cesnet
metacentrum

ÚVOD DO MOŽNOSTÍ VYUŽITÍ VÝPOČETNÍ INFRASTRUKTURY METACENTRUM

DATUM
23. 6. 2026, 13:00

PŘEDNÁŠEJÍCÍ
Jiří Vorel

DÉLKA
60 min + diskuze

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

OTÁZKY POKLÁDEJTE NA
sli.do/1443316

cesnet metacentrum

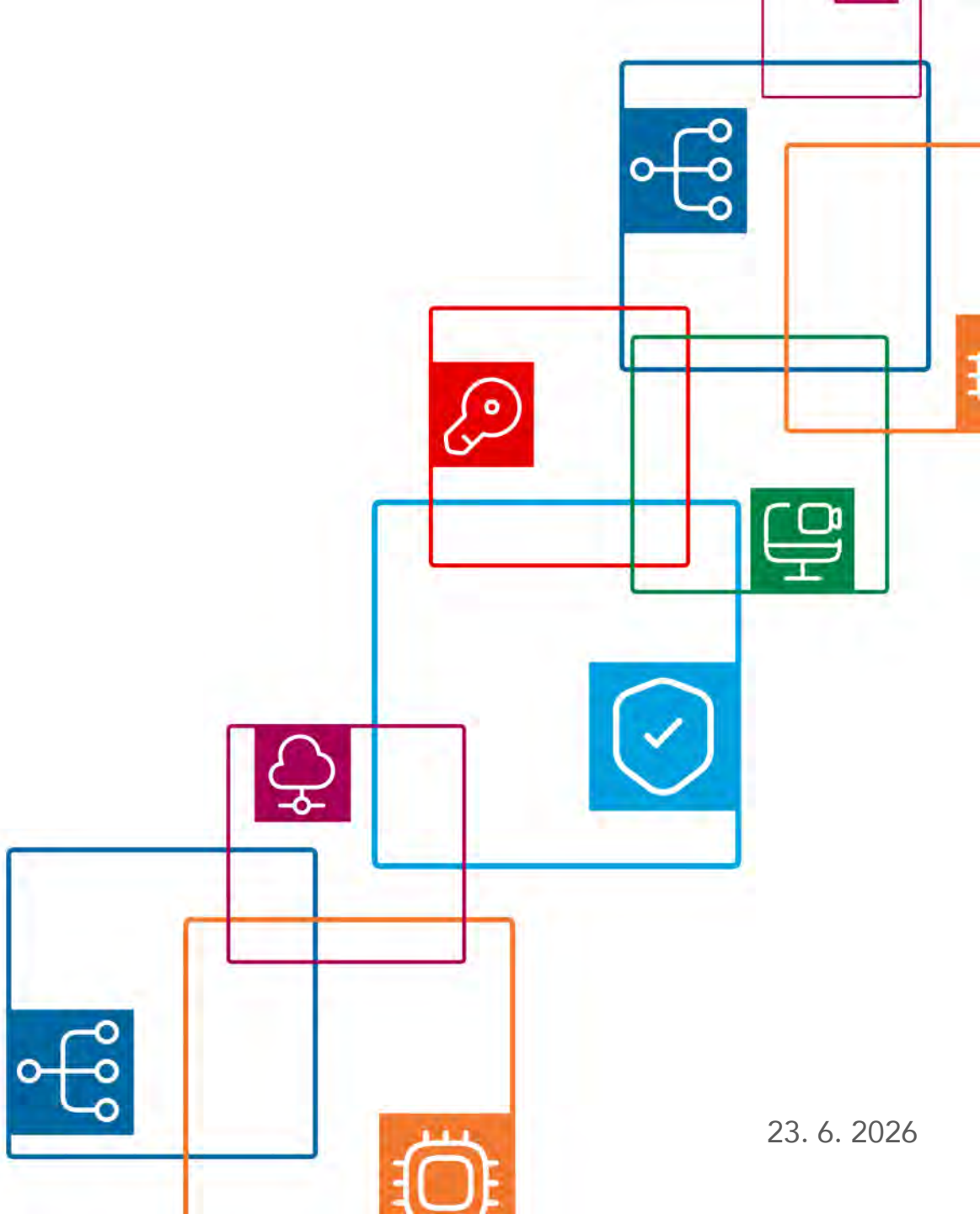
MetaCentrum NGI

The MetaCentrum webinar series

1. Introduction to MetaCentrum

Jiří Vorel

vorel@cesnet.cz meta@cesnet.cz



23. 6. 2026

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/ambasadors/
  - 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 in a nutshell

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

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

- MetaCentrum is
  - A national grid infrastructure (NGI)
  - The activity of the CESNET association
  - Part of the e-INFRA CZ e-infrastructure
  - A provider of computational resources, application software (both commercial and free/open source) and data storage
  - 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://docs.metacentrum.cz/en/docs/access/terms#acknowledgements-and-publications

