- Workflows
- Workflow Invocations
- Interactive Tools
- Visualization
- Histories
- History Multiview
- Datasets
- Pages
- Libraries
- Notifications
- More

Tools

statistics

Show Sections

Statistics on presence-absence of a numeric variable

Summary Statistics for any numerical column

FASTQ Summary Statistics by column

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Name
renamed_GCA_029291075.1_E_nip_genomic.fna.gz

Info
My genome file

Annotation - optional
Lorem ipsum dolor sit amet, consectetur adipiscing elit. Nullam justo enim, consectetur 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.

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unspecified (?)

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search datasets

Unnamed history

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Annotation (optional)

Add Tags

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295 MB

1: renamed_GCA_029291075.1_E_nip_genomic.fna.gz

Tools

statistics

Show Sections

Statistics on presence-absence of a numeric variable

Summary Statistics for any numerical column

FASTQ Summary Statistics by column

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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)

Run Tool

Tool Parameters

FASTA or Multi-FASTA file *

Select a dataset

accepted formats

FASTA dataset to get sta

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

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.

Run Tool

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 TotalNotN
- Number of sequences
- GC content

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

History

search datasets

Unnamed history

Unnamed history

Annotation (optional)

Add Tags

Save Cancel

295 MB

1

1: renamed_GCA_029291075.1_E_nip_genomic.fna.gz

Upload

Tools

Workflows

Workflow Invocations

Interactive Tools

Visualization

Histories

History Multiview

Datasets

Pages

Libraries

Notifications

More

Tools

statistics

Show Sections

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

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

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](#)

History

search datasets

Unnamed history

Unnamed history

Annotation (optional)

Add Tags

Save Cancel

295 MB 2 1

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

1: renamed_GCA_02929107_5.1_E_nip_genomic.fna.gz

- Upload
- Tools
- Workflows
- Workflow Invocations
- Interactive Tools
- Visualization
- Histories
- History Multiview
- Datasets
- Pages
- Libraries
- Notifications
- More

Tools

statistics

Show Sections

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

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Read length statistics from a set of FAST5 files

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Here is a link to the job: [83e4c30195971270](#)

History

search datasets

Unnamed history

1.25 GB

2 1

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

1: **renamed_GCA_02929107_5.1_E_nip_genomic.fna.gz**

- Upload
- Tools
- Workflows**
- Workflow Invocations
- Interactive Tools
- Visualization
- Histories
- History Multiview
- Datasets
- Pages
- Libraries
- Recent Exports
- Notifications
- More

Workflows

+ Create + Import

My workflows

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mbodova

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search datasets 📄 ✕

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🔍

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Upload

Tools

Workflows

Workflow Invocations

Interactive Tools

Visualization

Histories

History Multiview

Datasets

Pages

Libraries

Recent Exports

Notifications

More

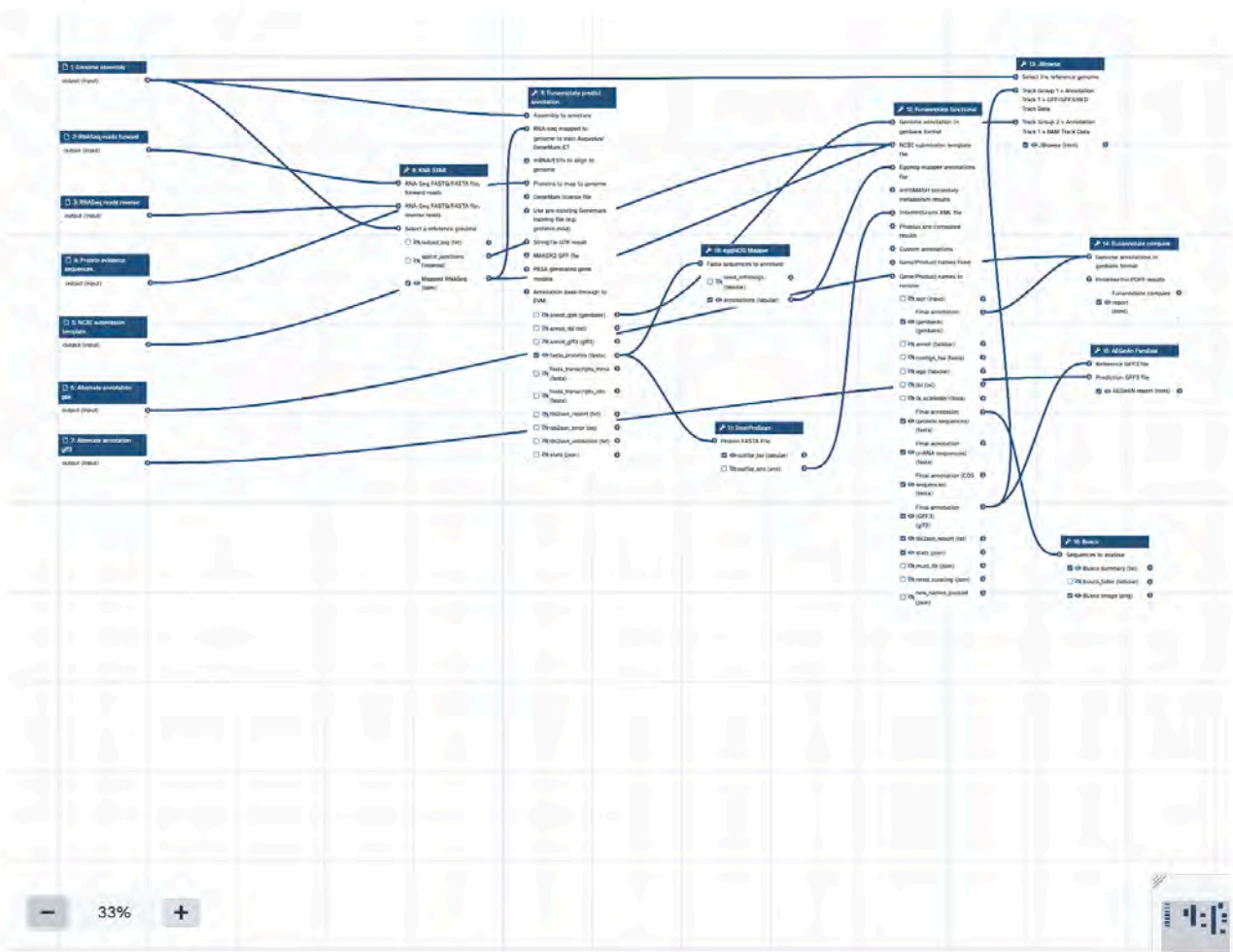
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+ Create + Import

History

search datasets

Workflow Preview



33%

Download Import Run

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

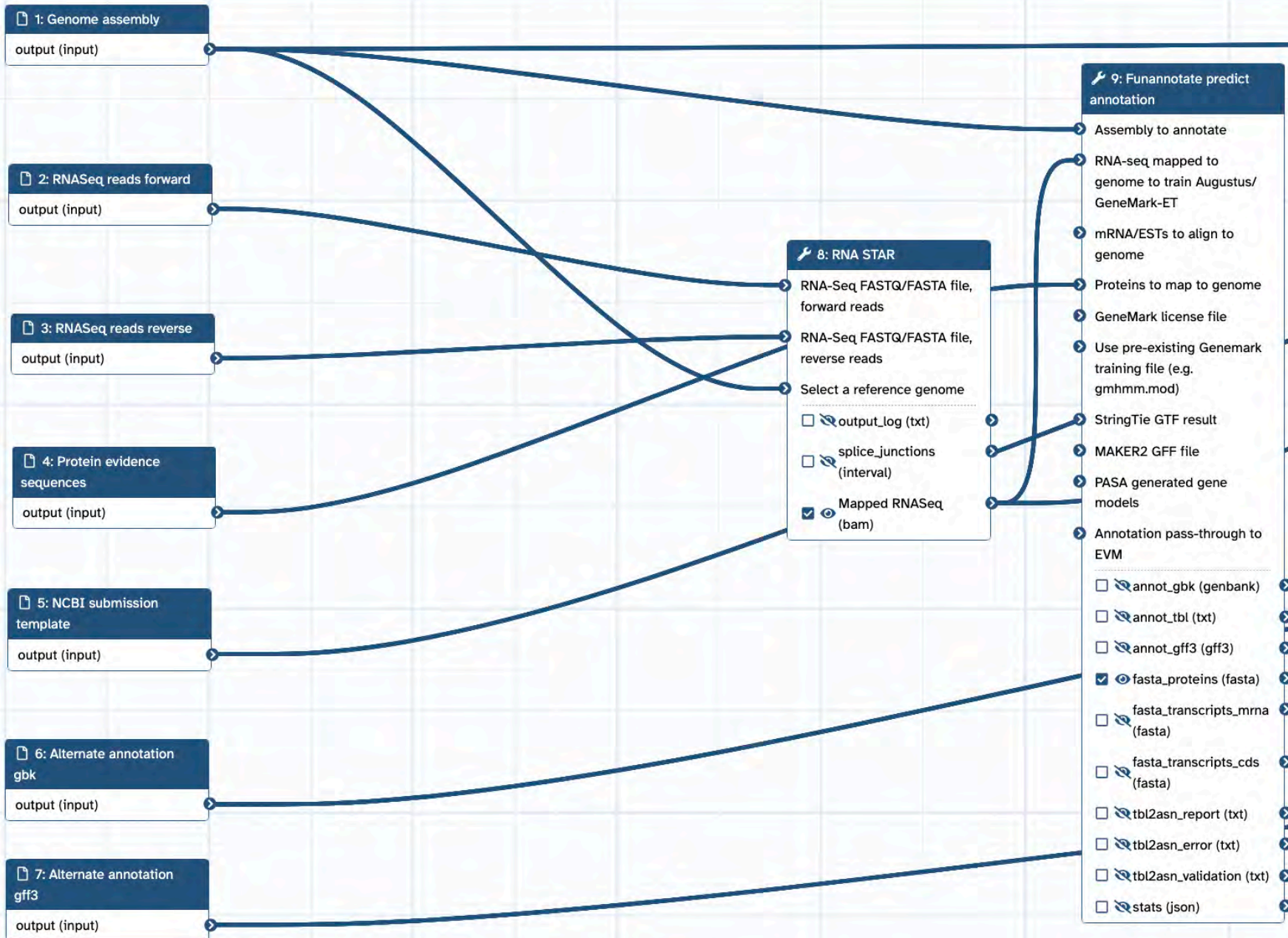
Last Updated

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

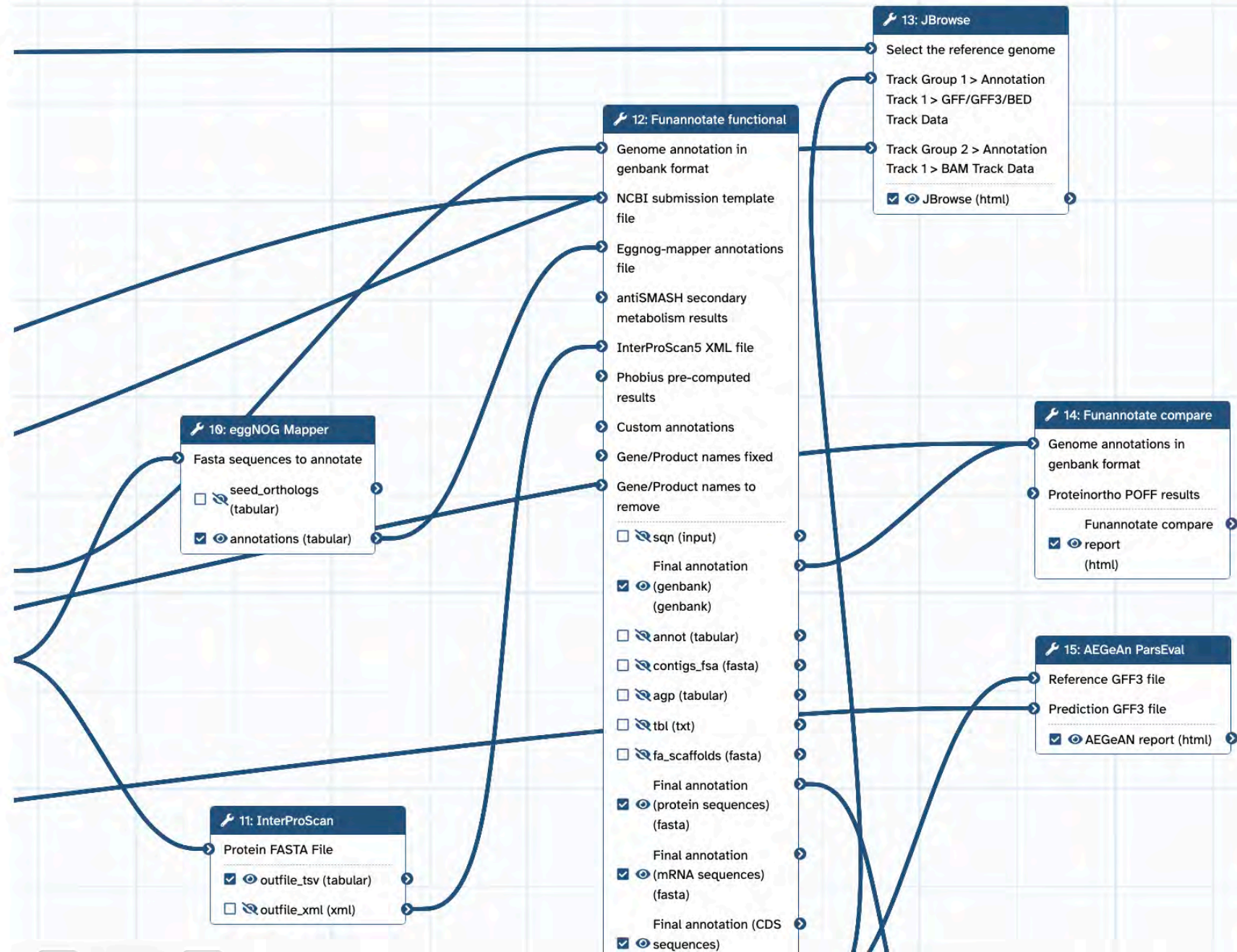
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Workflow Preview



Workflow Preview



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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!

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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!

[Start Learning](#)

Scientific Fields

Topic	Tutorials
Climate	14
Computational chemistry	9

Quickstart

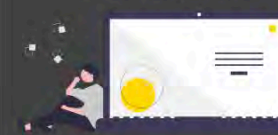
Learning Pathways



Galaxy for SysAdmins



Galaxy for Developers



Galaxy for Teachers



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

Introduction to Galaxy Analyses







Galaxy is a scientific workflow, data integration, and data and analysis persistence and publishing platform that aims to make computational biology accessible to research scientists that do not have computer programming experience.

Material





You can view the tutorial materials in different languages by clicking the dropdown icon next to the slides () and tutorial () buttons below.

