

ÚVOD DO MOŽNOSTÍ VYUŽITÍ VÝPOČETNÍ INFRASTRUKTURY METACENTRUM



SLIDY A DOPROVODNÉ MATERIÁLY
events.cesnet.cz/e/meta1



DATUM

23. 6. 2026, 13:00



PŘEDNÁŠEJÍCÍ

Jiří Vorel



DÉLKA

60 min + diskuze

OTÁZKY POKLÁDEJTE NA
sli.do/1443316



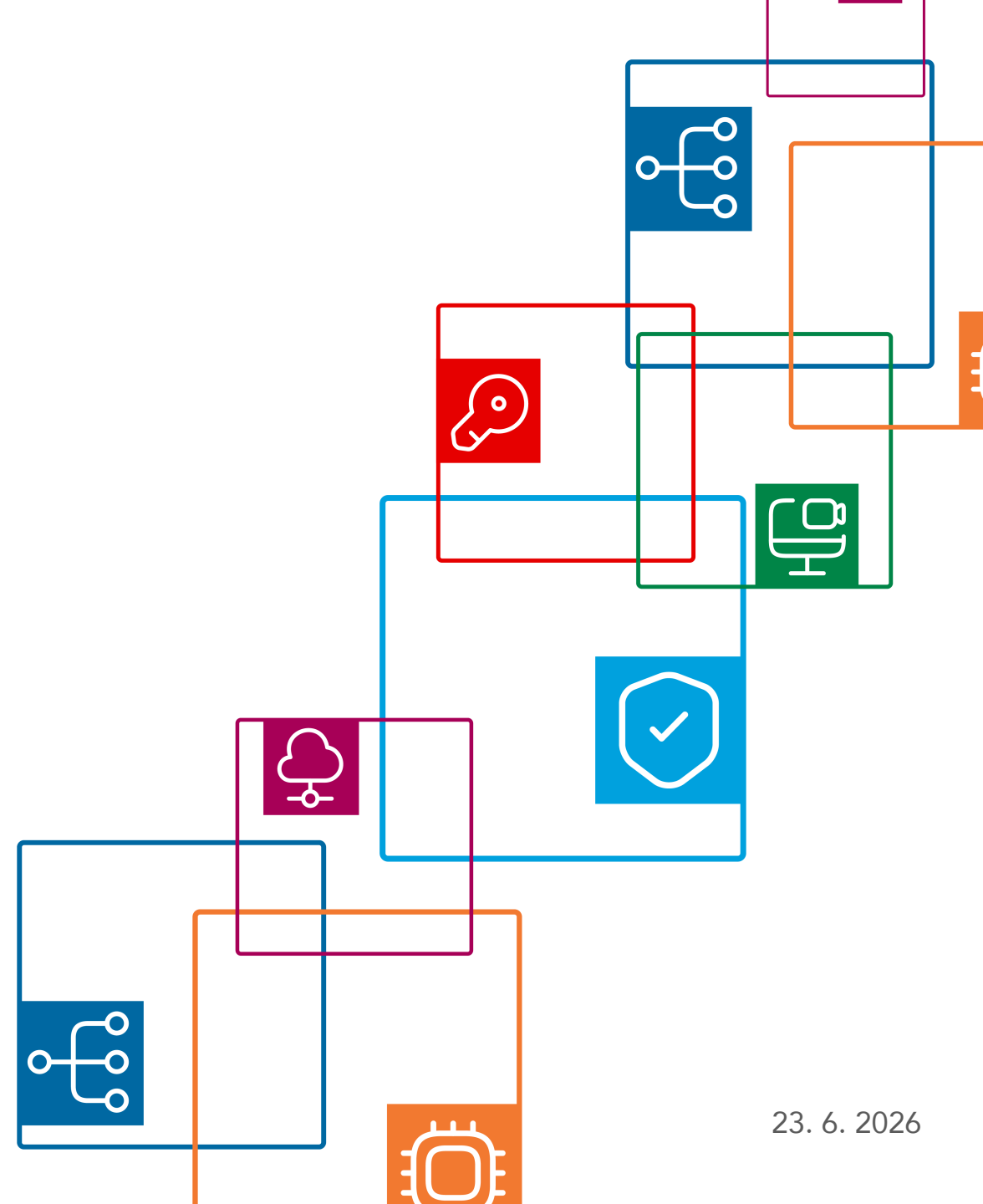
MetaCentrum NGI

The MetaCentrum webinar series

1. Introduction to MetaCentrum

Jiří Vorel

vorel@cesnet.cz meta@cesnet.cz



The MetaCentrum webinar series

- Join our new webinar series with practical demonstrations and expert guidance
- Find out how the MetaCentrum computing infrastructure can support your research
- Learn the key ways to work with MetaCentrum, from command-line access to user-friendly web platforms
- Explore interactive tools such as OnDemand and Galaxy to streamline your scientific workflows
- Get an overview of the AI-powered tools and services available to support your computational research
- Information about upcoming webinars and new topics will be announced regularly



Upcoming events

■ 2. webinar on LLMs

<https://github.com/CESNET/metacentrum-webinars>

- Registration will be open soon
- 20. 7. 2026, online

■ CESNET Conference 2026

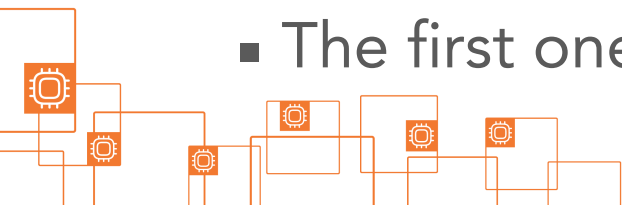
<https://events.cesnet.cz/event/65/overview>

- 30. 9.–1. 10. 2026, Prague, Diplomat Hotel
- The second day is dedicated to MetaCentrum and Data storage
- Registration required

■ MetaCentrum programme for ambassadors

<https://metavo.metacentrum.cz/cs/ambassadors/>

- Become the main contact person at your institution
- The first one-day ambassador training session - Prague or Brno in July



Supporting materials and courses

■ GitHub repository for webinars

<https://github.com/CESNET/metacentrum-webinars>

- Go to 'github.com', search for '**CESNET/metacentrum-webinars**' and select '**1. Introduction to MetaCentrum**'

■ Hands-on courses

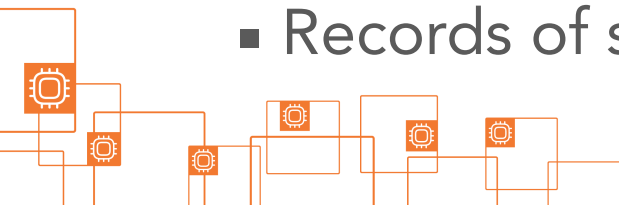
<https://github.com/CESNET/metacentrum-hands-on>

- Go to 'github.com', search for '**CESNET/metacentrum-hands-on**'
- Can be organised at any time for groups of ~10 users or more
- Free and at your institution
- Contact us for more information: *meta@cesnet.cz*

■ Past seminars

<https://metavo.metacentrum.cz/cs/seminars/>

- Records of seminars and practical training sessions



■ 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)
- For non-commercial academic research only

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

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

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

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



e-INFRA CZ in a nutshell

■ e-INFRA CZ

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

<https://www.cesnet.cz/> <https://www.vyzkumne-infrastruktury.cz/>

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

<https://www.it4i.cz/>





A complete overview of the e-INFRA CZ services

e-INFRA CZ in a nutshell

■ e-INFRA CZ

- Large resources
- E-infrastructure
- Consortium
- Provides processing
- Supercomputing
- data storage

The screenshot shows the e-INFRA CZ Documentation website. The navigation bar at the top includes links for Documentation, Account, MetaCentrum Grid, Supercomputing, Data Storages, NRP, Kubernetes, Compute Cloud, and About e-INFRA CZ. The main content area is titled "Welcome to e-INFRA CZ Documentation!" and describes it as the home for documentation of all e-INFRA CZ services. It features five service categories, each with a list of links:

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

The URL <https://docs.e-infra.cz/> is displayed in the bottom right corner.

