

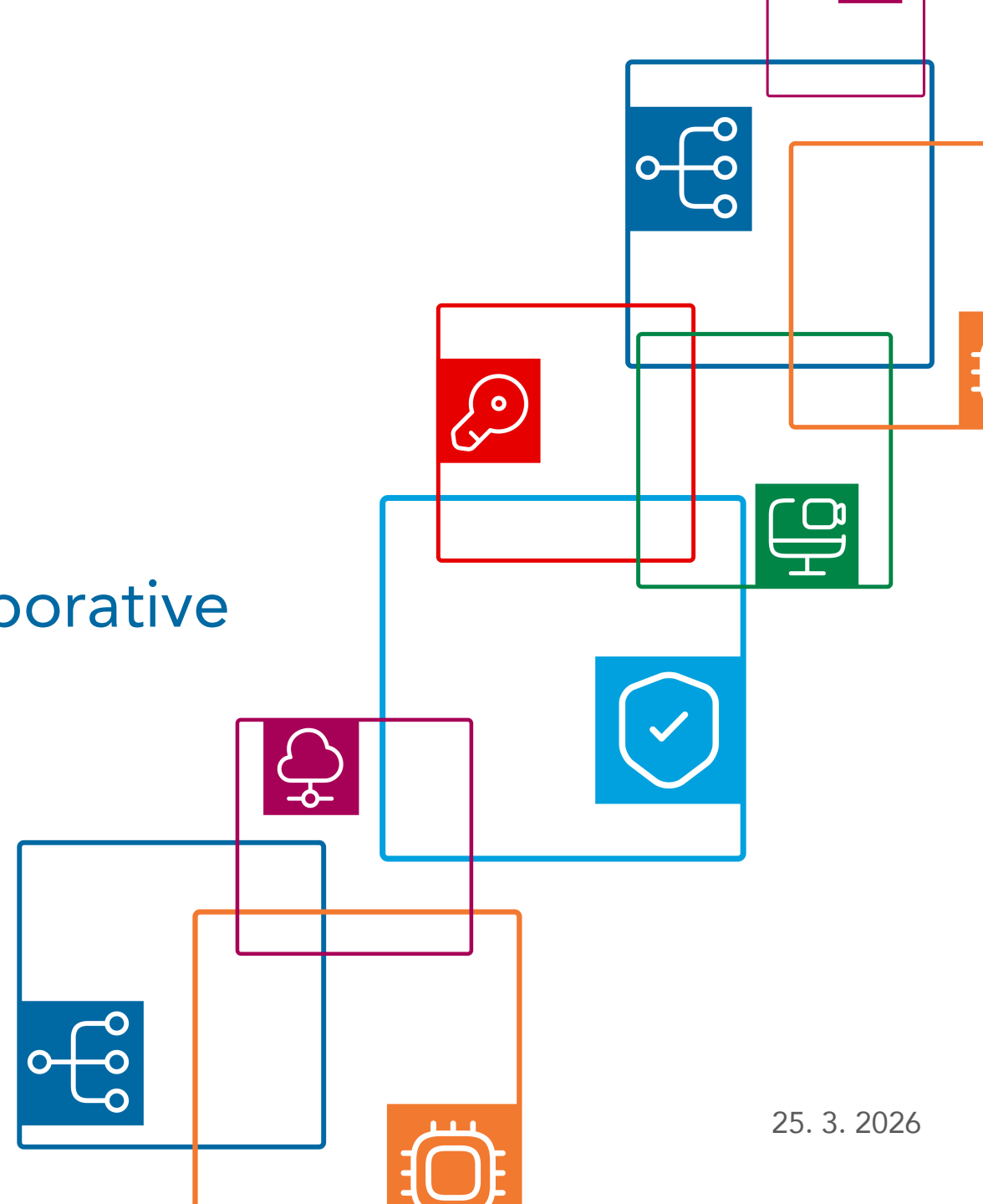
MetaCentrum NGI

For scientific computations, collaborative research and its support services

Jiří Vorel

Institute of Microbiology of the CAS, Prague

vorel@cesnet.cz meta@cesnet.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)

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

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

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

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



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



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

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

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

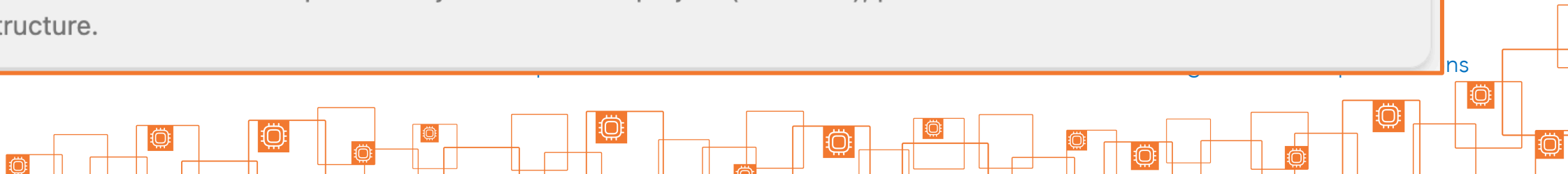


Acknowledgement formula for the MetaCentrum infrastructure

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

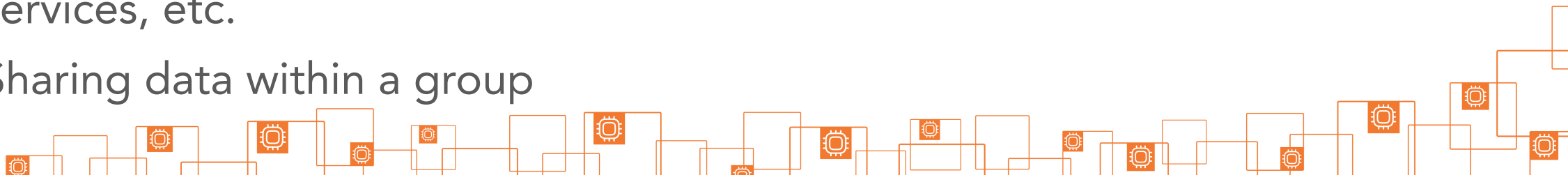
- Access without the grant competitions
- The possibility to apply for membership at any time
- Access to all resources without submitted projects (with one exception)
- Immediate access to hardware resources and licences (once an application has been approved)
- Grid (shared) usage principle (privileged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

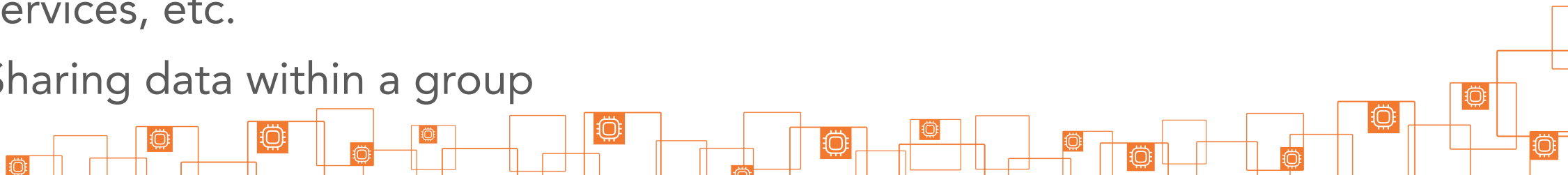
<https://www.metacentrum.cz/>

<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/>

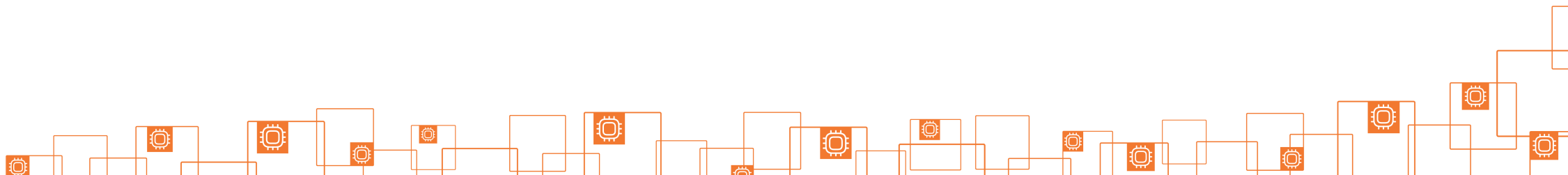
<https://www.e-infra.cz/>

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

<https://du.cesnet.cz>

cesnet
datacare
■■■■■

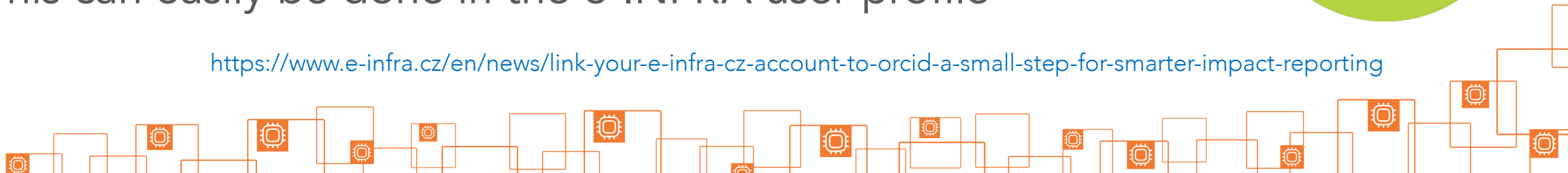
<https://www.cerit-sc.cz/>

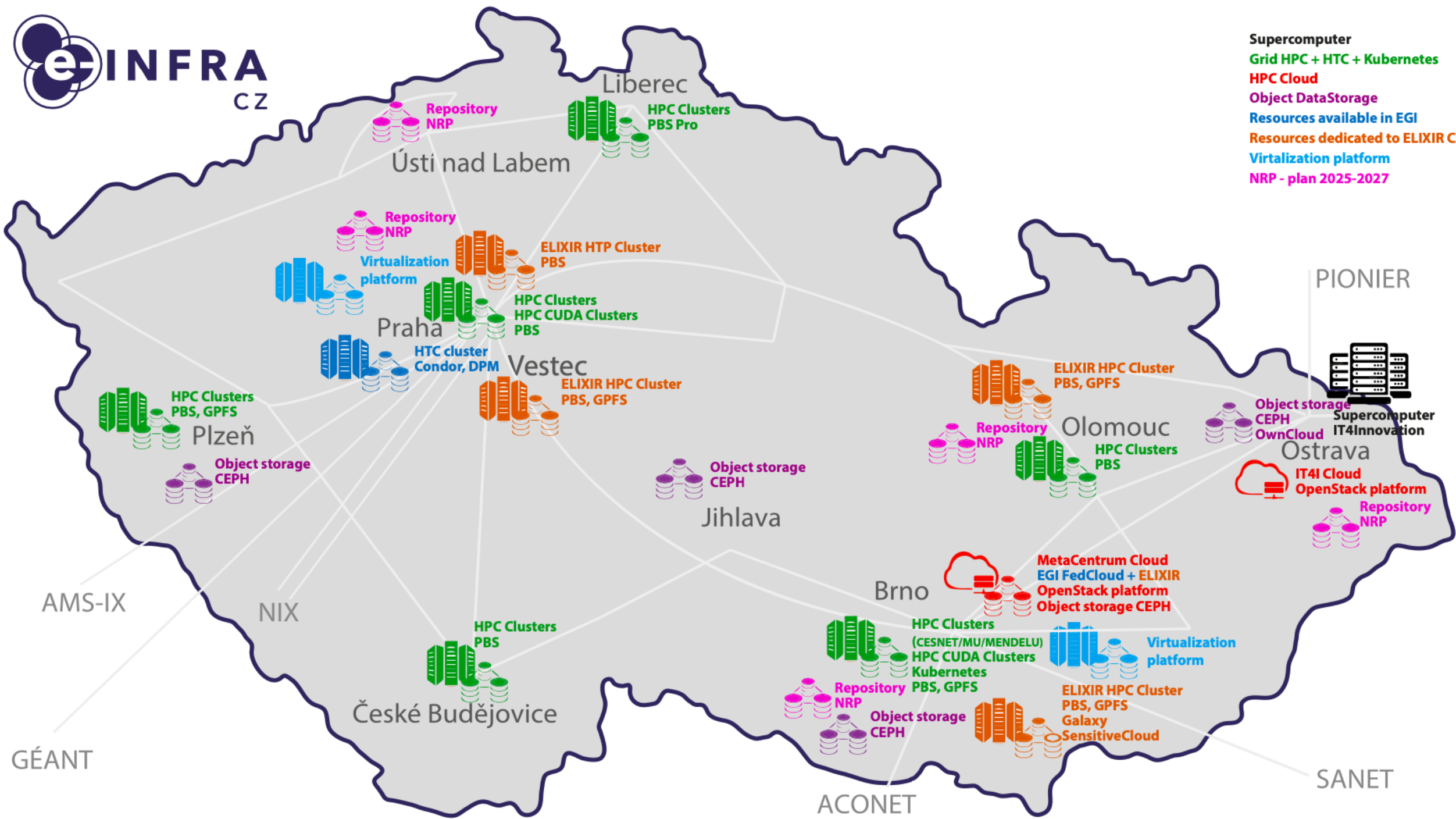


- **Link your e-INFRA CZ account to ORCID**
 - The future of national computing and storage services depends on demonstrating that researchers are truly using them
 - Currently, much of the valuable research output of e-INFRA CZ/MetaCentrum users is 'invisible' to our funders
 - We are developing a new 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>

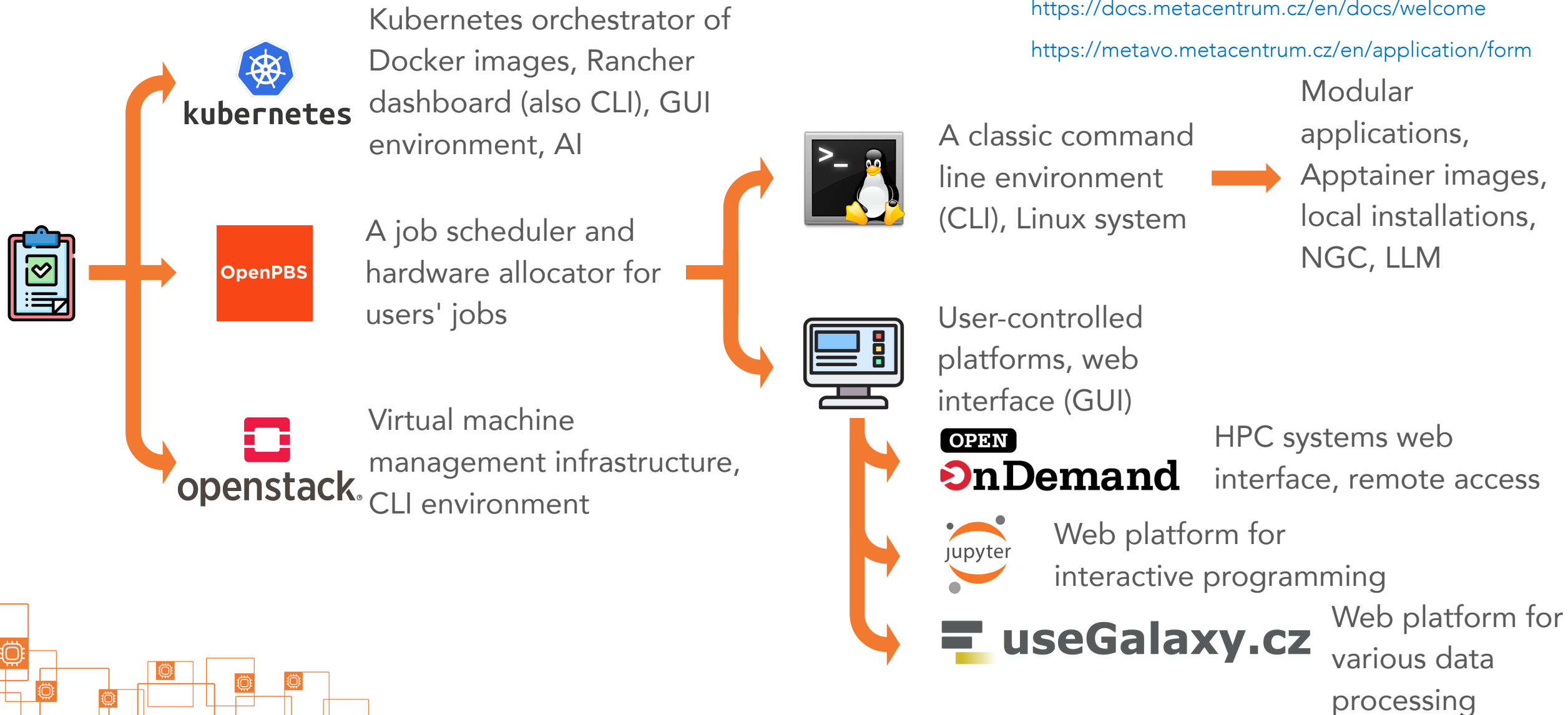





A close-up, high-angle shot of the One Ring from J.R.R. Tolkien's Middle-earth. The ring is positioned diagonally, showing its inner and outer surfaces. It is inscribed with the Elvish word 'Eärendil' in a golden, flowing script. The ring is set against a background of a golden, textured fabric, possibly silk or a similar material, which is draped and folded, creating deep shadows and bright highlights. 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 mystery and power.

