# metacentrum



## **MetaCentrum NGI**

For scientific computations, collaborative research & its support services

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## What is MetaCentrum

### MetaCentrum is

https://metacentrum.cz

... National Grid Infrastructure (NGI)

https://metavo.metacentrum.cz

... the activity of the CESNET association (coordinator)

https://docs.metacentrum.cz

- ... part of e-INFRA CZ
- ... a provider of computational resources, application software (commercial and free/open source) and data storage
- ... free of charge (users "pay" by acknowledgement in their publications)

### MetaCentrum is available for

- ... employees and students from Czech universities, the Czech Academy of Sciences, non-commercial research facilities, abroad partners, etc..
- industry users (non-profit and public research, upon individual request)



## What is MetaCentrum

### MetaCentrum targets

- ... individual users (we can offer resources)
- ... projects (cooperation, sharing data in a group)

https://metacentrum.cz

https://metavo.metacentrum.cz

https://docs.metacentrum.cz

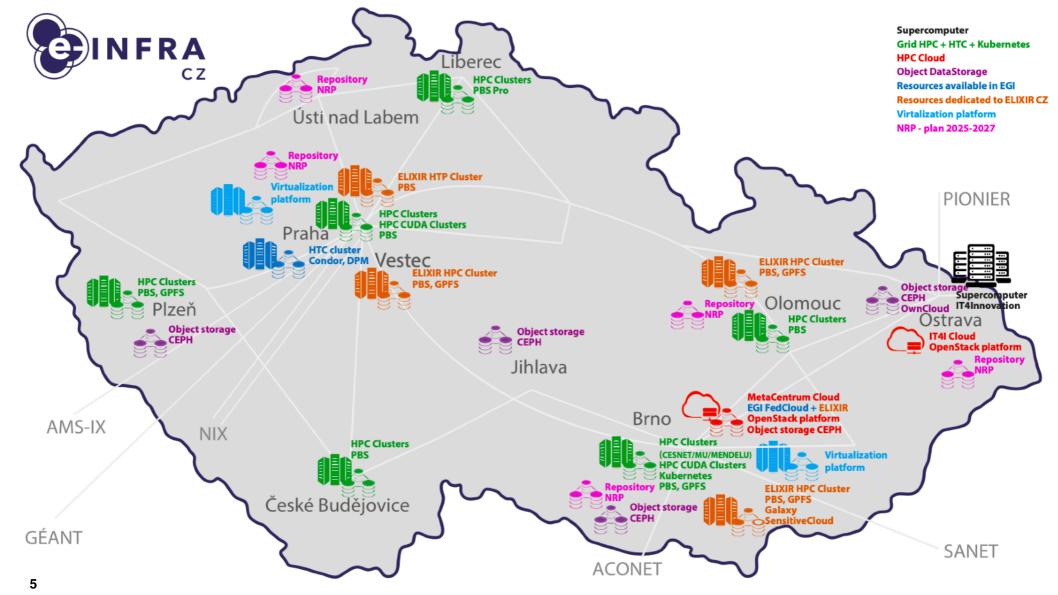
... organisations (incorporate their resources under central management)

### MetaCentrum offers

- ... possibility of applying at any time without grant competitions
- ... access without submitted projects (with one exception)
- ... immediate access to HW resources and licences
- ... the principle of grid (shared) usage (privileged access for cluster owners)
- ... various application software (commercial, free, open source)
- ... CPU/GPU resources, GUI applications and access, cloud services

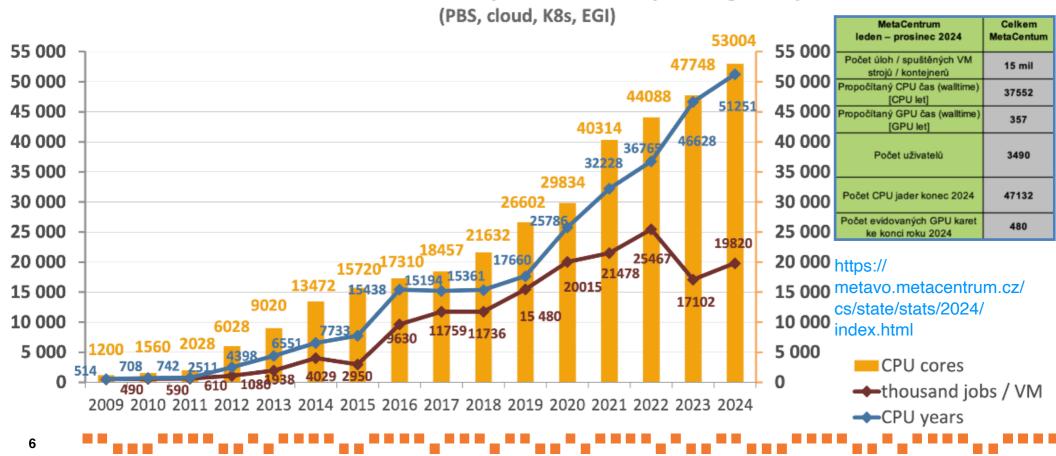
## Shared resources

- Compute resources are provided by the CESNET association and its partners (universities, CAS institutes), and
  - ... are freely available for research and academic usage
  - ... are shared among all users (community approach)
  - ... are with privileged access for cluster owners
  - ... can be used in case of urgent/heavy load extensively
  - ... are replaceable during an outage
  - ... are centrally managed (AAI)
  - ... are dedicated to grid HPC/HTC and containerised computing, cloud computing, and data storage capacities
  - ... are designed to process all types of data



## **Available computing power**

### Number of CPUs, executed jobs and corresponding CPU years



		Computer sciences			Biochemistry Molecular biology			
Chemistry	Material sciences		Plant scier	ices	Enviro nt scier Ecol	al nces		athemat ics
		Engineering	Microbiolo			Biophysics		
			gy	Gen	etics edity	Opt	ics	Pharma cology
Physics	Other topics	Astronomy Astrophysics	Cell biology		fe nces	Spe	ctro	scopy