First Time Using Galaxy













A quick look at using Galaxy

Lesson	Slides	Hands-on	Recordings	Input dataset	Workflows
Introduction to Galaxy	 ▾				
A short introduction to Galaxy	 ▾	 ▾	 ▾		

A short introduction to Galaxy

Author(s)   Anna Syme   Nicola Soranzo

Editor(s)   Bérénice Batut   Ahmed Hamid Awan   Phil Reed

Reviewers            

Overview



Questions:


- How to get started in Galaxy

Objectives:







- Learn how to upload a file
- Learn how to use a tool
- Learn how to view results
- Learn how to view histories
- Learn how to extract and run a workflow
- Learn how to share a history

Time estimation: 40 minutes

Level: Introductory  

Translations:  Español

Supporting Materials:

 Slides  Datasets  Workflows  FAQs  Recordings  Available on these Galaxies

Published: Aug 27, 2018

Last modification: Jan 23, 2026

License: Tutorial Content is licensed under [Creative Commons Attribution 4.0 International License](#). The GTN Framework is licensed under MIT

PURL: <https://gxy.io/GTN:T00190>

Rating: 4.9 (69 recent ratings, 771 all time)

Revision: 44



Workflows

What does Galaxy look like?

Overview

Create an account on a Galaxy instance/ server

What does Galaxy look like?

Key Galaxy actions

Conclusion

Frequently Asked Questions

Feedback

Citing this Tutorial

Hands On: Log in to Galaxy

1. Open your favorite browser (Chrome, Safari, Edge or Firefox as your browser, not Internet Explorer!)
2. Browse to your Galaxy instance
3. Log in or register

The screenshot shows a web browser window with the address bar containing 'usegalaxy.org.au'. An orange arrow points to the address bar with the text 'enter Galaxy address'. The browser displays the Galaxy Australia homepage. The navigation bar includes 'Workflow', 'Visualize', 'Data', 'Help', 'Log in or Register', and a user profile icon. A blue banner at the top of the page reads 'Galaxy Australia has been upgraded to release 24.1. Check the release notes for...'. Below this, the text 'Register or login' is highlighted with an orange arrow. The main content area features the Galaxy Australia logo and a blue box with the text 'Dude where's my ear tools? They're now in the new activity bar on the left of your screen! Get rapid, one click access to tools and other common functions:'. The left sidebar contains a 'Tools' section with a search bar and a list of tool categories: FILE AND META TOOLS (Get Data, Send Data, Collection Operations), GENERAL TEXT TOOLS (Text Manipulation, Filter and Sort, Join, Subtract and Group), and GENOMIC FILE MANIPULATION (FASTA/FASTQ, FASTQ Quality Control, SAM/BAM, BED, VCF/BCF, Nanopore). The right sidebar shows a 'History' section with a search bar and a message: 'This history is empty. You can load your own data or get data from an external source.'

Comment: Different Galaxy servers

This is an image of Galaxy Australia, located at usegalaxy.org.au

The particular Galaxy server that you are using may look slightly different and have a different web address.

You can also find more possible Galaxy servers at the top of this tutorial in **Available on these Galaxies**

Not sure where to start?

Try the NGS Basics Learning Path!

[Start Learning](#)

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

Upcoming Events

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Galaxy Beyond Basics: Mastering Workflows, Automation, and Scalability

[See all events](#)

[Add your event!](#)

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

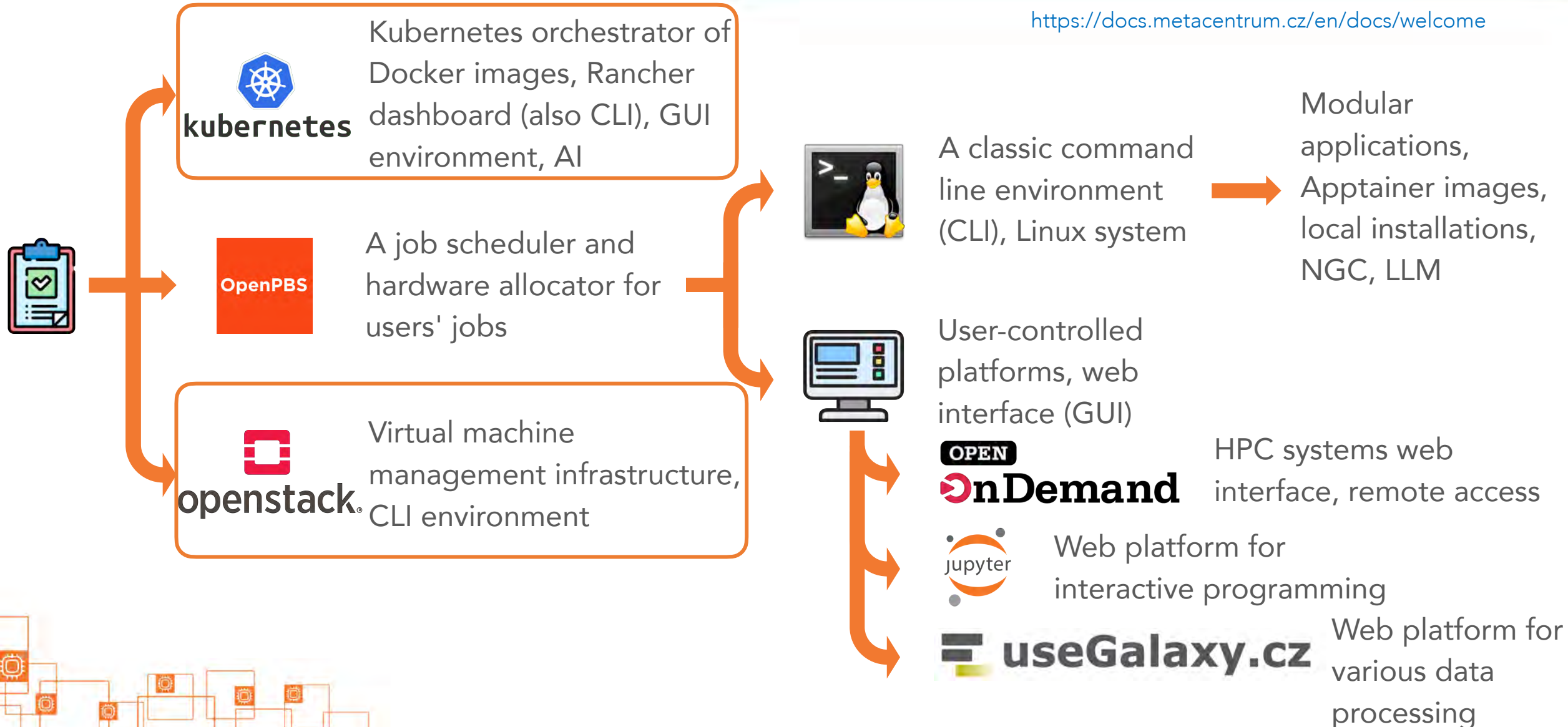
Sep 12, 2025

We want you to help us organize the Galaxy Training Academy 2026

Workflows

How to use it

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





Web hosting can be arranged, but please discuss this in advance



Kubernetes Container Platform

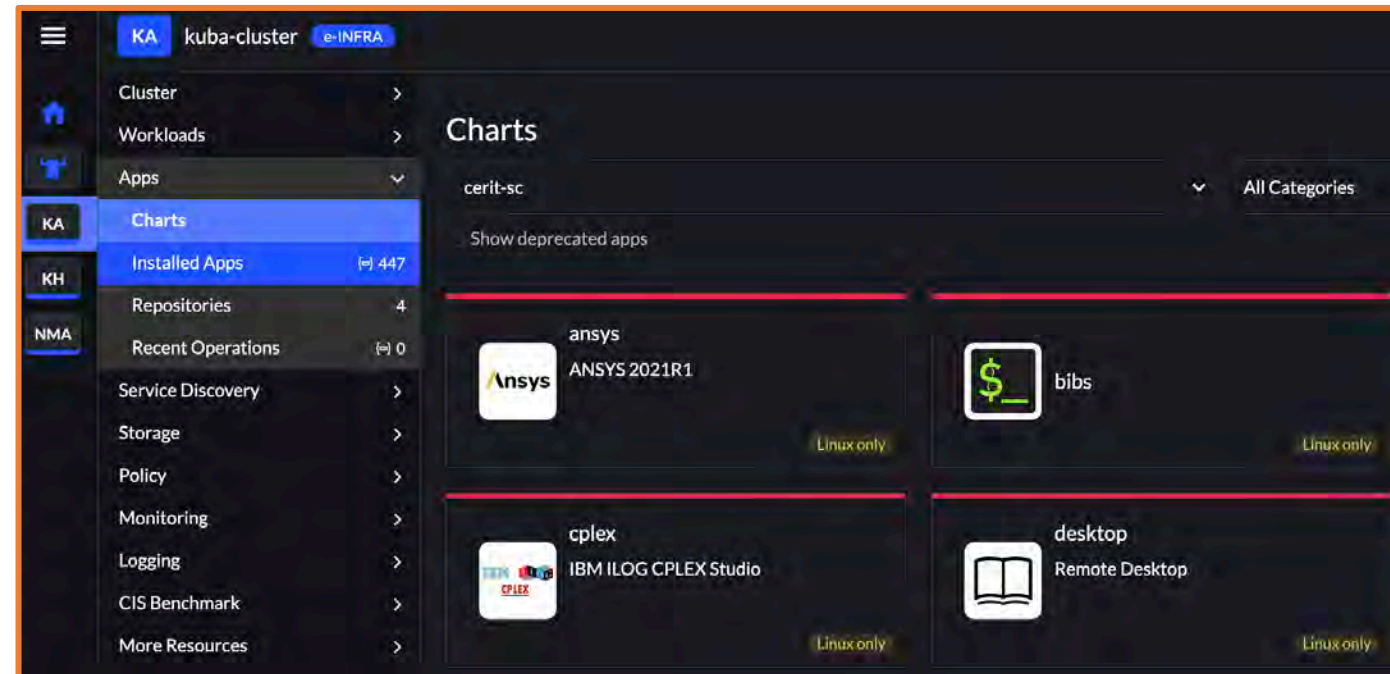
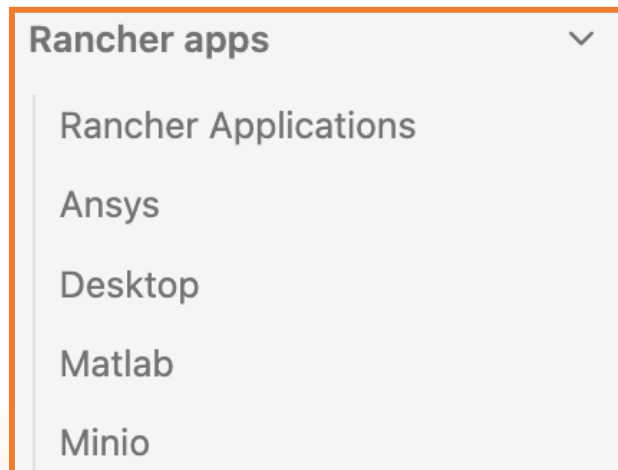
■ Kubernetes

MUNI | CERIT - SC

<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>





Web hosting can be arranged, but please discuss this in advance



Kubernetes Container Platform

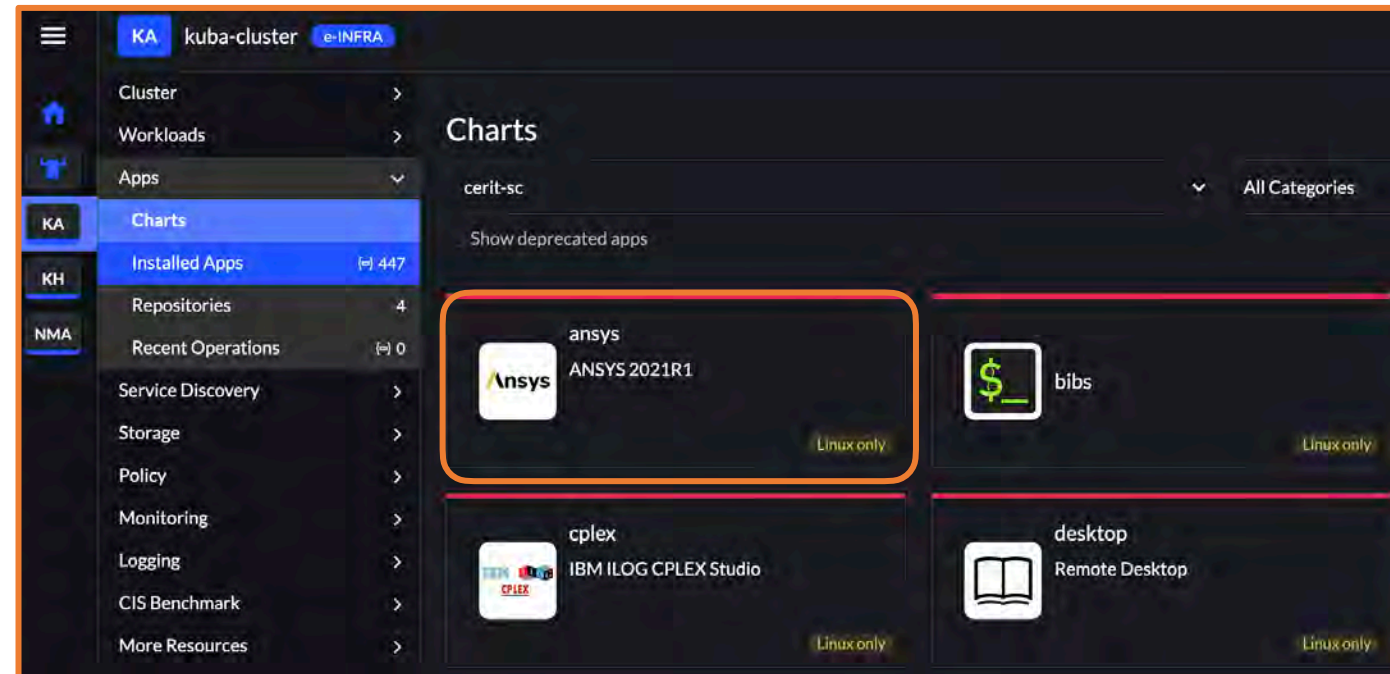
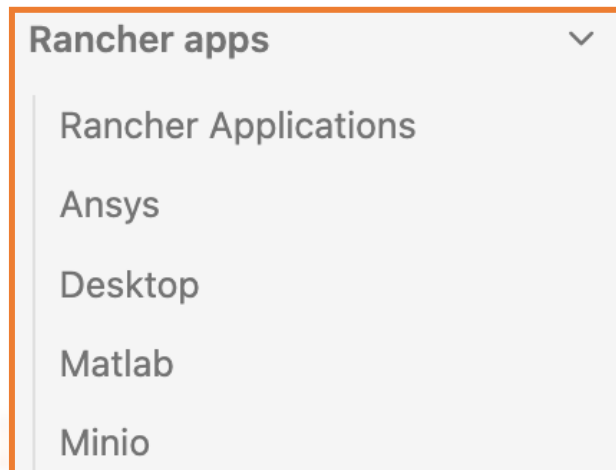
■ Kubernetes

MUNI | CERIT - SC

<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>



- File System
- Home
- FlexNet
- License Checker
- Google Chrome
- ANSYS FLUENT
- ANSYS Fluent
- FlexNet
- Licence Checker
- Firefox
- ANSYS CFX
- ANSYS CFX
- ANSYS Workbench

License Checker

Select license: (hold down CTRL to select multiple)

License name	Available
ansys	0
ansys-mcad	30

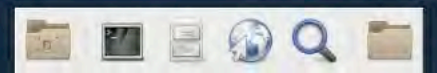
License Information

You must be the registered user of of national grid infrastructure of MetaCentrum to use this application.