e-INFRA CZ in a nutshell

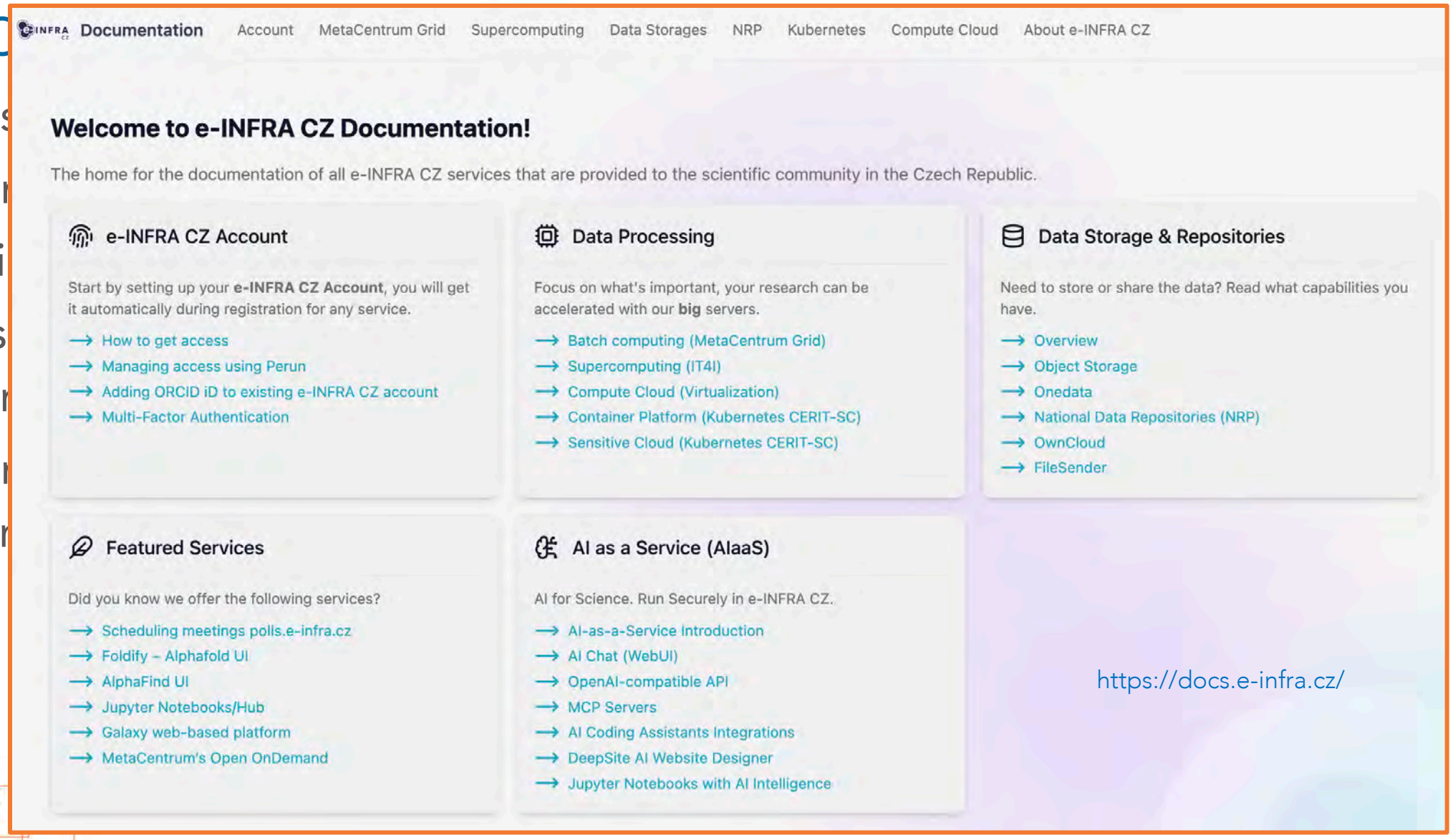
https://www.cesnet.cz/ https://www.vyzkumne-infrastruktury.cz/
https://www.e-infra.cz/ https://www.cerit-sc.cz/
https://www.it4i.cz/

- 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

A complete overview of the e-INFRA CZ services

e-INFRA CZ in a nutshell

- e-INFRA C
  - Large res
  - E-infrastr
  - Consorti
  - Provides
    processi
  - Supercor
    data stor