## metacentrum cesnet

## **Application software**

Hundreds of available SW tools in many versions (circa 5,000 different modules)
PAID LICENCE





## One application to rule them all





## One application to rule them all

- Submission of the application is conditional on academic affiliation (eduID)
- Access is granted to the MetaCentrum and its services
  - Grid computing (CLI, OpenPBS scheduler) https://docs.metacentrum.cz
  - Open OnDemand (GUI, remote web access) nbemand

https://ondemand.grid.cesnet.cz

- Galaxy (GUI, web-based platform for computational analyses) https://usegalaxy.cz
- Jupyter notebook (GUI) jupyter https://docs.cerit.io/en/docs/web-apps/jupyterhub





Cloud/Sensitive cloud computing (OpenStack, Kubernetes) https://

docs.platforms.cloud.einfra.cz/en/docs

Container platform Kubernetes (GUI, for Docker images)

Nextflow pipelines https://docs.cerit.io/en/docs/workflows/nextflow

https://docs.cerit.io



kubernetes



Al chatbot (on local HW)

https://docs.cerit.io/en/docs/web-apps/chat-ai





## Service overview

MetaCentrum Grid	Kubernetes	OpenStack Cloud			
Centrally managed infrastructure (restrictive in some cases)	Centrally managed infrastructure (containers can be modified)	Images provided by MetaCentrur EGI, projects, users,			
Batch/interactive (long) jobs with reserved resources (OpenPBS)	Individually started non-root containers with reserved HW	Long-term running VMs with HW reserved via specific flavours			
Compute nodes and storages are distributed across the CZE	Central localisation in Brno (CERIT-SC)	Central OpenStack installation in Brno			
Mainly CLI, also GUI approaches (OnDemand, Galaxy, Jupyter)	Considerable interactive support (mostly remote GUI applications)	CLI management			
Limitations given by OS and system libraries	Potentially problematic container incorporation to K8s/Rancher	High level of user freedom, independent work with VMs			
Easily supported	Easily supported	Problematic access into users' VM			
Kerberos authentication	Web application (AAI)	SSH keys			

## Where and how to start

### Fill out and submit the registration form

- Select your organisation (through the eduID)
- Use your local/institutional username and password
- Fill out the form and create a strong (and unique) MetaCentrum password
- Applications are approved manually (and almost immediately)
- All accounts are valid till 02. 02. YYYY
- Users must extend MetaCentrum membership from the beginning of each calendar year (during January)

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



## The old-fashioned way

Access through the CLI (command line interface)
 https://docs.metacentrum.cz/en/docs/welcome

```
L@MacBook ~$ ssh vorel@nympha.metacentrum.cz
vorel@nympha.metacentrum.cz's password:
Linux nympha.meta.zcu.cz 6.1.0-34-amd64 #1 SMP PREEMPT_DYNAMIC Debian 6.1.135-1+zs1 (2025-05-13) x86_64
10 updates could not be installed automatically. For more details,
see /var/log/unattended-upgrades/unattended-upgrades.log
Last login: Tue Jun 24 11:16:06 2025 from gtx121.cesnet.cz
Avail | DATA | FILES |Backup |Storage
 CPUs
 Free Used
                             META
 Contact
 E-mail
               meta@cesnet.cz
               http://www.metacentrum.cz/
```

```
(BOOKWORM)vorel@nympha:~$ module add orca/6.0.1
Loading orca/6.0.1
 Loading requirement: libiconv/1.16-gcc-10.2.1-jbvbjyi python/3.9.12-gcc-10.2.1-rg2lpmk xz/5.2.5-gcc-10.2.1-fteagxc
  zlib/1.2.12-gcc-10.2.1-7qmmk4c libxml2/2.9.13-gcc-10.2.1-42uofzw cuda/11.6.2-gcc-10.2.1-nwpmxyy
   libpciaccess/0.16-gcc-10.2.1-f4q3srx ncurses/6.2-gcc-10.2.1-h3werp5 hwloc/2.7.1-gcc-10.2.1-a7ilbqq
   libevent/2.1.12-gcc-10.2.1-dqblgi5 numactl/2.0.14-gcc-10.2.1-gasmwpx opa-psm2/11.2.206-gcc-10.2.1-q4gu6pl
   openjdk/11.0.14.1_1-gcc-10.2.1-21177ke pmix/4.1.2-gcc-10.2.1-enmnubp psm/2017-04-28-gcc-10.2.1-hrczaup
   libnl/3.3.0-qcc-10.2.1-oa4lipo rdma-core/39.1-qcc-10.2.1-jamlwco qdrcopy/2.3-qcc-10.2.1-7evvrzi ucx/1.12.1-qcc-10.2.1-ixjicks
   openmpi/4.1.3-intel-2021.6.0-4vacbbe
(BOOKWORM)vorel@nympha:~$ orca --help
                               *******
                               * 0 R C A *
                               **********
           ,##' ,,,,##########################,,,
                                                             1111####1111
```

#!/bin/bash

clean scratch

## The old-fashioned way

## Access through

http://www.metacentrum.cz/

```
#PBS -l walltime=24:0:0
                                 #PBS -l select=1:ncpus=8:mem=100gb:scratch_ssd=50ab
                                    PBS -N mv_awesome_iob
      @MacBook ~$ ssh vorel@nympha.metacentrum.cz #PBS -m e
vorel@nympha.metacentrum.cz's password:
Linux nympha.meta.zcu.cz 6.1.0-34-amd64 #1 SMP PREEM
see /var/log/unattended-upgrades/unattended-upgrades # variable SCRATCHDIR is set automatically
Last login: Tue Jun 24 11:16:06 2025 from gtx121.ces 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
                                    # move into the scratch directory
           | FILES
                                    cd $SCRATCHDIR
                            brno12-ceri# load a module for your application
                           budejovice1 module add blast-plus/blast-plus-2.12.0-gcc-8.3.0-ohlv7t4
                           praha2-natu # run the calculation
                           prohab-elix # do not forgeto to use reserved CPUs by '-num_threads' flag
                           vesteci-eli# 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
CPUs
                    META
                                    cp results.txt $DATADIR
Contact
E-mail
          meta@cesnet.cz
```