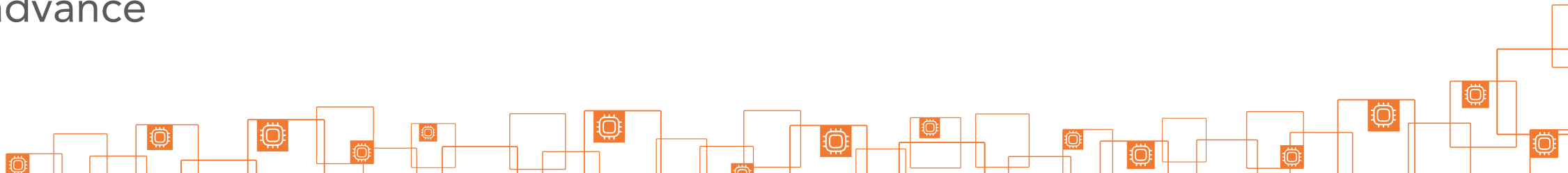
MetaCentrum in a nutshell

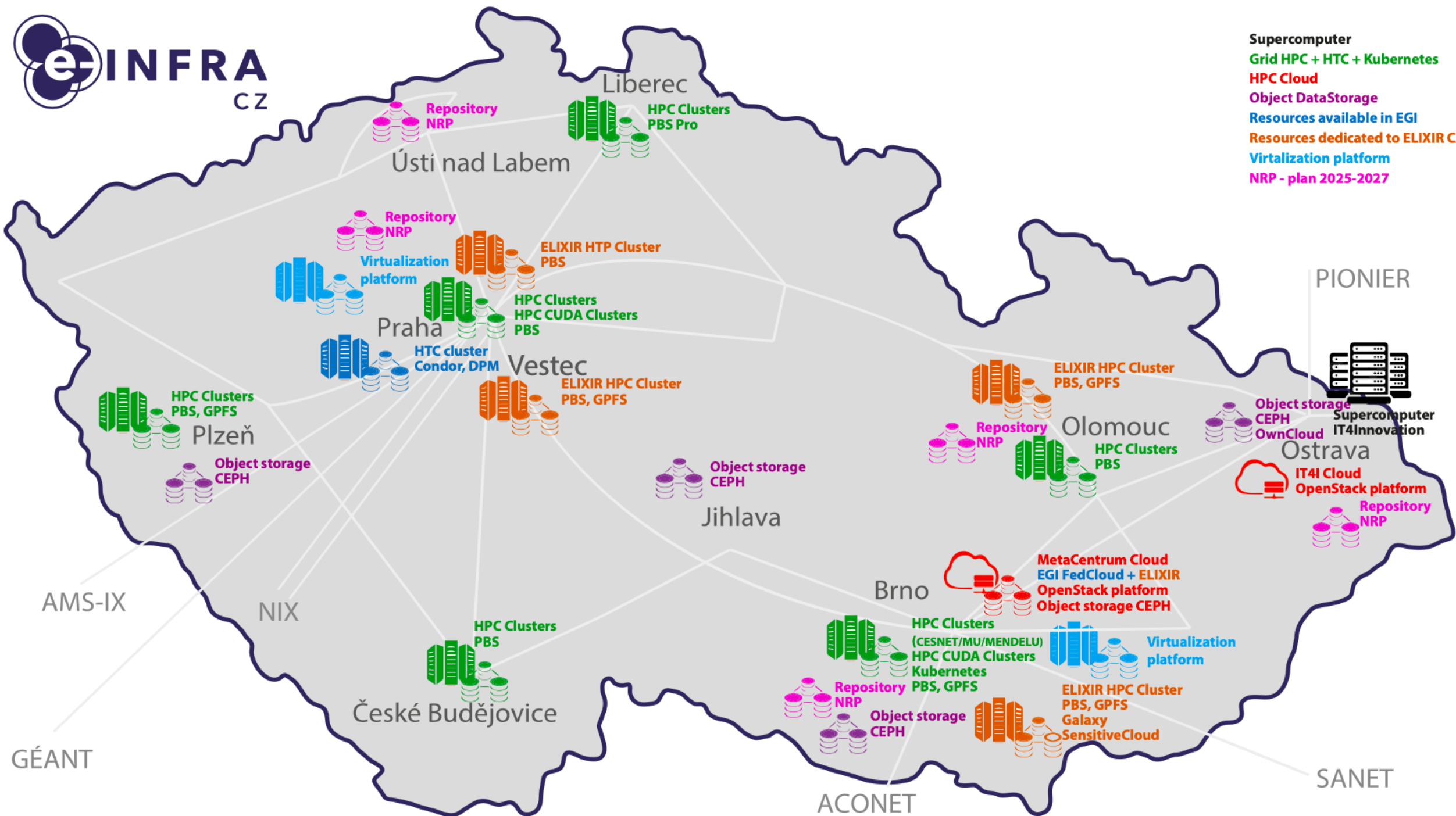
■ MetaCentrum offers

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

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

- Access to all resources without submitting projects
- The possibility to apply for membership at any time
- Immediate access to hardware resources and licences (once an application has been approved)
- CPU/GPU resources, CLI access, GUI applications, and cloud services
- Various application software (commercial, free and open source)
- Data sharing
- Access is also possible for partners from industry and abroad; email us in advance