All licenses are restricted to academical use only!

Cancel OK

Exit





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

■ Foldify

- A web application based on the Alphafold tools

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

The screenshot shows the Foldify web application interface. At the top left is the Foldify logo. The navigation bar includes a home icon, a document icon, and a menu with options: AlphaFold 3, AlphaFold 2, ColabFold, OmegaFold, and ESMFold. On the right of the navigation bar is the user name 'Mgr. Jiří Vorel Ph.D.' with a dropdown arrow. The main content area features a purple and white background with a large heading 'Protein Folding Platform'. Above the heading is a badge that says 'Powered by Advanced AI'. Below the heading are three icons with text: '3D Result Comparison', 'Multiple Tools', and 'Powerful Hardware'. At the bottom, there are two buttons: 'Get Started →' and 'View Examples'. Below these buttons are three statistics: '2000+' Predicted Proteins, '5' Prediction Tools, and '24/7' Processing.



AlphaFold 3

AlphaFold 2

ColabFold

OmegaFold

ESMFold

Mgr. Jiří Vorel Ph.D. ▾

Powered by Advanced AI

Protein Folding Platform

3D Result Comparison Multiple Tools Powerful Hardware

Get Started →

View Examples

2000+

Predicted Proteins

5

Prediction Tools

24/7

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.

Compare Tools

MultiFold

Compare multiple prediction tools

Latest

AlphaFold 3

Latest version with advanced capabilities

Stable

AlphaFold 2

Reliable and proven protein structure prediction

Fast 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.

Select jobs to compare

Search Jobs

Type job name...



View

My Jobs

Public Jobs



Visibility

Job Name

Service

Started

Status

Actions

[← Back to Dashboard](#)

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?

[JSON Guide](#)

1 Basic Information

Job Name *

test-job

Model Seeds *

1

2 Sequences and Ligands

1 Entity 1 • Protein

Type *

Protein

IDs *

A

Sequence *

```
MGSFAKMFVAASFVLCFCIIIGCFADQNESPFQKNFIINSNTASKGVDYVSQSWSMFKNFFKRNFFENAIEEGERFFFIFARNFFMIS
SHNAEYASGKKIYELTLNKFSDAKESELMKLRGYKAVMKKHKDAPKGSTYISPSVDFKLPDWDWRNDGAVTDVKNQGCQCGSC
WAFSTTGSLEGQHRKTGNLVSLEQQLVDCSSSYGNMGCNGLMDNAFAYIKATNGIDYEDKYPYVSGDTGSAEDTCYFKE
EDIGAVDTGYVDIPTDEFAALQEAANVGPVSVAINAGRADFMMYKOGIYKPDECPGQMNDLDHGVLVVGYSSENGODYWI
VKNSWGPDWGESGYIRMARNSGNLCGIATAASYPLV
```



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

3 Model Configuration

MSA and Templates ⓘ

Use precomputed MSA
Faster computation against public MMseqs2 server (unofficial).

Use precomputed templates
Enhanced structure prediction quality

4 Advanced Parameters

Bonded Atom Pairs

1 Bond Pair 1 · Covalent Bond

1 First Atom

Entity ID * ⓘ

A

Residue # ⓘ

1

Atom Name ⓘ

SG

— bond —

2 Second Atom

Entity ID * ⓘ

L

Residue # ⓘ

1

Atom Name ⓘ

C04

Entity IDs must match those defined in your sequences above. Define covalent bonds between atoms. Example: Chain A residue 145 atom SG bonded to ligand L residue 1 atom C04.



Add Atom Pair

Click to add bonded atom pair.

Custom Component Dictionary

Custom Component Dictionary

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

CCD File ⓘ

Procházet... Soubor nevybrán.

Requirements

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

Resources

[Download example](#) [Format guidelines](#)



Force Computation

Force re-computation even if results exist



Make Results Public

Allow others to view your results



Large Input

Process large molecular complexes

» **Submit Job**

You will receive an email notification when your job completes

* Required fields.



Operated by CERIT-SC, ICS MUNI

Developed by Romana Ďuračiová

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RESOURCES

[Documentation](#)

[Terms of use](#)

[✉ k8s@ics.muni.cz](mailto:k8s@ics.muni.cz)

TOOLS

[AlphaFold 3](#)

[AlphaFold 2](#)

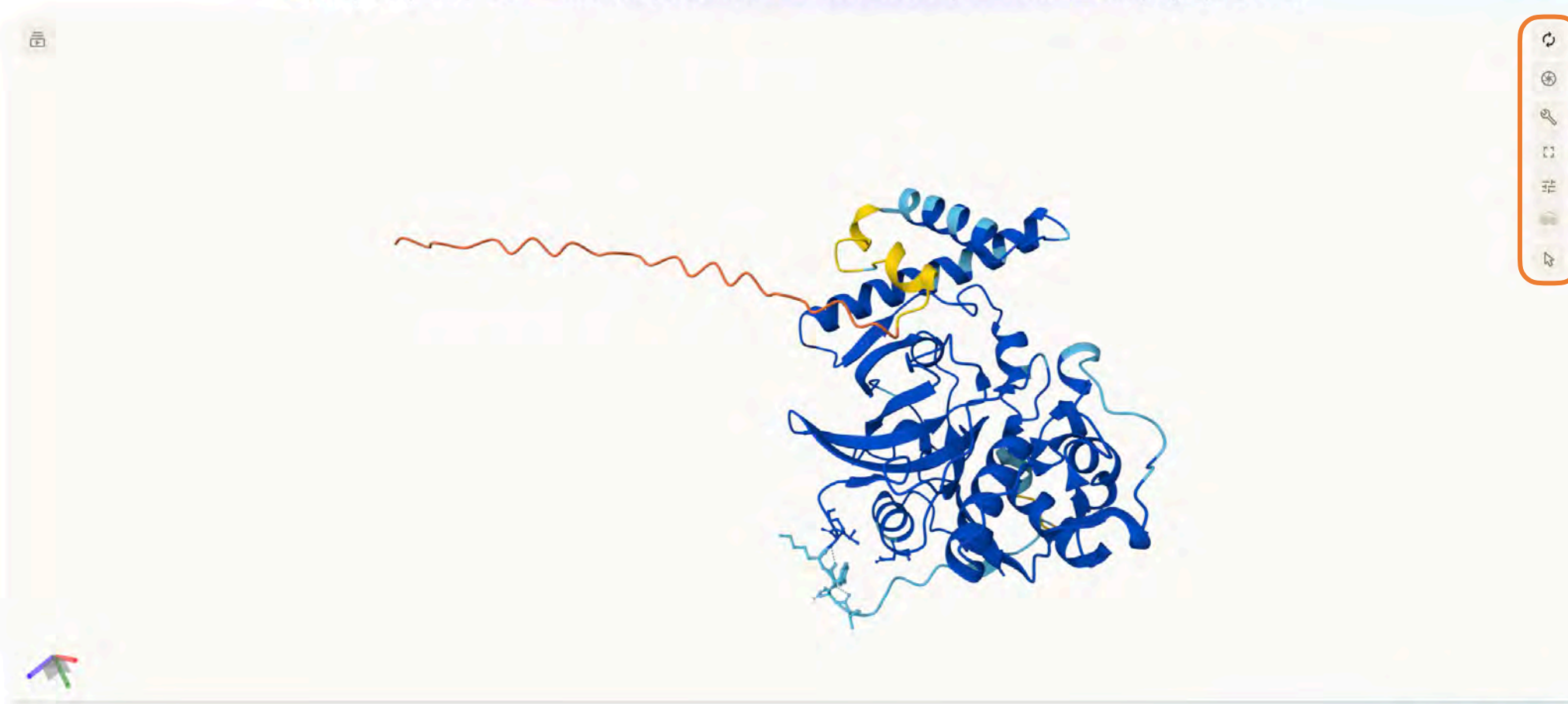
[ColabFold](#)



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)



Open in 

ⓘ PLDDT data not available.

MGSFAKMFVAASFVLCFCIIIGCFADQNESPFQKNFIINSNTASKGVYVSQSWSMFKNFFKRNFFENAIIEEGERFFIFARNFFMISSHNAEYASGKKIYELTLNKFSDAKESELMKLRGYKAVMKKHKDAPKGSTYISPSVDFKLPDWDWRNDGAVTDVK
NQGQCGSCWAFSTTGSLEGQHFRKTGNLVSLEQQLVDC...

▼ Show 168 more characters

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

Sequence of test-job Chain 1: A

1 11 21 31 41 51 61 71 81 91 101 111 121 131 141 151
MGSFAKMFVAASFVLCFCIIIGCFADQNESPFQKNFIINSNTASKGVYVSQSWSMFKNFFKRNFFENAIIEEGERFFIFARNFFMISSHNAEYASGKKIYELTLNKFSDAKESELMKLRGYKAVMKKHKDAPKGSTYISPSVDFKLPDWDWRND
161 171 181 191 201 211 221 231 241 251 261 271 281 291 301
GAVTDVKNQGQCGSCWAFSTTGSLEGQHFRKTGNLVSLEQQLVDCSSSYGNMGCNGGLMDNAFAYIKATNGIDYEDKYPYVSGDTGSAEDTCYFKEEDI GAVDTGYVDI PTEDEAALQEAVANVGPVSVAINAGRADEMMYKQGIYK PDECPG
311 321 331 341 351 361
QMNDLDHGVLVVGYGSENGQDYWIVKNSWGPDWGESGYIRMARNSGNLGIATAASYPLV

Structure Tools

Structure

test-job

Type Model

MET 1 | A [+ 14 other Residues]

Measurements

+ Add

Quick Styles

Apply Representation

Default Cartoon Spacefill Surface

Apply Style

Default Illustrative

Components test-job

Preset + Add

Polymer Cartoon

[Focus] Target Ball & Stick

[Focus] Surroundings (5 Å)

Export Models

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*

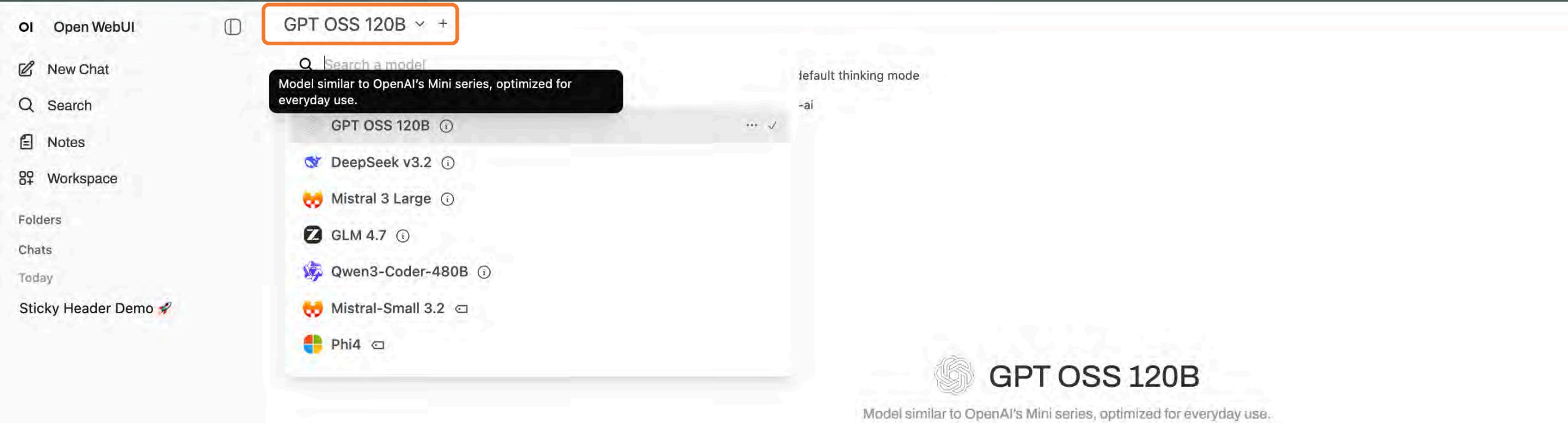
■ AI chatbot (Open WebUI, LLMs)

<https://docs.cerit.io/en/docs/ai-as-a-service/chat-ai>

<https://chat.ai.e-infra.cz/>

- The AI-powered chatbot interface runs strictly on local hardware
- Open WebUI itself logs at the 'INFO' level by default, meaning that request/response data is not logged
- Only system administrators have access to these logs, which are not transmitted anywhere else
- Image generator and picture editor included
- Can extract text from images
- Programming languages proficiency
- Visit documentation for the description of available models





You can select any available model and view its notes



The primary uses of different models vary. For general computing, coding, image creation, text processing, etc.

Guaranteed Models

Model	Model Name	Capability	Description	Context Size
GPT-OSS-120B	gpt-oss-120b	tool	A 120B language model from OpenAI. Superior performance.	128k
DeepSeek V3.2	deepseek-v3.2-thinking	coder, reasoning, tool	A 685B reasoning and instruct (selectable) language model from DeepSeek AI. Excels at complex tasks, including mathematics, logical reasoning, and code generation.	160k
Qwen3.5	qwen3.5-122b	multimodal, coder, tool	A 122B language model from Qwen. Succeeds the Qwen3-coder with significantly enhanced performance in coding tasks.	256k

120B

imized for everyday use.

Experimental Models

Model	Model Name	Capability	Description	Context Size
GLM 5	glm-5	multimodal, coder, tool	The 744B GLM 5 fp4 language model for advanced "agentic" reasoning and superior multi-step task handling	200k
Kimi K2.5	kimi-k2.5	agentic, multimodal, coder, tool	Large-scale MoE model with roughly 1 trillion parameters with significantly enhanced performance in coding tasks.	256k
Qwen 3.5	qwen3.5	agentic, multimodal, coder, tool	397B Multimodal advanced model for coding, tool use, and agentic workflows	262k
Mistral-small	mistral-small-4	multimodal, coder, tool	397B Multimodal advanced model for coding, tool use, and agentic workflows	262k



Please note that the available models may change over time

Open WebUI | GPT OSS 120B

Guaranteed Models

New Chat | Search | Model Name | Capability | Description | Context Size

Model similar to OpenAI's Mini series, optimized for everyday use.