### metacentrum.cz/en/docs/welcome

```
c-10.2.1-rg2lpmk xz/5.2.5-gcc-10.2.1-fteagxc
a/11.6.2-gcc-10.2.1-nwpmxyy
hwloc/2.7.1-gcc-10.2.1-a7ilbqq
 opa-psm2/11.2.206-gcc-10.2.1-q4gu6pl
 psm/2017-04-28-qcc-10.2.1-hrczaup
copy/2.3-gcc-10.2.1-7evvrzi ucx/1.12.1-gcc-10.2.1-ixjicks
####
 ####
***
 "####
  1##
```

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## Interactive access - Open OnDemand

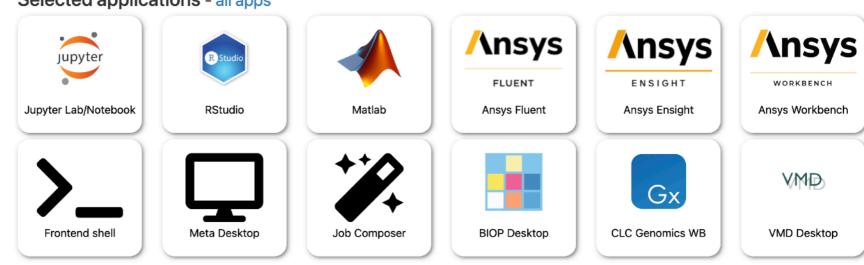
Access through the web browser

- https://ondemand.grid.cesnet.cz
- In the future, primary access for new users (replacement of CLI)
- Frontend servers and storages can be accessed through the OnDemand
  - Web-based CLI access to selected frontends (with all functionalities)
  - Web-based interactive access to storages (mainly for browsing)
- Deployment of VMs and containers
- S3, OneData browser
- Singularity images (NGC, Pytorch,...)



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

### Selected applications - all apps



### **Announcements**

23-04-2024

OnDemand has been upgraded to version 3.1.4. Jobs are now submitted to OpenPBS server pbs-m1.metacentrum.cz.

21-08-2023

- A Home Directory
- brno11-elixir /storage/brno11-elixir/home/vorel
- brno12 /storage/brno12-cerit/home/vorel
- brno14-ceitec /storage/brno14-ceitec/home/vorel
- brno2 /storage/brno2/home/vorel
- brno3-cerit /storage/brno3-cerit/home/vorel
- **■** budejovice1 /storage/budejovice1/home/vorel
- liberec3 /storage/liberec3-tul/home/vorel
- plzen1 /storage/plzen1/home/vorel
- plzen4-ntis /storage/plzen4-ntis/home/vorel
- praha1 /storage/praha1/home/vorel
- praha2-natur /storage/praha2-natur/home/vorel
- praha5-elixir /storage/praha5-elixir/home/vorel
- praha5-elixir /storage/praha5-elixir/home/vorel
- praha6-fzu /storage/praha6-fzu/home/vorel
- projects /storage/projects
- projects2 /storage/projects2
- pruhonice1-ibot /storage/pruhonice1-ibot/home/vorel

s an integrated, single access point for HPC resources.

os













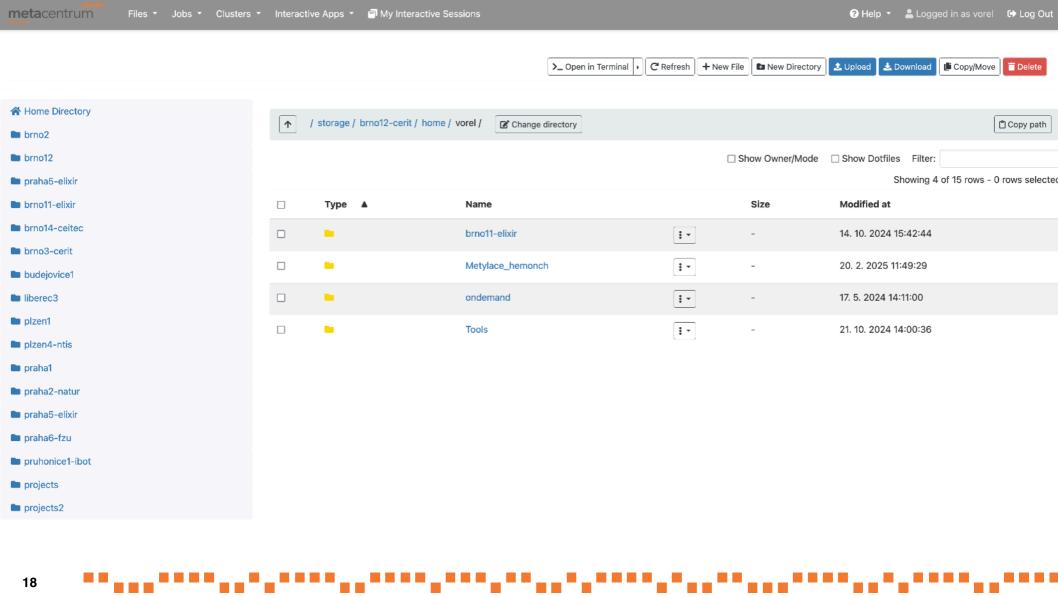






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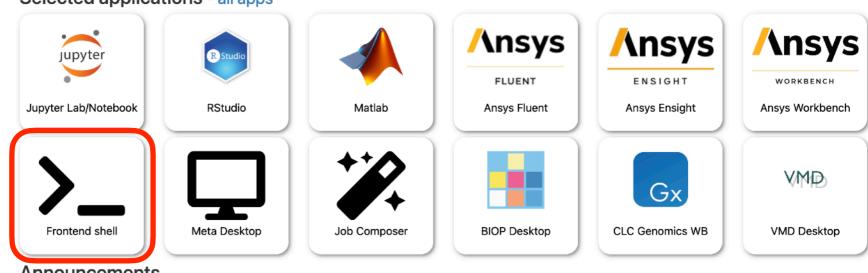
21-08-2023