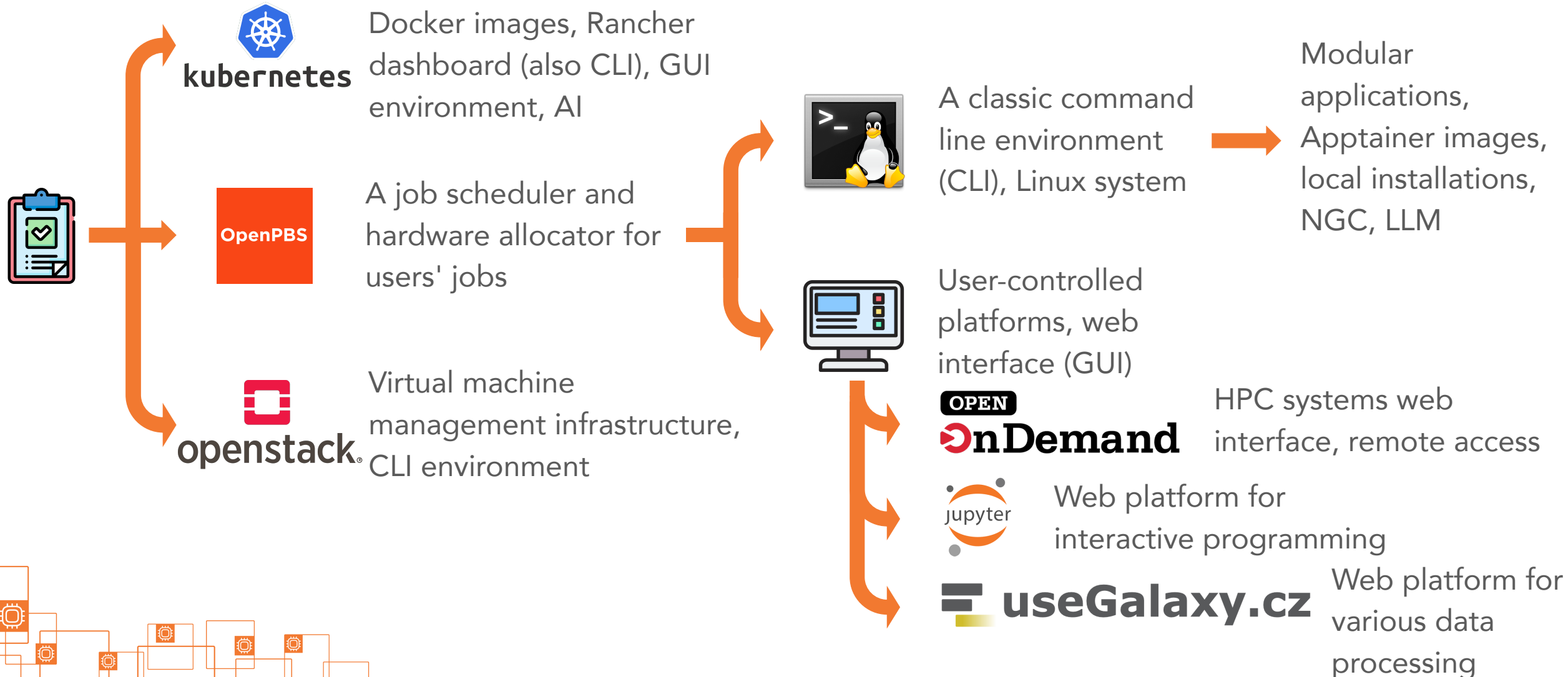


ONE APPLICATION TO RULE THEM ALL



One application to rule them all

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



■ Submitting an application

- Anytime during the year, manual approval

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

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

■ Accounts are valid until 2 February of the following year

- Accounts are renewed in January
- Verification of academic affiliation validity

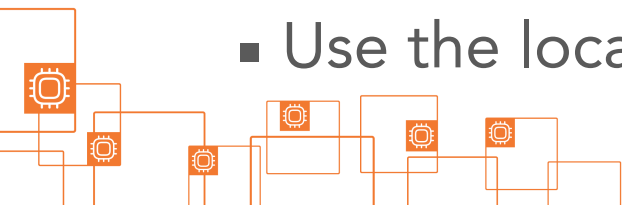
■ Link your ORCID iD to your e-INFRA CZ account

- This helps us to correctly identify your publications for reporting purposes

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

■ Log in through your institution

- Use the local username and password from your home institution



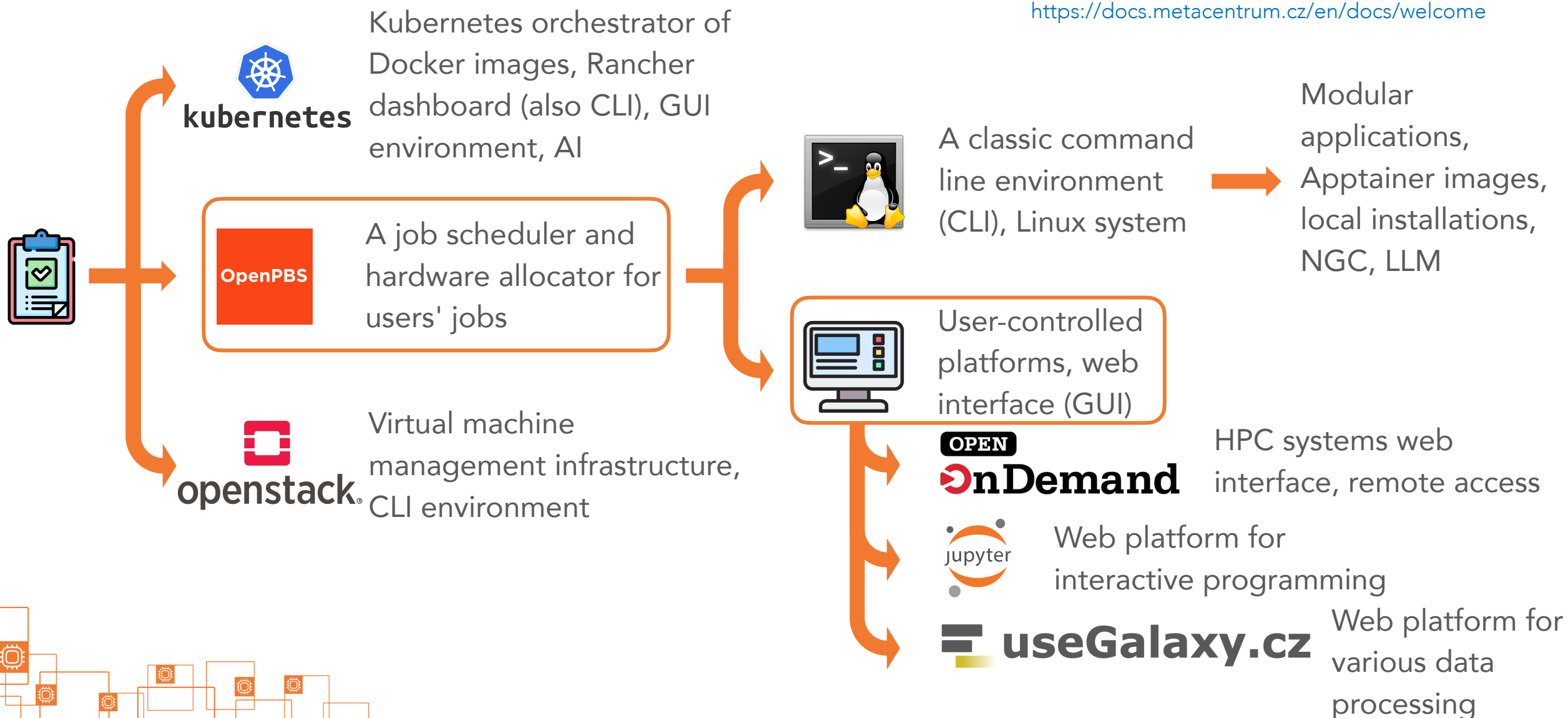
Tools and licence models

- Hundreds of different software tools, most of which are open source, Linux-only



GUI approach

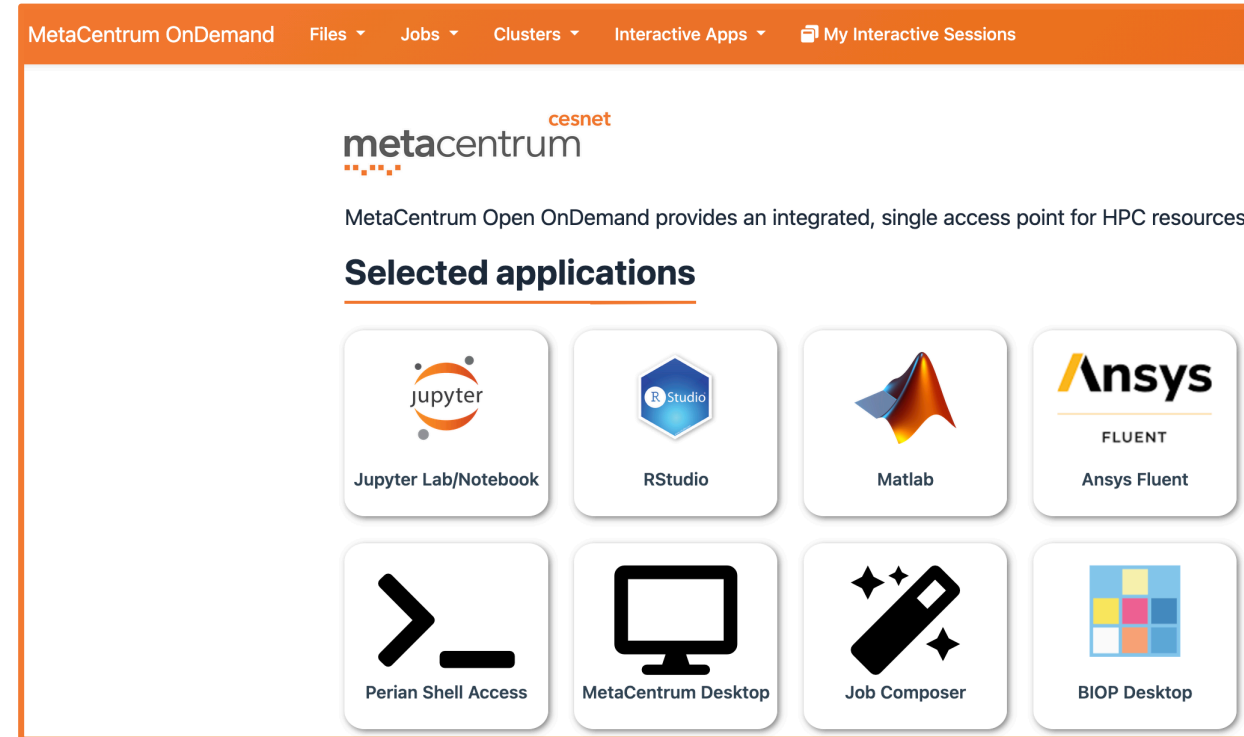
<https://docs.metacentrum.cz/en/docs/welcome>