Model Name	Capability	Description	Context Size
GPT OSS 120B
DeepSeek v3.2
GPT-oss-120b	tool	A 120B language model from OpenAI. Superior performance	128k

Czech Language Proficiency

We evaluated selected models using the [BenCzechMark](#) benchmark. Full results are available at the provided link. For reference, key scores are summarized below:

Model	Mean Score
DeepSeek-R1-0528	85.3
Command-A	82.8
LLaMA-3.3	73.5
LLaMA-4-Scout	71.5
Aya Expanse	63.5
Gemma 3	59.2
Phi-4	58.2

Context Size

ed "agentic" 200k

parameters with 256k

ks.

l use, and 262k

l use, and 262k

Programming Languages Proficiency

We evaluated selected models using [Aider Polyglot Benchmark](#). For reference, key scores are summarized below:

Model	C++ Score	Go Lang Score	Java Score	Javascript Score	Python Score	Rust Score
Qwen3-Coder-480B	61.5	59.0	63.8	53.1	50.0	53.3
Qwen3-Coder-Next	69.2	51.3	51.1	75.5	70.6	46.7
GPT-OSS-120B	50.0	59.0	40.4	61.2	70.6	53.3
DeepSeek-R1-0528	7.7	56.4	55.3	69.4	73.5	70.0
DeepSeek V3.2 (think)	88.5	84.6	66.0	89.9	82.4	76.7
DeepSeek V3.2 (nothink)	92.3	82.1	59.6	79.6	79.4	66.7
GLM 4.7 (think)	69.2	71.8	59.6	83.7	82.4	53.3
GLM 4.7 (nothink)	69.2	38.5	44.7	55.1	55.9	33.3
Kimi K2.5 (think)	92.3	84.6	74.5	93.9	91.2	90
Kimi K2.5 (nothink)	92.3	82.1	76.6	89.8	82.4	90

Mistral-small multimodal-coder, 397B Multimodal advanced model for coding, tool use, and agentic workflows 262k

Open WebUI



RedHatAI Scout ▼ +

Set as default

INFO Use <https://llm.ai.e-infra.cz/v1> as API endpoint

New Chat

Search

Notes

Workspace

Models

Folders

Chats



RedHatAI Scout

How can I help you today?



Upload Files

Capture

Attach Webpage

Attach Notes ➤

Attach Knowledge ➤

Reference Chats ➤



of a website's sticky header



New Chat

Search

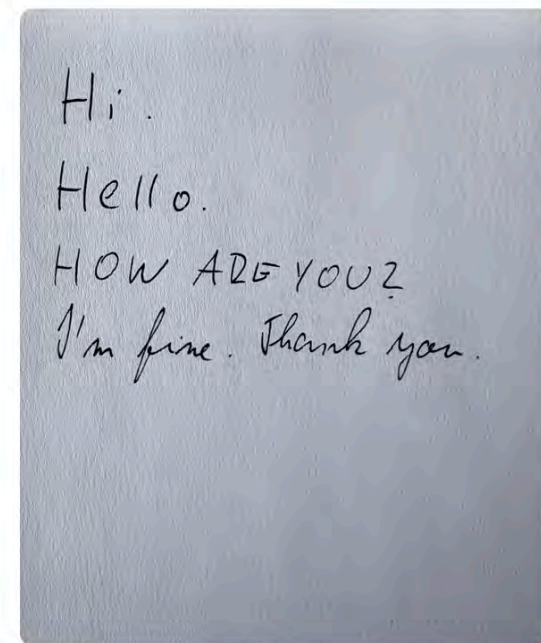
Notes

Workspace

Models

Folders

Chats



Read it.

**RedHatAI Scout**

The image presents a handwritten note on a gray background, featuring a mix of typed and written text. The note is divided into five lines:

- "Hi."
- "Hello."
- "HOW ARE YOU?"
- "I'm fine. Thank you."

The first three lines are written in black ink, with the first two lines in a smaller font and the third line in a larger font. The last line is written in cursive.

The background of the image is a light gray color, resembling paper or cardboard. The overall appearance of the image suggests that it may be a photograph of a handwritten note or a piece of artwork created using digital tools.

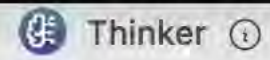


Thinker ▾ +

Set as default

INFO Use <https://llm.ai.e-infra.cz/v1> as API endpoint

Model for advanced reasoning and analytical tasks.



Thinker

Model for advanced reasoning and analytical tasks.

2025_Sreibr.pdf

9.4 MB

Do a short summary (max. 20 sentences) from the article.



Upload Files

Capture

Attach Webpage

Attach Notes

Attach Knowledge

Reference Chats



Open WebUI · v0.8.10

Do a short summary (max. 20 sentences) from the article.



Thinker

Retrieved 1 source

- Querying
- Retrieved 1 source

Thought for 9 seconds ▾

This study characterizes the activation of *Heterorhabditis bacteriophora* infective juveniles (IJs) and their release of excreted/secreted products (ESPs) in response to various stimuli ^{2025_Sreibr.pdf}. The researchers compared insect-derived activation materials—including homogenates from live larvae (H1), frozen larvae (H2), and heat-inactivated frozen larvae (H3)—with non-biological stimuli such as filtered water (H2O) and phosphate-buffered saline (PBS) ^{2025_Sreibr.pdf}. None of the tested materials induced complete recovery of the IJ population, consistent with the phased infectivity hypothesis observed in entomopathogenic nematodes ^{2025_Sreibr.pdf}. However, all activation materials triggered the release of ESPs, with comparable protein concentrations across treatments despite significant differences in protein composition ^{2025_Sreibr.pdf}. Notably, PBS exposure resulted in the highest number of identified proteins (over 200), whereas bioactive homogenates from live and frozen larvae yielded the fewest proteins (65 and 48, respectively) ^{2025_Sreibr.pdf}. The study identified several protein families associated with host-parasite interactions, including alpha-2-macroglobulins, trypsin inhibitor-like (TIL) domain proteins, and metalloendopeptidases, which were significantly upregulated in response to insect-derived materials ^{2025_Sreibr.pdf}. Heat-inactivated homogenate (H3) showed distinct characteristics, including lower protein content and altered protein profiles due to denaturation of host proteins during heating ^{2025_Sreibr.pdf}. Interestingly, nematodes exposed to water also released numerous proteins, though these reflected stress responses rather than host-parasite interaction mechanisms ^{2025_Sreibr.pdf}. The findings demonstrate that both host-derived cues and non-biological stressors can induce IJ activation and ESP release, revealing a complex interplay between environmental stimuli and nematode physiology ^{2025_Sreibr.pdf}. These insights into the molecular mechanisms of *H. bacteriophora* parasitism may contribute to optimizing mass production and biocontrol applications ^{2025_Sreibr.pdf}.

1 Source



Follow up



Do a short summary (max. 20 sentences) from the article.



Thinker

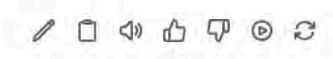
Retrieved 1 source

- Querying
- Retrieved 1 source

Thought for 9 seconds ▾

This study characterizes the activation of *Heterorhabditis bacteriophora* infective juveniles (IJs) and their release of excreted/secreted products (ESPs) in response to various stimuli ^{2025_Sreibr.pdf}. The researchers compared insect-derived activation materials—including homogenates from live larvae (H1), frozen larvae (H2), and heat-inactivated frozen larvae (H3)—with non-biological stimuli such as filtered water (H2O) and phosphate-buffered saline (PBS) ^{2025_Sreibr.pdf}. None of the tested materials induced complete recovery of the IJ population, consistent with the phased infectivity hypothesis observed in entomopathogenic nematodes ^{2025_Sreibr.pdf}. However, all activation materials triggered the release of ESPs, with comparable protein concentrations across treatments despite significant differences in protein composition ^{2025_Sreibr.pdf}. Notably, PBS exposure resulted in the highest number of identified proteins (over 200), whereas bioactive homogenates from live and frozen larvae yielded the fewest proteins (65 and 48, respectively) ^{2025_Sreibr.pdf}. The study identified several protein families associated with host-parasite interactions, including alpha-2-macroglobulins, trypsin inhibitor-like (TIL) domain proteins, and metalloendopeptidases, which were significantly upregulated in response to insect-derived materials ^{2025_Sreibr.pdf}. Heat-inactivated homogenate (H3) showed distinct characteristics, including lower protein content and altered protein profiles due to denaturation of host proteins during heating ^{2025_Sreibr.pdf}. Interestingly, nematodes exposed to water also released numerous proteins, though these reflected stress responses rather than host-parasite interaction mechanisms ^{2025_Sreibr.pdf}. The findings demonstrate that both host-derived cues and non-biological stressors can induce IJ activation and ESP release, revealing a complex interplay between environmental stimuli and nematode physiology ^{2025_Sreibr.pdf}. These insights into the molecular mechanisms of *H. bacteriophora* parasitism may contribute to optimizing mass production and biocontrol applications ^{2025_Sreibr.pdf}.

1 Source



Follow up





Thinker Today at 17:01

Retrieved 1 source

- Querying
- Retrieved 1 source

Thought for 9 seconds ^

"The user wants a short summary (max. 20 sentences) from the article provided in the context.

First, I need to identify the key points of the article:

1. The study investigates the activation of *Heterorhabditis bacteriophora* infective juveniles (IJs) and their release of excreted/secreted products (ESPs).
2. They tested various activation materials: H1 (homogenate from live larvae), H2 (homogenate from frozen larvae), H3 (heat-inactivated homogenate from frozen larvae), H2O (filtered water), and PBS (phosphate-buffered saline).
3. None of the materials induced 100% recovery, but all triggered ESP release.
4. Protein concentrations were consistent across treatments, but protein composition varied significantly.
5. PBS induced the highest number of proteins (over 200), while insect-derived materials (H1, H2) induced the fewest.
6. Key proteins identified include alpha-2-macroglobulins, trypsin inhibitor-like proteins, and metalloendopeptidases, which are important for host-parasite interactions.
7. Heat inactivation (H3) reduced protein content and altered protein profiles compared to live/frozen homogenates.
8. The study reveals that both host-derived and non-biological stimuli can trigger IJ activation and ESP release.
9. ESPs play roles in immune suppression, melanization inhibition, and tissue migration.
10. The findings provide insights for optimizing biocontrol strategies.

Now I need to condense this into maximum 20 sentences, using inline citations [id] only when the <source> tag includes an explicit id attribute. Looking at the context, all sources have id="1", so I should cite as 2025_Sreibr.pdf when referencing specific information.

2025_Sreibr.pdf 9.4 MB

20 sentences) from the article.

and their release of excreted/
d insect-derived activation
f frozen larvae (H3)—with non-
. None of the tested materials
is observed in entomopathogenic
comparable protein concentrations
PBS exposure resulted in the
frozen larvae yielded the fewest
sociated with host-parasite
metalloendopeptidases, which
vated homogenate (H3) showed
uration of host proteins during
ns, though these reflected stress
strate that both host-derived
interplay between environmental
f *H. bacteriophora* parasitism

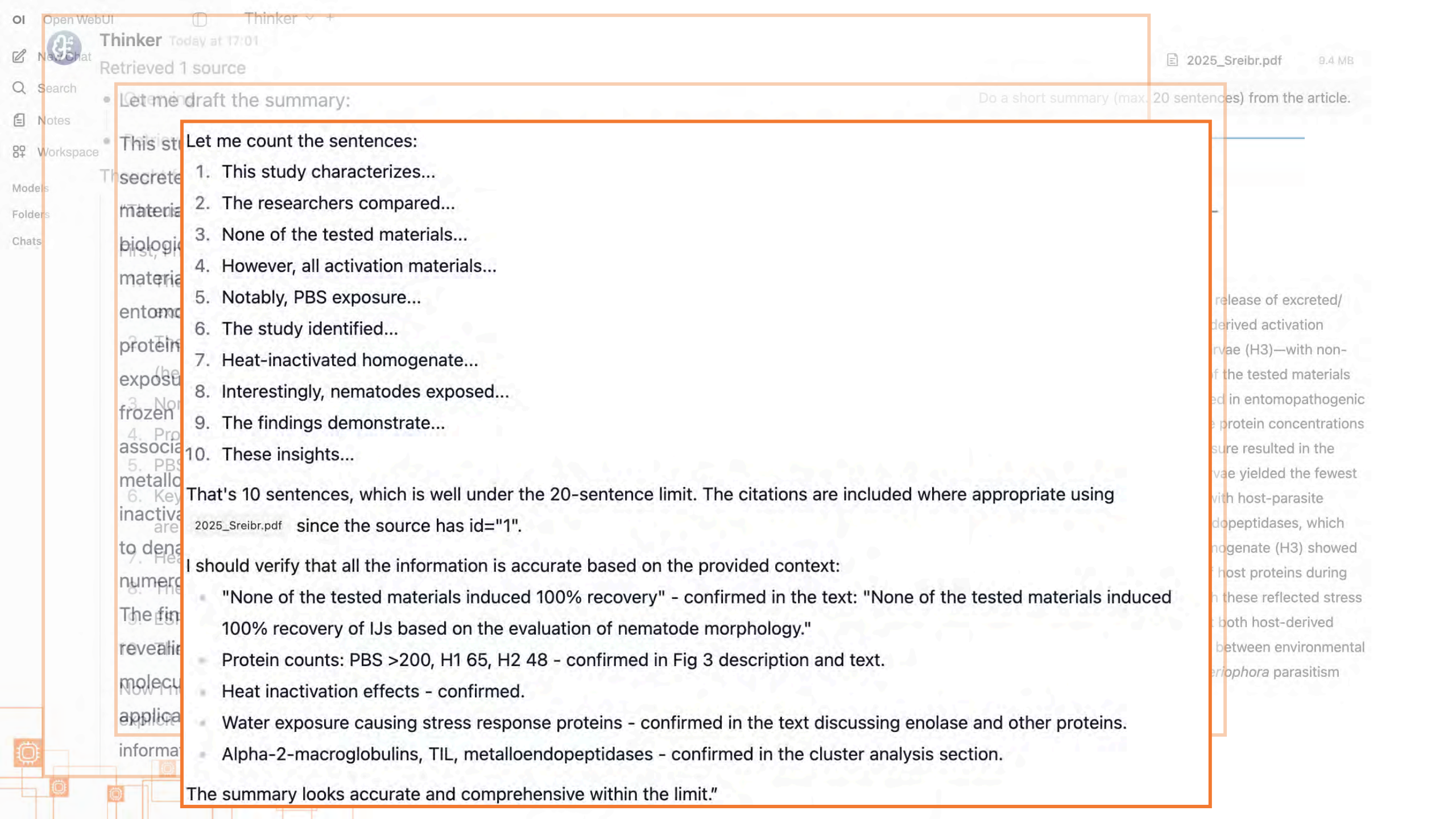
- Search
- Notes
- Workspace
- Models
- Folders
- Chats

Let me draft the summary:

This study characterizes the activation of *Heterorhabditis bacteriophora* infective juveniles (IJs) and their release of excreted/secreted products (ESPs) in response to various stimuli. The researchers compared insect-derived activation materials—including homogenates from live larvae (H1), frozen larvae (H2), and heat-inactivated frozen larvae (H3)—with non-biological stimuli such as filtered water (H2O) and phosphate-buffered saline (PBS). None of the tested materials induced complete recovery of the IJ population, consistent with the phased infectivity hypothesis observed in entomopathogenic nematodes. However, all activation materials triggered the release of ESPs, with comparable protein concentrations across treatments despite significant differences in protein composition. Notably, PBS exposure resulted in the highest number of identified proteins (over 200), whereas bioactive homogenates from live and frozen larvae yielded the fewest proteins (65 and 48, respectively). The study identified several protein families associated with host-parasite interactions, including alpha-2-macroglobulins, trypsin inhibitor-like (TIL) domain proteins, and metalloendopeptidases, which were significantly upregulated in response to insect-derived materials. Heat-inactivated homogenate (H3) showed distinct characteristics, including lower protein content and altered protein profiles due to denaturation of host proteins during heating. Interestingly, nematodes exposed to water also released numerous proteins, though these reflected stress responses rather than host-parasite interaction mechanisms. The findings demonstrate that both host-derived cues and non-biological stressors can induce IJ activation and ESP release, revealing a complex interplay between environmental stimuli and nematode physiology. These insights into the molecular mechanisms of *H. bacteriophora* parasitism may contribute to optimizing mass production and biocontrol applications.

es) from the article.

release of excreted/
rived activation
ae (H3)—with non-
he tested materials
in entomopathogenic
rotein concentrations
re resulted in the
e yielded the fewest
h host-parasite
eptidases, which
genate (H3) showed
ost proteins during
hese reflected stress
oth host-derived
etween environmental
ophora parasitism



Let me draft the summary:

This study Let me count the sentences:

1. This study characterizes...
2. The researchers compared...
3. None of the tested materials...
4. However, all activation materials...
5. Notably, PBS exposure...
6. The study identified...
7. Heat-inactivated homogenate...
8. Interestingly, nematodes exposed...
9. The findings demonstrate...
10. These insights...