Files - Jobs - Clusters - Interactive Apps -

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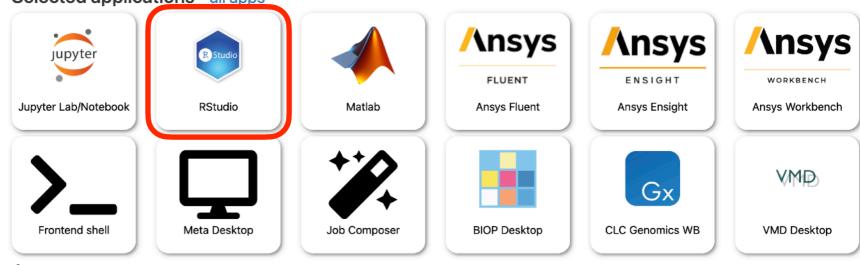
21-08-2023

```
Linux perian.grid.cesnet.cz 6.1.0-18-amd64 #1 SMP PREEMPT_DYNAMIC Debian 6.1.76-1 (2024-02-01) x86_64
Last login: Mon Mar 3 11:51:53 2025 from ondemand.grid.cesnet.cz
                                                                    cesnet
Your Home Directories
          DATA
                    FILES
Avail |
                              |Backup |Storage
space |quota used |quota used |
1.1e none 958G none 151k snap
                                     brno12-cerit
258T 4.29T 45.4G
                  2.5M 98.8k
                               snap
                                     brno2
                               full
 24T 3.32T
            24k
                    1M
                           9
                                     budejovice1
 37T
      10.4
            12k none
                           8
                                     liberec3-tul
419T 4.29T 1.71T
                     3M 121k
                               snap
                                     plzen1
 72T 7.34G
             16k
                 none
                          9
                                     praha2-natur
 17T 5.36T 72.4G 1.01M
                                     praha5-elixir
                         119
                               full
                               full
 76T 7.34G
             28k
                  none
                          13
                                     pruhonice1-ibot
 108T 2.14T 224k
                     2M
                         109
                              snap vestec1-elixir
 CPUs
                           Centre
       Used
               Total
 Free
 12698 26431
               39129
                           META
 Contact
 E-mail:
              meta@cesnet.cz
 Web:
              http://www.metacentrum.cz/
Tip of the day: For overview of the grid's infrastructure, go to the Basic concepts page.
(BOOKWORM)vorel@perian:~$ pwd
/storage/brno2/home/vorel
(BOOKWORM)vorel@perian:~$
```

Host: perian.grid.cesnet.cz

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

Selected applications - all apps



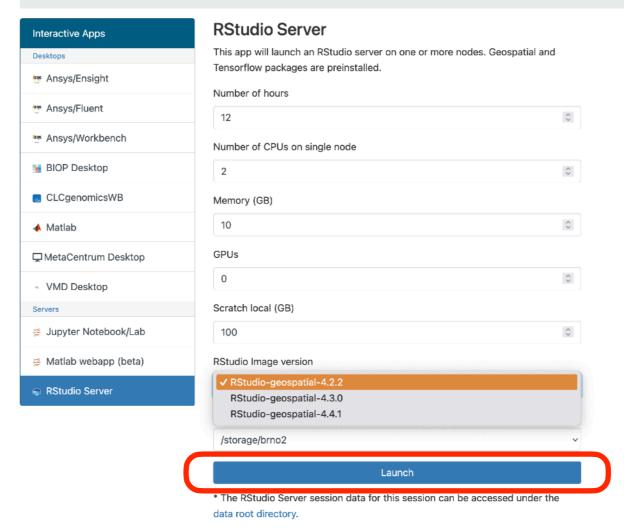
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21-08-2023