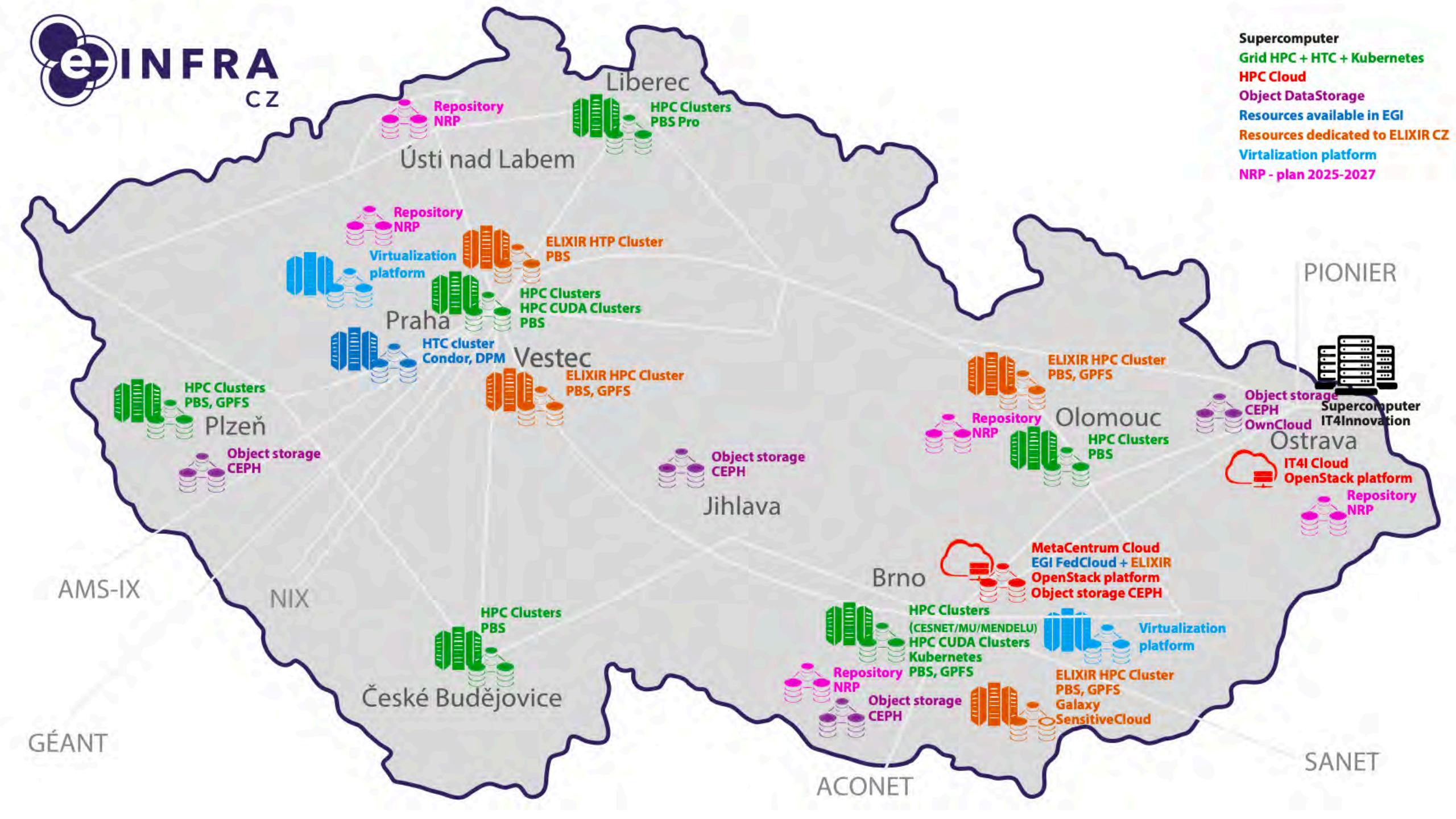
https://docs.e-infra.cz/

MetaCentrum in a nutshell

https://www.metacentrum.cz/

https://docs.metacentrum.cz/

- MetaCentrum offers
  - 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


e-INFRA CZ
Supercomputer
Grid HPC + HTC + Kubernetes
HPC Cloud
Object DataStorage
Resources available in EGI
Resources dedicated to ELIXIR CZ
Virtalization platform
NRP - plan 2025-2027
Liberec
Repository NRP
HPC Clusters PBS Pro
Ústí nad Labem
Repository NRP
Virtualization platform
ELIXIR HTP Cluster PBS
HPC Clusters HPC CUDA Clusters PBS
Praha
HTC cluster Condor, DPM
Vestec
ELIXIR HPC Cluster PBS, GPFS
HPC Clusters PBS, GPFS
Plzeň
Object storage CEPH
Object storage CEPH
Jihlava
PIONIER
ELIXIR HPC Cluster PBS, GPFS
Repository NRP
Olomouc
HPC Clusters PBS
Object storage CEPH OwnCloud
Supercomputer IT4Innovation
Ostrava
IT4I Cloud OpenStack platform
Repository NRP
AMS-IX
NIX
MetaCentrum Cloud
EGI FedCloud + ELIXIR
OpenStack platform
Object storage CEPH
Brno
HPC Clusters (CESNET/MU/MENDELU)
HPC CUDA Clusters
Kubernetes
PBS, GPFS
Virtualization platform
Repository NRP
Object storage CEPH
ELIXIR HPC Cluster PBS, GPFS
Galaxy SensitiveCloud
HPC Clusters PBS
České Budějovice
GÉANT
ACONET
SANET


ONE APPLICATION TO RULE THEM ALL

One application to rule them all

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

kubernetes

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

OpenPBS

A job scheduler and hardware allocator for users' jobs

openstack

Virtual machine management infrastructure, CLI environment

A classic command line environment (CLI), Linux system

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

User-controlled platforms, web interface (GUI)

OPEN OnDemand

HPC systems web interface, remote access

jupyter

Web platform for interactive programming

useGalaxy.cz

Web platform for various data processing

Application

- 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

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

Tools and licence models

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

Paid licence

For registered individuals

For all users

Free licence

WIEN2k
VASP
CRYSTAL23
COMSOL MULTIPHYSICS
CASTEP
CLC bio
geneious biologics
Ansys
TURBOMOLE
MATLAB
Gaussian, Inc.
The Amber Project
NAMD Scalable Molecular Dynamics
ORCA
cuDNN
AlphaFold
GAMESS
R
RStudio
NCBI BLAST
Mamba
FAST. FLEXIBLE. FREE. GROMACS
TensorFlow
jupyter
julia
CONDA
PyTorch
Beast2 Bayesian evolutionary analysis by sampling trees