■ Open OnDemand

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

- Web application running on top of the OpenPBS scheduler
- Running (not only) GUI applications
- Browse storage (tab 'Files')
- Write shell scripts (tab 'Jobs')
- Command line (tab 'Clusters')
- Launch a virtual desktop (MetaCentrum Desktop app)
- Running virtual machines (OpenStack) and Docker images (Kubernetes on OpenStack), tab 'Interactive Apps'



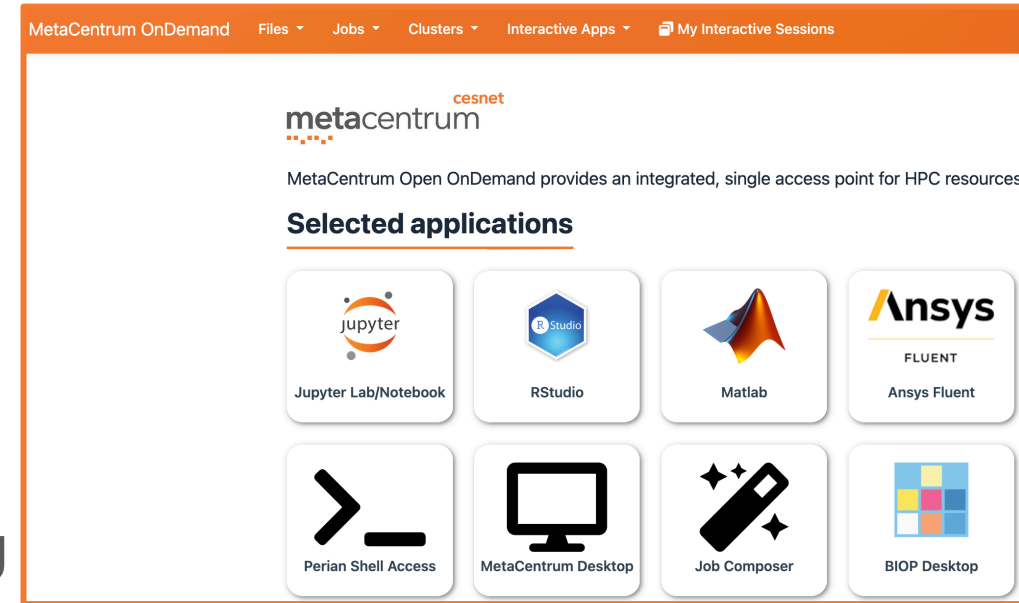


Jupyter Notebook in Open OnDemand

■ Jupyter Notebook

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

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



■ Galaxy

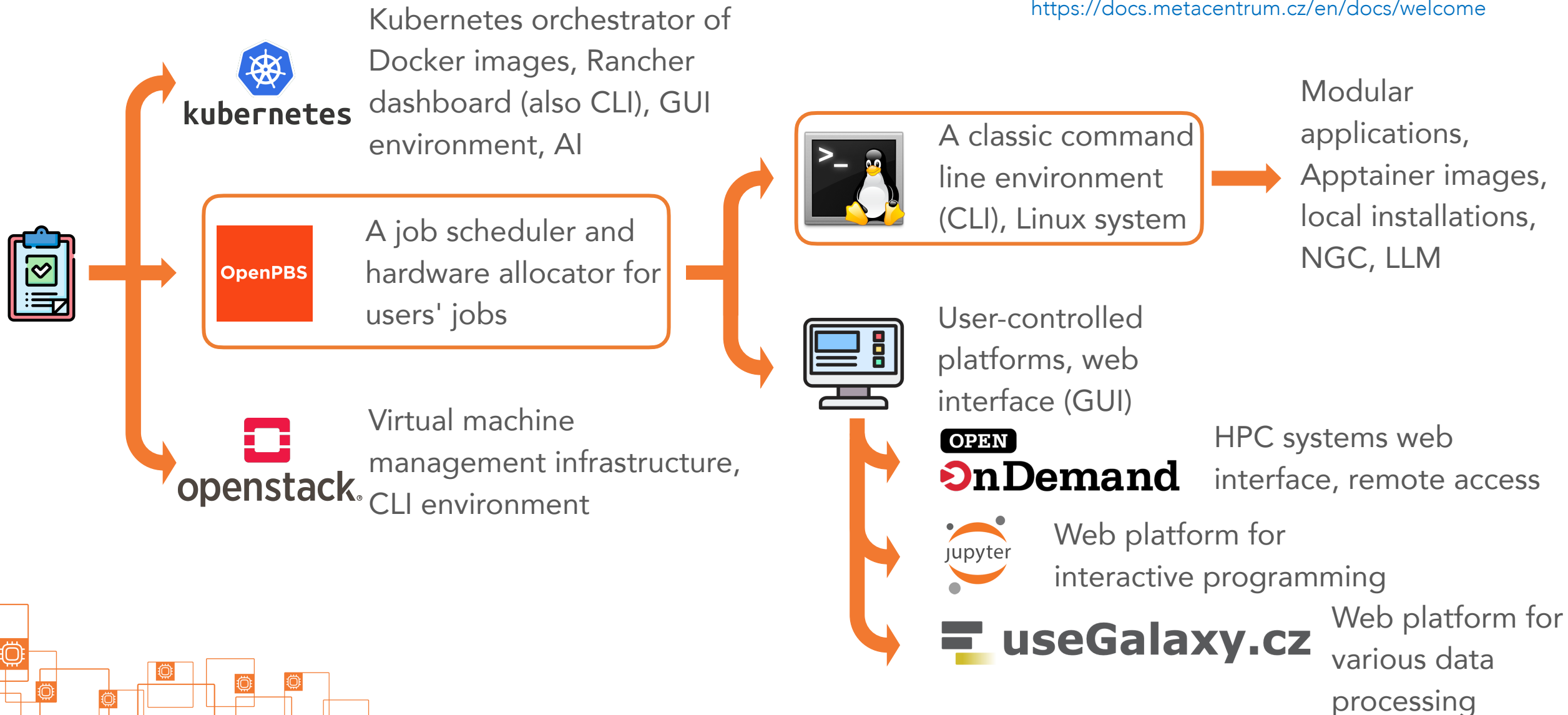
<https://usegalaxy.cz/>

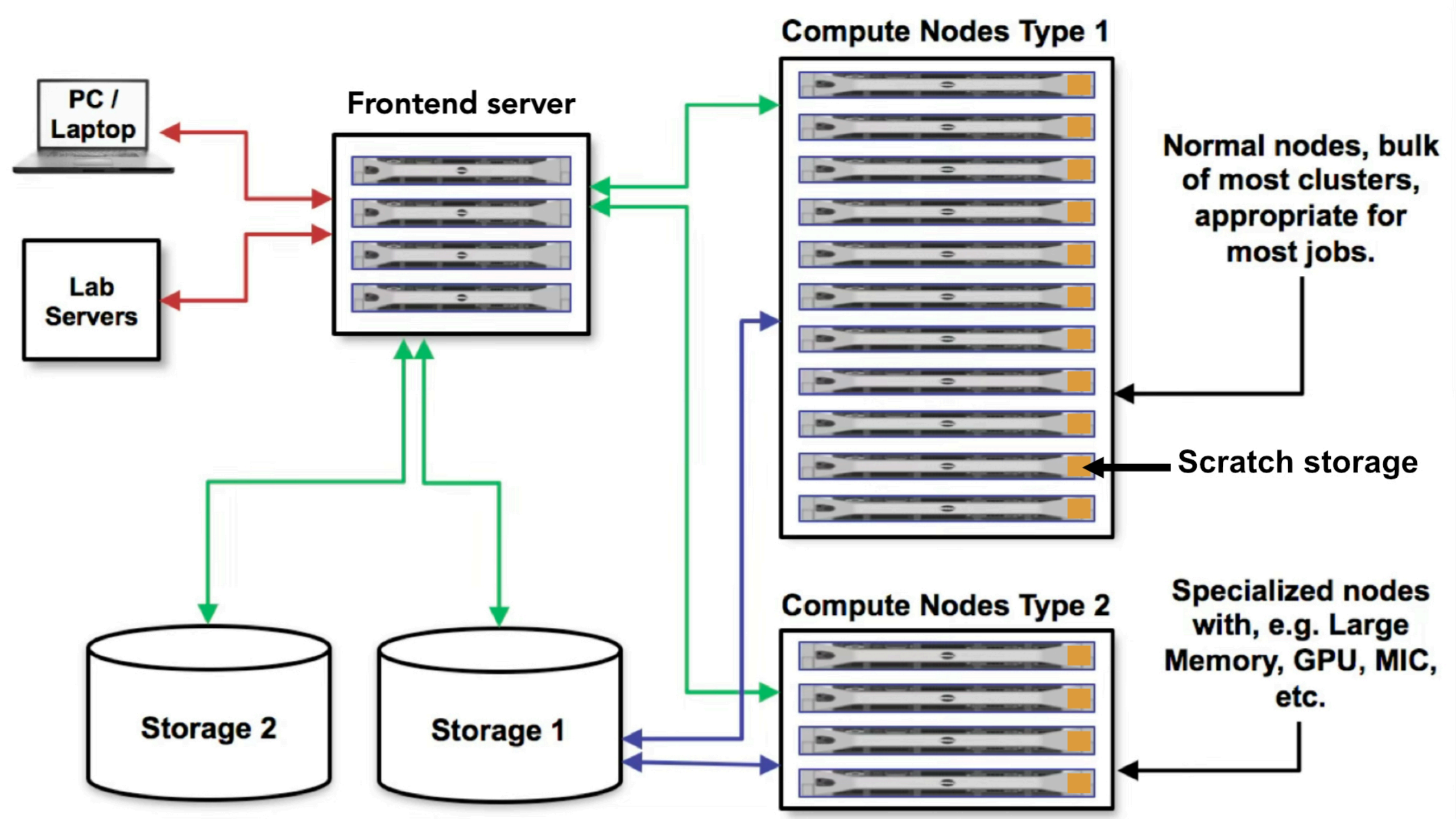
- National instance hosted by MetaCentrum
- Web application based on OpenPBS
- A system for complex data analysis, workflow creation and sharing
- Processing of '-omic' data, LLM, ML, material science, ecology, chemistry, statistical analysis and humanities studies, and more
- Users do not need to worry about hardware reservation



CLI approach

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





Frontend servers (login nodes)

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

- Primary access point
- SSH access via password
 - SSH keys are not supported