That's 10 sentences, which is well under the 20-sentence limit. The citations are included where appropriate using 2025_Sreibr.pdf since the source has id="1".

I should verify that all the information is accurate based on the provided context:

- "None of the tested materials induced 100% recovery" - confirmed in the text: "None of the tested materials induced 100% recovery of IJs based on the evaluation of nematode morphology."
- Protein counts: PBS >200, H1 65, H2 48 - confirmed in Fig 3 description and text.
- Heat inactivation effects - confirmed.
- Water exposure causing stress response proteins - confirmed in the text discussing enolase and other proteins.
- Alpha-2-macroglobulins, TIL, metalloendopeptidases - confirmed in the cluster analysis section.

The summary looks accurate and comprehensive within the limit."

release of excreted/
derived activation
ryae (H3)—with non-
of the tested materials
ed in entomopathogenic
e protein concentrations
sure resulted in the
vae yielded the fewest
with host-parasite
dopeptidases, which
nogenate (H3) showed
of host proteins during
n these reflected stress
t both host-derived
between environmental
eriphora parasitism

■ OpenAI API

<https://docs.cerit.io/en/docs/ai-as-a-service/introduction>

- Integrate LLMs into local applications, scripts, or AI workflows

■ AI coding assistant (Claude Code)

- A coding tool that lives in your terminal, understands your codebase and helps you code faster by executing routine tasks and explaining complex code

■ Vibe Coding (DeepSite)

- Web-based AI web page and application generator that creates fully functional websites directly from your descriptions, powered by DeepSeek 3.2



Local [Solver](#)

Answers from AI may be inaccurate, please verify the information.

Ask a direct question or paste an error—only the first question searches the documentation; **for a new topic, use the button below.**

You

How to prepare a shell script for a batch job?

Jarvis

To prepare a shell script for a batch job in **MetaCentrum** using **PBS (Torque)** scheduler (submitted via `qsub`), follow the structure and best practices shown in your documentation (especially the *job example* and *scratch usage* sections). Here's a step-by-step guide:

✓ 1. Script Header: PBS Directives

Place required PBS resource requests and job options at the top of the script (they must appear **before** any executable commands, typically as comments starting with `#`):

```
#!/bin/bash
#PBS -N job_name           # Job name (visible in qstat, output files)
#PBS -l select=1:ncpus=4:mem=4gb:scratch_local=10gb  # Resource request
#PBS -l walltime=02:00:00  # Max runtime (HH:MM:SS)
#PBS -q standard          # (optional) Specify queue if needed
```

🚨 Important:

- *Do not specify queue unless necessary — omit `-q` to let the scheduler route to default.*
- *`select=1` means 1 node; `ncpus`, `mem`, `scratch_local` are mandatory for most jobs.*
- *`scratch_local` is strongly recommended — it defines size (e.g., `10gb`) and sets `$SCRATCHDIR`.*

✓ 2. Set up environment & scratch directory

Ensure `$SCRATCHDIR` is set and use it for I/O-intensive operations:



An AI assistant is also available in the MetaCentrum documentation



openstack®



kubernetes

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 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





■ FileSender

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

- 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

■ 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

Preferovaný jazyk cs

Nahrávání Pozvánky Mé přenosy Můj profil

Nápověda Soukromí Odhlášení

Sem přetáhněte soubory k nahrání

Vložit vše

Vybrat soubory

Od : vorel@cesnet.cz

Příjemce :

Předmět (volitelné) :

Zpráva (volitelné) :

Zašifrování souborů (beta)

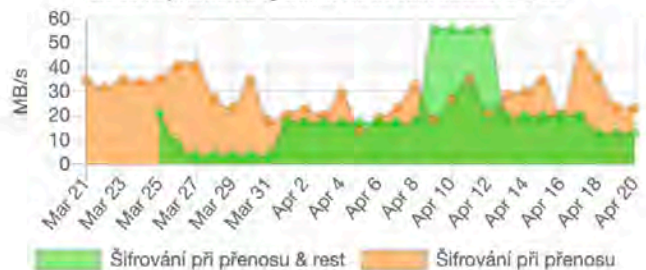
Datum expirace:

- Zaslát mi denní statistiku
- Zahrň mě jako příjemce

[Pokročilá nastavení](#)

 Odeslat

Globální průměrná rychlost nahrávání souborů 1 GB



■ 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
- S3 storage can be accessed via the command line or a GUI client (for Windows, Linux, Mac)
- 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)

<https://access.du.cesnet.cz/>



■ 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>



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.



[Open in Terminal](#) [Refresh](#) [New File](#) [New Directory](#) [Upload](#) [Download](#) [Copy/Move](#) [Delete](#)

Home Directory

- brno2
- brno12
- praha5-elixir
- brno11-elixir
- brno14-ceitec
- brno3-cerit
- budejovice1
- liberec3
- plzen1
- plzen4-ntis
- praha1
- praha2-natur
- praha5-elixir
- praha6-fzu
- pruhonice1-ibot
- projects
- projects2
- projects-du-praha
- cesnet_s3

cesnet_s3: / [Change directory](#) [Copy path](#)

Show Owner/Mode Show Dotfiles Filter: Showing 1 rows - 0 rows selected

Type	Name	Size	Modified at
<input type="checkbox"/>	meta-archive	-	20. 8. 2024 17:59:00

Open in Terminal Refresh New File New Directory Upload Download Copy/Move Delete

- Home Directory
- brno2
- brno12
- praha5-elixir
- brno11-elixir
- brno14-ceitec
- brno3-cerit
- budejovice1
- liberec3
- plzen1
- plzen4-ntis
- praha1
- praha2-natur
- praha5-elixir
- praha6-fzu
- pruhonice1-ibot
- projects
- projects2
- projects-du-praha
- cesnet_s3

cesnet_s3: / meta-archive / Change directory Copy path

Show Owner/Mode Show Dotfiles Filter: Showing 12 rows - 0 rows selected

Type	Name	Size	Modified at
Folder	03_E_nip_genom	-	17. 4. 2026 10:19:50
Folder	03_E_nip_trans	-	17. 4. 2026 10:19:50
Folder	04_Viremie_AV_Kapr_Karas	-	17. 4. 2026 10:19:50
Folder	04_Viremie_AV_Plotice_Cejn	-	17. 4. 2026 10:19:50
Folder	05_Nikol_Kmentova	-	17. 4. 2026 10:19:50
Folder	06_Kasa_mansoni_hepatica_vejce	-	17. 4. 2026 10:19:50
Folder	07_Haem_cont_metylaseDNA	-	17. 4. 2026 10:19:50
Folder	08_JI_hetero_trans	-	17. 4. 2026 10:19:50
File	01_Echo.tar.gz	662.80 GB	9. 10. 2022 15:21:53
File	02_TomasPakosta.tar.gz	3.56 GB	14. 11. 2020 18:46:42
File	02_TomasPakosta_posledni_vymysl.zip	13.46 GB	19. 3. 2025 14:40:50
File	Kapentagyrus_July2022.tar.gz	473.75 GB	11. 12. 2023 19:47:56

- 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

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: [REDACTED]

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_metylacDNA	--	Unknown	--
> 08_JI_hetero_trans	--	Unknown	--
Kapentagyryus_July2022.tar.gz	473.7 GB	21.08.2024, 2:00	--

✓ /meta-archive

Filename /

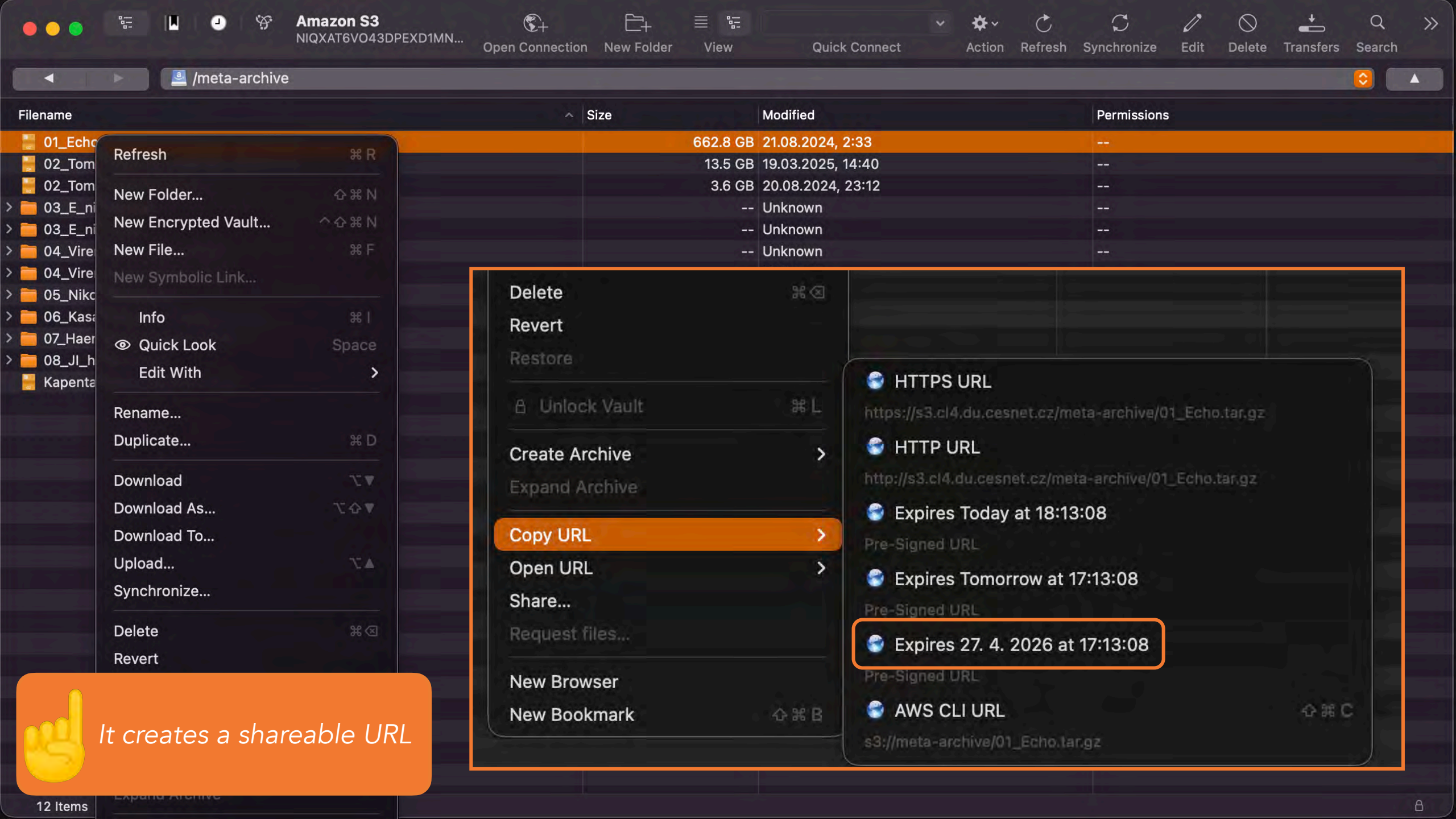
01_Echo.tar.gz	662.8 GB	21.08.2024, 2:33	--
02_TomasPakosta_posledni_vymysl.zip	13.5 GB	19.03.2025, 14:40	--
02_TomasPakosta.tar.gz	3.6 GB	20.08.2024, 23:12	--
> 03_E_nip_genom	--	Unknown	--
> 03_E_nip_trans	--	Unknown	--
> 04_Viremie_AV_Kapr_Karas	--	Unknown	--
> 04_Viremie_AV_Plotice_Cejn	--	Unknown	--
> 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	--

Filename	Size	Modified	Permissions
01_Echo.tar.gz	662.8 GB	21.08.2024, 2:33	--
02_TomasPakosta_posledni	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_Ceji	--	Unknown	--
> 05_Nikol_Kmentova	--	Unknown	--
> 06_Kasa_mansoni_hepatica	--	Unknown	--
> 07_Haem_cont_metylaceDN	--	Unknown	--
> 08_JI_hetero_trans	--	Unknown	--
Kapentagyrus_July2022.tar.	473.7 GB	21.08.2024, 2:00	--

- Refresh ⌘ R
- New Folder...
- New Encrypted Vault... ⌘ ⌘ N
- New File... ⌘ F
- New Symbolic Link...
- Info ⌘ I
- Quick Look Space
- Edit With >
- Rename...
- Duplicate... ⌘ D
- Download ⌘ ⌘
- Download As... ⌘ ⌘
- Download To...
- Upload... ⌘ ⌘
- Synchronize...
- Delete ⌘ ⌘
- Revert
- Restore
- Unlock Vault ⌘ L
- Create Archive >
- Expand Archive

Filename	Size	Modified	Permissions
01_Echo	662.8 GB	21.08.2024, 2:33	--
02_Tom	13.5 GB	19.03.2025, 14:40	--
02_Tom	3.6 GB	20.08.2024, 23:12	--
03_E_ni	--	Unknown	--
03_E_ni	--	Unknown	--
04_Vire	--	Unknown	--
04_Vire	--	Unknown	--
05_Nikc	--	Unknown	--
06_Kasa	--	Unknown	--
07_Haer	--	Unknown	--
08_JI_h	--	Unknown	--
Kapenta	473.7 GB	21.08.2024, 2:00	--

- Refresh ⌘ R
- New Folder... ⌘ N
- New Encrypted Vault... ⌘ N
- New File... ⌘ F
- New Symbolic Link...
- Info ⌘ I
- Quick Look Space
- Edit With >
- Rename...
- Duplicate... ⌘ D
- Download ⌘ V
- Download As... ⌘ V
- Download To...
- Upload... ⌘ A
- Synchronize...
- Delete ⌘ ⌫
- Revert
- Restore
- Unlock Vault ⌘ L
- Create Archive >
- Expand Archive



It creates a shareable URL

- Refresh
- New Folder...
- New Encrypted Vault...
- New File...
- New Symbolic Link...
- Info
- Quick Look
- Edit With
- Rename...
- Duplicate...
- Download
- Download As...
- Download To...
- Upload...
- Synchronize...
- Delete
- Revert

Filename	Size	Modified	Permissions
01_Echo	662.8 GB	21.08.2024, 2:33	--
02_Tom	13.5 GB	19.03.2025, 14:40	--
02_Tom	3.6 GB	20.08.2024, 23:12	--
03_E_ni	--	Unknown	--
03_E_ni	--	Unknown	--
04_Vire	--	Unknown	--
04_Vire	--	Unknown	--
05_Nikc	--	Unknown	--
06_Kasa	--	Unknown	--
07_Haer	--	Unknown	--
08_JI_h	--	Unknown	--
Kapenta	--	Unknown	--

- Delete
- Revert
- Restore
- Unlock Vault
- Create Archive
- Expand Archive
- Copy URL
- Open URL
- Share...
- Request files...
- New Browser
- New Bookmark

- HTTPS URL
https://s3.cl4.du.cesnet.cz/meta-archive/01_Echo.tar.gz
- HTTP URL
http://s3.cl4.du.cesnet.cz/meta-archive/01_Echo.tar.gz
- Expires Today at 18:13:08
Pre-Signed URL
- Expires Tomorrow at 17:13:08
Pre-Signed URL
- Expires 27. 4. 2026 at 17:13:08
Pre-Signed URL
- AWS CLI URL
s3://meta-archive/01_Echo.tar.gz

■ 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 needs to be configured with access keys



■ CESNET S3 service

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 = xxxxxxxxxxxxxxxxxxxxxxxx
secret_key = xxxxxxxxxxxxxxxxxxxxxxxx
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.