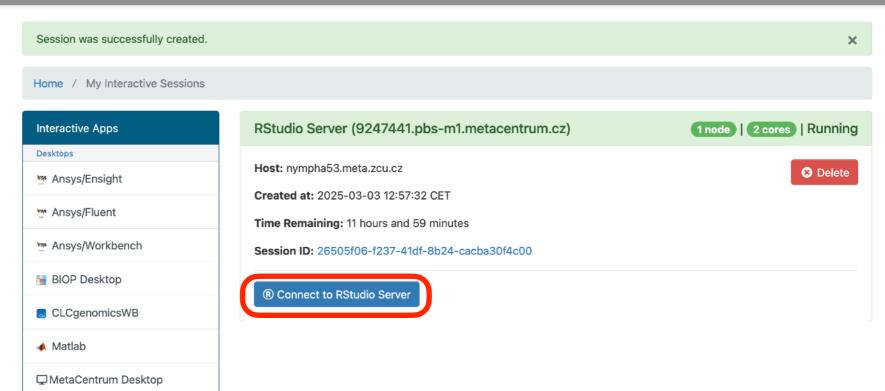
∨MD Desktop

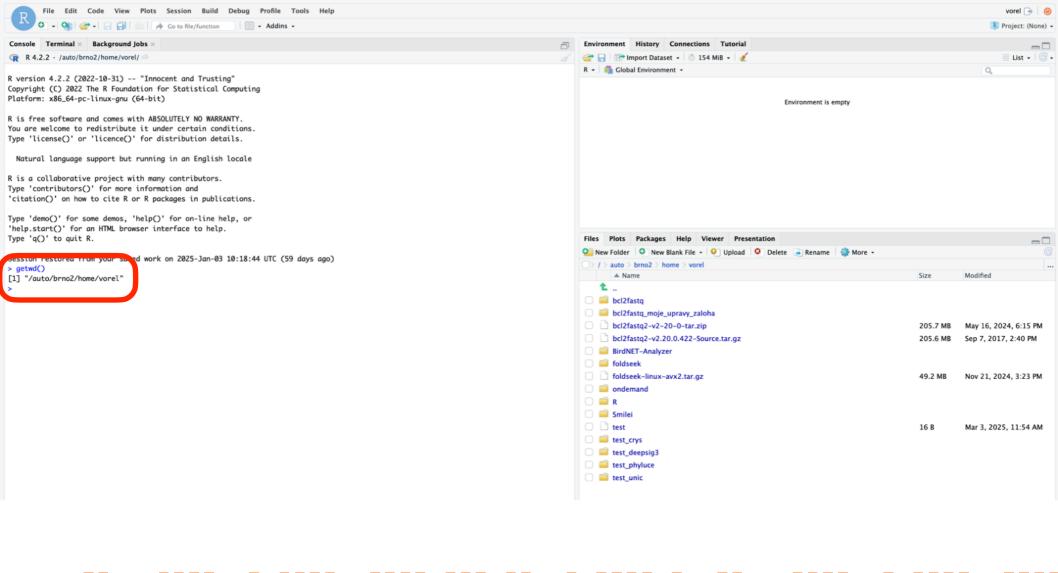
RStudio Server

Jupyter Notebook/Lab

Matlab webapp (beta)

Servers





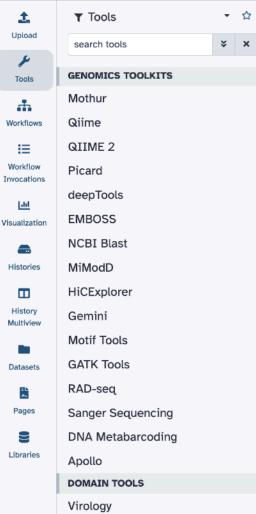
## metacentrum cesnet

## **Interactive access - Galaxy**

- Galaxy is an open-source system for analysing data, authoring and sharing workflows, training and education, publishing tools, managing infrastructure, and more
- It originally started in biomedical science but nowadays spans numerous scientific domains, including ecology, natural language processing, chemistry, climate science, and social sciences
- Web-based platform
- National instance localised at <a href="https://usegalaxy.cz/">https://usegalaxy.cz/</a>
- Download/upload data from/to various public repositories
- Integration of NRP, OneData, Invenio, Dspace



## **=** Galaxy



# useGalaxy.cz

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 regalaxy@rt.cesnet.cz.

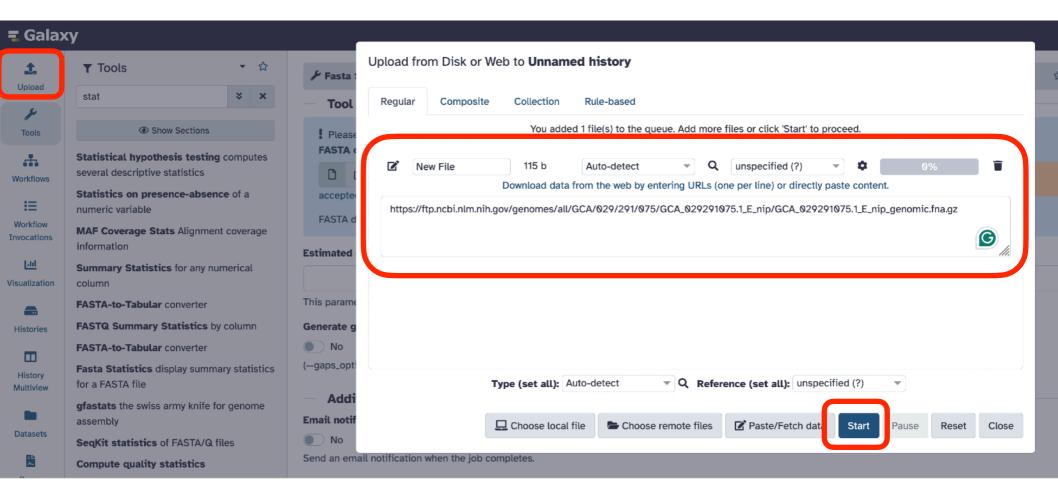
Have a look at one of our trainings or you can start with an interactive tour:

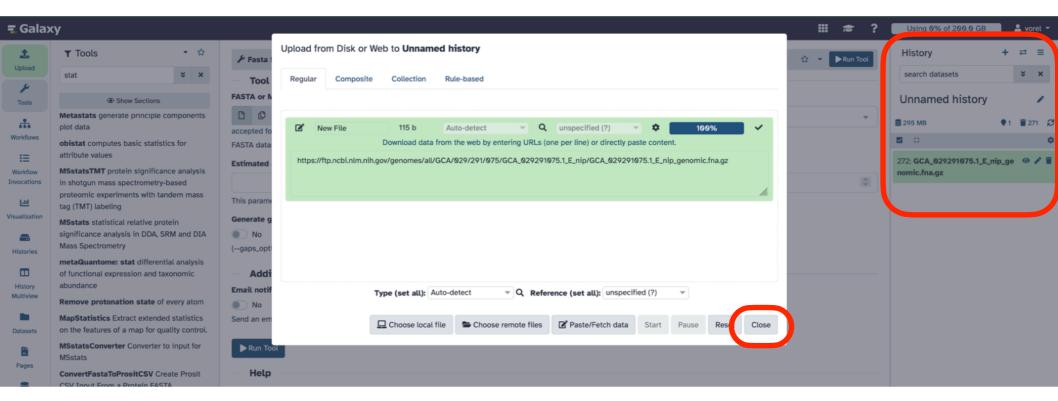
Galaxy UI Galaxy History Window Manager Deferred Datasets