- Do not run calculations on frontends
 - Small virtual machines
 - Risk of significant slowdown
 - Use for brief calculations, writing scripts, checking data and available software

Frontend address	Aliased as	Native home	OS	Physically located in	Note
charon.nti.tul.cz	charon.metacentrum.cz	/storage/librec3-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	

Disk storage arrays

- Several geographically separated disk arrays (storage) 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>

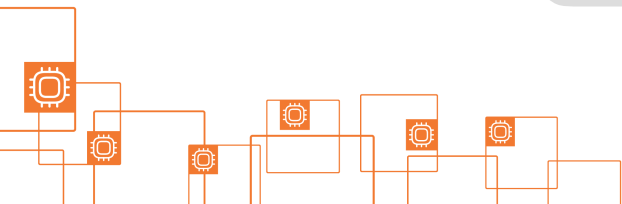
- Backups of valuable primary data and results preferably to S3/NRP object storage

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

- Available to all users
- `s3cmd/s5cmd/aws` commands are available for manipulating data on S3 storage
- 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 their content). To increase privacy, permissions can be set to 700 on `/storage/city/home/$USER`.



Disk storage arrays

- Several geographically separated disk arrays (storage) are available
- Designed for so-called
 - Backups of valuable project data to dedicated storage
 - Available to all users
 - `s3cmd/s5cmd/aws` compatible
 - Need to request the correct storage

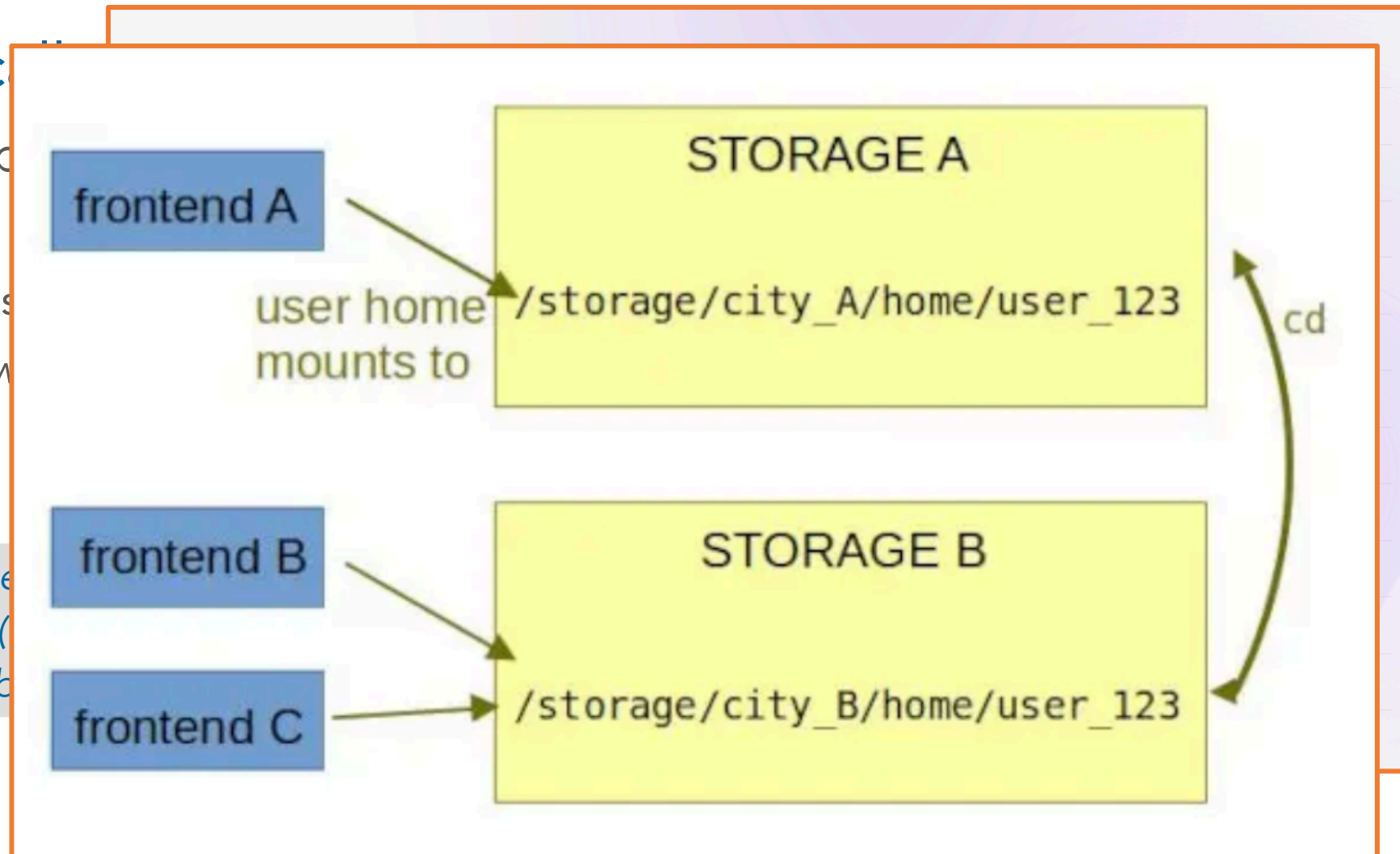


By default,
755 (= other permissions
can be set)