■ C S5cmd for Ultra-Fast Transfers

/s3-service

Co

If you have a fast connection of around 1-2 Gbps and want to maximize its potential for data transfers, you can use the s5cmd tool. This tool optimizes data transfers for maximum efficiency. It is available as compiled binaries for Windows, Linux, and macOS, as well as in source code and Docker image formats. For more detailed information, visit [the project Github page](#).

Add

[d

Please add the following options to your `.aws/credentials`.

```
[default]
aws_access_key_id = xxxxxxxxxxxxxxxxxxxxxxxx
aws_secret_access_key = xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
max_concurrent_requests = 200
max_queue_size = 20000
multipart_threshold = 128MB
multipart_chunksize = 32MB
```

the

acce

`aws_access_key_id` and `aws_secret_access_key` has been provided by admins while creating the S3 account.

<https://docs.du.cesnet.cz/en/docs/object-storage-s3/s3cmd#basic-s3cmd-commands>

```
(BOOKWORM)vorel@nympha:~$ cat ~/.s3cfg
[default]
host_base = https://s3.cl4.du.cesnet.cz
use_https = True
access_key = 
secret_key = 
host_bucket = s3.cl4.du.cesnet.cz
```



```
(BOOKWORM)vorel@nympha:~$ s3cmd ls
2024-08-20 15:59  s3://meta-archive
(BOOKWORM)vorel@nympha:~$
(BOOKWORM)vorel@nympha:~$ s3cmd ls s3://meta-archive
DIR s3://meta-archive/03_E_nip_genom/
DIR s3://meta-archive/03_E_nip_trans/
DIR s3://meta-archive/04_Viremie_AV_Kapr_Karas/
DIR s3://meta-archive/04_Viremie_AV_Plotice_Cejn/
DIR s3://meta-archive/05_Nikol_Kmentova/
DIR s3://meta-archive/06_Kasa_mansoni_hepatica_vejce/
DIR s3://meta-archive/07_Haem_cont_metylanceDNA/
DIR s3://meta-archive/08_JI_hetero_trans/
2024-08-21 00:33 662801231434 s3://meta-archive/01_Echo.tar.gz
2024-08-20 21:12 3555354858 s3://meta-archive/02_TomasPakosta.tar.gz
2025-03-19 13:40 13457631873 s3://meta-archive/02_TomasPakosta_posledni_vymysl.zip
2024-08-21 00:00 473749416845 s3://meta-archive/Kapentagyrus_July2022.tar.gz
```



```
(BOOKWORM)vorel@nympha:~$ s3cmd mb s3://test-bucket
Bucket 's3://test-bucket/' created
(BOOKWORM)vorel@nympha:~$
(BOOKWORM)vorel@nympha:~$ s3cmd ls
2024-08-20 15:59 s3://meta-archive
2026-04-20 15:56 s3://test-bucket
(BOOKWORM)vorel@nympha:~$
(BOOKWORM)vorel@nympha:~$ s3cmd rb s3://test-bucket
Bucket 's3://test-bucket/' removed
(BOOKWORM)vorel@nympha:~$
(BOOKWORM)vorel@nympha:~$ s3cmd ls
2024-08-20 15:59 s3://meta-archive
```

jce/

mysl.zip

Z



<https://docs.du.cesnet.cz/en/docs/object-storage-s3/s3cmd#basic-s3cmd-commands>

```
(BOOKWORM)vorel@nympha:~$ s3cmd put MHC3_S3_L001_R1_001.fastq s3://meta-archive
upload: 'MHC3_S3_L001_R1_001.fastq' -> 's3://meta-archive/MHC3_S3_L001_R1_001.fastq' [part 1 of 28, 15MB] [1 of 1]
15728640 of 15728640 100% in 0s 16.12 MB/s done
upload: 'MHC3_S3_L001_R1_001.fastq' -> 's3://meta-archive/MHC3_S3_L001_R1_001.fastq' [part 2 of 28, 15MB] [1 of 1]
15728640 of 15728640 100% in 1s 13.61 MB/s done
upload: 'MHC3_S3_L001_R1_001.fastq' -> 's3://meta-archive/MHC3_S3_L001_R1_001.fastq' [part 3 of 28, 15MB] [1 of 1]
15728640 of 15728640 100% in 0s 21.67 MB/s done
upload: 'MHC3_S3_L001_R1_001.fastq' -> 's3://meta-archive/MHC3_S3_L001_R1_001.fastq' [part 4 of 28, 15MB] [1 of 1]
15728640 of 15728640 100% in 0s 32.40 MB/s done
upload: 'MHC3_S3_L001_R1_001.fastq' -> 's3://meta-archive/MHC3_S3_L001_R1_001.fastq' [part 5 of 28, 15MB] [1 of 1]
15728640 of 15728640 100% in 0s 29.93 MB/s done
```

```
Bucket 's3://test-bucket/' removed
2024-08-21 00:33 662801231434 s3://meta-archive/08_JI_hetero_trans/
2024-08-20 21:22 5555551818 s3://meta-archive/01_Echo.tar.gz
(BOOKWORM)vorel@nympha:~$ s3cmd ls
2024-08-21 00:00 473749416845 s3://meta-archive/02_TomasPakosta.tar.gz
(BOOKWORM)vorel@nympha:~$ s3cmd ls
2024-08-21 00:00 473749416845 s3://meta-archive/02_TomasPakosta_posledni_vymysl.zip
2024-08-21 00:00 473749416845 s3://meta-archive/Kapentagyryus_July2022.tar.gz
2024-08-20 15:59 s3://meta-archive
```



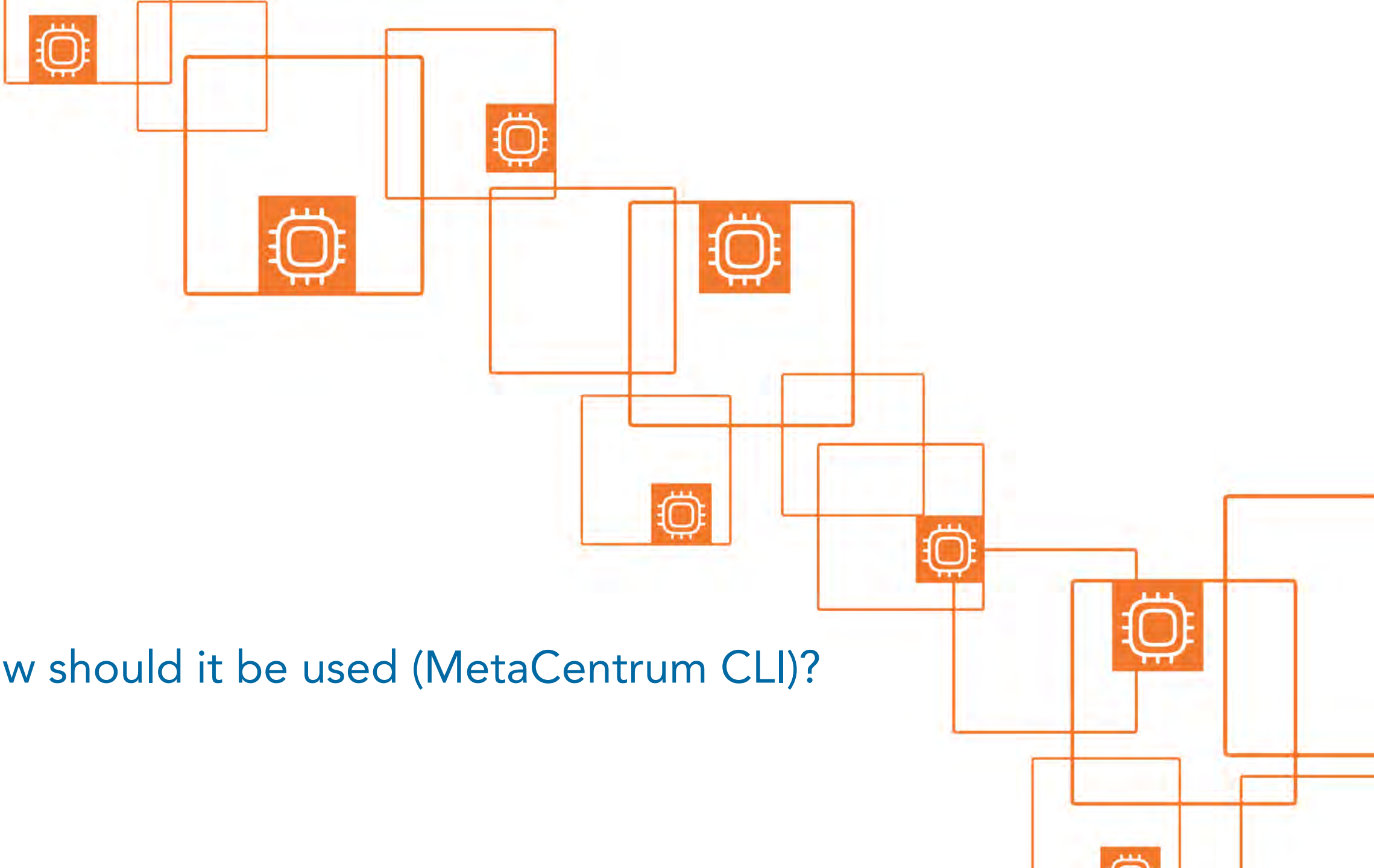
```
(BOOKWORM)vorel@nympha:~$ s3cmd ls s3://meta-archive
DIR s3://meta-archive/03_E_nip_genom/
DIR s3://meta-archive/03_E_nip_trans/
DIR s3://meta-archive/04_Viremie_AV_Kapr_Karas/
DIR s3://meta-archive/04_Viremie_AV_Plotice_Cejn/
DIR s3://meta-archive/05_Niko1_Kmentova/
DIR s3://meta-archive/06_Kasa_masoni_hepatica_vejce/
DIR s3://meta-archive/07_Haem_cont_metylacedNA/
DIR s3://meta-archive/08_JI_hetero_trans/
2024-08-21 00:33 662801231434 s3://meta-archive/01_Echo.tar.gz
2024-08-20 21:12 3555354858 s3://meta-archive/02_TomasPakosta.tar.gz
2025-03-19 13:40 13457631873 s3://meta-archive/02_TomasPakosta_posledni_vymysl.zip
2024-08-21 00:00 473749416845 s3://meta-archive/Kapentagyryus_July2022.tar.gz
2026-04-20 16:03 437260288 s3://meta-archive/MHC3_S3_L001_R1_001.fastq
```

```
(BOOKWORM)vorel@nympha:~$ s3cmd get s3://meta-archive/MHC3_S3_L001_R1_001.fasta
download: 's3://meta-archive/MHC3_S3_L001_R1_001.fasta' -> './MHC3_S3_L001_R1_001.fasta' [1 of 1]
437260288 of 437260288 100% in 3s 126.39 MB/s done
(BOOKWORM)vorel@nympha:~$ s3cmd del s3://meta-archive/MHC3_S3_L001_R1_001.fasta
delete: 's3://meta-archive/MHC3_S3_L001_R1_001.fasta'
(BOOKWORM)vorel@nympha:~$ s3cmd ls s3://meta-archive/
DIR s3://meta-archive/03_E_nip_genom/
DIR s3://meta-archive/03_E_nip_trans/
DIR s3://meta-archive/04_Viremie_AV_Kapr_Karas/
DIR s3://meta-archive/04_Viremie_AV_Plotice_Cejn/
DIR s3://meta-archive/05_Nikol_Kmentova/
DIR s3://meta-archive/06_Kasa_mansoni_hepatica_vejce/
DIR s3://meta-archive/07_Haem_cont_metylanceDNA/
DIR s3://meta-archive/08_JI_hetero_trans/
2024-08-21 00:33 662801231434 s3://meta-archive/01_Echo.tar.gz
2024-08-20 21:12 3555354858 s3://meta-archive/02_TomasPakosta.tar.gz
2025-03-19 13:40 13457631873 s3://meta-archive/02_TomasPakosta_posledni_vymysl.zip
2024-08-21 00:00 473749416845 s3://meta-archive/Kapentagyrus_July2022.tar.gz
```

```
(BOOKWORM)vorel@nymph:~$ s3cmd --help
Usage: s3cmd [options] COMMAND [parameters]

S3cmd is a tool for managing objects in Amazon S3 storage. It allows for
making and removing "buckets" and uploading, downloading and removing
"objects" from these buckets.

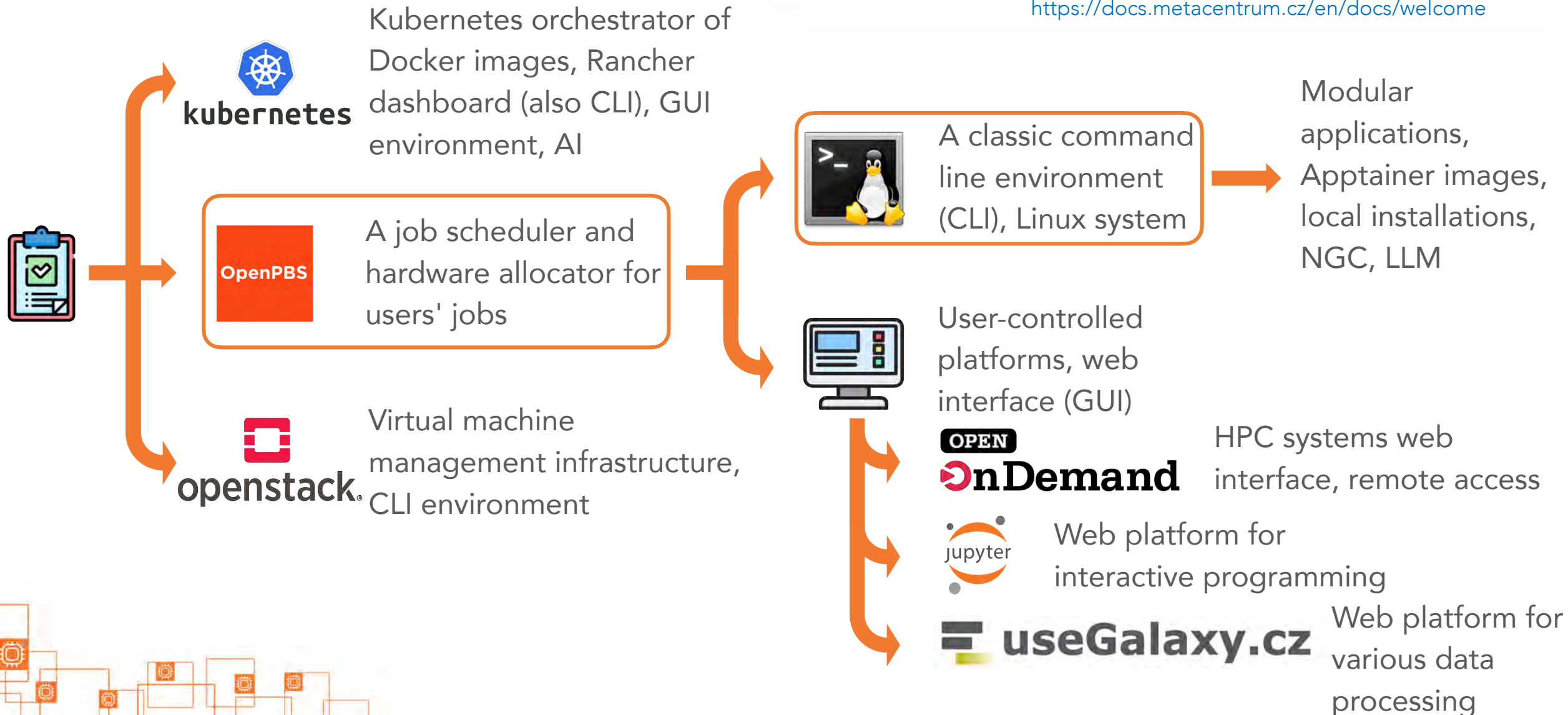
Options:
  -h, --help                show this help message and exit
  --configure                Invoke interactive (re)configuration tool. Optionally
                             use as '--configure s3://some-bucket' to test access
                             to a specific bucket instead of attempting to list
                             them all.
  -c FILE, --config=FILE    Config file name. Defaults to $HOME/.s3cfg
  --dump-config              Dump current configuration after parsing config files
                             and command line options and exit.
  --access_key=ACCESS_KEY   AWS Access Key
  --secret_key=SECRET_KEY   AWS Secret Key
```



How should it be used (MetaCentrum CLI)?