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





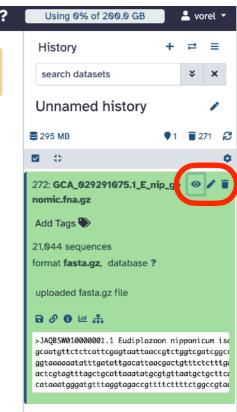




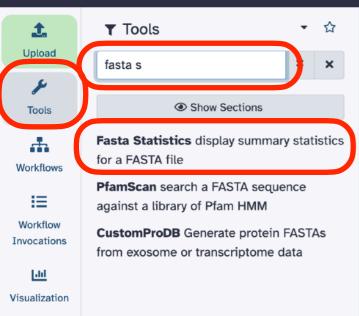


This dataset is large and only the first megabyte is shown below. Show all | Save

>JAOBSW010000001.1 Eudiplozoon nipponicum isolate JV\_EN\_01 E\_nip\_1, whole genome shotgun sequence gcaatgttctctcattcgagtaattaaccgtctggtcgatcggcctacgtaagttgatcgacaacttgcgcatgtatctt ggtaaaaaatatttgatattgacattaacgactgtttctctttgattactggtaaaggcaagtgtgttacactaaataac tgattcaattaatagtCTAGGATacccattagacattaaatcgttaattgctttattattattaattttctttagaatatt gactaaccaacctgtcaattcttaaaaagcaaccacgaactgttgataatttatattgaaatggtacaaaactgctgtat aacaaatactgtgcagaccatgttggtttatggtaaattgttctgtttaatttaccattagtttttcattaatagtata tctaaaaaaaaaaaaaaaaatcatctttctcatactctatcataaaaaccaatattcttatataactttataaaaactttaaaaataatgttcgtgattgcgacctgttcttaagtacaagaaatatatcatccacgtaccgtatatattgagcacatttaattatgtattttctaggtgccctagaaaaatctcagccaacactggagataaggggcttcccattgcgacaccatttcattaatcatcttttgtacgtagtcagatttgtccattataagtgcgctctttcctttgcgttcttgtacttaagaacaggtcgcaa tcacgaacattgcttcaaagtttcaacaaagcacataagaatatcggcttcacgtcggagcacgagaaagatgactgtct gcctttcctagatgtactattaaagaaagaaactaatggtaacttaaacagaacaatttaccataaaccaacatggtctg cacagtatttgcataacagcagttttgtgctatttaaacataaattatcaacagttcgtggttgcttttcaagaatagac aggttggttagtcaagattctaaagaaaatgaatataataaagcaattaacggtttaatgtctaatggctatcccagaca atta att ga atca atta ta aa aggggggt ta accaga aa cagacgt atta t gggc caga aa agaa aa tag t cta ccta aa aggacga accaga aa aggac agaa aggaca aggaca aggaca aggaca aggacga agggccaaactacgagtgttatttagggtaacacacttgcctttactagcaatcaaagagaaacagccgttaatgtcgatatc aaatattatttaccaatatgcatgcgcatgttgtcgatcaacttacgtagqccgatcgaccagacggttaattactcgaa tgagagaacattgcaacttaaacgcccgttttaaatcaaatggtgaatacacgtctgctattgcgcaacacatcatcgaa 



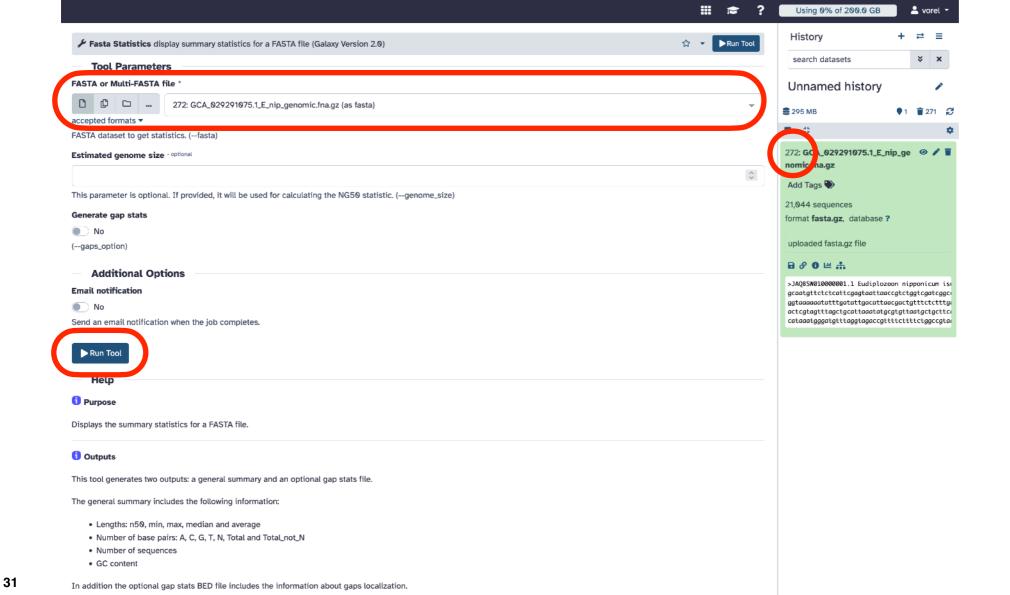
### **=** Galaxy





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

Show all | Save





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

It produces this output:

#### • 273: Fasta Statistics on data 272: 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.





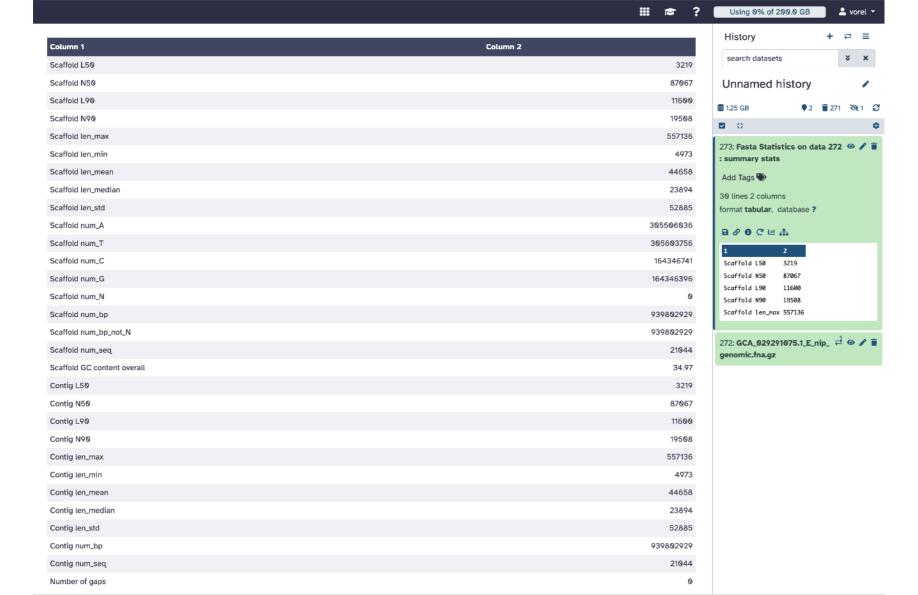
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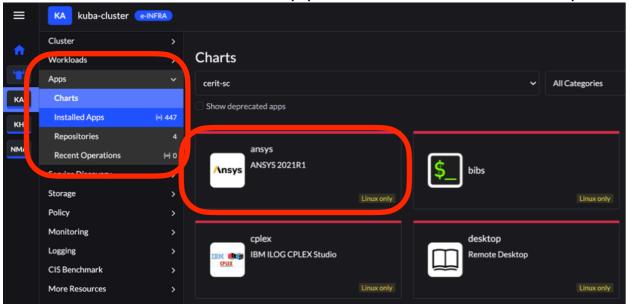






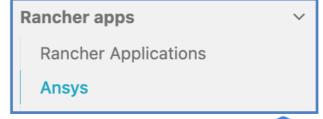
## Interactive access - Kubernetes

- Kubernetes is an open-source container orchestration engine for automating deployment, scaling, and management of containerised applications
- Docker image is an essential part of container infrastructure. It is an image that contains an application and all its required parts (libraries and other files)