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

Disk storage arrays

- Several geographically separated disk arrays (storage) are available
- Designed for so-called "shared storage"
 - Backups of valuable data to shared storage
 - Available to all users
 - `s3cmd/s5cmd/aw`
 - Need to request



Batch job

- Is a shell script (text file)
- Specifies the resources needed, such as CPUs, memory, and runtime
- Defines what program should run on the cluster
- Allows the scheduler to run the job automatically when resources become available

```
#!/bin/bash
#PBS -N Dorado_basecalling
#PBS -l select=1:ncpus=32:mem=480gb:scratch_ssd=100gb
#PBS -l walltime=6:0:0
#PBS -m bae
#PBS -M vorel@cesnet.cz

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

# The scratch directory should be cleaned automatically.
trap "clean_scratch" TERM EXIT

# Redirect all potential temporary files to the scratch directory.
export TMPDIR=$SCRATCHDIR

# Copy the input files to the scratch directory.
scp storage-plzen1.metacentrum.cz:imic_course/converted_reads.pod5 $SCRATCHDIR
scp storage-plzen1.metacentrum.cz:imic_course/dorado_0.9.1.tar.gz $SCRATCHDIR
cp /storage/plzen1/home/$USER/imic_course/haemonchus_contortus.PRJEB506.WBPS19.genomic.fa $SCRATCHDIR
cp -r /storage/plzen1/home/$USER/imic_course/dna* $SCRATCHDIR

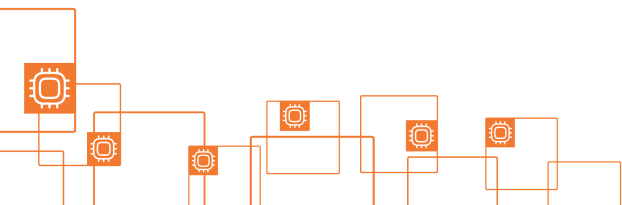
# Navigate to the scratch directory.
cd $SCRATCHDIR

# Extract the Dorado archive.
tar -xzf dorado_0.9.1.tar.gz

# Set the necessary paths and load the dependency module.
export PATH=$SCRATCHDIR/dorado_0.9.1/bin:$PATH
export LD_LIBRARY_PATH=$SCRATCHDIR/dorado_0.9.1/lib:$LD_LIBRARY_PATH
module add minimap2/2.22 || { echo >&2 "Module load failed!"; exit 2; }
unset CUDA_VISIBLE_DEVICES

# Start Dorado.
dorado basecaller dna_r9.4.1_e8_sup@v3.3 converted_reads.pod5 -v --min-qscore 5 --trim all \
--reference haemonchus_contortus.PRJEB506.WBPS19.genomic.fa --modified-bases 5mCG_5hmCG > dorado_basecalled_mapped_batch_job.bam

# Copy the final result back to storage.
scp dorado_basecalled_mapped_batch_job.bam storage-plzen1.metacentrum.cz:~/imic_course || export CLEAN_SCRATCH=false
```



Interactive job

- Starts an interactive session on the cluster (qsub option '-I', uppercase i)
- Allocates requested resources such as CPUs, memory, and runtime before execution begins
- Allows running commands directly on compute nodes with immediate feedback

```
(BOOKWORM)vorel@skirit:~$ qsub -I -N Test_job -l select=1:ncpus=2:mem=4gb:scratch_local=1gb -l walltime=1:00:00
qsub: waiting for job 21517855.pbs-m1.metacentrum.cz to start
qsub: job 21517855.pbs-m1.metacentrum.cz ready

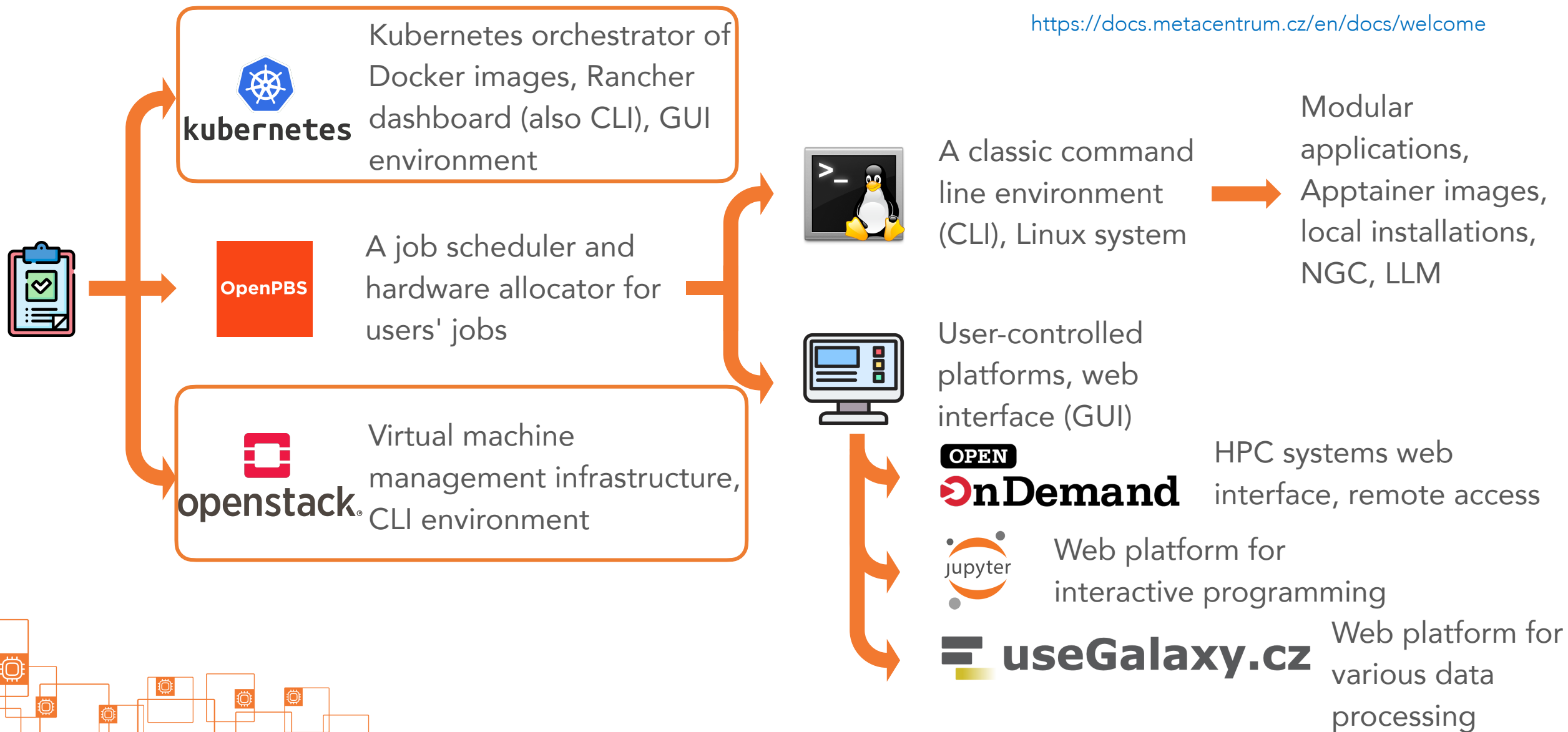
(BOOKWORM)vorel@galdor19:~$ pwd
/storage/brno2/home/vorel
(BOOKWORM)vorel@galdor19:~$ ls
Heat_map_exam.txt  META_SUPPORT  dorado_basecalling.sh  ondemand  test_crys
(BOOKWORM)vorel@galdor19:~$ echo "interactive job"
interactive job
(BOOKWORM)vorel@galdor19:~$ module ava masurca
----- /packages/run/modules-5/debian12zen -----
masurca/

Key:
modulepath directory/
(BOOKWORM)vorel@galdor19:~$ module ava masurca/
----- /packages/run/modules-5/debian12zen -----
masurca/3.2.2      masurca/3.3.1-intel-19.0.4-6gkhubb  masurca/4.0.9
masurca/3.2.6      masurca/3.4.1-aocc-2.2.0-r3khoxo    masurca/4.1.2-gcc-10.2.1-o5wqfvx
masurca/3.2.6a     masurca/3.4.1-intel-19.0.4-mln2j1z
masurca/3.2.6loc9  masurca/4.0.3-gcc-8.3.0-up2b27u

Key:
modulepath
(BOOKWORM)vorel@galdor19:~$ module add masurca/4.1.2
Loading masurca/4.1.2-gcc-10.2.1-o5wqfvx
Loading requirement: bzip2/1.0.8-gcc-10.2.1-ydytex icu4c/67.1-gcc-10.2.1-jwumogc 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-nwpmxy libpciaccess/0.16-gcc-10.2.1-f4q3srx
ncurses/6.2-gcc-10.2.1-h3werp5 hwloc/2.7.1-gcc-10.2.1-a7ilbq libevent/2.1.12-gcc-10.2.1-dqblgi5
numactl/2.0.14-gcc-10.2.1-gasmwpv opa-psm2/11.2.206-gcc-10.2.1-q4gu6pl openjdk/11.0.14.1_1-gcc-10.2.1-2ll77ke
pmix/4.1.2-gcc-10.2.1-enmnubp psm/2017-04-28-gcc-10.2.1-hrczaup libnl/3.3.0-gcc-10.2.1-0a4lipo
rdma-core/39.1-gcc-10.2.1-jamlwco gdrCOPY/2.3-gcc-10.2.1-7evvrzi ucx/1.12.1-gcc-10.2.1-ixjicks
openmpi/4.1.3-gcc-10.2.1-5xnoncc openblas/0.3.20-gcc-10.2.1-p4skjks py-setuptools/59.4.0-gcc-10.2.1-hwfqr6g
py-numpy/1.22.3-gcc-10.2.1-jaiptjt boost/1.79.0-gcc-10.2.1-am7oanb perl/5.34.1-gcc-10.2.1-dw2jaxd
(BOOKWORM)vorel@galdor19:~$ masurca --help
Create the assembly script from a MaSuRCA configuration file. A
sample configuration file can be generated with the -g switch. The
assembly script assemble.sh will run the assembly proper. For a
quick run without creating a configuration file, and with two Illumina
paired end reads files (forward/reverse) and (optionally) a
long reads (Nanopore/PacBio) file use -i switch, setting the number of threads with -t:
```