How to use it

<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 keys are not supported
 - A valid Kerberos ticket enables you to submit tasks and browse the infrastructure
 - Beware of leaving sessions open for too long – ticket validity is only 10 hours
 - You can generate Kerberos tickets on a local PC and log in without a password

<https://docs.metacentrum.cz/en/docs/access/security/kerberos>





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

Frontend servers (login nodes)

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

- Primary access point
- SSH access via password (credentials)
 - SSH keys are not supported
 - A valid Kerberos ticket enables access to the infrastructure
 - Beware of leaving sessions open
 - You can generate Kerberos tickets

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	



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 keys are not supported
- A valid Kerberos ticket enables you to submit tasks and browse the infrastructure
- Beware of leaving sessions open for too long – ticket validity is only 10 hours
- You can generate Kerberos tickets on a local PC and log in without a password

<https://docs.metacentrum.cz/en/docs/access/security/kerberos>

■ Do not run calculations on frontends

- They are small virtual machines
- They are at risk of significant slowdown or crashing
- Automatic mechanisms terminate demanding and/or long processes
 - Even for short tests, an interactive task is more suitable

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



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-called "cold" storage
 - Backups of valuable production data
 - Available to all users
 - `s3cmd/s5cmd` commands
 - Need to request the correct storage



By default, the storage ID is 755 (= other storages can be set to other IDs)

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/

Disk storage arrays

- Several geographically separated disk arrays (storages) are available
- Designed for so-called live data
 - Backups of valuable primary data and results preferably to S3/NRP object storage
 - 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
- User quotas are set for the total volume of data and the number of files
 - Storage capacity is not unlimited (keep only needed data)
 - Disk storages come in different sizes and quotas are set the same for everyone
 - Some disk storages have owners with higher quotas
 - Manipulating many small files is more problematic (use archives)

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

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

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





Only members of the project Elixir CZ have a high quota on the storage praha5-elixir

Disk storage arrays

Several geographically separated disk arrays (storages) are available


user	dir	space				files			
		used	soft quota	hard quota	grace	used	soft limit	hard limit	grace
vorel	/storage/brno12-cerit/home/vorel	200.55728 GB	-	-	none	35	-	-	none
vorel	/storage/brno2/home/vorel	40.40222 GB	4294.967296 GB	4294.967296 GB	none	31062	2500000	2550000	none
vorel	/storage/budejovice1/home/vorel	24 kB	3323.625472 GB	5522.30912 GB		9	1000000	1100000	
vorel	/storage/liberec3-tul/home/vorel	12 kB	10.48576 GB	15.72864 GB		8	-	-	
vorel	/storage/plzen1/home/vorel	1714.056364 GB	4294.967296 GB	6442.450944 GB	none	133431	3000000	3100000	none
vorel	/storage/praha2-natur/home/vorel	44 kB	7.340032 GB	10.48576 GB		18	-	-	
vorel	/storage/praha5-elixir/home/vorel	940.99644 GB	5369.757696 GB	6014.107648 GB		113327	1010000	1212000	
vorel	/storage/pruhonice1-ibot/home/vorel	32 kB	7.340032 GB	10.48576 GB		12	-	-	
vorel	/storage/vestec1-elixir/home/vorel	80 kB	2147.483648 GB	2202.0096 GB	none	33	2000000	2100000	none

storages
department
service

- Disk storages come in different sizes and quotas are set the same for everyone
- Some disk storages have owners with higher quotas
 - Manipulating many small files is more problematic (use archives)



The concept of multiple home directories and disk storages


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

 All frontend servers can also be reached in the domain 'metacentrum.cz'


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	



The concept of multiple home directories and disk storages

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

 All frontend servers can also be reached in the domain 'metacentrum.cz'

 Although disk storage servers cannot be accessed interactively, it is possible to send specific commands to them

Frontend address	Aliased as	Native home	OS	Physically located in	Note
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/
zenith.cerit-sc.cz	zenith.metacentrum.cz	/storage/brno12-cerit	Debian 12	Brno	

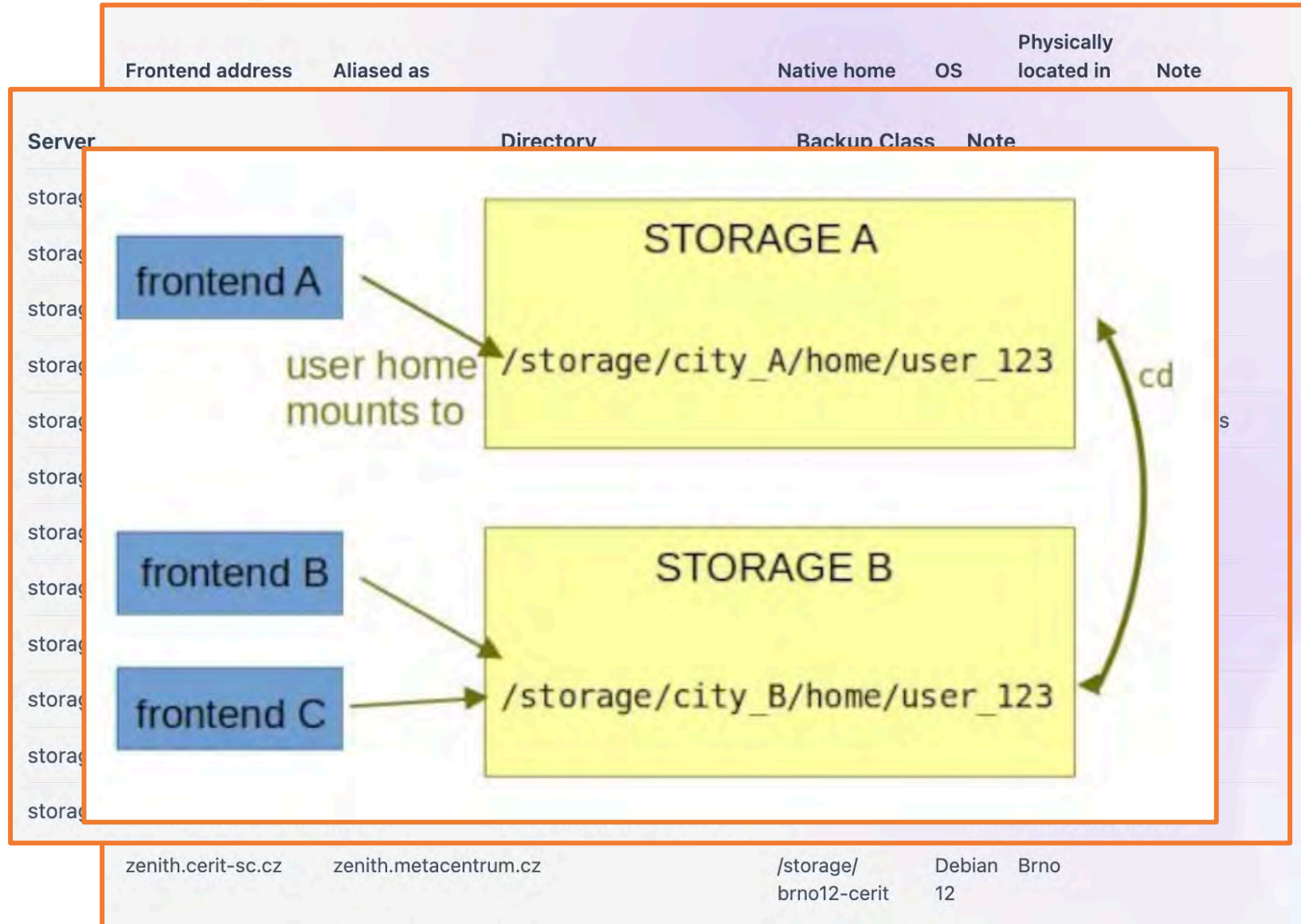


The concept of multiple home directories and disk storages

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

All frontend servers can also be reached in the domain 'metacentrum.cz'

Although disk storage servers cannot be accessed interactively, it is possible to send specific commands to them



```
name@my_pc:~$ ssh vorel@perian.metacentrum.cz
```

```
vorel@perian.metacentrum.cz's password:
```

← Type a password

```
vorel@perian:~$ pwd
```

← Where am I?

```
/storage/brno2/home/vorel
```

```
vorel@perian:~$ cd /storage/plzen1/home/vorel
```

```
vorel@perian:~$ pwd
```

← Hmm, I forgot that my data is on different storage...

```
/storage/plzen1/home/vorel
```

```
name@my_pc:~$ ssh vorel@minos.metacentrum.cz
```

```
vorel@minos.metacentrum.cz's password:
```

← Direct access to the same storage through different frontend

```
vorel@minos:~$ pwd
```

```
/storage/plzen1/home/vorel
```



The concept of multiple home directories and disk storages

- Comes from the nature of the grid (distributed) infrastructure
- Generally, with a group of compute clusters in each geographical location there is also a disk storage
- Compute nodes also have a mounted some native home directory
- Compute jobs can run on clusters with a different home directory
- Users cannot rely on the same data being on all nodes
 - Because of different home directories...
 - But everything is accessible, you just need to specify correct path



The concept of multiple home directories and disk storages

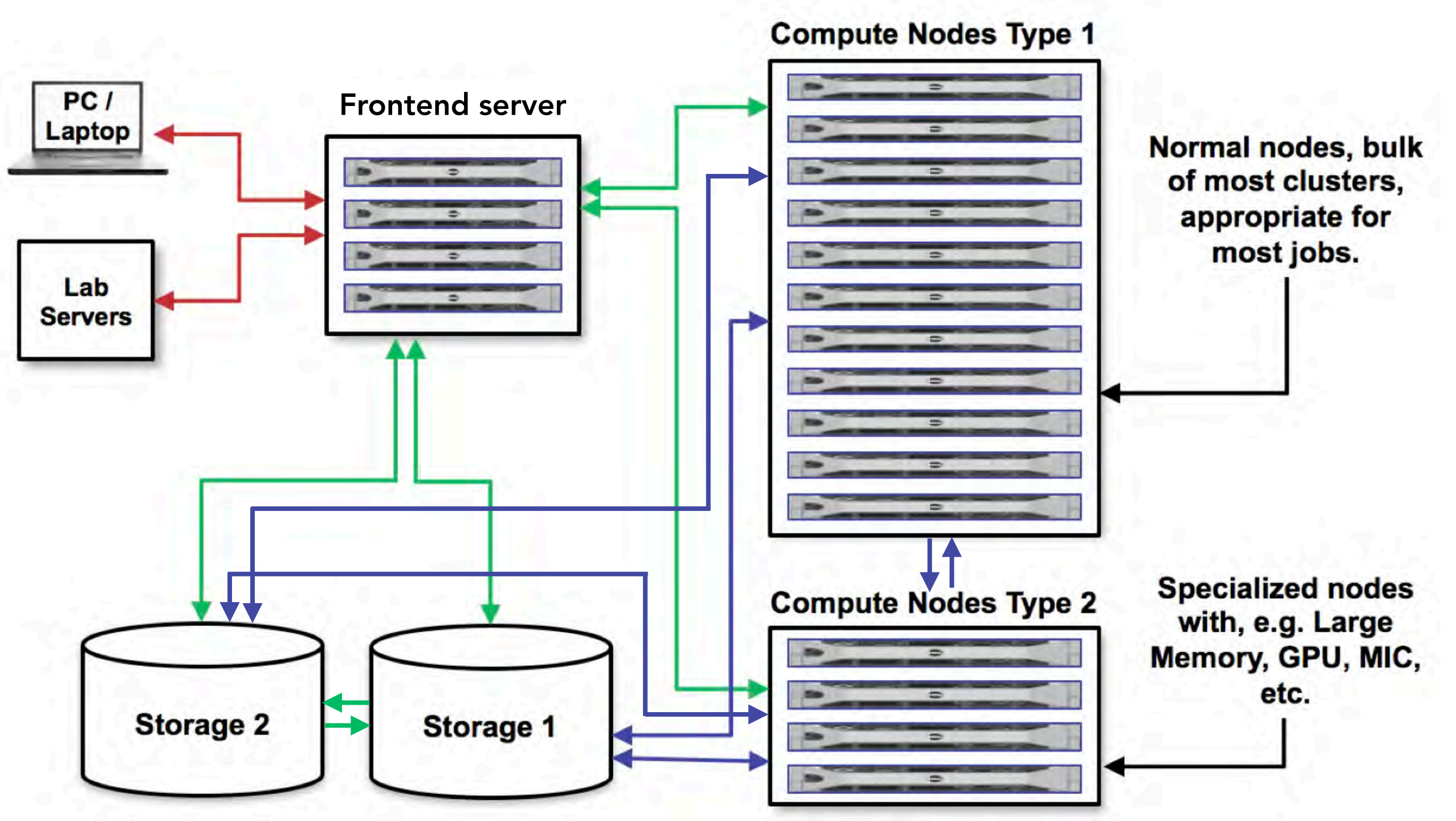
```
[(BOOKWORM)vorel@skirit:~$ ls
CASTEP-25.12 META_SUPPORT ondemand OpenMolcas pcangsd Smilei test_crys test_CZ_shift test_phyluce test_unic
[(BOOKWORM)vorel@skirit:~$ pwd
/storage/brno2/home/vorel
[(BOOKWORM)vorel@skirit:~$ ssh adan1
Linux adan1.grid.cesnet.cz 6.1.0-38-amd64 #1 SMP PREEMPT_DYNAMIC Debian 6.1.147-1+zs2 (2025-08-22) x86_64

5 updates could not be installed automatically. For more details,
see /var/log/unattended-upgrades/unattended-upgrades.log

The programs included with the Debian GNU/Linux system are free software;
the exact distribution terms for each program are described in the
individual files in /usr/share/doc/*/copyright.

Debian GNU/Linux comes with ABSOLUTELY NO WARRANTY, to the extent
permitted by applicable law.
Last login: Tue Aug 12 12:57:42 2025 from nympha.meta.zcu.cz
[(BOOKWORM)vorel@adan1:~$ pwd
/storage/praha1/home/vorel
[(BOOKWORM)vorel@adan1:~$ ls
geometry.in inp.xyz ondemand xyz_to_aims.py
[(BOOKWORM)vorel@adan1:~$
```







By default, data in the scratch directory cannot be read by other users (the main directory has 700 permissions).