GUI approach

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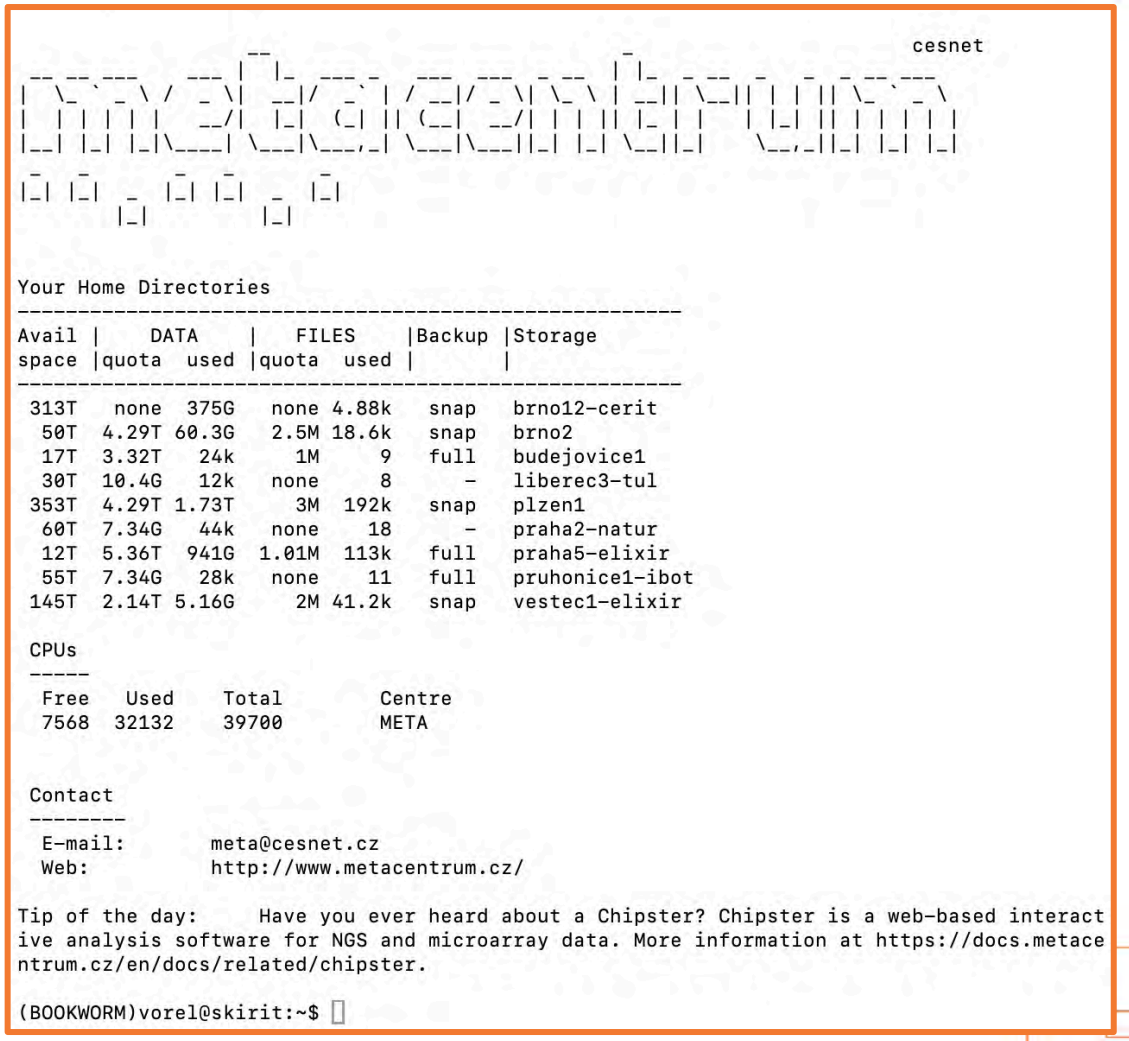
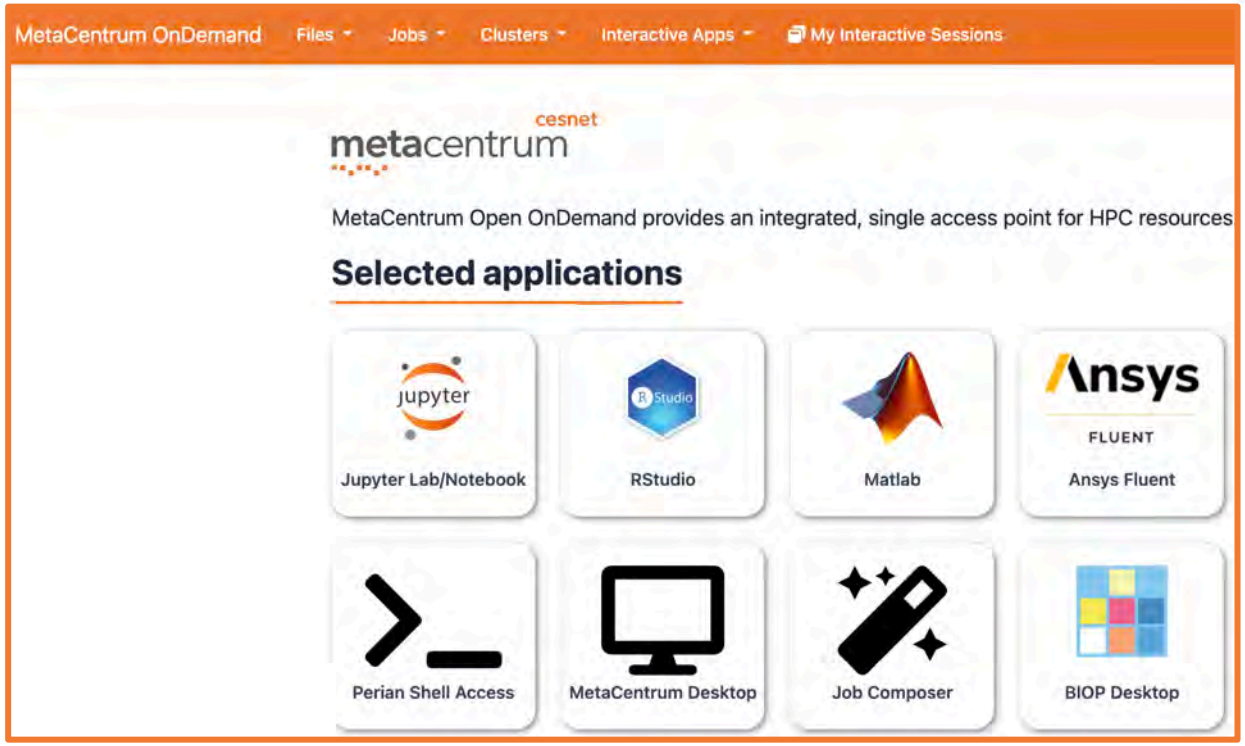
Grid computing