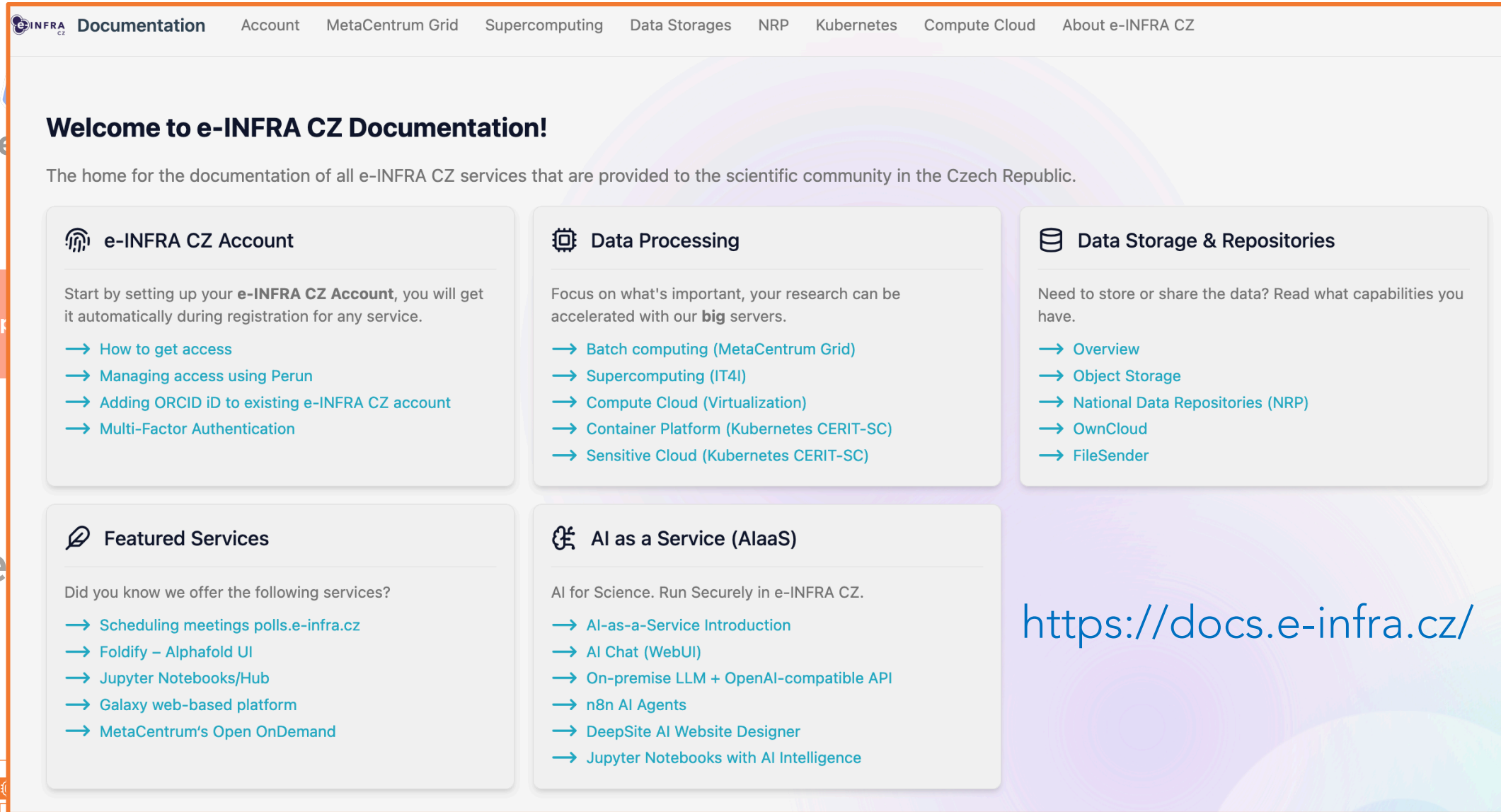
ONE APPLICATION TO RULE THEM ALL

One application to rule them all



 A complete overview of e-INFRA CZ services

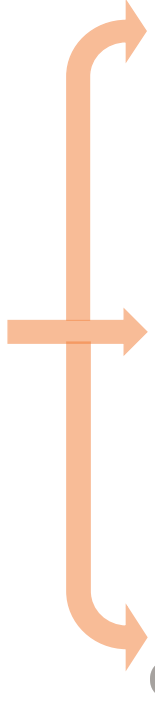
One application to rule them all



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 heading is "Welcome to e-INFRA CZ Documentation!". Below this is a sub-heading: "The home for the documentation of all e-INFRA CZ services that are provided to the scientific community in the Czech Republic." The content is organized into five main sections, each with a list of links:

- e-INFRA CZ Account**
 - [How to get access](#)
 - [Managing access using Perun](#)
 - [Adding ORCID iD to existing e-INFRA CZ account](#)
 - [Multi-Factor Authentication](#)
- Data Processing**
 - [Batch computing \(MetaCentrum Grid\)](#)
 - [Supercomputing \(IT4I\)](#)
 - [Compute Cloud \(Virtualization\)](#)
 - [Container Platform \(Kubernetes CERIT-SC\)](#)
 - [Sensitive Cloud \(Kubernetes CERIT-SC\)](#)
- Data Storage & Repositories**
 - [Overview](#)
 - [Object Storage](#)
 - [National Data Repositories \(NRP\)](#)
 - [OwnCloud](#)
 - [FileSender](#)
- Featured 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-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](#)

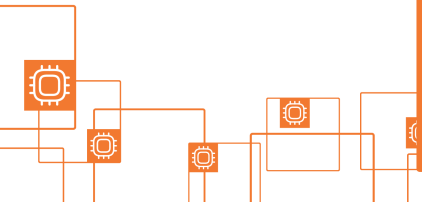
On the right side of the screenshot, the URL <https://docs.e-infra.cz/> is displayed.



kube

op

ope





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

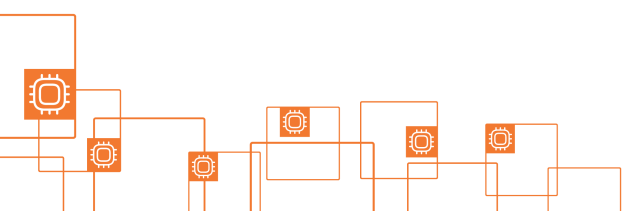


For registered individuals

For all users



Free licence

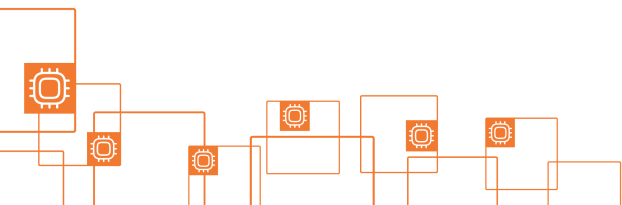
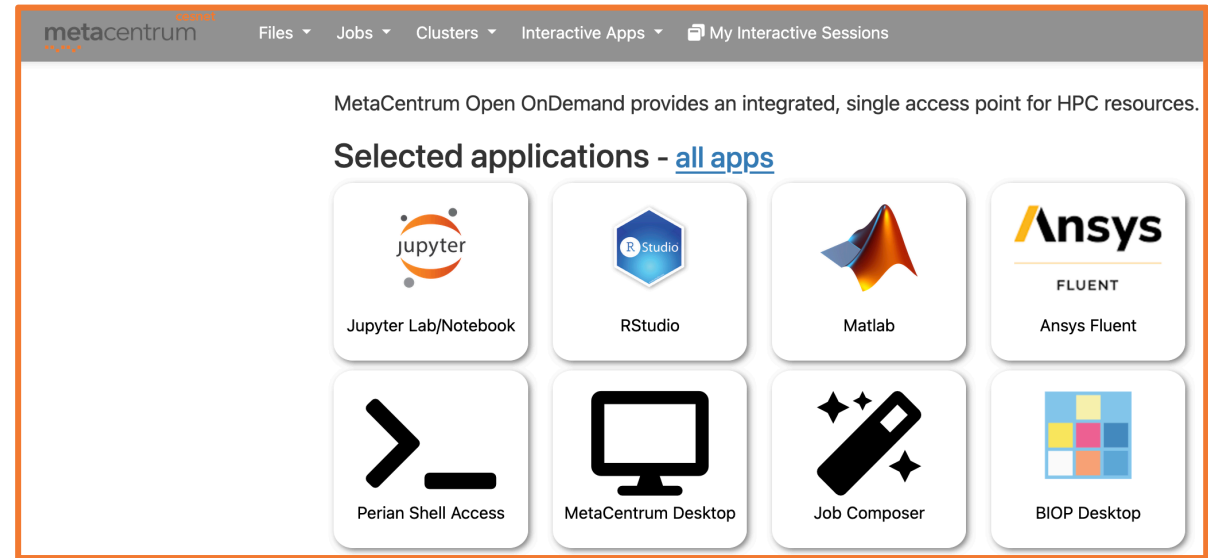


■ Open OnDemand



<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

A screenshot of the Open OnDemand login page. The page has a grey header with the "metacentrum" logo and navigation links for "Files", "Jobs", "Clusters", "Interactive Apps", and "My Interactive Sessions". The main content area is titled "Log in with" and contains four login options, each with a text label and a logo: "CESNET" with the "cesnet" logo, "Institute of Archeology of the Czech Academy of Sciences, Brno" with its crest, "Institute of Microbiology AS CR" with the "MBU" logo, and "Masaryk University" with the "MUNI" logo. Below these is a button labeled "Another account". At the bottom, there is a row of flags representing different countries and a "CESNET" user profile icon with a "Personal data processing" notice.

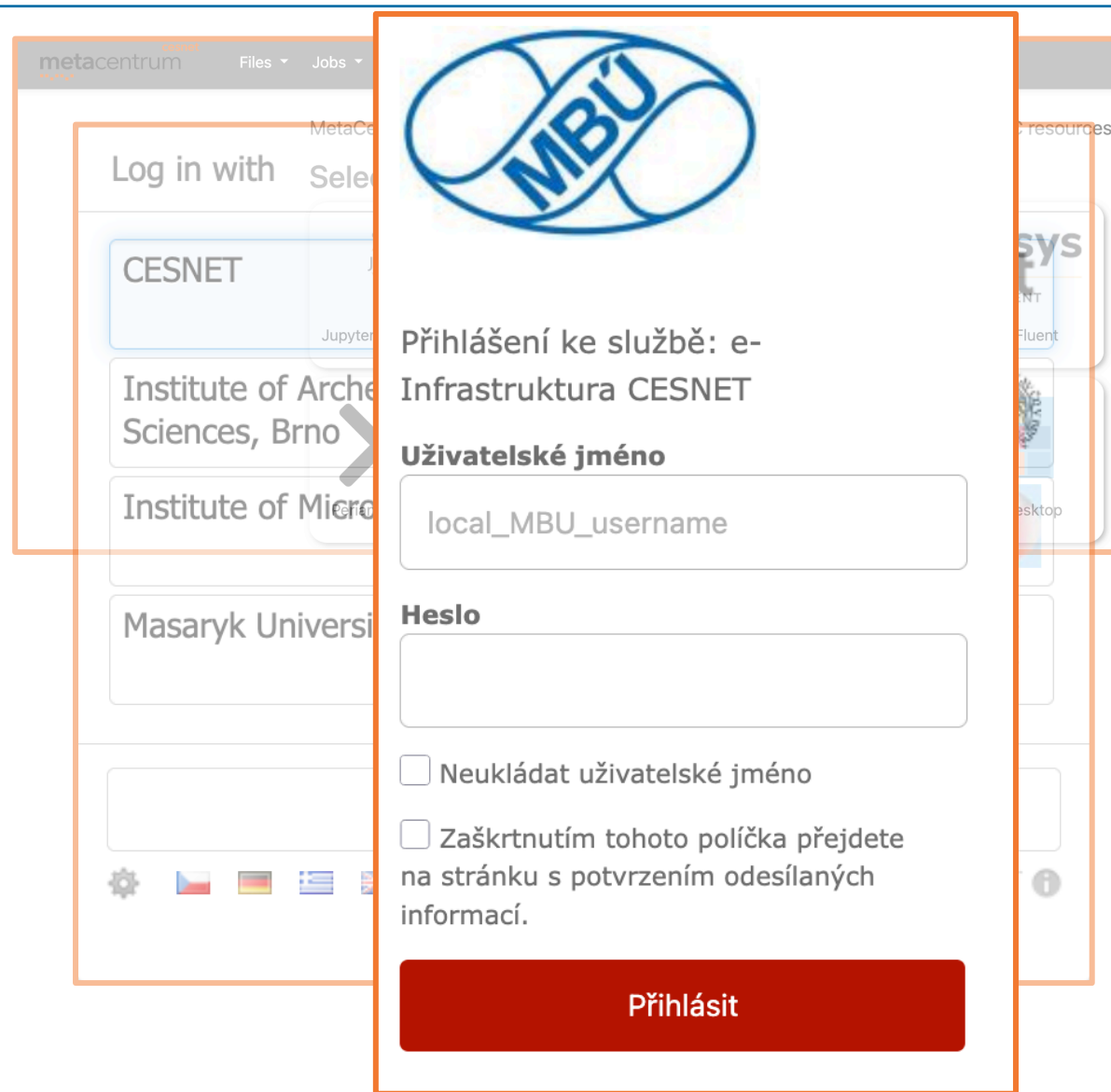
Open OnDemand

■ Open OnDemand



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

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

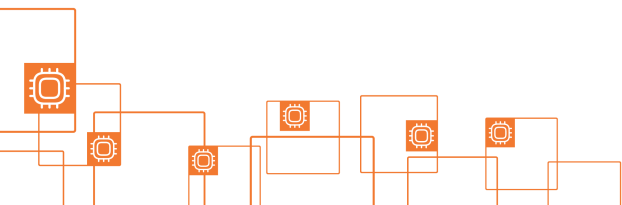
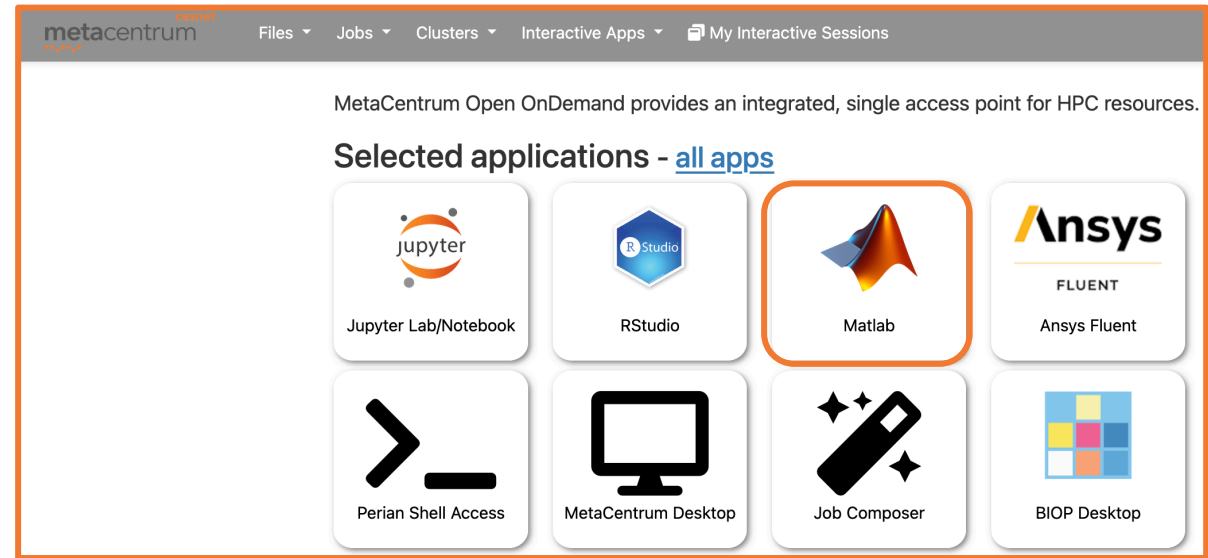
A screenshot of the Open OnDemand login page. The page is titled "metacentrum" and has a navigation bar with "Files" and "Jobs" menus. The main content area is titled "Log in with" and lists several institutions: "CESNET", "Institute of Arche Sciences, Brno", "Institute of Micro", and "Masaryk Universi". A red box highlights the login form for "MBÚ". The form includes the MBÚ logo, the text "Přihlášení ke službě: e-Infrastruktura CESNET", a label "Uživatelské jméno" with a text input field containing "local_MBU_username", a label "Heslo" with a password input field, and two checkboxes: "Neukládat uživatelské jméno" and "Zaškrtnutím tohoto políčka přejdete na stránku s potvrzením odesílaných informací.". A red "Přihlásit" button is at the bottom of the form.