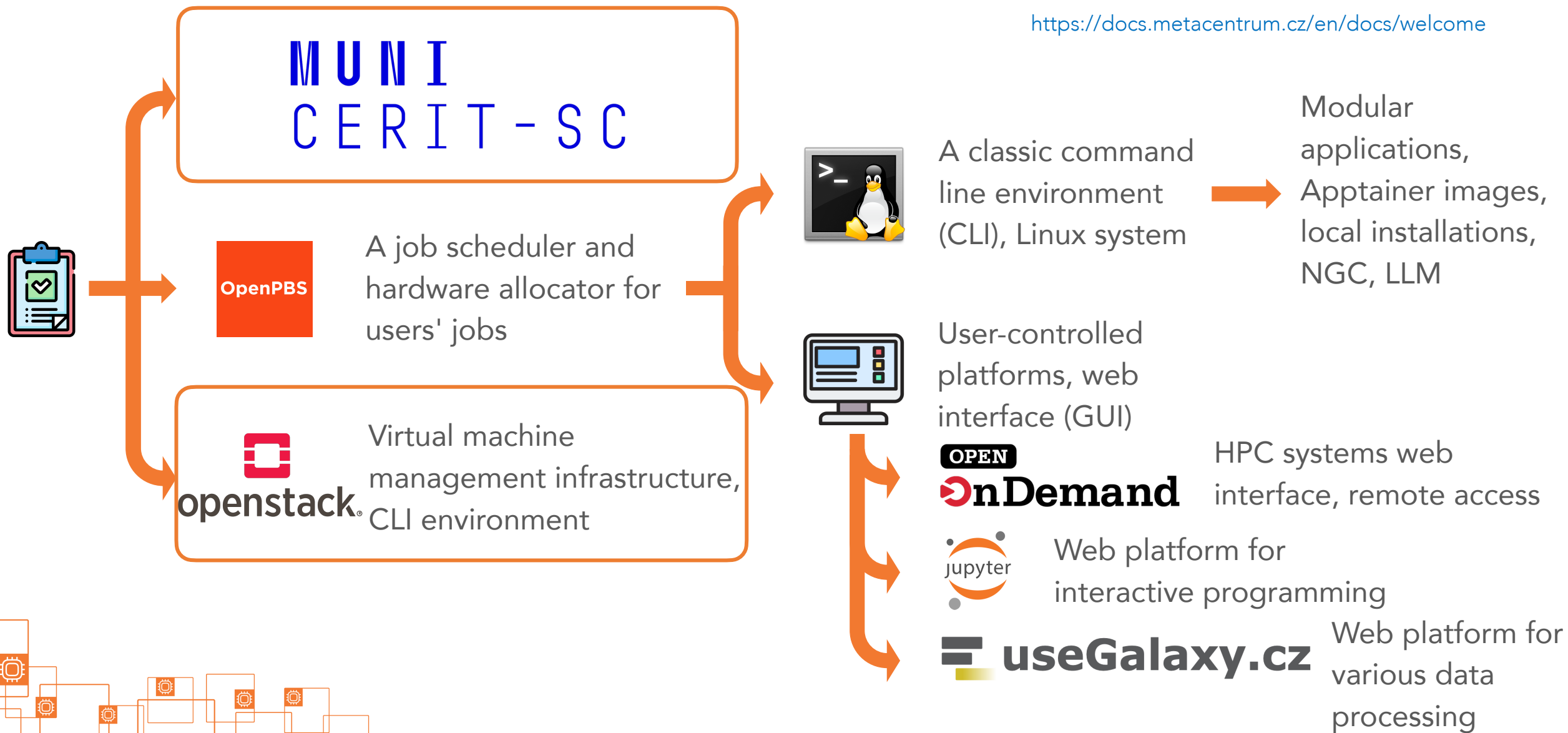

Other services

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



Other services

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



■ Build a personalised computing environment

<https://brno.openstack.cloud.e-infra.cz/>

- Based on OpenStack infrastructure
- Create virtual machines with your preferred OS (Ubuntu, Debian, AlmaLinux, etc.)
- Full administrator (root) access and control over networking, storage, and software

■ Flexible resources for research

- Choose CPU, memory, GPU, and storage configurations that match your needs
- Deploy services, databases, web applications, Kubernetes clusters, or long-running environments

■ Cloud vs. grid computing

- Grid: Submit jobs to shared computing clusters managed by scheduler
- Cloud: Provision and manage your own virtual machine for greater flexibility and customisation