- OpenPBS scheduler
  - Allocation of hardware resources
  - Centrally managed HTC/HPC clusters
  - Classic command line environment (CLI)
  - GUI platforms
  - Long batch jobs (days/weeks)
  - Interactive jobs (hours)
  - Parallel and multi-node computing
  - GPU acceleration (NVIDIA H100 NVL)



- Open OnDemand

https://ondemand.metacentrum.cz/



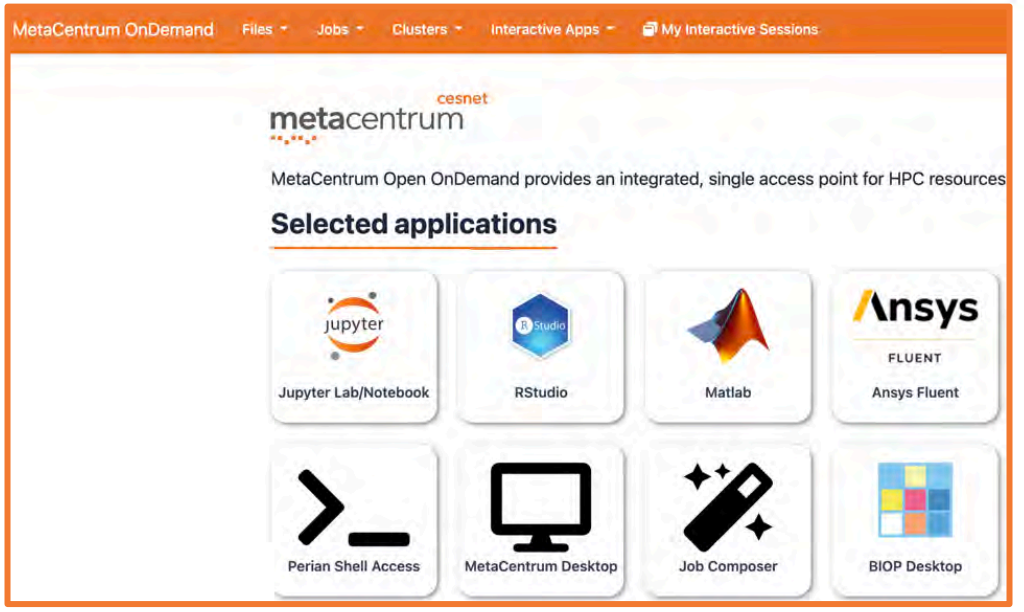
- Web application running on top of the OpenPBS scheduler
- Running (not only) GUI applications
- Browse storage (tab 'Files')
- Write shell scripts (tab 'Jobs')
- Command line (tab 'Clusters')
- Launch a virtual desktop (MetaCentrum Desktop app)
- Running virtual machines (OpenStack) and Docker images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