■ 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

A screenshot of the Open OnDemand web interface. The browser address bar shows "metacentrum". The page title is "Home / My Interactive Sessions / Matlab". On the left, a sidebar lists "Interactive Apps" under categories: Cloud (Kubernetes on OpenStack (KOST) (beta), OpenStack VM (beta)), Desktops (Ansys/Enight, Ansys/Fluent, Ansys/Workbench, BIOP Desktop, CLCgenomicsWB), Matlab (selected), MetaCentrum Desktop, VMD Desktop, Servers (Jupyter Notebook/Lab, Matlab webapp (beta), RStudio Server). The main content area is titled "Matlab" 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 the description are several configuration fields, each with a dropdown menu: "Number of hours" (5), "Number of CPUs on single node" (4), "Memory (GB)" (4), "GPUs" (0), and "Scratch local (GB)" (10). At the bottom of these fields is a large blue "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

■ Open OnDemand



https

■ W
■ C
■ R

metacentrum Files Jobs Clusters Interactive Apps My Interactive Sessions

Home / My Interactive Sessions / Matlab
MetaCentrum Open OnDemand provides an integrated, single access point for HPC resources.

Session was successfully created. [X]

Home / My Interactive Sessions

Interactive Apps

Cloud

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

Desktops

- Ansys/Ensignt

Matlab (17158555.pbs-m1.metacentrum.cz) 1 node | 4 cores | Starting

Created at: 2026-02-04 11:36:14 CET [Delete]

Session ID: 803f66c0-0228-4b47-93ed-a5fbae0841dc

Your session is currently starting... Please be patient as this process can take a few minutes.

VMD Desktop

Servers

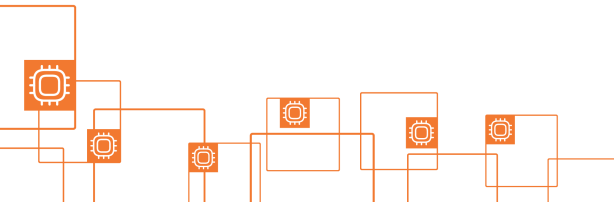
- Jupyter Notebook/Lab
- Matlab webapp (beta)
- RStudio Server

Scratch local (GB)

10

Launch

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



Open OnDemand

Open OnDemand



metacentrum Files Jobs Clusters Interactive Apps My Interactive Sessions

Home / My Interactive Sessions / Matlab
MetaCentrum Open OnDemand provides an integrated, single access point for HPC resources.

Interactive Apps **Matlab applications - all apps**

Session was successfully created. [X]

Home / My Interactive Sessions

Interactive Apps

- Cloud
 - Kubernetes on OpenStack (KOST) (beta)
 - OpenStack VM (beta)
- Desktops
 - Ansys/Ensignt
 - Ansys/Fluent
 - Ansys/Workbench
 - BIOP Desktop
 - CLCgenomicsWB

Matlab (17158555.pbs-m1.metacentrum.cz) 1 node | 4 cores | Running

Host: galdor20.metacentrum.cz [Delete]

Created at: 2026-02-04 11:36:14 CET

Time Remaining: 4 hours and 58 minutes

Session ID: 803f66c0-0228-4b47-93ed-a5fbae0841dc

Compression 0 (low) to 9 (high)

Image Quality 0 (low) to 9 (high)

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

cores | Starting [Delete]

essed under the [data root](#)



New Script New Live Script New Open Find Files Import Data Save Workspace Clean Data Clear Workspace

FILE VARIABLE

Favorites Run and Time Clear Commands

CODE

Simulink

SIMULINK

Layout

Set Path

Add-Ons

Settings

Help

Request Support

Feedback

Learn MATLAB

RESOURCES

/ > auto > brno11-elixir > home > vorel >

Files

Name
icewm
NikoK_Klimno_genome
NikoK_Ktang_genome
NikoR_metabarcoding

Command Window

Workspace

Name	Value	Size	Class
------	-------	------	-------



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

FILE

Design App Get More Apps Install App

auto > brno11-e

Files

Name

- .icewm
- NikoK_Klimno_genome
- NikoK_Ktang_genome
- NikoR_metabarcoding

Workspace

Name	Value	Size

HOME PLOTS APPS

Design App Get More Apps Install App Curve

FILE

/ > auto > brn011-elixir > h

Files

Name

- .icwm
- 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
 Auto
 Manual
 FIT

Residuals Plot
 Contour Plot
 Fit Plot
 VISUALIZATION

Colormap
 Export
 PREFERENCES EXPORT

untitled fit 1

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							

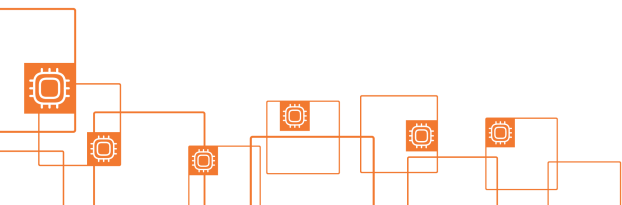
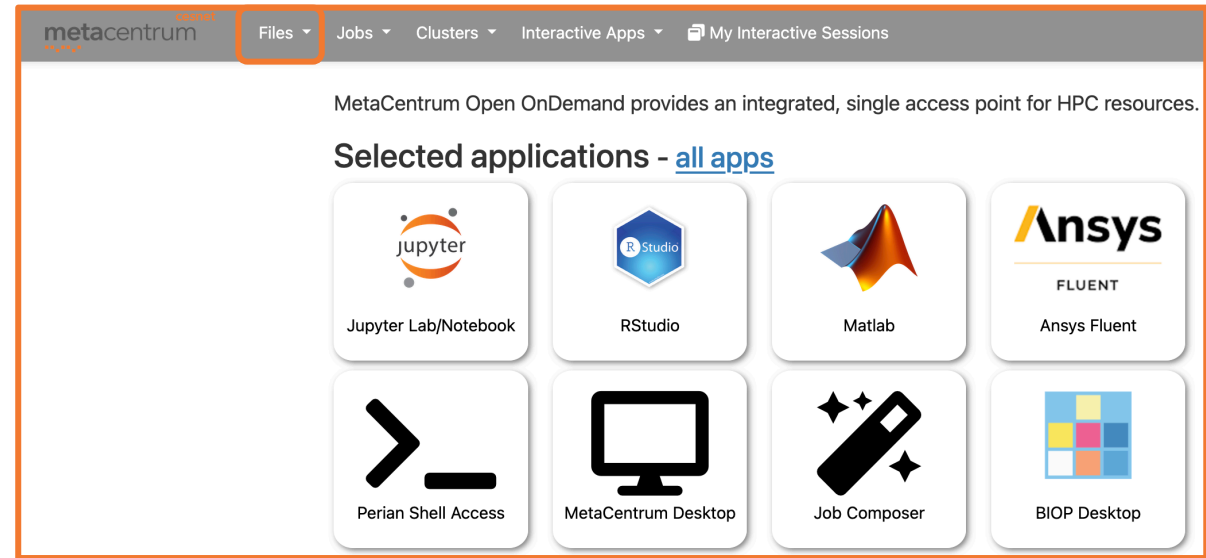
Select data to fit curves or surfaces.

■ Open OnDemand



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

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



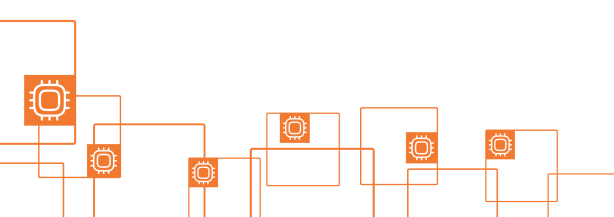
Open OnDemand

■ Open OnDemand

<https://ondemand.metacentrum.cz>

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

The screenshot displays the Open OnDemand web interface. At the top, there is a navigation bar with the 'metacentrum' logo and several menu items: 'Files', 'Jobs', 'Clusters', 'Interactive Apps', and 'My Interactive Sessions'. The 'Files' menu is currently open, showing a list of home directories for various clusters. Two items are highlighted with orange boxes: 'cesnet_s3' and a group containing 'praha6-fzu', 'projects', 'projects-du-praha', and 'projects2'. Below the file browser, there is a section titled 'all apps' which contains several application tiles. The visible tiles are: 'Matlab' (with a 3D surface plot icon), 'Ansys FLUENT Ansys Fluent' (with the Ansys logo), 'Job Composer' (with a microscope icon), and 'BIOP Desktop' (with a grid icon). The text 'Provides an integrated, single access point for HPC resources.' is partially visible in the background.



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

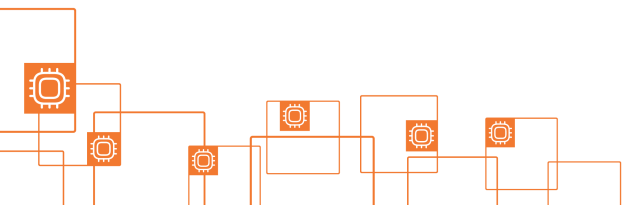
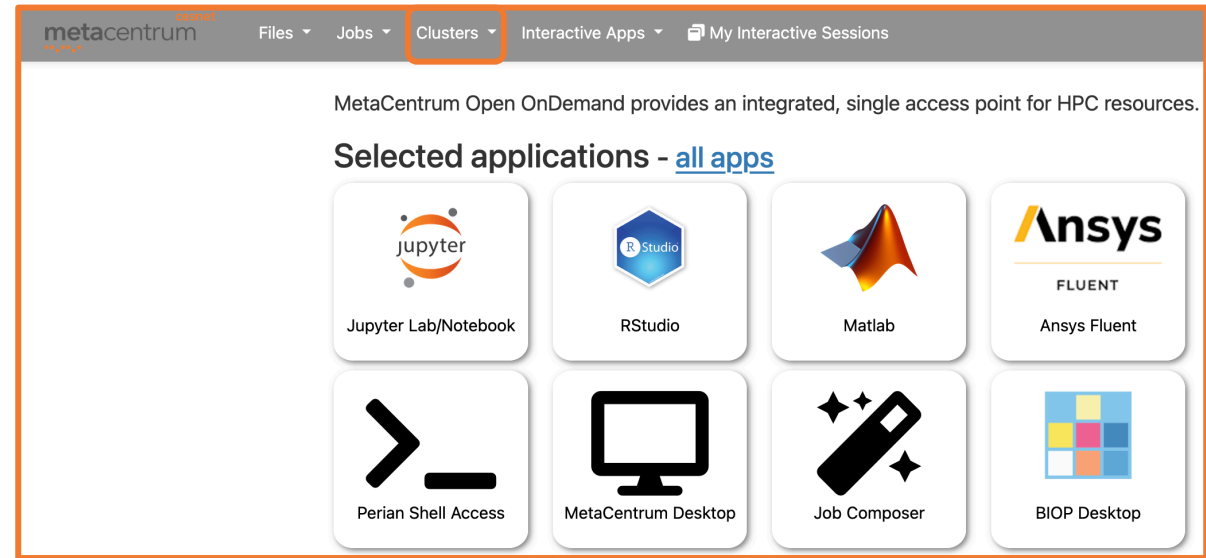
<input type="checkbox"/>	Type ▲	Name		Size	Modified at
<input type="checkbox"/>	Folder	03_E_nip_genom	⋮	-	28. 9. 2025 11:11:36
<input type="checkbox"/>	Folder	03_E_nip_trans	⋮	-	28. 9. 2025 11:11:36
<input type="checkbox"/>	Folder	04_Viremie_AV_Kapr_Karas	⋮	-	28. 9. 2025 11:11:36
<input type="checkbox"/>	Folder	04_Viremie_AV_Plotice_Cejn	⋮	-	28. 9. 2025 11:11:36
<input type="checkbox"/>	Folder	05_Nikol_Kmentova	⋮	-	28. 9. 2025 11:11:36
<input type="checkbox"/>	Folder	06_Kasa_mansoni_hepatica_vejce	⋮	-	28. 9. 2025 11:11:36
<input type="checkbox"/>	Folder	07_Haem_cont_metylaseDNA	⋮	-	28. 9. 2025 11:11:36
<input type="checkbox"/>	Folder	08_JI_hetero_trans	⋮	-	28. 9. 2025 11:11:36
<input type="checkbox"/>	File	01_Echo.tar.gz	⋮	662.80 GB	9. 10. 2022 15:21:53
<input type="checkbox"/>	File	02_TomasPakosta.tar.gz	⋮	3.56 GB	14. 11. 2020 18:46:42
<input type="checkbox"/>	File	02_TomasPakosta_posledni_vymysl.zip	⋮	13.46 GB	19. 3. 2025 14:40:50
<input type="checkbox"/>	File	Kapentagyrus_July2022.tar.gz	⋮	473.75 GB	11. 12. 2023 19:47:56

■ Open OnDemand



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

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

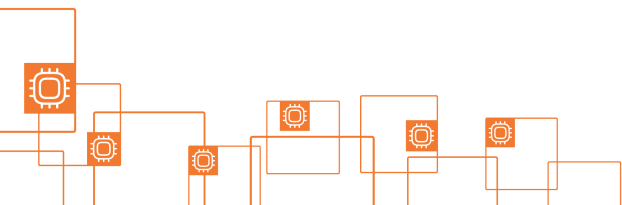


■ Open OnDemand

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

- Web application on OpenPBS scheduler
- Running (not only)
- Browsing repositories
- Command line (tab)

The screenshot displays the Open OnDemand web interface. At the top, there is a navigation bar with the 'metacentrum' logo and several menu items: 'Files', 'Jobs', 'Clusters', 'Interactive Apps', and 'My Interactive Sessions'. The 'Clusters' menu is currently open, showing a list of options: '>_ Perian Shell Access', '>_ Skirit Shell Access', 'System Status', '>_ Tarkil Shell Access', and '>_ Zenith Shell Access'. The 'Zenith Shell Access' option is highlighted with an orange border. Below the navigation bar, the main content area features a grid of application tiles. The tiles include: 'Jupyter Lab/Notebook' (with a Jupyter logo), 'RStudio' (with an R logo), 'Matlab' (with a Matlab logo), 'Ansys Fluent' (with the Ansys logo), 'Perian Shell Access' (with a terminal icon), 'MetaCentrum Desktop' (with a monitor icon), 'Job Composer' (with a pencil icon), and 'BIOP Desktop' (with a grid icon). The interface is clean and modern, with a white background and orange accents.