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

■ A container platform for research

- Deploy applications and scientific workflows in containers on Kubernetes platform
- Run personal Docker images, web services, databases, and scalable research environments and workflows (Snakemake, Nextflow)

■ Interactive computing and data analysis

- Access ready-to-use tools such as Jupyter notebooks, RStudio, Ansys, Scipion, Matlab, Binder, and domain-specific scientific applications
- Analyse data in a web-based environment without setting up software or servers (Foldify, AlphaFind)
- SensitiveCloud for sensitive data processing and research

■ AI and advanced research services

- Use large language models and generative AI via web interfaces or APIs



- Foldify is a web application based on Alphafold tools

Protein Folding Platform

👁 3D Result Comparison 🧰 Multiple Tools ⚡ Powerful Hardware

Get Started →

View Examples

Select Prediction Tool & Start Your Computation

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

Compare Tools

MultiFold

Compare multiple prediction tools

Latest

AlphaFold 3

Latest version with advanced capabilities

Stable

AlphaFold 2

Reliable and proven protein structure prediction

Fast Prediction

ColabFold

Fast and efficient protein predictions

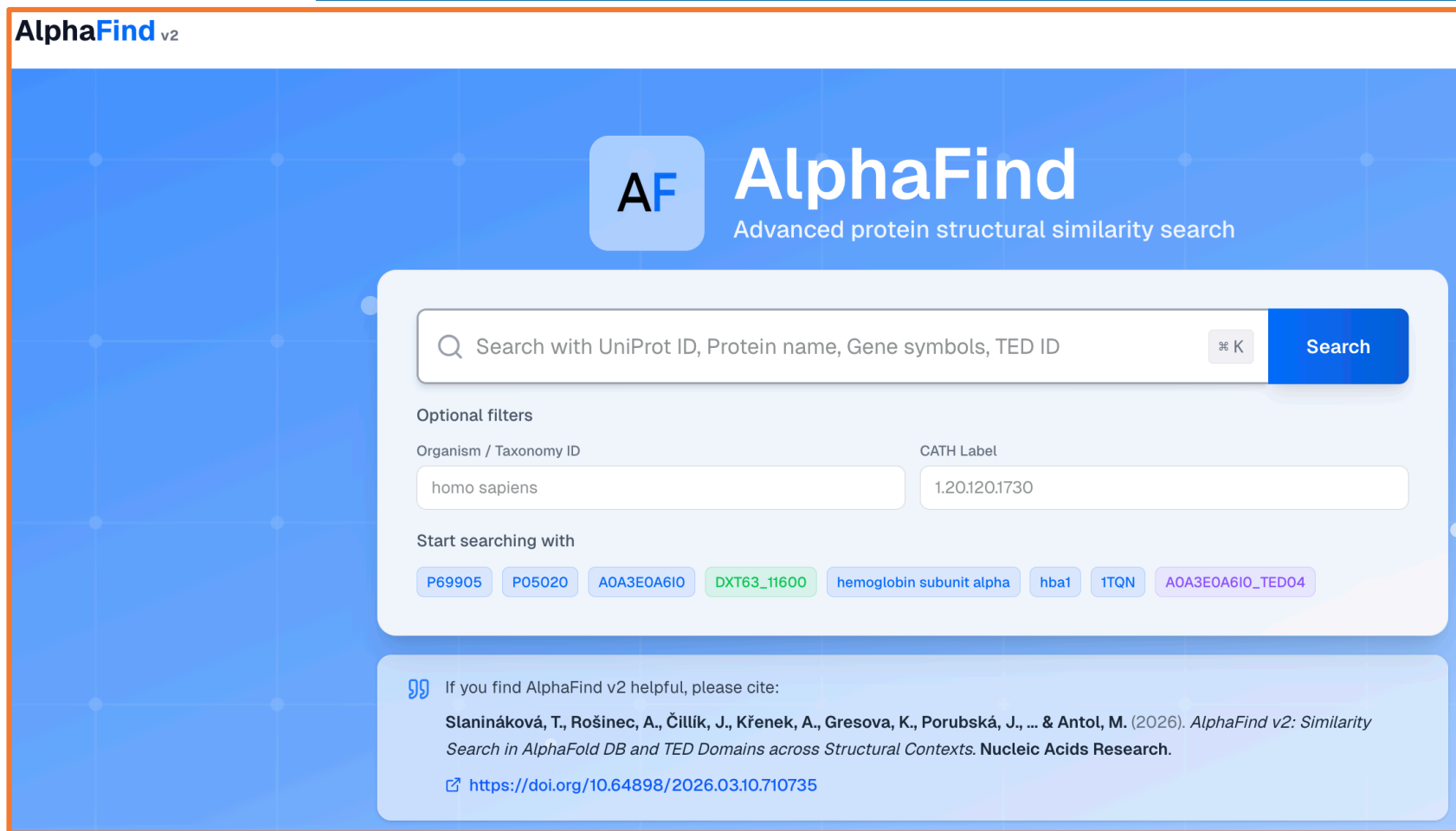
OmegaFold

End-to-end protein structure prediction

ESMFold

Fast folding with language models

- AlphaFind is a web application based for advanced protein structural similarity search
- It searches for structurally similar proteins in the AlphaFold Database



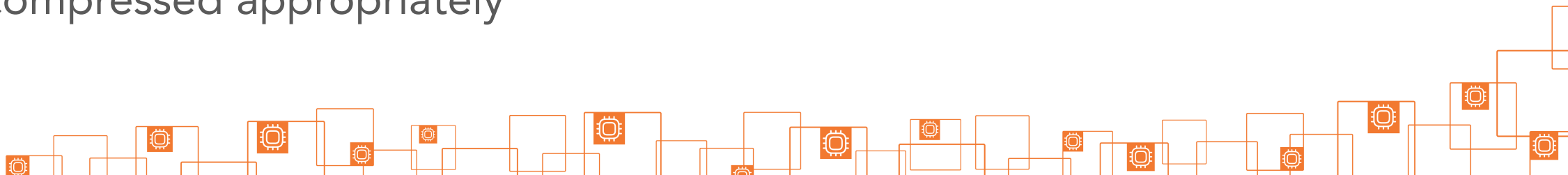
The screenshot shows the AlphaFind v2 web application interface. At the top left, it says "AlphaFind v2". The main header features the "AF" logo and the text "AlphaFind Advanced protein structural similarity search". Below this is a search bar with the placeholder text "Search with UniProt ID, Protein name, Gene symbols, TED ID" and a "Search" button. Under the search bar, there are "Optional filters" for "Organism / Taxonomy ID" (with "homo sapiens" entered) and "CATH Label" (with "1.20.120.1730" entered). Below the filters, there is a section "Start searching with" containing several buttons: "P69905", "P05020", "A0A3E0A6I0", "DXT63_11600", "hemoglobin subunit alpha", "hba1", "1TQN", and "A0A3E0A6I0_TED04". At the bottom, there is a citation notice: "If you find AlphaFind v2 helpful, please cite: Slanináková, T., Rošinec, A., Čillík, J., Křenek, A., Gresova, K., Porubská, J., ... & Antol, M. (2026). AlphaFind v2: Similarity Search in AlphaFold DB and TED Domains across Structural Contexts. Nucleic Acids Research. https://doi.org/10.64898/2026.03.10.710735".

■ CESNET S3 service

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

- Provided by the CESNET Data Storage Department
- Long-term and secure storage for valuable scientific data (archive, backup)
- Users must be registered and have generated keys (credentials) to configure any S3 client
- S3 storage can be accessed via the command line or a GUI client (for Windows, Linux, Mac)
- The documentation provides step-by-step descriptions of all scenarios
- Any archived/backed up data should be free of unnecessary clutter and compressed appropriately

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



■ CESNET S3 service

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

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

■ How to access it?

- Get credentials (key pair) to access the storage
- Save configuration file on any MetaCentrum frontend server
- Configure any of your favourite SFTP client



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

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

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

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

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

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