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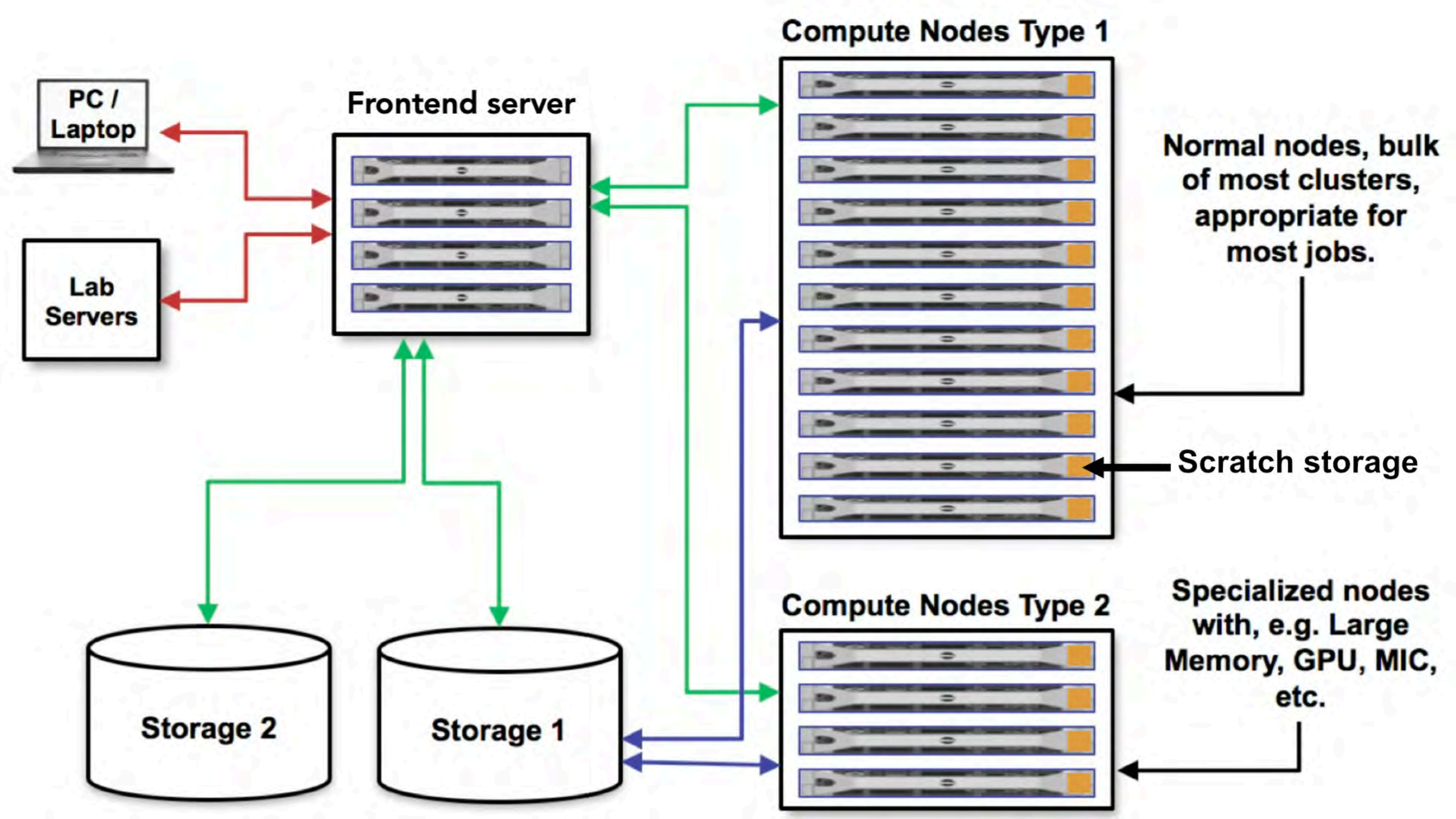

Compute Nodes Type 1
PC / Laptop
Frontend server
Lab Servers
Normal nodes, bulk of most clusters, appropriate for most jobs.
Scratch storage
Compute Nodes Type 2
Specialized nodes with, e.g. Large Memory, GPU, MIC, etc.
Storage 2
Storage 1

Frontend servers (login nodes)

- 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

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

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	

Disk storage arrays

- Several geographically separated disk arrays (storage) are available
- Designed for so-called live data

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

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

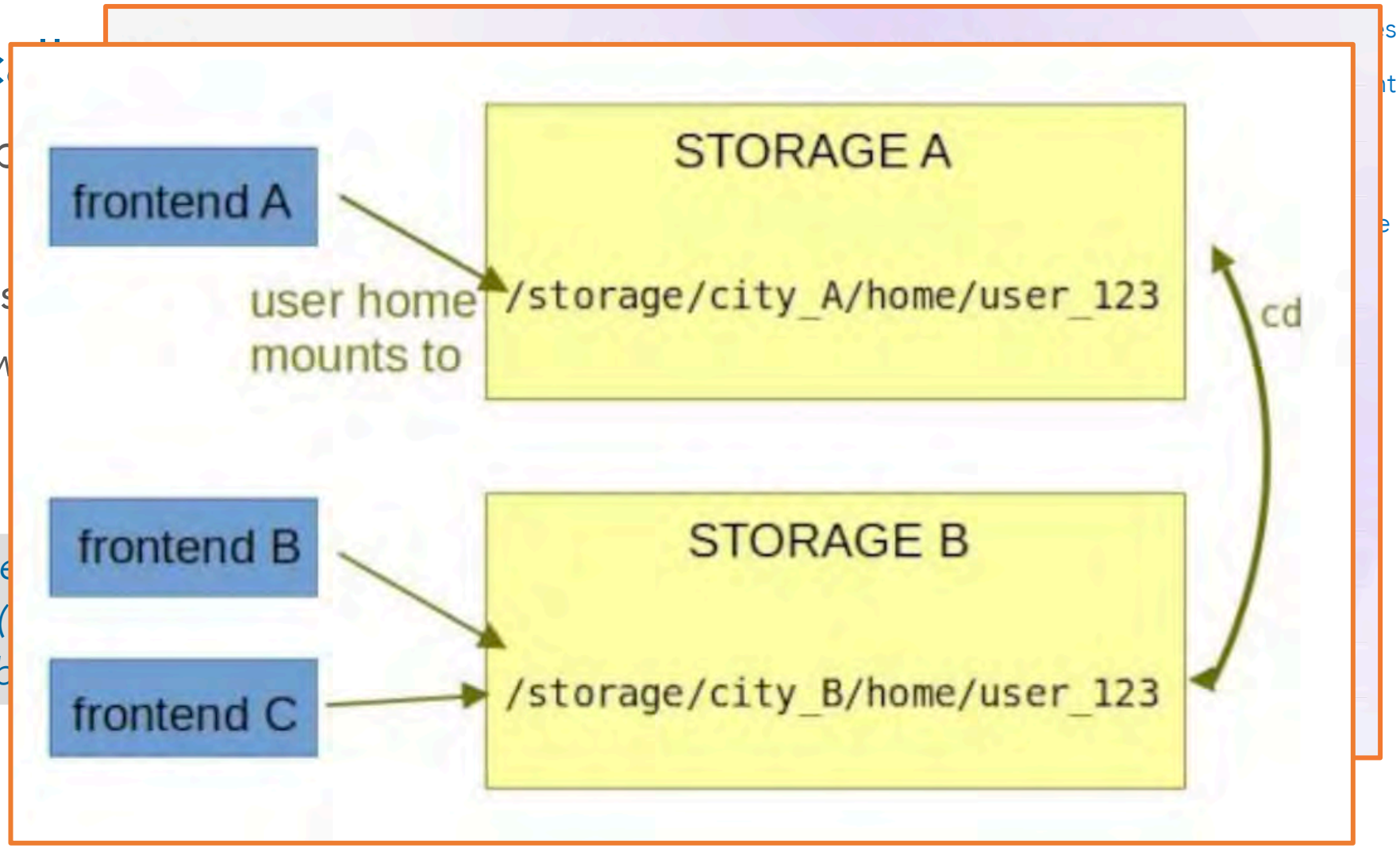
- Several geographically separated disk arrays (storage) are available
- Designed for so-calle
  - Backups of valuable p
    storage
    - Available to all users
    - *s3cmd/s5cmd/aws* cor
    - Need to request the c