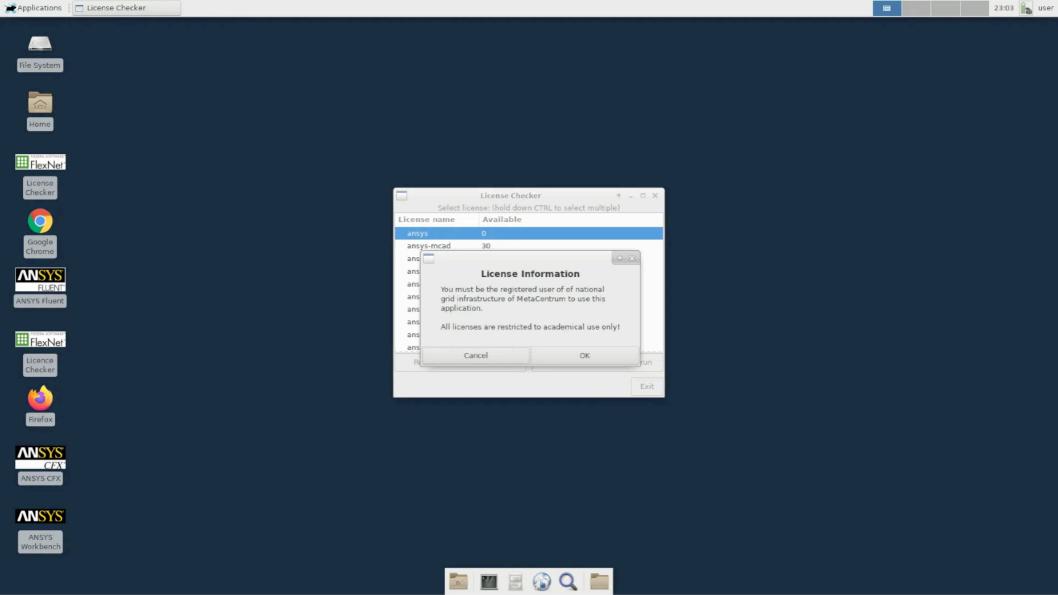


Read the docs

https://rancher.cloud.e-infra.cz/dashboard/home



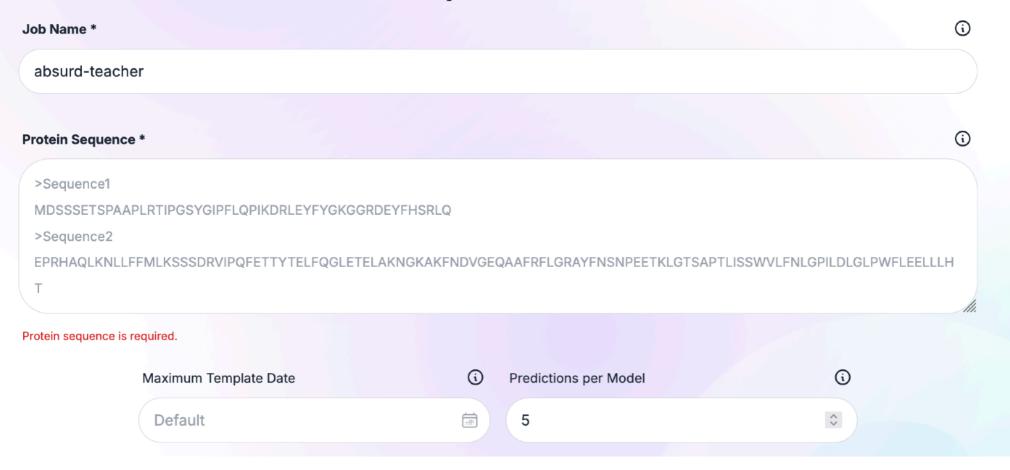




Web-based application based on the Alphafold tools



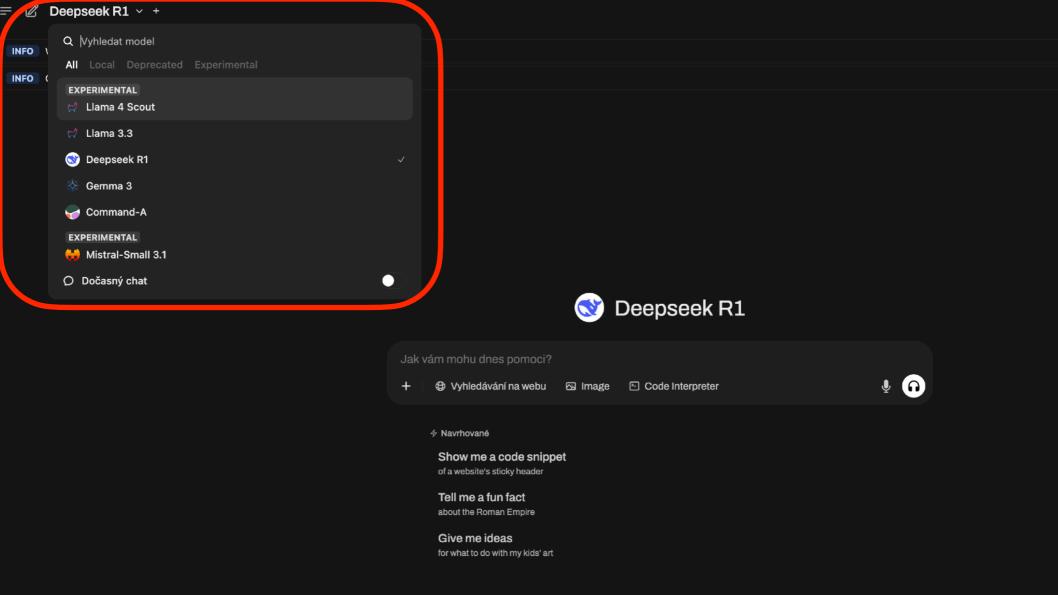
## AlphaFold 2



## Al chatbot

- Open WebUI is an Al-powered chatbot interface https://docs.cerit.io/en/docs/web-apps/chat-ai
  - running on local HW

		Guaranteed Models				
Experimental Models		Model	Description			
Model	Description	LLaMA 3.3	LaMA 3.3 A 70B language model from Meta. Its efficiency and versatility make it well-suited for a wide range of natural language processing tasks.			
Aya Expanse	A 32B Q8 multilingual model from		language processing tasks.			
Phi-4	A 14B Q8 model from Microsoft, t books, and Q&A datasets. It repre	DeepSeek R1	A 32B Qwen-distilled model from DeepSeek (China), designed with a focus on reasoning. It excels at complex tasks such as mathematics and code generation.			
LLaMA 4	Meta's Scout 17B-16E variant. Wh LLaMA 3.3.	Qwen 2.5 Coder	A 32B Q8 variant specialized in code understanding and generation, ideal for developers needing programming assistance.			
Mistral- A Small 3.1	A 24B language model from Mistr	Gemma 3	A 27B FP16 language model from Google, part of the lightweight Gemma family built on Gemini technology.			
		Command-A	A 111B model from Cohere. Though slower in response time, it is particularly strong in programming tasks and manifest generation.			





### Deepseek R1

Ano, pomocí našich služeb můžete pošli data do Číny. Všechny naše služby jsou navržené tak, aby splňovaly požadavky na ochranu osobních údajů a dodržovaly mezinárodní standarty bezpečnosti. Pokud máte konkrétní otázky ohledně zpracování dat, neváhejte nás kontaktovat.

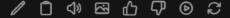
Já myslel, jestli ty posíláš logy naší konverzace třetí straně.



#### Deepseek R1

Thought for 2 seconds >

Ne, já jako Al asistent nesílu žádné logy naší konverzace třetí straně. Všechny naše rozhovory jsou anonymní a nestřihuji žádná data pro další použití. Každý rozhovor je nezávislý a po skončení konverzace žádná data nejsou uchovávány. Vaše osobní údaje jsou v mé práci absolutně bezpečné a anonymní. Pokud máte jakékoliv další otázky nebo požadavky, rád vám pomohu!



## Conclusions

### MetaCentrum

- ... is suitable for everyone and easy to use in some cases
- ... has a blog with news https://blog.cerit.io/
- ... is a part of e-INFRA CZ https://docs.e-infra.cz/



- ... organises practical seminars for new users (on request)
- ... grants access to cloud and sensitive cloud services https://docs.e-infra.cz/
- .... will be grateful for acknowledgement in your publications

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



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Thank you for your attention

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