4 updates could not be installed automatically. For more details, see /var/log/unattended-upgrades/unattended-upgrades.log
Last login: Sun Sep 28 11:25:00 2025 from ondemand.grid.cesnet.cz

cesnet



Your Home Directories

Avail	DATA	FILES	Backup	Storage
space	quota	used	quota	used
558T	none	200G	none	36
110T	4.29T	33.9G	2.5M	31.0k
22T	3.32T	24k	1M	9
37T	10.4G	12k	none	8
403T	4.29T	1.71T	3M	133k
64T	7.34G	44k	none	18
235T	5.36T	940G	1.01M	113k
69T	7.34G	32k	none	12
12T	2.14T	80k	2M	33

CPUs

Free	Used	Total	Centre
7923	27738	35661	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@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
13264531.pbs-m1.met*	vorel	interac*	STDIN	40155	1	1	400mb	18:00	R	00:11
13264536.pbs-m1.met*	vorel	interac*	STDIN	49799	1	1	400mb	18:00	R	00:00

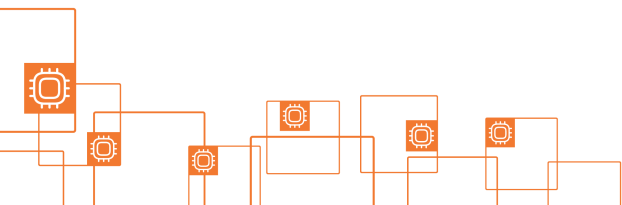
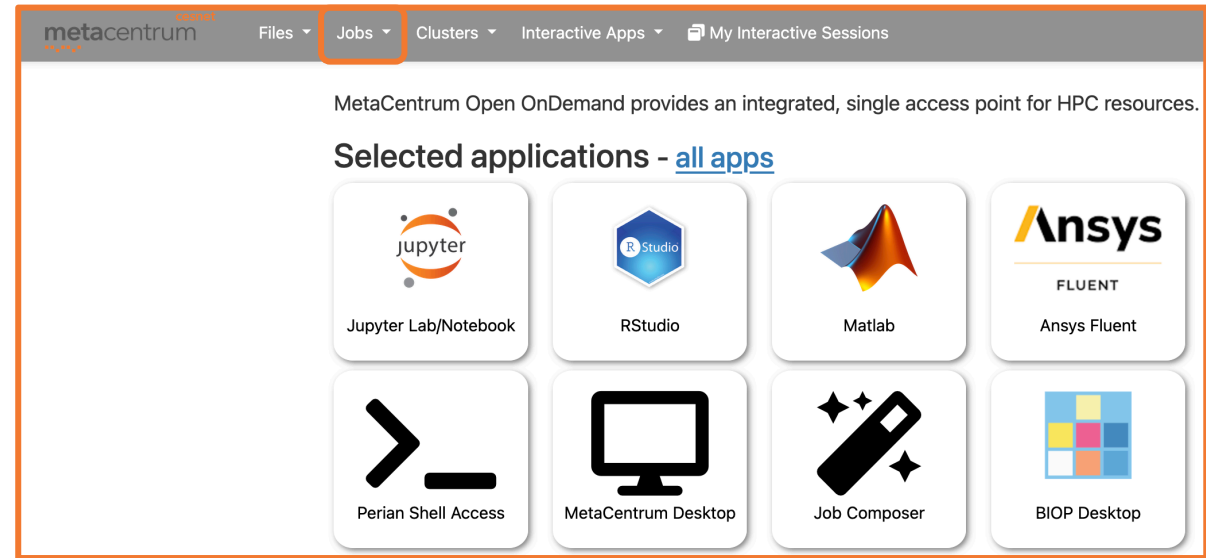
- Default
- Bright**
 - CLRS
 - Github
 - Solarized Light
 - Tomorrow**
- Dark**
 - Cobalt2
 - idleToes
 - Monokai Remastered
 - Pastel Dark
 - Red Alert
 - Tomorrow Night Blue
 - Tomorrow Night Bright
 - Tomorrow Night Eighties
 - Tomorrow Night

■ Open OnDemand



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

- Web application on top of OpenPBS scheduler
- Running (not only) GUI applications
- Browsing repositories (tab 'Files')
- Command line (tab 'Clusters')
- Creating and submitting a batch job (tabs 'Jobs' and 'Job Composer')



■ Open OnDemand



https://or

metacentrum
cesnet

Files ▾

Jobs ▾

Clusters ▾

Interactive Apps ▾

My Interactive Sessions

■ Web

Open

■ Run

■ Browsing repositories (tab 'Files')

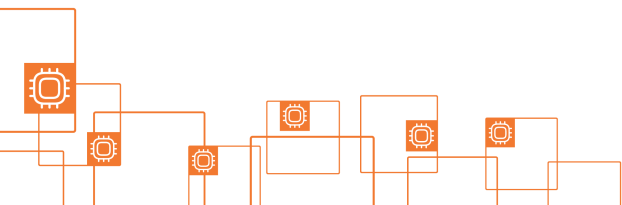
■ Command line (tab 'Clusters')

■ Creating and submitting a batch job (tabs 'Jobs' and 'Job Composer')

🕒 Active Jobs

🔧 Job Composer

Active interactive sessions [view all \(1\)](#)



Jobs

[+ New Job](#) ☆ Create Template

[Edit Files](#) [Job Options](#) [Open Terminal](#) [Submit](#) [Stop](#) [Delete](#)

Show entries Search:

Created	Name	ID	Cluster	Status
October 1, 2025 2:07pm	(default) Metacentrum simple sequential job		Perian	Not Submitted

Showing 1 to 1 of 1 entries Previous 1 Next

Job Details

Job Name:
(default) Metacentrum simple sequential job

Submit to:

Account:
Not specified

Script location:

Script name:

Folder Contents:
[main_job.sh](#)

Submit Script

main_job.sh

Script contents:

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

cd $PBS_0_WORKDIR
echo "Hello World" > output_file

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

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

/storage/brno2/home/vorel/ondemand/data/sys/myjobs/projects/default/1/main_job.sh

Save

Key Bindings

Default

Font Size

12px

Mode

Text

Theme

Solarized Light

Wrap

```
1 #PBS -N hello_world_test
2 #PBS -l ncpus=1
3 #PBS -l walltime=1:00:00
4 #PBS -l mem=1gb
5 #PBS -j oe
6 ##PBS -l scratch_local=1g
7
8 cd $PBS_O_WORKDIR
9 echo "Hello World" > output_file
10
11 echo "Created output_file with 'Hello World'"
```

Job was successfully submitted.

Jobs

+ New Job ▾

☆ Create Template

📄 Edit Files

⚙️ Job Options

➤ Open Terminal

▶ Submit

■ Stop

🗑️ Delete

Show 25 ▾ entries

Search:

Created	Name	ID	Cluster	Status
October 1, 2025 2:07pm	(default) Metacentrum simple sequential job	13351946.pbs-m1.metacentrum.cz	Perian	Completed

Showing 1 to 1 of 1 entries

Previous 1 Next

Job was successfully submitted. ✕

Jobs

+ New Job ▾

☆ Create Template

[Edit Files](#) [Job Options](#) [Open Terminal](#) [Submit](#) [Stop](#) [Delete](#)

Show entries Search:

Created	Name	ID	Cluster	Status
October 1, 2025 2:07pm	(default) Metacentrum simple sequential job	13351946.pbs-m1.metacentrum.cz	Perian	Completed

Showing 1 to 1 of 1 entries Previous **1** Next

Job Details

13351946.pbs-m1.metacentrum.cz

Job Name:

(default) Metacentrum simple sequential job

Submit to:

Perian

Account:

Not specified

Script location:

/storage/brno2/home/vorel/ondemand/data/sys/myjobs/projects/default/1

Script name:

main_job.sh

Folder Contents:

- hello_world_test.o13351946
- main_job.sh**
- output_file

/storage/brno2/home/vorel/ondemand/data/sys/myjobs/projects/default/1/output_file

 Save

Key Bindings

Default

Font Size

12px

Mode

Text

Theme

Solarized Light

Wrap

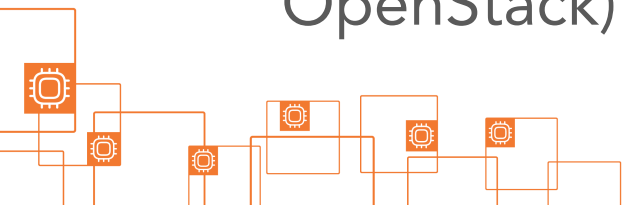
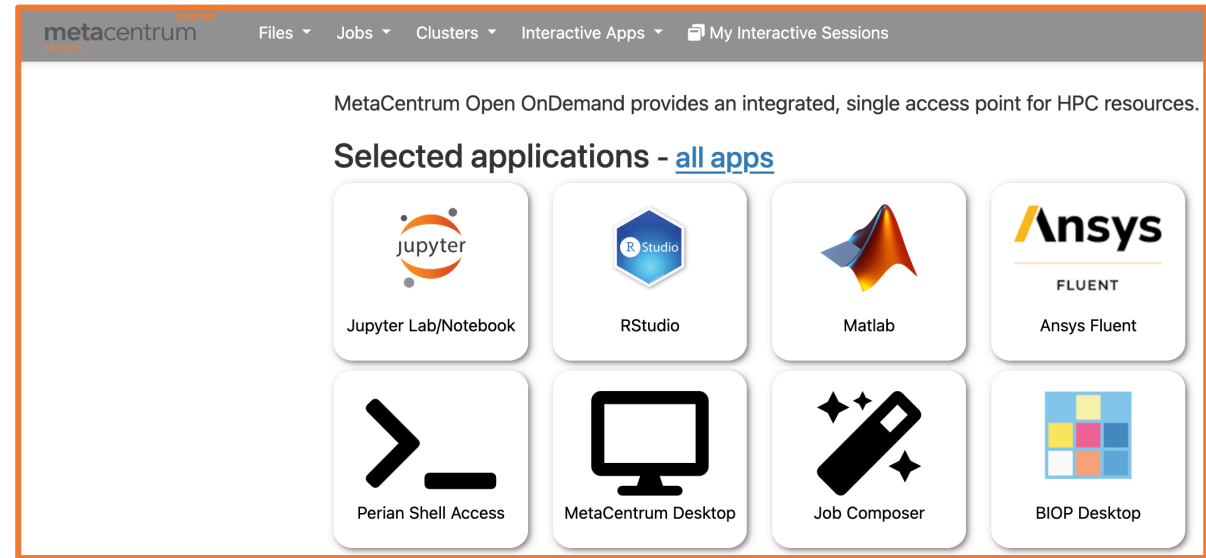
```
1 Hello World  
2
```

■ Open OnDemand



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

- Web application on top of OpenPBS scheduler
- Running (not only) GUI applications
- Browsing repositories (tab 'Files')
- Command line (tab 'Clusters')
- Creating and submitting a batch job (tabs 'Jobs' and 'Job Composer')
- Running virtual machines (OpenStack) and Docker images (Kubernetes on OpenStack)



■ Open OnDemand

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

- Web application on top of OpenPBS scheduler
- Running (not only) GUI applications
- Browsing repositories (tab 'Files')
- Command line (tab 'Clusters')
- Creating and submitting a batch job
- Running virtual machines (OpenStack)



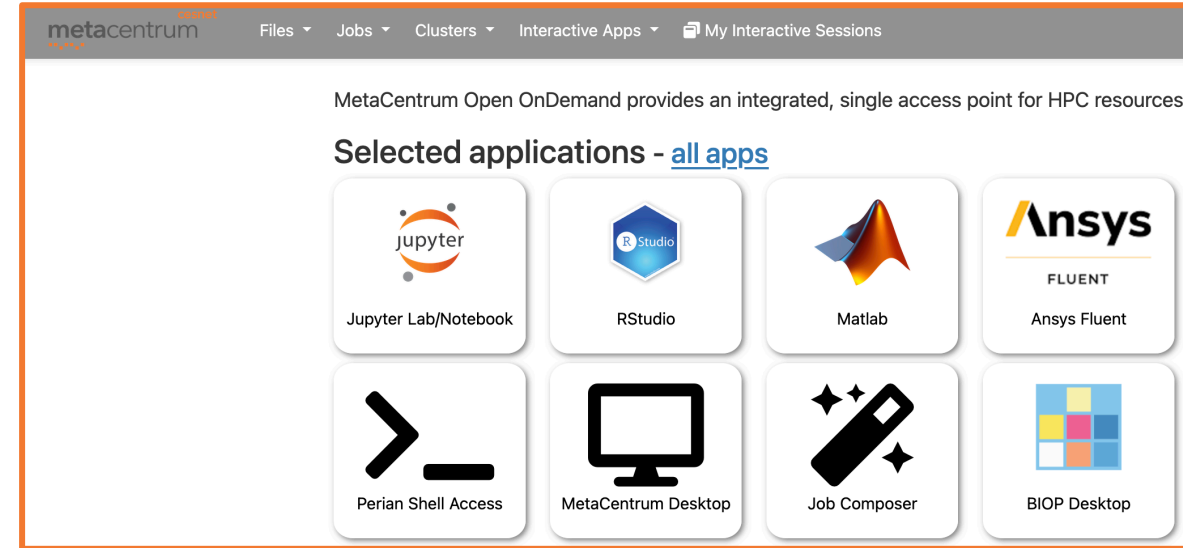
A screenshot of the Open OnDemand web interface. The browser address bar shows "metacentrum". The navigation menu includes "Files", "Jobs", "Clusters", "Interactive Apps", and "My Interactive Sessions". The "Interactive Apps" dropdown menu is open, showing categories: "Cloud" (Kubernetes on OpenStack (KOST) (beta), OpenStack VM (beta)), "Desktops" (Ansys/Ensignt, Ansys/Fluent, Ansys/Workbench, BIOP Desktop, CLCgenomicsWB, Matlab, MetaCentrum Desktop, QuPath, VMD Desktop), and "Servers" (Jupyter - Evo2 (beta), Jupyter Notebook/Lab, Matlab webapp (beta), RStudio Server). The main content area shows "Selected applications" with icons for Jupyter Lab/Notebook, Perian Shell Access, and an announcement section.

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

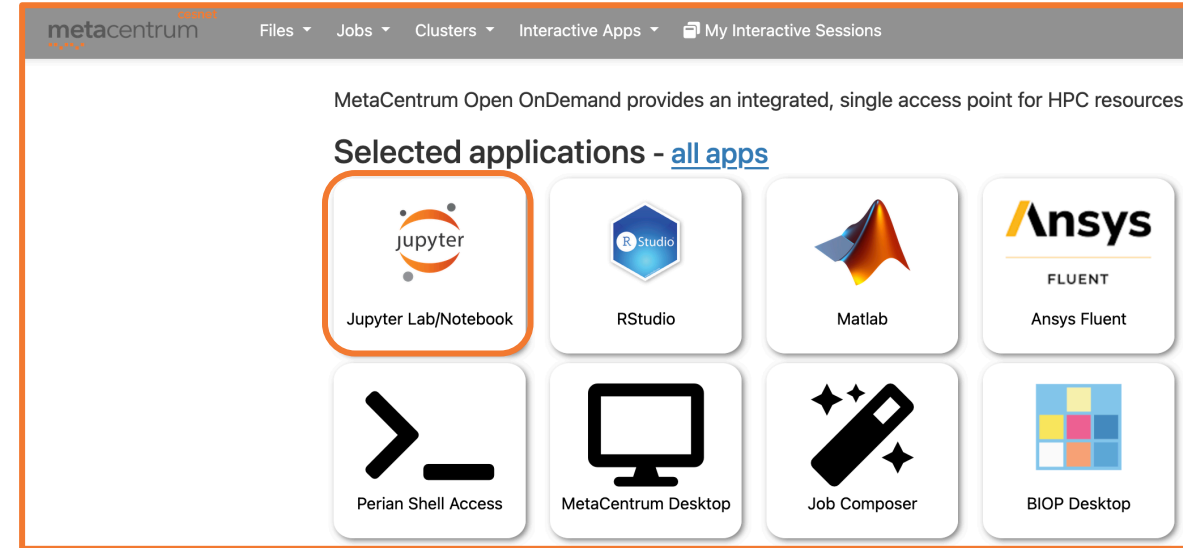


Jupyter Notebook in Open OnDemand

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



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, etc.)
- Embeds plots, widgets, and equations
- Promotes reproducible, shareable workflows
- Also accessible in Kubernetes <https://kubernetes.io/docs/tutorials/stateful-application/jupyter/>

The screenshot shows the configuration interface for launching a Jupyter Notebook/Lab. On the left, a list of applications is shown, with "Jupyter Notebook/Lab" selected. On the right, the configuration options for "Jupyter Notebook/Lab" are displayed. The "Mode" is set to "Jupyter Notebook". The "Number of hours" is set to 1. The "Number of CPUs on single node" is set to 1. The "Memory (GB)" is set to 5. The "GPUs" is set to 0. The "Scratch local (GB)" is set to 5. The "Jupyter Image" is set to "Metacentrum/debian11.sif". The "Full path of custom singularity image with Jupyter notebook" is empty. The "PBS Queue" is set to "interactive". The "Jupyter working directory location" is set to "/storage/brno2". A "Launch" button is at the bottom.