By default,
755 (= oth
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-c
  - Backups of valuab
    storage
    - Available to all us
    - *s3cmd/s5cmd/aw*
    - Need to request



By de
755 (
can b

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-mln2jlz
masurca/3.2.6loc9  masurca/4.0.3-gcc-8.3.0-up2bz7u

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-ydytecx 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-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-10.2.1-2ll77ke
    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-oa4lipo
    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

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

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OPEN OnDemand — HPC systems web interface, remote access

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CERIT-SC

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MetaCentrum cloud

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

- Build a personalised computing environment
  - 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

- A container platform for research

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

  - 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

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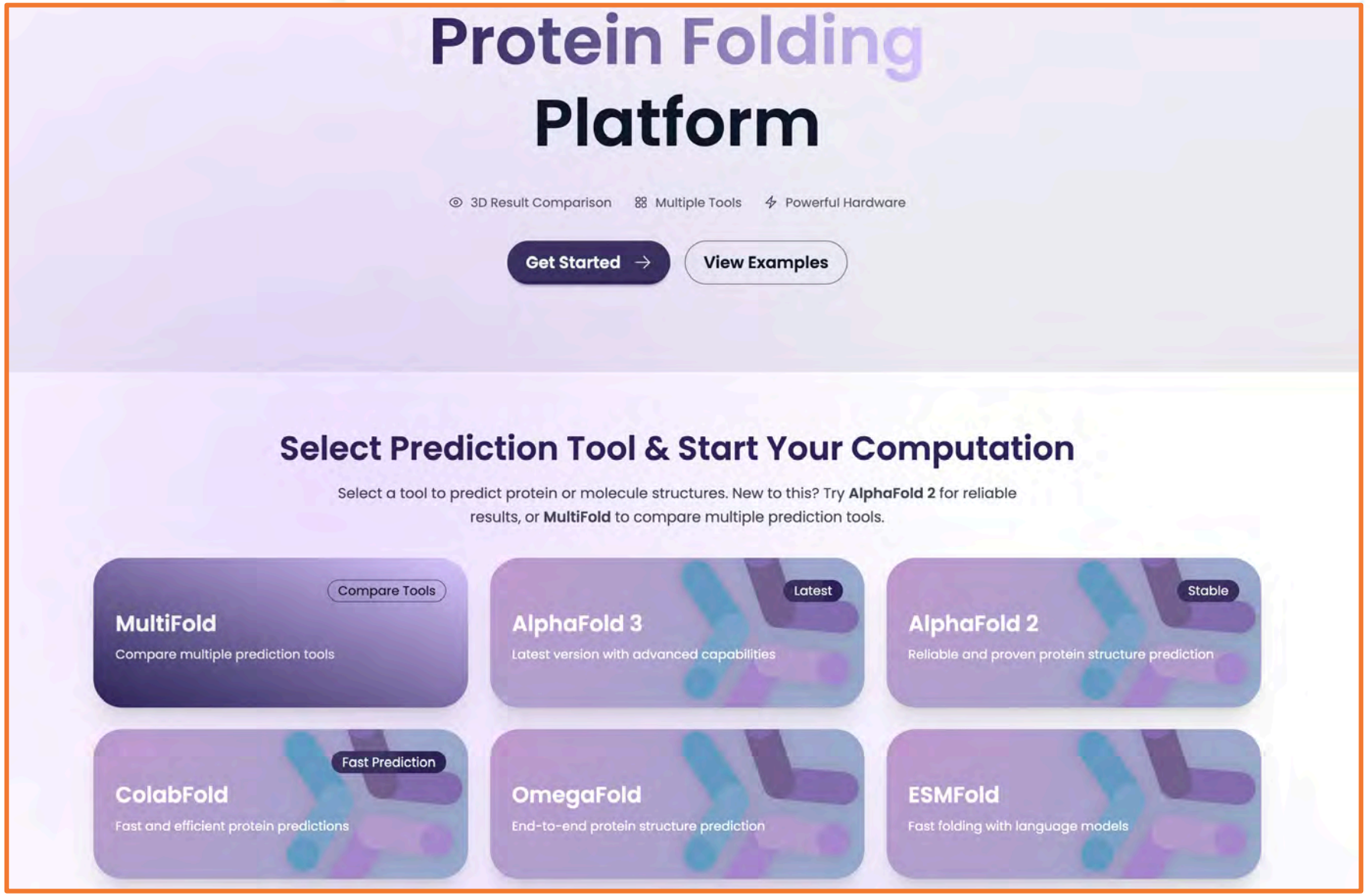
https://foldify.cloud.e-infra.cz

