

# METACENTRUM

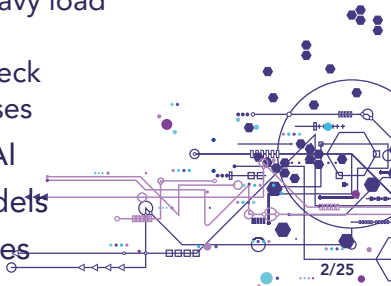
Miroslav Ruda

April 2024

# MetaCentrum I

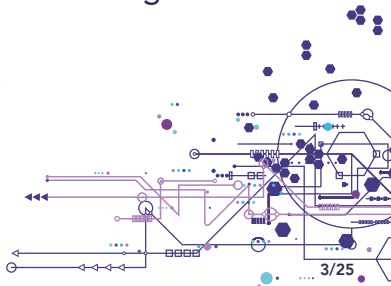
National distributed computing environment, coordinated by CESNET

- resources both by CESNET and CERIT-SC (48.000 CPU cores)
- clusters located at CESNET, universities, CAS
  - original motivation of resource sharing (HW) still valid
  - providing temporarily free resources for remote users
  - usage of remote resources in case of urgent/heavy load
  - use other resources during an outage
  - resources for project start-up, HW suitability check
  - idea works also for expensive commercial licenses
- community access, central management and AAI
- grid, IaaS cloud and PaaS cloud computing models
- virtualization platform for highly available services



# MetaCentrum II

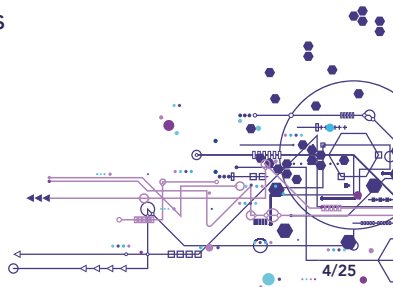
- distributed model useful for different use-cases
  - integration of resources owned by other RIs (ELIXIR)
  - big-data use-cases - no need for remote transfer
  - architecture compatible with data repositories in EOSC CZ NDI
- NGI in European e-infrastructure EGI, EOSC mandated org.
- targeted support for large projects (VI, ESFRI)
- umbrella for development of new services/tools
  - OnDemand, Jupyter, Galaxy
  - Kubernetes platform
  - support for processing of sensitive data



# Cooperation with partners

Collaboration with projects = motivation to develop new services

- High Energy Physics, Astrophysics – LHC, Auger, CTA, Belle
  - original motivation of the grid, still active in EGI
- Life Science – ELIXIR (OpenScreen, CCT, Czech Bioimaging)
  - collaborating VIs, resources integrated into MetaCentrum
  - cooperation in the operation of ELIXIR services
  - life-science is the largest consumer of resources
- ELI, BBMRI, LINDAT/CLARIN, ICOS
  - especially at international/project/EGI level
- research centres CzechGlobe, CEITEC, Recetox
  - long term users, link through CERIT-SC (MU)
- ESA – CollGS, Data Relay Hub
  - various groups/project using Copernicus data

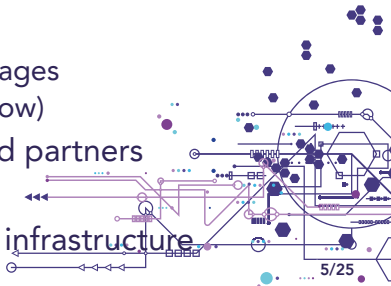




# MetaCentrum computational models I

Grid, centrally managed HTC, HPC clusters

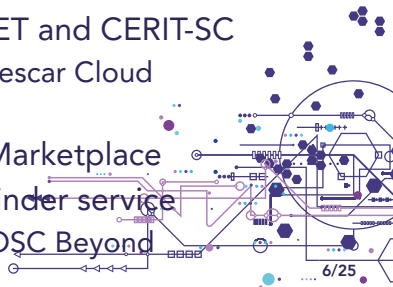
- batch, long (days/weeks) jobs, both HTC and HPC/parallel computing
- including interactive tasks, GUI
  - Galaxy, Jupyter, OnDemand
- semi-permanent storage (GPFS+NFS) and local/shared scratch
- computations also in containers (Singularity)
  - HPC approach, support for non-root Docker images
  - NVIDIA GPU Cloud software (PyTorch, TensorFlow)
- distributed clusters of e-INFRA CZ members and partners
  - origins of Perun development (AAI)
- subset of resources available also in WLCG/EGI infrastructure



# MetaCentrum computational models II

## MetaCentrum cloud - virtual machine instead of tasks

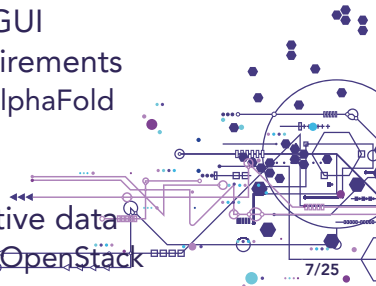
- images provided by MetaCentrum, EGI, projects, users
- scientific computing and services for computing (OpenStack)
  - but also training, teaching, KYPO security polygon
- Terraform or EGI Infrastructure Manager for virtual clusters/K8s
- central installation in Brno, joint effort of CESNET and CERIT-SC
  - development of new OpenStack distribution, Bescar Cloud
  - second installation in IT4I in 2023
- site access also through EGI FedCloud, EOSC Marketplace
- group is also responsible for EGI Jupyter and Binder service
  - including EOSC EU Node, ENVRI-Hub Next, EOSC Beyond