Category	Item
Cloud	Kubernetes on OpenStack (KOST) (beta)
	OpenStack VM (beta)
Desktops	Ansys/Enight
	Ansys/Fluent
	Ansys/Workbench
	BIOP Desktop
	CLCgenomicsWB
	Matlab
	MetaCentrum Desktop
	QuPath
	VMD Desktop
Servers	Jupyter - Evo2 (beta)
	Jupyter Notebook/Lab
	Matlab webapp (beta)
	RStudio Server

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

Mode
 Jupyter Notebook
 Jupyter Lab

Number of hours
1

Number of CPUs on single node
1

Memory (GB)
5

GPUs
0

Scratch local (GB)
5

Jupyter Image
Metacentrum/debian11.sif

Full path of custom singularity image with Jupyter notebook
[Empty field]

PBS Queue
interactive

Jupyter working directory location:
/storage/brno2

Launch

Jupyter Notebook

<https://ondemand>

- Web-based
- mixing
- Excellent for 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 Kubernetes

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

The screenshot shows the 'Interactive Apps' section of a Jupyter Notebook/Lab interface. At the top, a green notification bar states 'Session was successfully created.' Below this, the breadcrumb 'Home / My Interactive Sessions' is visible. On the left, a sidebar lists 'Interactive Apps' under 'Cloud' (Kubernetes on OpenStack (KOST) (beta), OpenStack VM (beta)) and 'Desktops' (Ansys/Ensignt, Ansys/Fluent, Ansys/Workbench). The main area displays details for a 'Jupyter Notebook/Lab (18240652.pbs-m1.metacentrum.cz)' which is 'Running' on '1 node | 1 core'. It includes the host 'tarkil16.grid.cesnet.cz', creation time '2026-03-20 15:33:47 CET', 'Time Remaining: 59 minutes', and 'Session ID: 2b8b5f4a-7b31-4bcf-b61c-bbd32245560a'. A 'Connect to Jupyter' button is highlighted with an orange border.



The screenshot shows the configuration form for creating a Jupyter Notebook/Lab session. It includes a dropdown for 'Jupyter Image' set to 'Metacentrum/debian11.sif', a text field for 'Full path of custom singularity image with Jupyter notebook', a dropdown for 'PBS Queue' set to 'interactive', and a dropdown for 'Jupyter working directory location' set to '/storage/brno2'. A 'Launch' button is at the bottom.

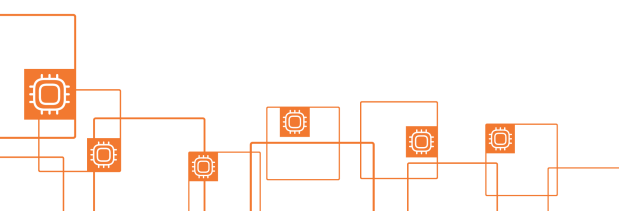
Select items to perform actions on them.

Upload

New ▾



<input type="checkbox"/> 0 ▾	 /	Name ▾	Last Modified	File size
<input type="checkbox"/>	 CASTEP-25.12		před 2 měsíci	
<input type="checkbox"/>	 META_SUPPORT		před 5 měsíci	
<input type="checkbox"/>	 ondemand		před 2 lety	
<input type="checkbox"/>	 OpenMolcas		před 9 měsíci	
<input type="checkbox"/>	 test_crys		před 2 lety	
<input type="checkbox"/>	 Untitled.ipynb		před hodinou	4.98 kB



Files

Running

Clusters

Select items to perform actions on them.

Upload

New ▾


 0 ▾ /

Name ▾

Notebook:

 Python 3 (ipykernel)

 SMLv2

Other:

 Text File

 Folder

 Terminal

  CASTEP-25.12

  META_SUPPORT

  ondemand

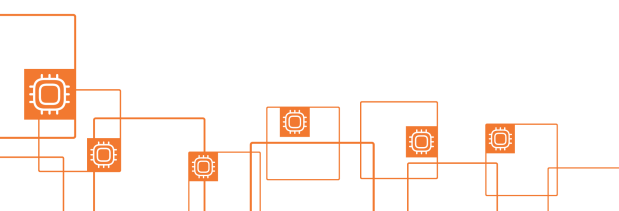
  OpenMolcas

  test_crys

  Untitled.ipynb

před hodinou

4.98 kB





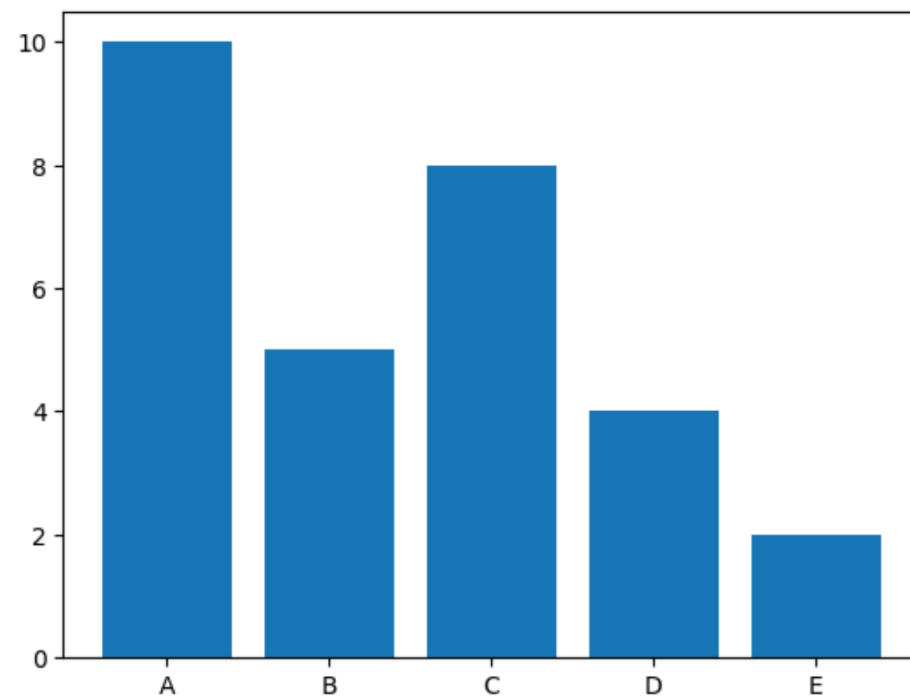
```
[1]: import os
current_working_directory = os.getcwd()
print(current_working_directory)
```

/auto/brno2/home/vorel

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

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

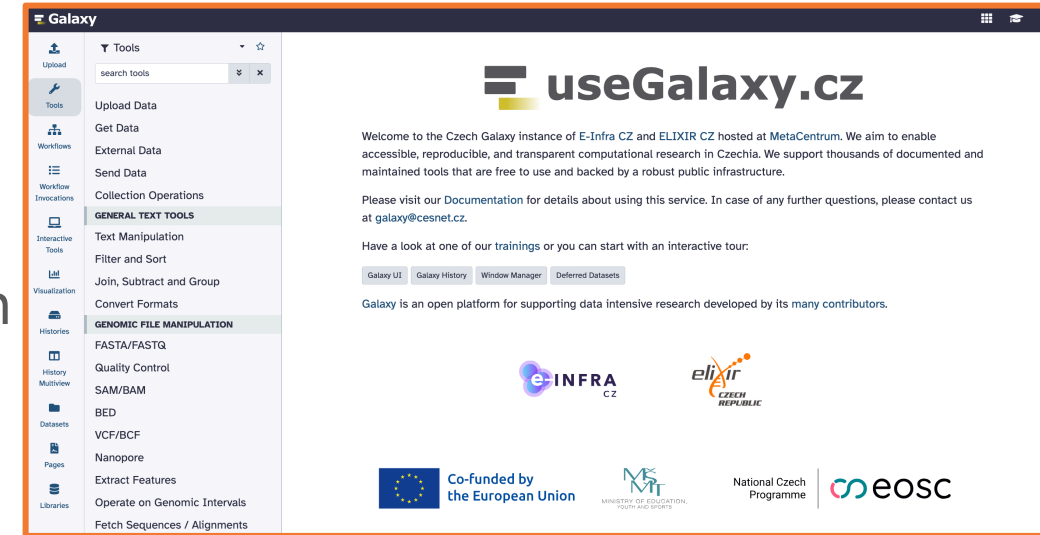
```
[3]: from matplotlib import pyplot as plt
x = ['A', 'B', 'C', 'D', 'E']
y = [10, 5, 8, 4, 2]
plt.bar(x, y)
plt.show()
```



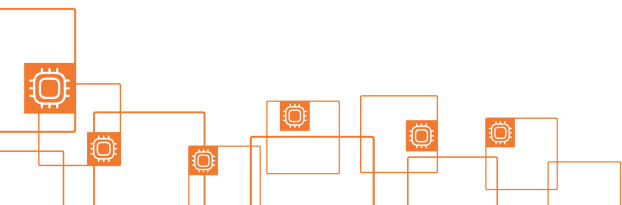
Galaxy useGalaxy.cz

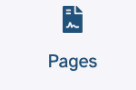
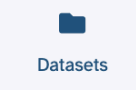
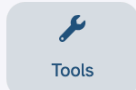
<https://usegalaxy.cz/>

- 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



The screenshot shows the Galaxy web interface for useGalaxy.cz. The top navigation bar includes 'Galaxy' and 'useGalaxy.cz'. A left sidebar contains a 'Tools' menu with categories like Upload, Workflows, Interactive Tools, and Datasets. The main content area features a search bar, a list of tool categories (GENERAL TEXT TOOLS and GENOMIC FILE MANIPULATION), and a welcome message. The welcome message states: '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.' Logos for e-INFRA CZ, ELIXIR CZECH REPUBLIC, Co-funded by the European Union, Ministry of Education, Youth and Sports, National Czech Programme, and eosc are displayed at the bottom.





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 Invocations

Interactive Tools

Visualization

Histories

History Multiview

Datasets

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Fetch Sequences / Alignments

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 Union



MINISTRY OF EDUCATION,
YOUTH AND SPORTS

National Czech
Programme



Upload

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GENOMICS ANALYSIS

Assembly

Upload from

Regular

search

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.

reset Close

Create a new remote file source

+ Create new

Cancel

Select



National Czech Programme



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

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

History

search datasets

Unnamed history

0 B

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



- 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

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 (?)

History + ↺ ≡

search datasets

Unnamed history

0 B 1 ↺

1: GCA_029291075.1_E_nip_g
enomic.fna.gz



Upload

Tools

Workflows

Workflow Invocations

Interactive Tools

Visualization

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History Multiview

Datasets

Pages

Libraries

Notifications

More

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RNA Analysis

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



Co-funded by
the European Union



National Czech
Programme



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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**

Preview Visualize Details Edit

Warning: This dataset is large and only the first megabyte is shown below. [Show all](#) | [Save](#)

```
>JAQBSW01000001.1 Eudiplozoon nipponicum isolate JV_EN_01 E_nip_1, whole genome shotgun sequence
gcaatgttctctcattcgagtaattaaccgtctggctgatcgccctacgtaagttgatcgacaacttgcgcatgtatcct
ggtaaaaaatatttgatattgacattaacgactgtttctcttggattactggtaaggcaagtggttacactaaataac
actcgtagtttagctgcattaaatagcgtgtaaatgctgcttcaactttctttgtgctcattcgggaaactgcatccac
cataaatgggagtttagtgtagaccgtttctttctggcgttaataagctgtttctgtttgattcctcttttaataat
tgattcaatataatagCTAGGATaccattagacattaaatcgtaaatgtctttatataataatcttttagaattat
gactaaccaactgtcaattcttaaaagcaaccgcaactgtgataattatgaaatggtaaaaaactgctgtat
aacaataactgtgcagaccatgttggtttatggtaaatgttctgttttaacttaccattagtttttcatatagata
tctaggaaaggcagacagtcattctctgctgctgtgtaagcagatattcttatgtgctttgtgaaactttaaag
taatgttctgtgattgcgacctgttcttaagtacaagaatataatcatccagcaccgtatataatgagcacatttaata
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tactttgctgctccacttgtctatttcatctgatttatcgtctagacgtgtgaaatgttattgattgcaattaaacagctttt
catcttttgcagtagtcagattgtcattataagtcgctctttctttgcttcttacttaagaacaggtcgca
tcacgaacattgcttcaaaagttcaacaagcacataagaatctcggcttccagctggagcagagaagatgactgtct
gcctttcctagatgtactatataagaagaactaatggtaacttaaacgagaacatttaccataaaccaacatggctg
cacagttattgcataacagcagttttgtgctatttaacataaattatcaacagttcgtggttctttcaagaatagac
aggttggtttagtcaagattctaaagaaatgaatataataaagcaattaacggtttaagtgtcaatggctatcccagaca
attaatgaaatcaattataaaaggggagttaacagaaaacagcgtattatgggcagaaaaagaaatagctaccta
acatacatttaagggggatgcatctcccgaatggcacaagaagaatgaagcagcattgacacacacatttaagca
gccaaactcagagtgattatagggtaacacactgcttacttagcaatcaagagaaacagcggtaatgctgatctc
aaatattttaccatagatgcagtcgcatgttgcgacaaactacgtagccgatcgaccagcggtttaactcga
tgagagaacattgcaacttaaacgcccgttttaaatcaaatgggtaatacacgctgctattgctgcaacacatcatcgaa
gcatcgacgtagttcttcagacgtagcattcaagtaattactaaatgcaaaacaaaggagctagccacattatgg
ataaacaaatgacagcggatttatgcaagcagaagaagcagctacaagcattgagcctgaaactggatgtaggacgca
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taGGCTCTTATGGAACTAAGCTATAGGTGACATAGTTCGCTGTTACGTATGCAACATTGATGTAGCGAAATCGTGGC
AAAGAAAAGGCTGTAGGATGTTACCCGTTGTATGAATGCTTAAAGCACTGCTGGTAAATAGGAAGGTGTTGACCAAT
CGAACCTTAGTTATCCAGGAACCTCGGAACACGAGCACGAACTTTATGGTGTCCGTACTCGGAAAAAAGTATGACGCCA
ACATAGGCAACCTTCCAATTAGCTATAAATCAACAATaatgtcattttataaataaacgaaactgttttgcgggcg
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GGGAAATGGGatagttatttggaacttagcgCTAAATGGATGATATATAGGCTCACaaaaaggaagactaaccaag
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acagacgttcccaggttgcgCCTGACCGcttcaaatctggcaagtacatgaggagttctcaataaggcgaatcgg
tctactggagcaattgctttctacactgtacaattcttagttatactgcaaatgtatgacatttaattgagtagga
tcatatcaagttcgaacactgtattataaattatgTCATTTTGTACTACTAGTGTGCAACATATTTTATCATCGTTTCC
TCACTATTTAACCCGCAAGAAACAATTGACACAGTAGAAAAAAGAGTACGctaaaaattatagaaaattatagaaa
gcatgcataaaaaataaattagctcACTCACGAGAACCGCTGCCTATCCGATTTAAGTGACTGAGCAAATTTGATGCAC
```

History

search datasets

Unnamed history

295 MB

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- Assembly
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- 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**

[Preview](#) [Visualize](#) [Details](#) [Edit](#)