<https://docs.metacentrum.cz/en/docs/computing/concepts#scratch-directory>

Scratch storage

- A different type of storage (than the classic home directories)
- An internal part of each compute node
- ONLY for data that is used in a running job
 - Old, unused data can be deleted at any time without warning
- Each job automatically defines a `$SCRATCHDIR` variable
- Direct access to data for CPU/GPU (=faster calculation)
- Every job that reads input data more than once should scratch
 - Reduces network traffic
 - Does not overload the disk storage
 - The task is faster and more robust (e.g. network outages)





By default, data in the scratch directory cannot be read by other users (the main directory has 700 permissions).

<https://docs.metacentrum.cz/en/docs/computing/concepts#scratch-directory>

Scratch storage

- A different type of storage (than the classic home directories)

```
(BOOKWORM)vorel@nympha:~$ qsub -I -l scratch_local=10gb
qsub: waiting for job 19226822.pbs-m1.metacentrum.cz to start
qsub: job 19226822.pbs-m1.metacentrum.cz ready
```

```
(BOOKWORM)vorel@tarkil16:~$ cd $SCRATCHDIR
(BOOKWORM)vorel@tarkil16:/scratch/vorel/job_19226822.pbs-m1$ pwd
/scratch/vorel/job_19226822.pbs-m1
```

Every job that reads input data more than once should scratch

- Reduces network traffic
- Does not overload the disk storage
- The task is faster and more robust (e.g. network outages)



■ Different types of scratch can be reserved

■ scratch_local

- On every node, mostly SSH, but can also be HDD, TBs
- Located in `/scratch/USERNAME/job_JOBID`

■ scratch_ssd

- Explicitly requires SSD, not on all nodes, TBs
- Ideal for intensive IO calculations
- Located in `/scratch.ssd/USERNAME/job_JOBID`

■ scratch_shm

- Scratch in RAM, on all nodes, the fastest solution, GBs/TBs
- The RAM reservation (PBS 'mem' parameter) is the sum of data volume (input and output) and memory requirements of the calculation
- Located in `/dev/shm/scratch.shm/USERNAME/job_JOBID`
- Boolean (true/false), reservation via the qsub parameter 'mem'

```
:scratch_local=100gb
```

```
:scratch_ssd=100gb
```

```
:mem=50gb:scratch_shm=true
```



■ scratch_shared

`:scratch_shared=10tb`

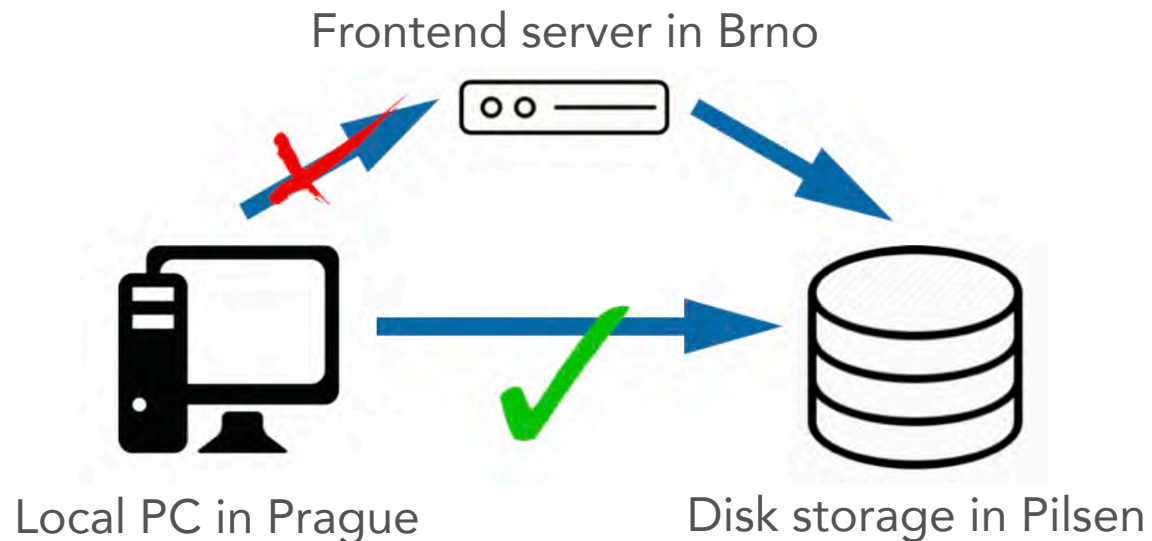
- Scratch shared by all the cluster's nodes, TBs, PBb
- Currently only available on Bee (BeeGFS) and Galdor GPU clusters
- No auto-delete policy
- Different directory naming policy in `/scratch.shared/USERNAME/some_folder_name`, it must not start with 'job_'.
- Suitable for tasks that process one large dataset/database
- Initialisation job copying data, other purely computational

```
qsub -l select=1:ncpus=1:mem=4gb:scratch_local=10gb -l walltime=1:00:00
cp my_input_data.txt $SCRATCHDIR
cd $SCRATCHDIR
...
cp $SCRATCHDIR/my_results.txt /storage/city/home/user_name/
```



- Do not copy (move) large amounts of data (up to 10 GB) via the frontend servers
- Copy (move) the data directly onto the disk storage server
- It's faster, more stable, does not overload network and servers
- SFTP clients are available for Windows users (WinSCP, CyberDuck, FileZilla, etc.)

<https://docs.metacentrum.cz/en/docs/data/large-data>





Users cannot browse disk storage interactively after logging in.
 Only individual commands can be sent on them
 \$ ssh storage-brno2.metacentrum.cz 'ls'

Copying data

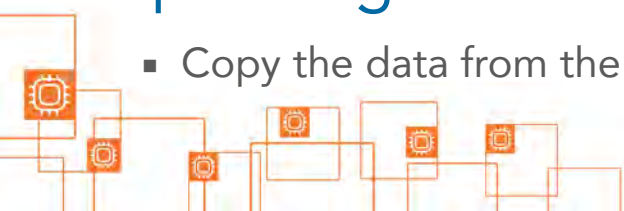
- Do not copy from frontend servers
- Copy (move) data to backup servers
- It's faster, more reliable
- SFTP clients: WinSCP, FileZilla, etc.

<https://docs.metacentrum.cz/en/>

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/



- `localUSER@localPC$ scp data.gz username@skirit.metacentrum.cz:~`
 - Copy the data from the local PC to the users' home on the frontend skirit (storage brno2) from the local PC. Small data sets
- `localUSER@localPC$ scp data.gz username@storage-brno2.metacentrum.cz:~`
 - Copy the data to the users' home on the brno2 storage server from the local PC. Suitable for large data sets
- `mv $SCRATCHDIR/results.txt /storage/brno2/home/username/`
 - Move the data from the scratch directory to the users' home on the brno2 storage (via the mounted path). Small data sets
- `scp -r $SCRATCHDIR/results storage-brno2.metacentrum.cz:~`
 - Copy folder recursively from the scratch directory to the users' home on the brno2 storage server. Large data sets
- `scp -r storage-brno2.metacentrum.cz:~/input_data $SCRATCHDIR`
 - Copy the data (folder, recursively) from the users' home on the brno2 storage server to the scratch directory. Large data sets
- `scp storage-brno2.metacentrum.cz:~/text.txt storage-plzen1.metacentrum.cz:~`
 - Copy the data from the users' home on the brno2 storage server to home on plzen1 storage server. Large data sets



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

skirit.metacentrum.cz - SFTP - brno2

SFTP (SSH File Transfer Protocol)

Nickname: skirit.metacentrum.cz - SFTP - brno2

Labels:

URL: sftp://skirit.metacentr...rage/brno2/home/vorel

Server: skirit.metacentrum.cz Port: 22

Username: vorel

Anonymous Login

Password: ●●●●●●●●

SSH Private Key: None

Client Certificate: None

More Options

Path: /storage/brno2/home/vorel

Web URL: http://skirit.metacentrum.cz/

Download Folder: Downloads

Transfer Files: Default

Timezone: UTC

Encoding: UTF-8

Connect Mode: Default

Notes:

storage-brno11 – SFTP
vorel@storage-brno11-elixi...

- 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

storage-brno11 – SFTP

SFTP (SSH File Transfer Protocol)

Nickname: storage-brno11 – SFTP

Labels:

URL: sftp://storage-brno11-elixir.metacentrum.cz

Server: storage-brno11-elixir.metacent Port: 22

Username: vorel

Anonymous Login

Password: ●●●●●●●●

SSH Private Key: None

Client Certificate: None

More Options

Path: Folder

Web URL: http://storage-brno11-elixir.metacentrum.cz

Download Folder: Downloads

Transfer Files: Default

Timezone: UTC

Encoding: UTF-8

Connect Mode: Default

Notes:

Refresh Synchronize Edit Delete Transfers Search

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/vore1/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-ohl7t4

# 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 avail *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 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)



- GPU
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- Spe
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- Spe
-
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-

Cluster	Nodes	GPUs per node	Compute capability	Mem [GB]	CuDNN
alfrid.meta.czu.cz	afrid[1-4].meta.czu.cz	2x L40	8.9	46	YES
alfridll.meta.czu.cz	afrid[6-9].meta.czu.cz	4x L40s	8.9	48	YES
bee.cerit-sc.cz	bee[1-10].cerit-sc.cz	2x H100 NVL	9.0	96	YES
copy.cerit-sc.cz	copy.cerit-sc.cz	8x H100	9.0	82	YES
cha.natur.cuni.cz	cha.natur.cuni.cz	8x GeForce RTX 2080 Ti	7.5	12	YES
elbi1.hw.elixir-czech.cz	elbi1[1].hw.elixir-czech.cz	2x NVIDIA A100	8.0	40	YES
fau.natur.cuni.cz	fau[1-3].natur.cuni.cz	8x Quadro RTX 5000	7.5	16	YES
fer.natur.cuni.cz	fer[1-3].natur.cuni.cz	8x RTX A4000	8.6	16	YES
fobos.metacentrum.cz	fobos[1-20].metacentrum.cz	4x L40s	8.9	46	YES
galdor.metacentrum.cz	galdor[1-20].metacentrum.cz	4x A40	8.6	46	YES
glados.cerit-sc.cz	glados[1-2].cerit-sc.cz	2x GeForce RTX 2080	7.5	8	YES
grimbold.metacentrum.cz	grimbold.metacentrum.cz	2x Tesla P100	6.0	12	YES
konos.fav.zcu.cz	konos[1-8].fav.zcu.cz	4x GeForce GTX 1080 Ti	6.1	12	YES
luna2022.fzu.cz	luna[201-206].fzu.cz	1x A40	8.6	46	YES
zia.cerit-sc.cz	zia[1-5].cerit-sc.cz	4x A100	8.0	40	YES

Cluster	Nodes	GPUs per node	Compute capability	Mem [GB]	CuDNN
alfrid.meta.czu.cz	afrid[1-4].meta.czu.cz	2x L40	8.9	46	YES
alfridll.meta.czu.cz	afrid[6-9].meta.czu.cz	4x L40s	8.9	48	YES

```
#!/bin/bash
#PBS -N run1_dorado_mod
#PBS -l select=1:ncpus=4 ngpu=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:~/Metylance_hemonch/RUN_1_IRE/02_run1_IRE_reads.pod5 $SCRATCHDIR
scp -r storage-brno12-cerit.metacentrum.cz:~/Metylance_hemonch/SOFT/dorado_0.9.1/models/dna_r9.4.1_e8_sup@v3.3* $SCRATCHDIR
cp /storage/brno12-cerit/home/vorel/Metylance_hemonch/Haemonch_refer/haemonchus_contortus.PRJEB506.WBPS19.genomic.fa $SCRATCHDIR

export PATH=/storage/brno12-cerit/home/vorel/Metylance_hemonch/SOFT/dorado_0.9.1/bin/:$PATH
export LD_LIBRARY_PATH=/storage/brno12-cerit/home/vorel/Metylance_hemonch/SOFT/dorado_0.9.1/lib/:$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
```

konos.fav.zcu.cz	konos[1-8].fav.zcu.cz	4x GeForce GTX 1080 Ti	6.1	12	YES
luna2022.fzu.cz	luna[201-206].fzu.cz	1x A40	8.6	46	YES
zia.cerit-sc.cz	zia[1-5].cerit-sc.cz	4x A100	8.0	40	YES

- Apptainer (formerly Singularity) is an alternative to Docker, primarily used for HPC with non-root access
 - Apptainer can work with Docker images and offers GPU and MPI support
- MetaCentrum offers some pre-built (ready-to-use) Singularity images. For example, NGC (NVIDIA GPU Cloud, with Kaldi, PyTorch and TensorFlow), Trinity (an RNA-seq assembler) and OpenFOAM (a numerical solver)
 - NGC images are highly optimised for GPU-accelerated calculations
- Users can also build their own SIFs
- Prevents conflicts

<https://docs.metacentrum.cz/en/docs/software/containers>



The most straightforward way to transfer highly optimised environments, complete with all dependencies and tuned libraries.

■ There are so many different ways

- Binary distributions (precompiled form, download them and use them)
- R, Python, Rust, Perl, Julia, Debian, etc. libraries
- Package managers like Mamba (recommended, fully automated, easy to use)
- Docker (Kubernetes, cloud) and Singularity/Apptainer images (grid, conversion Docker to Singularity)
- Snapshots of entire VMs (cloud, OnDemand)
- Local compilation (GCC, Intel compilers, BLAS/LAPACK math libraries, CUDA support and so on...)



As users do not have root access, installations must be placed in their home directories or in the scratch directory.



<https://www.cesnet.cz/>

<https://www.metacentrum.cz/>

<https://www.e-infra.cz/>

<https://docs.metacentrum.cz/>

- Is suitable for everyone and easy to use in the most cases
- Has user support <https://docs.metacentrum.cz/en/docs/support>
- Has documentation <https://docs.metacentrum.cz/en/docs/welcome>
- Has a blog with news <https://blog.e-infra.cz/>
- Is a part of e-INFRA CZ <https://www.e-infra.cz/>
- Is not just about the command line



- Take a look at our past trainings <https://github.com/CESNET/metacentrum-hands-on>
- Requests to add acknowledgements in publications

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