Foldify

- Foldify is a web application based on Alphafold tools



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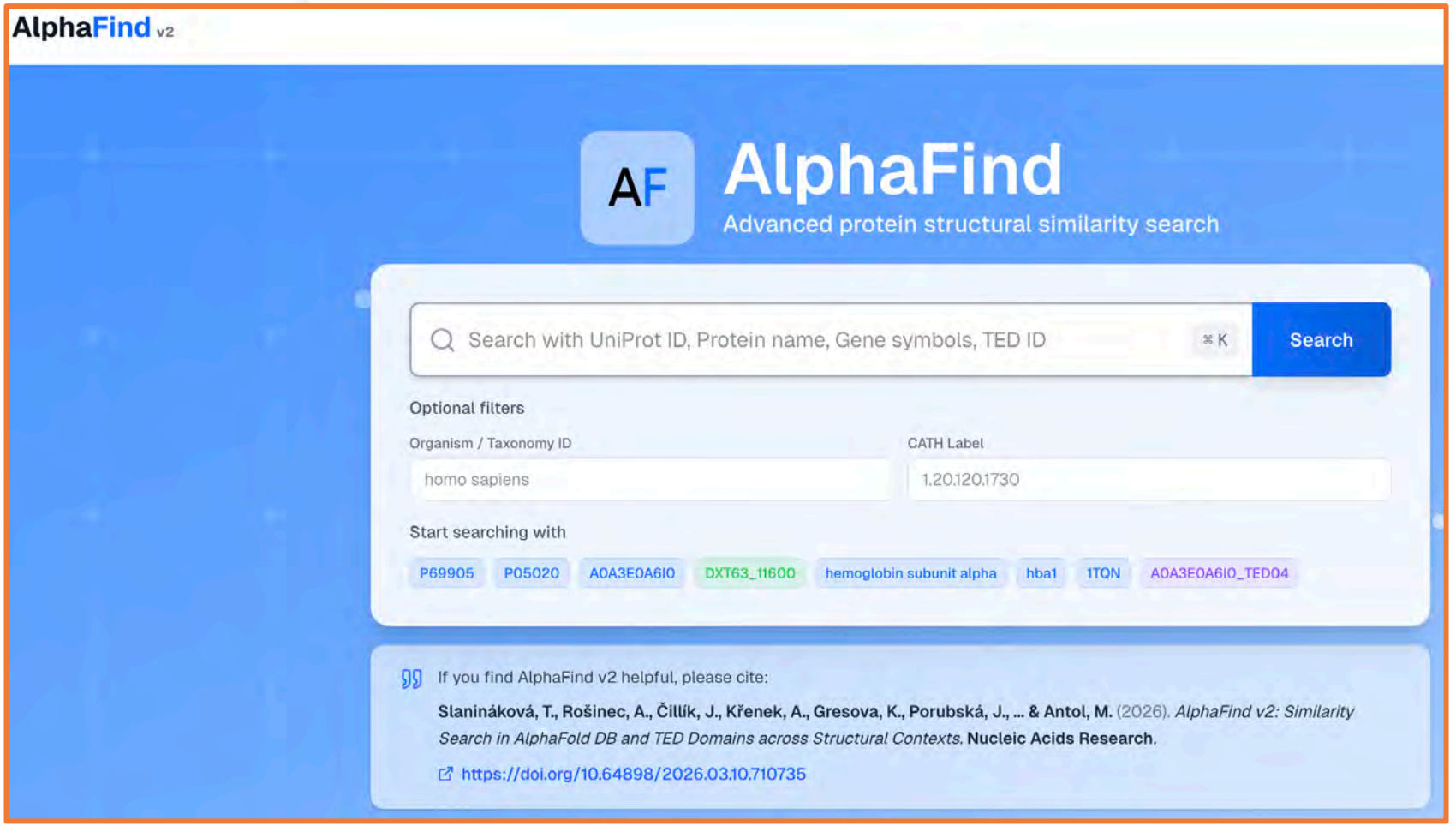
https://alphafind.ics.muni.cz/

AlphaFind

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



cesnet datacare

CESNET S3 storage

- CESNET S3 service

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

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

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

  - S3 storage can be accessed via the command line or a GUI client (for Windows, Linux, Mac)
  - The documentation provides step-by-step descriptions of all scenarios
  - Any archived/backed up data should be free of unnecessary clutter and compressed appropriately

CESNET S3 storage

- CESNET S3 service

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

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

Conclusions

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

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

- Free and immediately accessible, no grant proposals
- All we ask: acknowledge e-INFRA CZ (ID:90254) in your publications
- For everyone, no programming skills required
- Scales with your needs, from a small interactive session to large and long-term parallel jobs
- 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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