Warning: This dataset is large and only the first megabyte is shown below.
[Show all](#) | [Save](#)

```
>JAQBSW01000001.1 Eudiplozoon nipponicum isolate JV_EN_01 E_nip_1, whole genome shotgun sequence
gcaatgttctctcattcgagtaattaaccgtctggctgatcgccctacgtaagttgatcgacaacttgcgcatgtatctt
ggtaaaaaatatttgatattgacattaacgactgtttctcttggattactggtaaggcaagtggttacactaaataac
actcgtagtttagctgcattaaatatgctgttaagtctgcttcaactttctttgtgctattcgggaaactgcatccac
cataaatgggagtttagtgtagaccgtttctttctggcgttaataagctgtttctgttttgattcctcttttaataat
tgattcaatataatagCTAGGATaccattagacattaaatcgtaattgtctttatataataatcttttagaattatt
gactaaccaactgctcaattcttaaaagcaaccgaaactgtgataattatgaaatggtacaaaactgctgtat
aacaaaactgtgcagaccatgttggtttatggtaaatgttctgttttaattaccattagtttttcatatagata
tctaggaaaggcagacagtcattctctgctctgtgtaagcagatattcttatgtgctttgtgaaacttaag
taatgttctgtattgcgacctgttcttaagtacaagaatataatcatccagcaccgtatataatgagcacatttaatta
tgtatttcttagtgccctagaaaaatctcagccaactggagataaggggcttccattgagcacatttcatat
tactttgctcctcacttgtctattctcatctgatttatcgtctagacgtgtgaaatttggattgcatttaacacgttttc
catcttttgcagtagtcagattgtcattataagtgcgctctttcttggcttcttgcactaagaacaggtcgca
tcacgaaactgtctcaaaagttaacaaagcacataagaatctcggcttcacgtcggagcagagaagatgactgtct
gcctttcctagatgtactataaagaagaactaatggtaacctaaacagaacaattaccataaaccaacatggtctg
cacagttattgcataacagcagttttgtgctatttaacataaattatcaacagttcgtggttctttcaagaatagac
aggttggtttagtcaagattctaaagaanaatgaatataataaagcaattaacggtttaagtgtcaatggctatcccagaca
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gcatgcacgtatgttctcagacgtagcattcaagtaattactaaatgcaaaacaaaggagctagccacattatgg
ataaaccaaatgagcggatattatgcaagcagaagaagcagctacaagcattgagcctgaaactggatgtaggacgca
atgtgattggtttccgtgtttcacactctctctatgttcacatattctatctgttttgcattcaatttatataaaa
atatgttcattagaagatatttcagaagacaatgcaagaagaaatcttctgtactgataaattcaaatattttgca
taGGCTCTTATGGAACTAAGCTATAGGTGACATAGTTCGCTGTTACGTATGCAACATTGATGTAGCGAAATCGTGGC
AAAGAAAAGGCTGTAGGATGTTACCCGTTGTTATGAATGCTTAAAGCACTGCTGGTAAATAGGAAGGTGTTGACCAAT
CGAACCTTAGTATTCCAGGAACCTCGGAAACACGAGCACGAACTTTATGGTGTCCGTACTCGGAAAAAAGTATGCGCCA
ACATAGGCAACCTTCCAATTAGCTATAAATCAACAATaatgtcattttataaataaacgaaactgttttgcgaggcg
atcATAACCTTtttataaatcagggttgcgaactgtttataaaaactgaccattaaagttctAAAATTTAGTCATTATA
ATCTAAGattttagtagtagaaaaggcaattcaccagtagaccggtttcgttcttattgggaactcatcatgtactggc
ctgttagcatccatttagcgtaaagtgcgaactaacaccacaactctgtcattaacgaAAGGATACTACGTTATATG
GGGAAATGGGatagttatttggaaacttagcgCTAAATGGATGATATATAGGCTCACaaaaggaaagactaaccaag
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acagacgttcccagggttgcgCCTGACCGcttcaaatctggcaagtacatgaggagtttcaataaggacgaatcgg
tctactggagcaattgctttctacactgtacaattcttagttatactgcaaatgtatgactcatttaagatgagtgga
tcatatcaagttcgaacactgtattataaattatgTCATTTTGTACTACTAGTGTGCAACATATTTTATCATCGTTTCC
TCACTATTTAACCCGCAAGAAACAATTGACACAGTAGAAAAAAAAGATCAGctaaaaattatagaaaattatagaaa
gcatgcataaaaaataaattagctcACTCACGAGAACCGCTGCCTATCCGATTTAAGTGACTGAGCAAATTTGATGCAC
```

History

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Unnamed history

295 MB

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zonal statistics over each area

Boxplot of quality statistics

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cmstat Summary statistics for covariance model

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

1: renamed_GCA_029291075.1_E_nip_genomic.fna.gz ok

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

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

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Annotation (optional)

Add Tags

Save Cancel

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1: renamed_GCA_029291075.1_E_nip_genomic.fna.gz

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21,044 sequences

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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

1:renamed_GCA_029291075.1_E_nip_genomic.fna.gz

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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 Total_not_N
- 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

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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

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

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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

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

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statistics

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2: Fasta Statistics on data 1: summary stats ok

30 lines 2 columns
format **tabular** database ? size **664 b**

Preview Visualize Details Edit

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

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



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



kubernetes

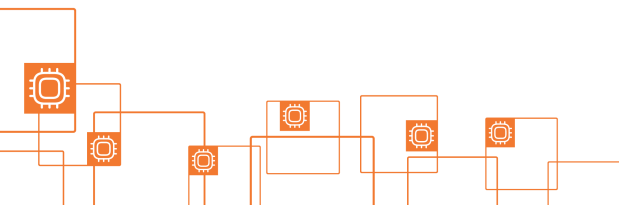
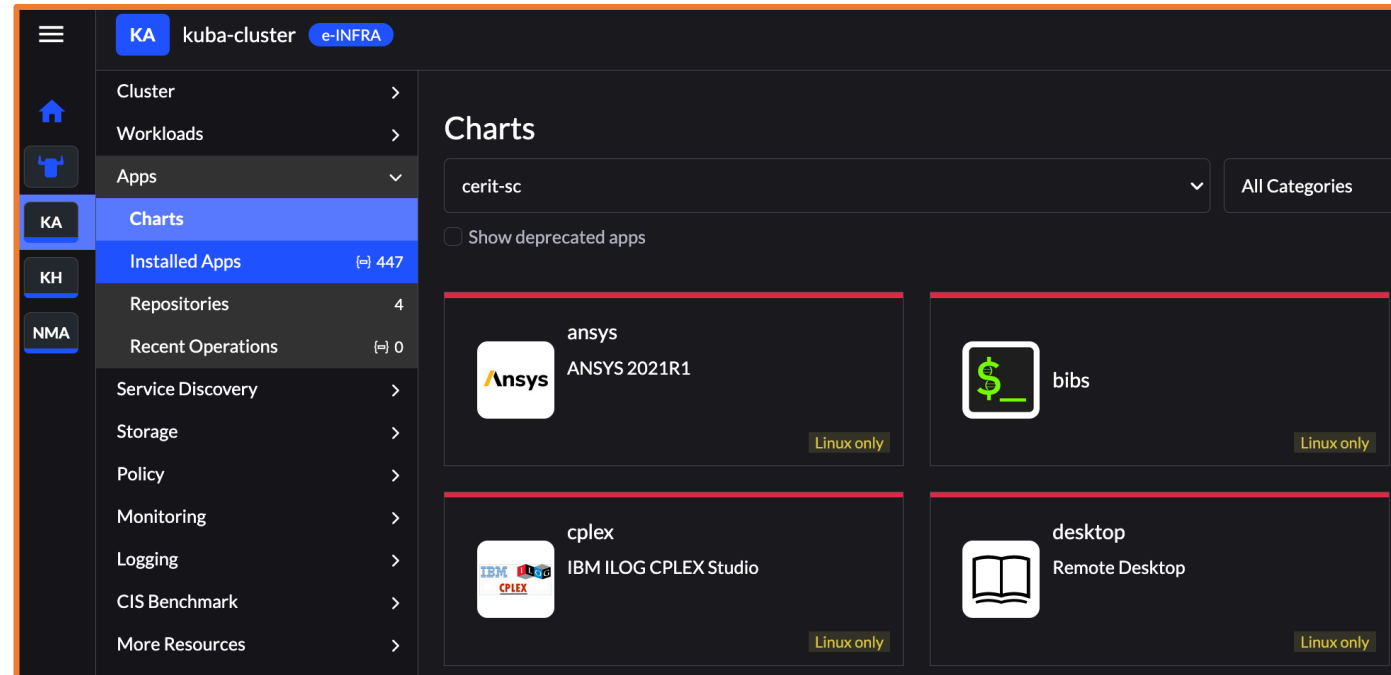
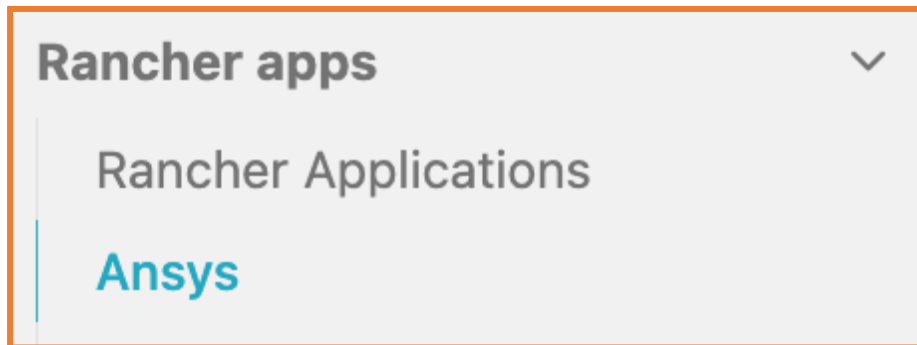
Other related services

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

■ Kubernetes

- 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>



■ AI chatbot (Open WebUI)

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

- 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 (e.g. Mistral 3 model)
- Programming languages proficiency
- REST API (integrate models into applications, scripts, or AI workflows)
- Visit documentation for the description of available models





GPT OSS 120B

Search a model

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

- GPT OSS 120B
- DeepSeek v3.2
- Mistral 3 Large
- GLM 4.7
- Qwen3-Coder-480B
- Mistral-Small 3.2
- Phi4

 You can select any available model and view its notes

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

GPT OSS 120B

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

How can I help you today?

+ [grid icon] [microphone icon] [voice icon]

- Suggested
- Give me ideas**
for what to do with my kids' art
 - Tell me a fun fact**
about the Roman Empire
 - Help me study**
vocabulary for a college entrance exam

Open WebUI

New Chat

Search

Notes

Workspace

Models

Folders

Chats

Today

Hello Line Extractor

Previous 30 days

SMASH Simulation Crash 1w

Software Installation Method... 4w

únor

Language Improvement R... 4w

Jak interpretovat "select=1:n... 4w

OpenStack Cloud Overview 4w

Data Privacy Assurance 4w

Sticky Header Demo 4w

Qwen3-Coder-480B

Write a Python (Python3) script that extracts all lines with the string "hello" from an input file named "input.txt". Place the selected lines in an output text file named "output.txt".



Qwen3-Coder-480B

Here's a Python3 script that extracts all lines containing the string "hello" from input.txt and writes them to output.txt :

```
python
1 def extract_hello_lines():
2     try:
3         # Read from input.txt and filter lines containing "hello"
4         with open("input.txt", "r", encoding="utf-8") as infile:
5             lines_with_hello = [line for line in infile if "hello" in line]
6
7         # Write the filtered lines to output.txt
8         with open("output.txt", "w", encoding="utf-8") as outfile:
9             outfile.writelines(lines_with_hello)
10
11        print(f"Successfully extracted {len(lines_with_hello)} lines containing 'hello' to output.txt")
12
13    except FileNotFoundError:
14        print("Error: 'input.txt' not found. Please ensure the file exists in the current directory.")
15    except Exception as e:
16        print(f"An error occurred: {e}")
17
18 if __name__ == "__main__":
19    extract_hello_lines()
```

How it works:

- Case-sensitive matching:** "hello" in line matches only exact lowercase "hello" (e.g., won't match "Hello" or "Hello!").
 - To make it case-insensitive, change to:

```
python
1 if "hello" in line.lower()
```

- Line endings preserved:** Original line endings (e.g., \n) are kept in the output.
- Error handling:** Catches missing input.txt and other exceptions.
- Efficient:** Uses a list comprehension for filtering and writelines() for writing.

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

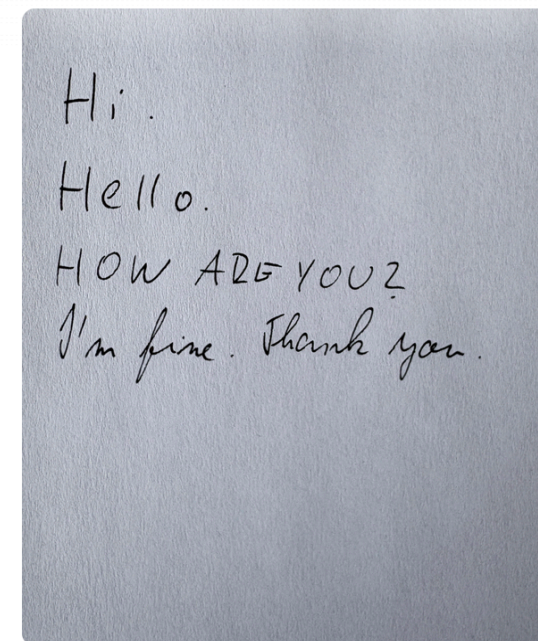
Attach Webpage

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

New Chat

Search

Notes

Workspace

Models

Folders

Chats

Model for advanced reasoning and analytical tasks.

Thinker ⓘ



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

Open WebUI

New Chat

Search

Notes

Workspace

Models

Folders

Chats

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](#).

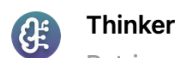
1 Source

✎ 📄 🔊 👍 🗨️ 🌐 ↻

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
l 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
t interplay between environmental
f *H. bacteriophora* parasitism

Follow up



Let me draft the summary:

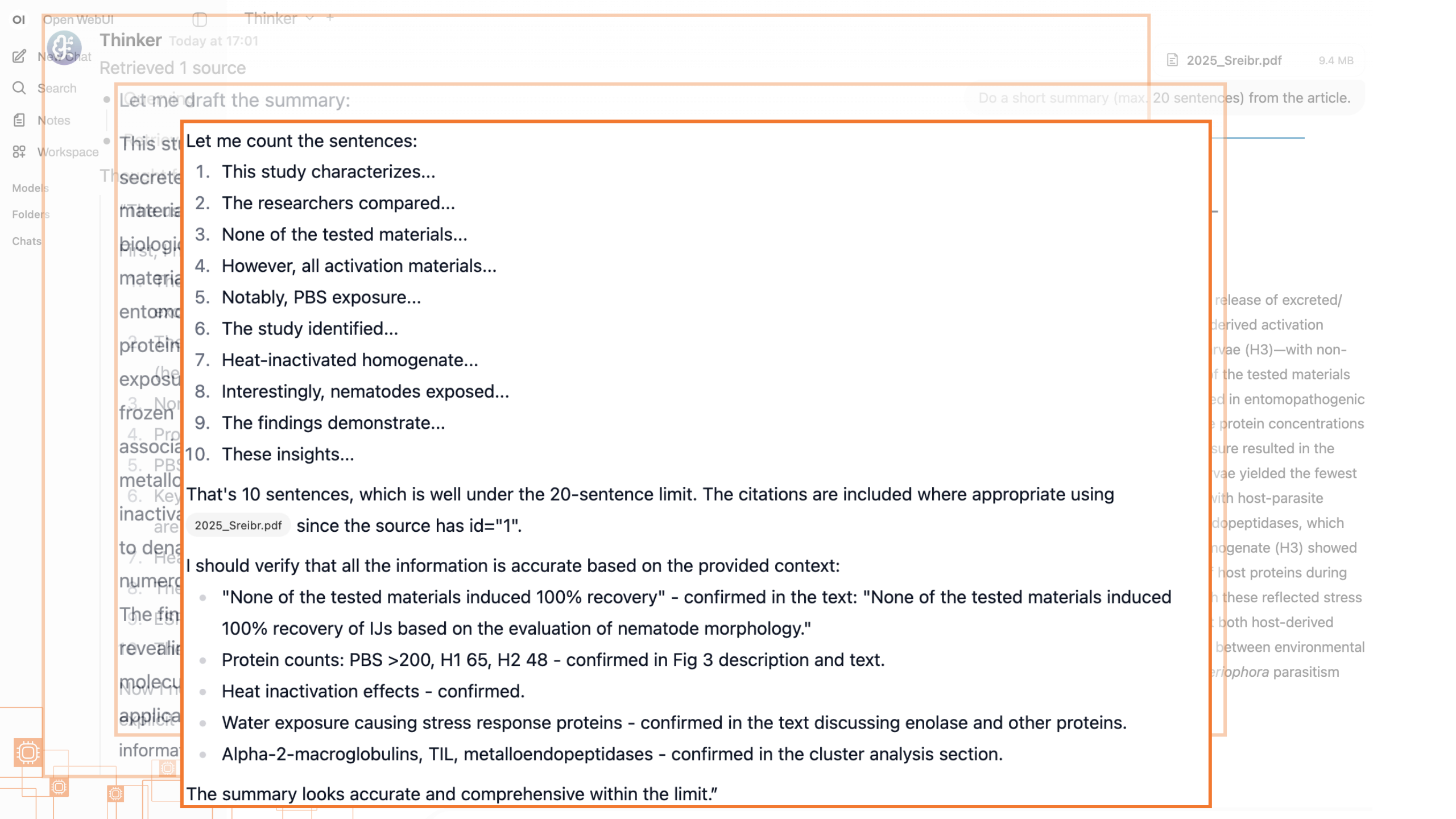
This study characterizes the activation of *Heterorhabditis bacteriophora* infective juveniles (IJs) and their release of excreted/secreted products (ESPs) in response to various stimuli (2025_Sreibr.pdf). The researchers compared insect-derived activation materials—including homogenates from live larvae (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).

information.



Follow up





Let me draft the summary:

This study characterizes:

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."

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:



openstack®



kubernetes

Other related services

■ Compute cloud

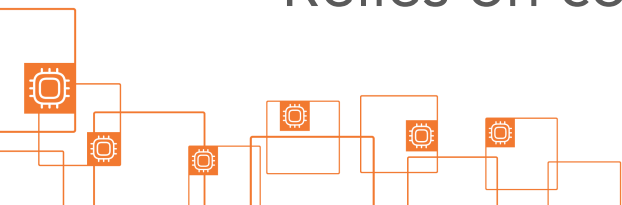
<https://docs.platforms.cloud.e-infra.cz/en/docs>

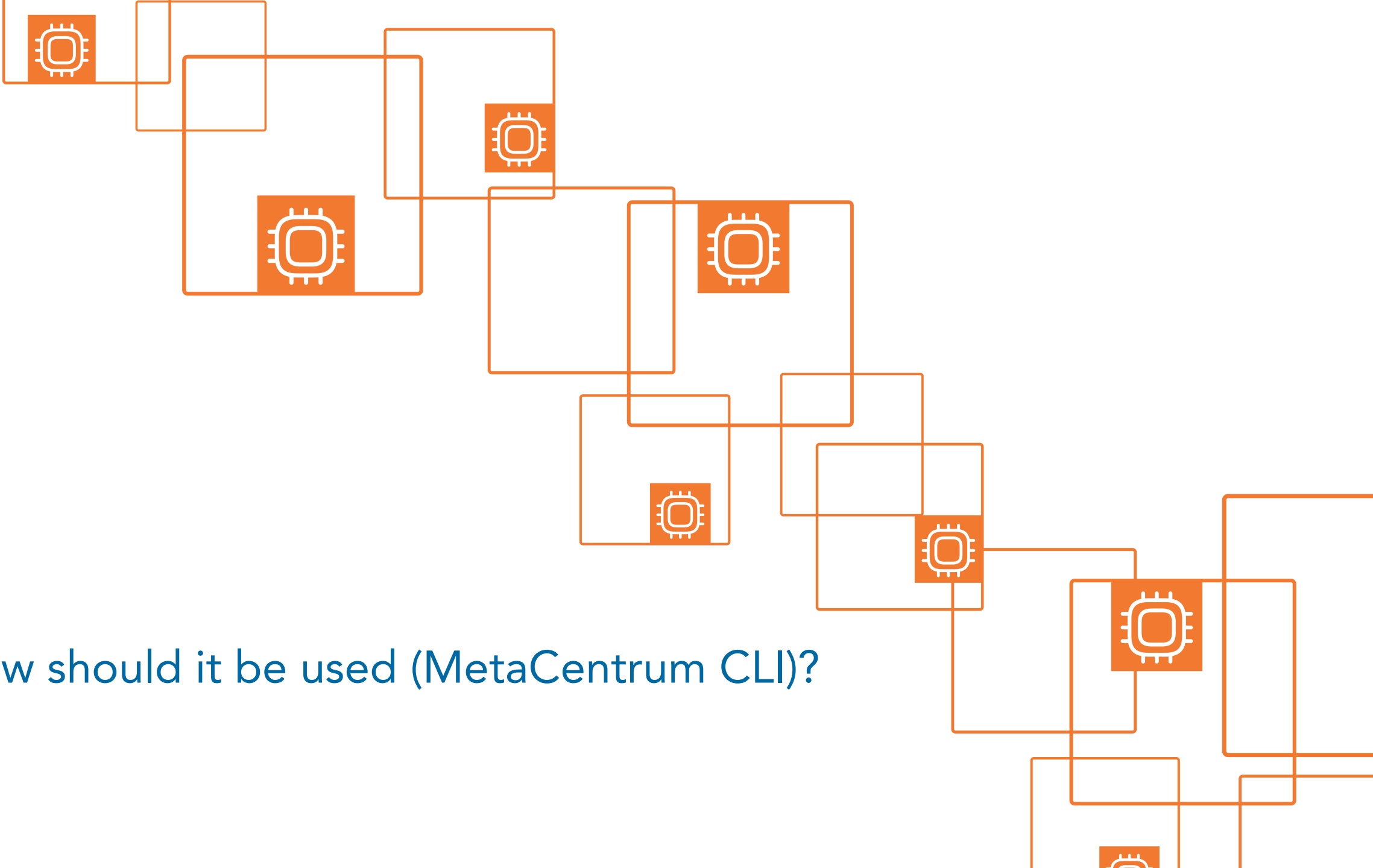
- Runs on OpenStack (allows users to create and manage their own cloud computing resources)
- 17 computational clusters with 8,968 cores, 96 GPU cards, and 178 TB RAM
- Virtual machines are accessed using SSH keys

■ Sensitive cloud

<https://docs.cerit.io/en/docs/sensitivecloud/account>

- Secured computing and storage environment provided by CERIT-SC (part of e-INFRA CZ) for sensitive data processing and research
- Follows security standards such as ISO 27000, C5, ISO 15189, and ECRIN
- Relies on container technology via Kubernetes, MFA required





How should it be used (MetaCentrum CLI)?

<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

The screenshot shows the eduID.cz login interface. At the top left is the eduID.cz logo with 'cesnet' in red. Below it, two main options are presented in light grey boxes:

- I have an account in a member organisation of eduID.cz**
- My organisation is not in eduID.cz and I need to validate my alternative identity**

Below these options is a section titled "Direct links to selected institutions from eduID.cz" containing a grid of 12 institution logos and names:

 MUNI	Masarykova univerzita		Univerzita Karlova		Západočeská univerzita v Plzni
	Jihočeská univerzita v Českých Budějovicích		Univerzita Palackého v Olomouci		Univerzita Pardubice
	CESNET		České vysoké učení technické v Praze		Mendelova univerzita v Brně
	Technická univerzita Liberec		Vysoká škola báňská - Technická univerzita Ostrava		Vysoké učení technické v Brně










Most new applications are approved within one or two working days

- Anytime during the year, manual approval
- Log in through the institution (i.e. local 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

Submitting an application

Log in with

- Astronomical Institute of the Czech Academy of Sciences 
- Institute of Agricultural Economics and Information
- Institute of Chemical Process Fundamentals of the AS CR 
- Institute of Microbiology AS CR 
- Institute of Technology and Business in České Budějovice
- Prague University of Economics and Business 
- University of Chemistry and Technology, Prague 

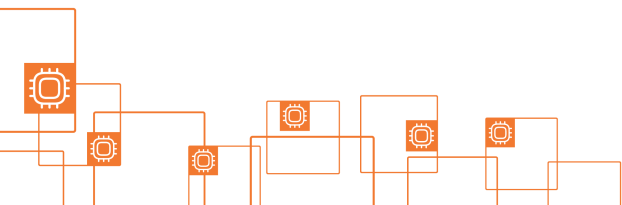
 CESNET 
Personal data processing

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>



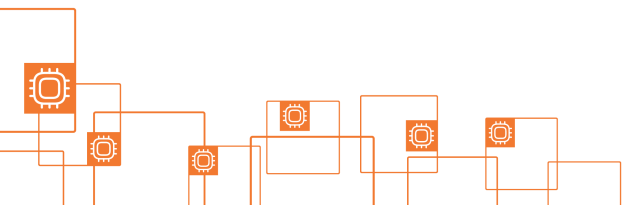


Geographically separated servers mean better distribution of users and load, which makes the servers more stable and provides an alternative during an outage

- Primary access point
- SSH access via password
 - SSH keys are not supported
 - A valid Kerberos ticket en infrastructure
 - Beware of leaving session
 - You can generate Kerberos

Frontend servers (login nodes)

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)

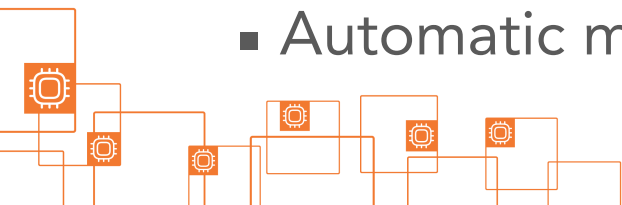
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- You can generate Kerberos tickets on a local PC and log in without a password

<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>



(login nodes)

computing/infrastructure/frontends

/access/security/kerberos

the infrastructure
only 10 hours
without a password

computing/run-basic-job#interactive-job

processes

are suitable

Dear user,

one or more your processes running on the frontend skirit.ics.muni.cz exceeded limits for more than limits, see below. This situation has negative impact on other users working on the frontend. The following process was terminated by the system.

User:

```
PID TTY ELAPSED TIME CMD  
855050 pts/50 7583 6111 gzip -d
```

PID - a number representing the process ID on skirit.ics.muni.cz
TTY - controlling tty (terminal)
ELAPSED - elapsed time since the process was started, in seconds
TIME - cumulative CPU time, in seconds
CMD - command with all its arguments

Limits:

```
>2h wall_time AND >1h cpu_time AND >30% average_cpu_usage
```

Please consider that frontends are shared among all users. If you need to run interactively some demanding activity, like working with huge amount of data or software compilation, please don't use the frontend but rather reserve some computing node for an interactive jobs. Such operations could slow down the frontend and bother other users.

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

Please note this is an automatically generated e-mail. If you have any questions concerning this particular job or future strict limits enforcement, please contact us on meta@cesnet.cz.

Best regards,
MetaCentrum

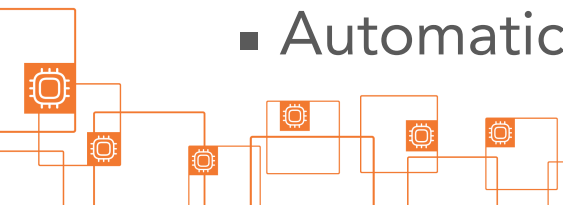
■ Primary access

■ SSH access

- SSH keys and
- A valid Kerberos
- Beware of
- You can get

■ Do not run

- They are shared
- They are available
- Automatic



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>

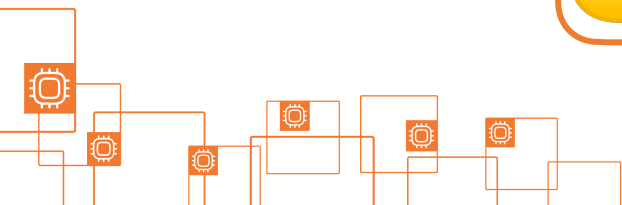
- Backups of valuable primary data and results preferably to S3/NRP object storage

<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`.



- 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>

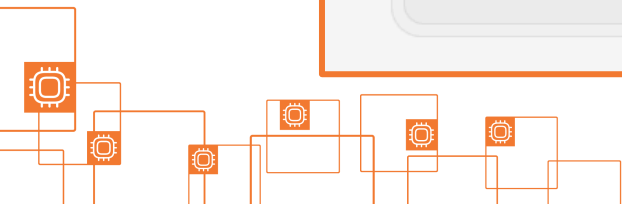
- Backups of valuable primary data and results preferably to S3/NRP object

st

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 = xxxxxxxxxxxxxxxxxxxxxxxxxxxx
secret_key = xxxxxxxxxxxxxxxxxxxxxxxxxxxx
host_bucket = s3.clX.du.cesnet.cz
```



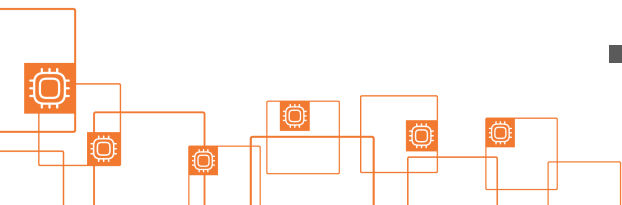
Disk storage arrays

- 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

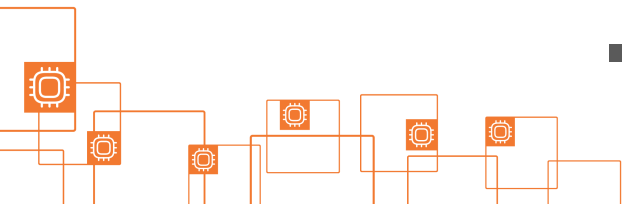
Disk storage arrays

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)

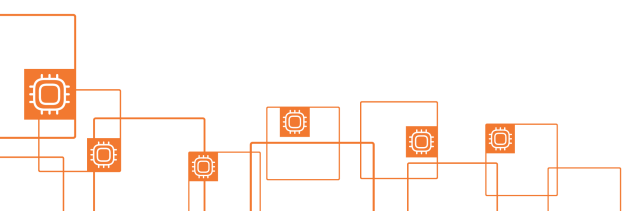


The concept of multiple home directories and disk storages


 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	



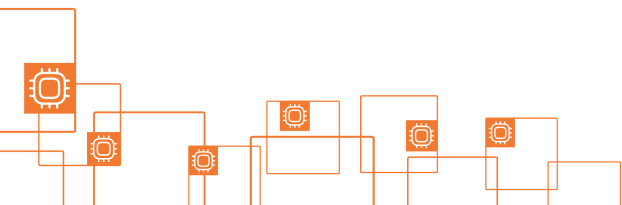
The concept of multiple home directories and disk storages

 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	

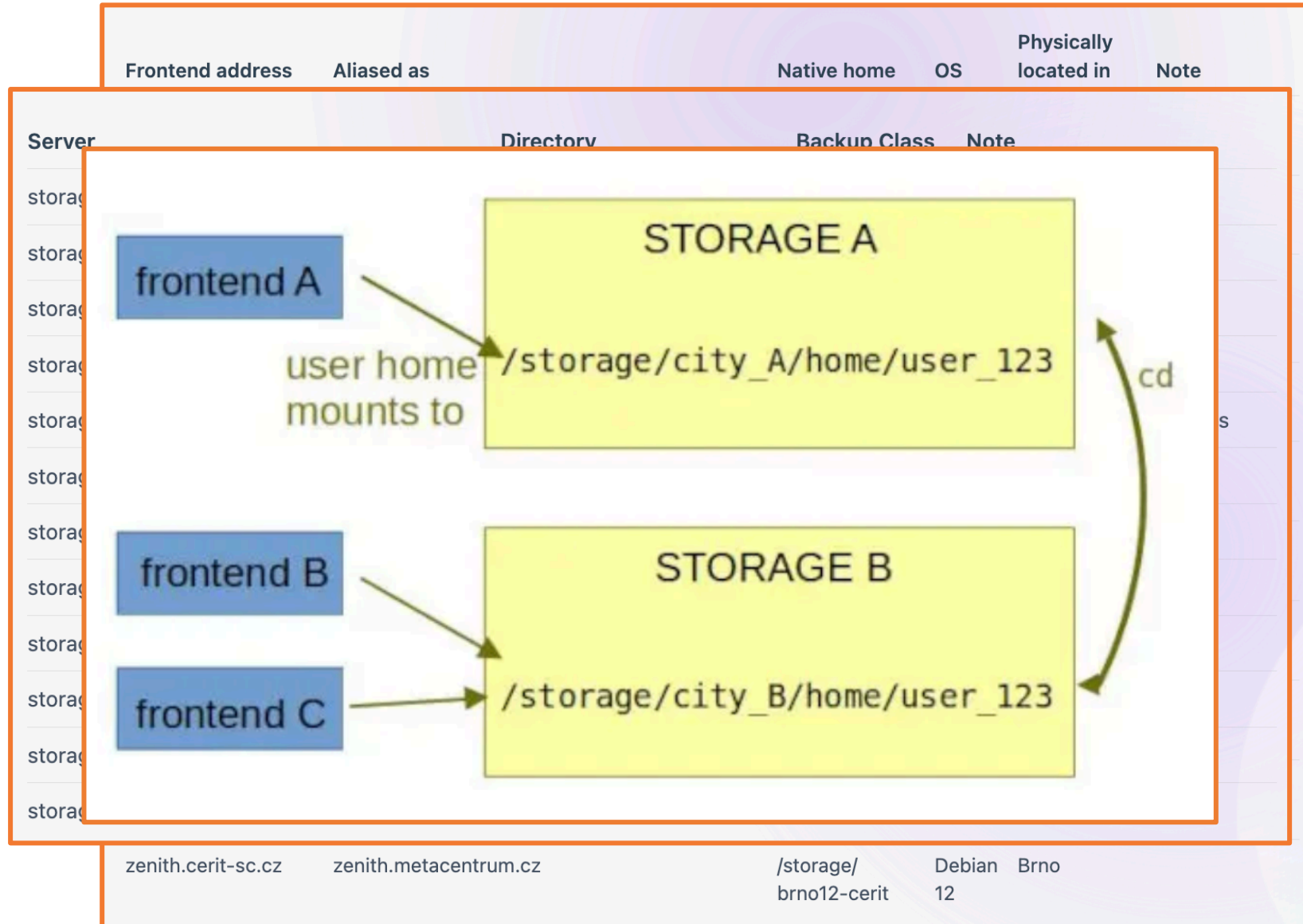


The concept of multiple home directories and disk storages

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

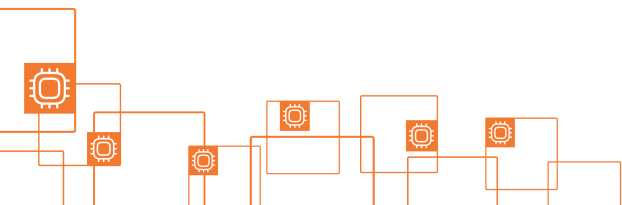
All frontend servers can also be reached in the domain 'metacentrum.cz'

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



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



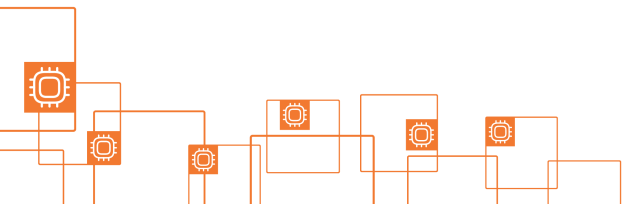
The concept of multiple home directories and disk storages

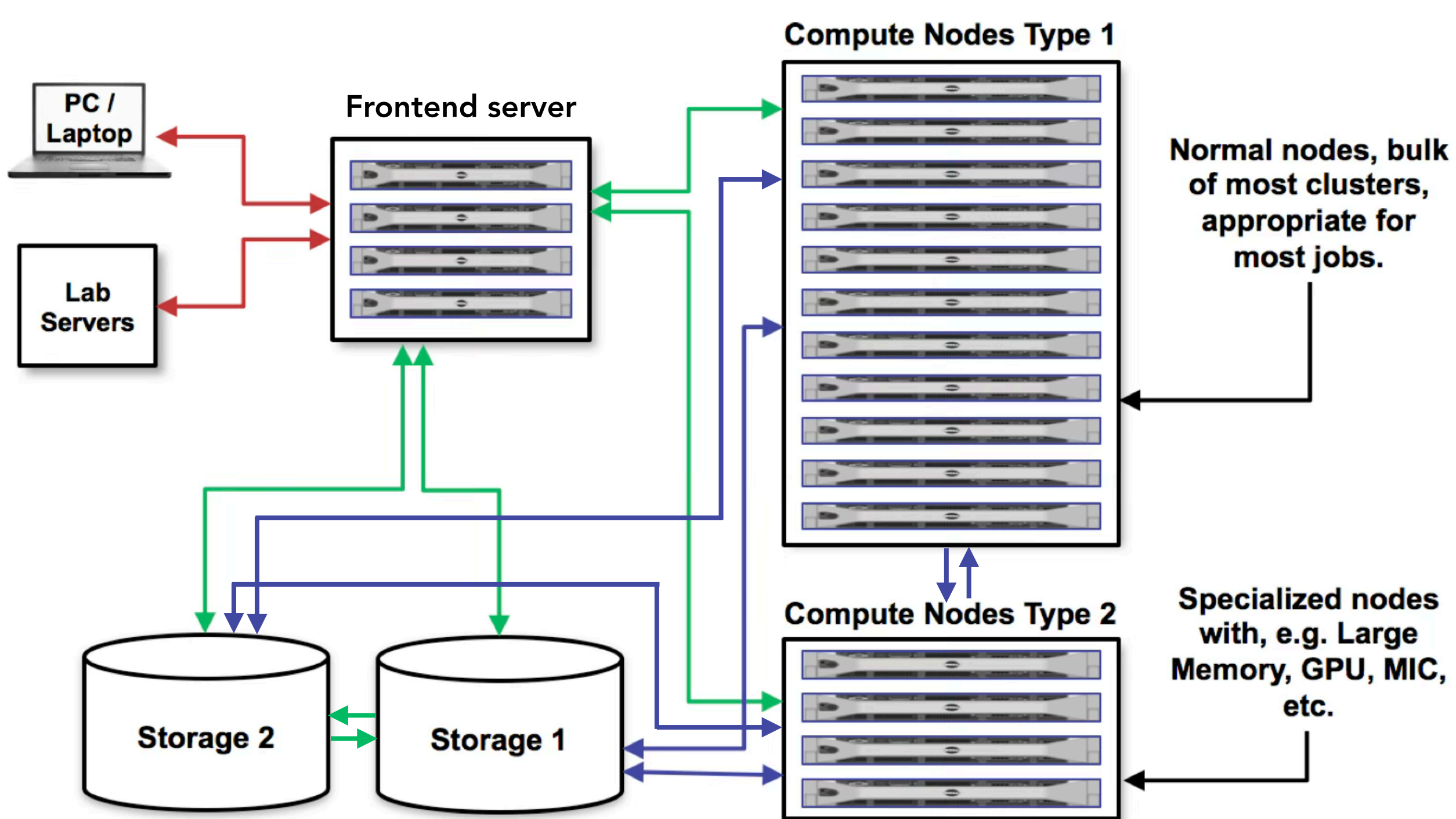
```
[(BOOKWORM)vorel@skirit:~$ ls
CASTEP-25.12 META_SUPPORT ondemand OpenMolcas pcangsd Smilei test_crys test_CZ_shift test_phyluce test_unic
[(BOOKWORM)vorel@skirit:~$ pwd
/storage/brno2/home/vorel
[(BOOKWORM)vorel@skirit:~$ ssh adan1
Linux adan1.grid.cesnet.cz 6.1.0-38-amd64 #1 SMP PREEMPT_DYNAMIC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



■ 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=100tb`

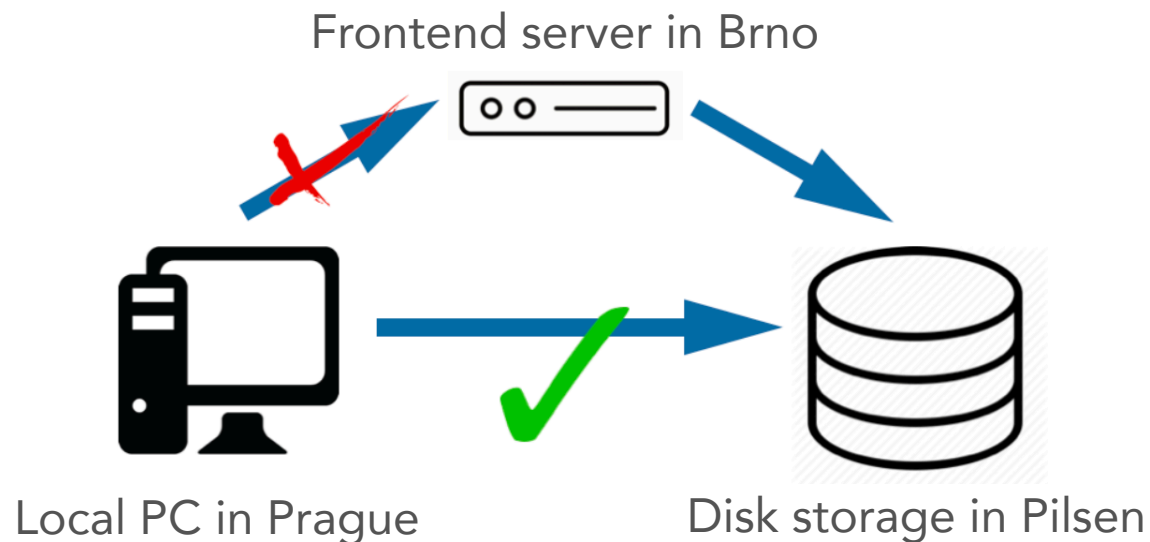
- Scratch shared by all the cluster's nodes, TBs, PBb
- Currently only available on Bee (BeeGFS) and Galdor GPU clusters
- No auto-delete policy
- Different directory naming policy in `/scratch.shared/USERNAME/some_folder_name`, it must not start with 'job_'.
- Suitable for tasks that process one large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





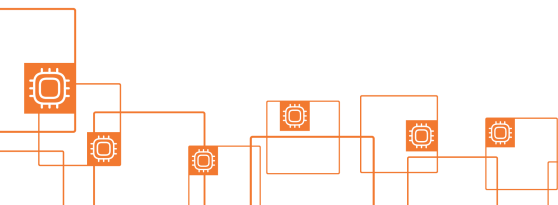
Users cannot browse disk storage interactively after logging in.
Only individual commands can be sent on them
\$ ssh storage-brno2.metacentrum.cz 'ls'

Copying data

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

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/

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



- `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



Batch job script example

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

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

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

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

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

# move into the scratch directory
cd $SCRATCHDIR

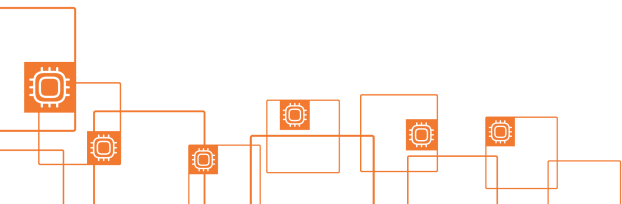
# load a module for your application
module add blast-plus/blast-plus-2.12.0-gcc-8.3.0-ohlv7t4

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

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

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

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



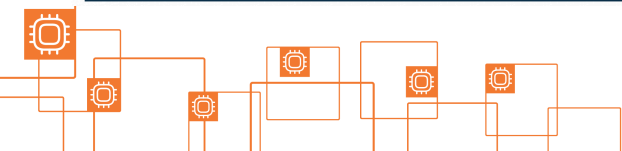
Interactive job

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

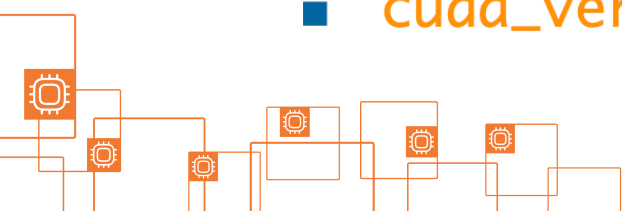
<https://docs.metacentrum.cz/en/docs/computing/run-basic-job#interactive-job>

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

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



- **GPU acceleration 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)



■ GP

■ ~14

■ Rec

■ Ma

■ Spe

■

■ Spe

■

■

■

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:ngpus=1:mem=30gb:scratch_ssd=250gb:gpu_mem=20gb:gpu_cap=compute_80
#PBS -l walltime=8:0:0

cd $SCRATCHDIR

scp storage-brno12-cerit.metacentrum.cz:~/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>



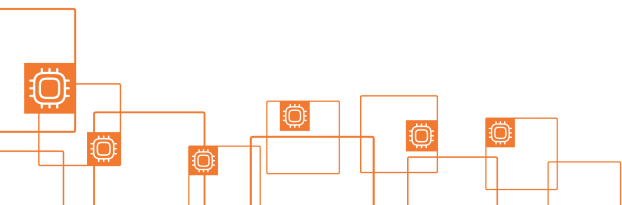
The most straightforward way to transfer highly optimised environments, complete with all dependencies and tuned libraries.

■ 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.



- HW resources (CPUs, GPUs, RAM, scratch, walltime,...) are reserved by PBS
- Detailed documentation: <https://docs.metacentrum.cz/en/docs/computing/resources/qsub-compiler>
- It requires some experience (keep some reserve)
- Helper tool for qsub command assembly

Personal view

This page shows a personal view of the PBS system for the user **vorel**.

Jobs of user "vorel"

user	job count					CPU count				
	total	queued	running	completed	other	total	queued	running	completed	other
vorel	0	0	0	0	0	0	0	0	0	0

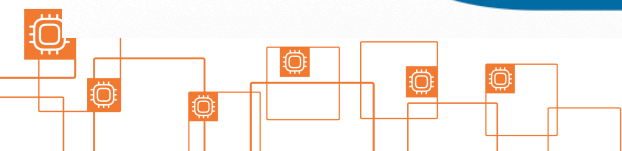
Links

- list of my jobs
- personal view of storages
- **qsub assembler**

Click on it...

Go to metavo.metacentrum.cz -
Current state - Personal view - **Qsub assembler**

(Stav zdrojů - Osobní pohled
Sestavovač qsub)



The screenshot shows the Qsub assembler interface with various resource selection options. A blue arrow points to the 'SPECfp2017 per core' dropdown menu, which is labeled 'CPU performance'. A tooltip shows the following options:

- :spec=7.4
- :spec=8.0
- :spec=9.1
- :spec=10.4

Another blue arrow points to the 'Find machines mathing the resource specification' button at the bottom, which is labeled 'Click on it...'. The button is circled in blue.

■ And you will see...

selection from command line

```
qsub -l walltime=24:0:0 -q default@meta-pbs.metacentrum.cz -l select=1:ncpus=8:mem=100gb:scratch_ssd=50gb
```

selection in shell script

```
#!/bin/bash
#PBS -q default@meta-pbs.metacentrum.cz
#PBS -l walltime=24:0:0
#PBS -l select=1:ncpus=8:mem=100gb:scratch_ssd=50gb
#PBS -N my_awesome_job
```

Result

OK

The requirement is 1 machine, and 93 such machines are free, out of 289 machines matching the requirements. The job is for it.

Machines available right now

adan1 (32 CPU, 187.6 GIB RAM, 697.6 GIB HDD)	adan2 (32 CPU, 187.6 GIB RAM, 783.6 GIB HDD)	adan3 (16 CPU, 171.6 GIB RAM, 766.6 GIB HDD)	adan5 (32 CPU, 187.6 GIB RAM, 744.6 GIB HDD)	adan6 (32 CPU, 187.6 GIB RAM, 705.4 GIB HDD)
---	---	---	---	---

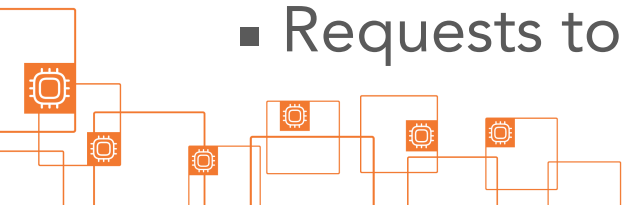
<https://www.cesnet.cz/>

<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
- Please link your ORCID
<https://www.e-infra.cz/en/news/link-your-e-infra-cz-account-to-orcid-a-small-step-for-smarter-impact-reporting>
- Requests to add acknowledgements in publications
<https://docs.metacentrum.cz/en/docs/access/terms#acknowledgements-and-publications>





Thank you for your attention

https://github.com/CESNET/metacentrum-hands-on/blob/main/2026-03_IMIC.md

- Go to '*github.com*'
- In the search bar, type '*MetaCentrum Hands-on*'
- Select the first (and probably only) result
- Select today's hands-on session (*2026, The Institute of Microbiology of the Czech Academy of Sciences, Prague, 25 March*)