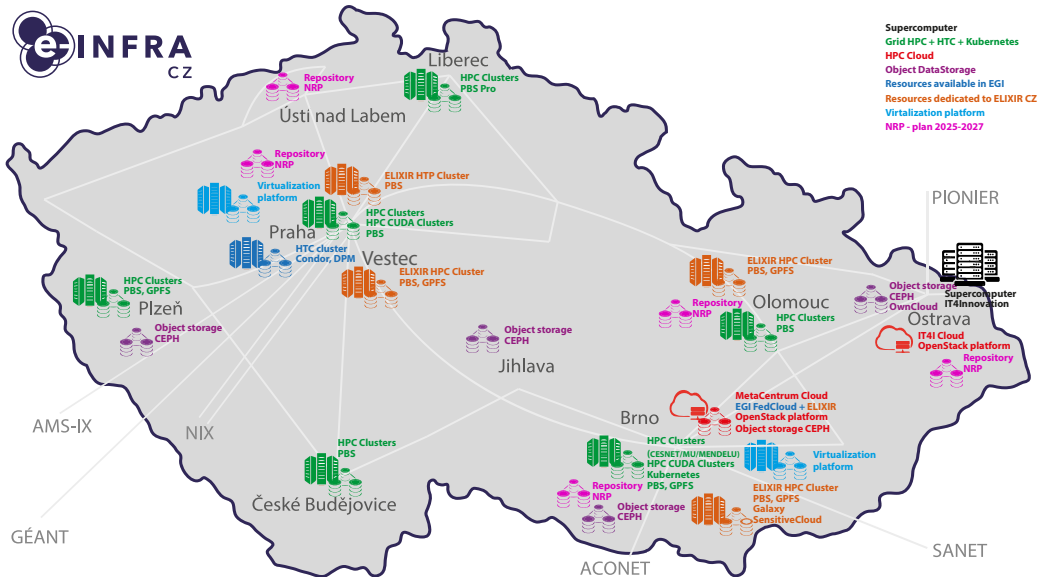


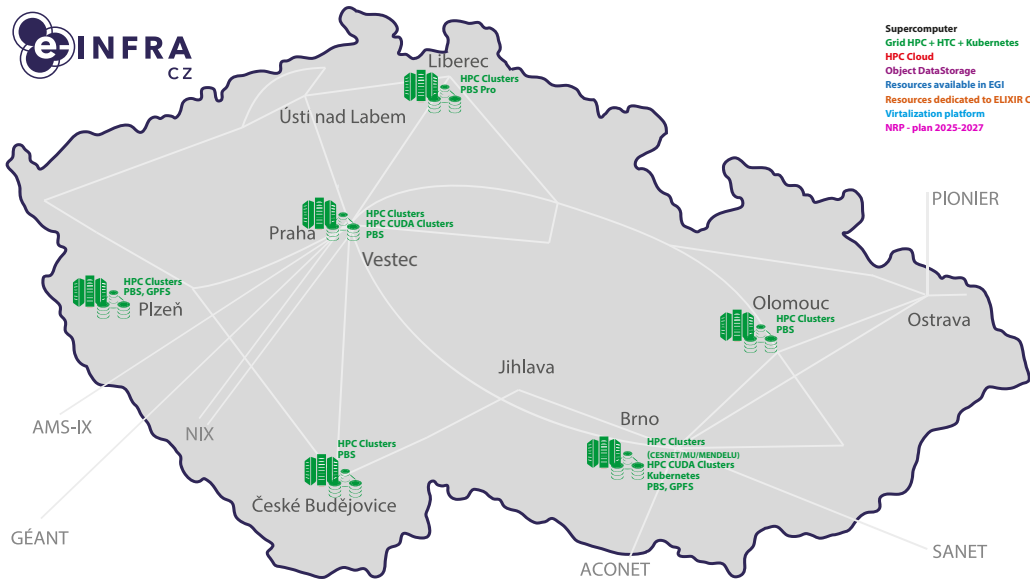
# MetaCentrum computational models III

## Containerized cloud, PaaS platform

- containers instead of jobs/virtual machines
  - packaging of software tools, encapsulation of services
  - reproducibility, provenance
  - both in HPC (Singularity) and cloud (Docker, Kubernetes)
- Kubernetes for micro-services, managing virtual environments
- managed service, non-root containers, Rancher GUI
- strong support for interactive and workflow requirements
  - SaaS approach for Matlab, RStudio, NextFlow, AlphaFold
- development in area of converged computing
  - integration of batch system and Kubernetes
- work on use-cases related to processing of sensitive data
  - Sensitive Cloud: currently Kubernetes, later also OpenStack



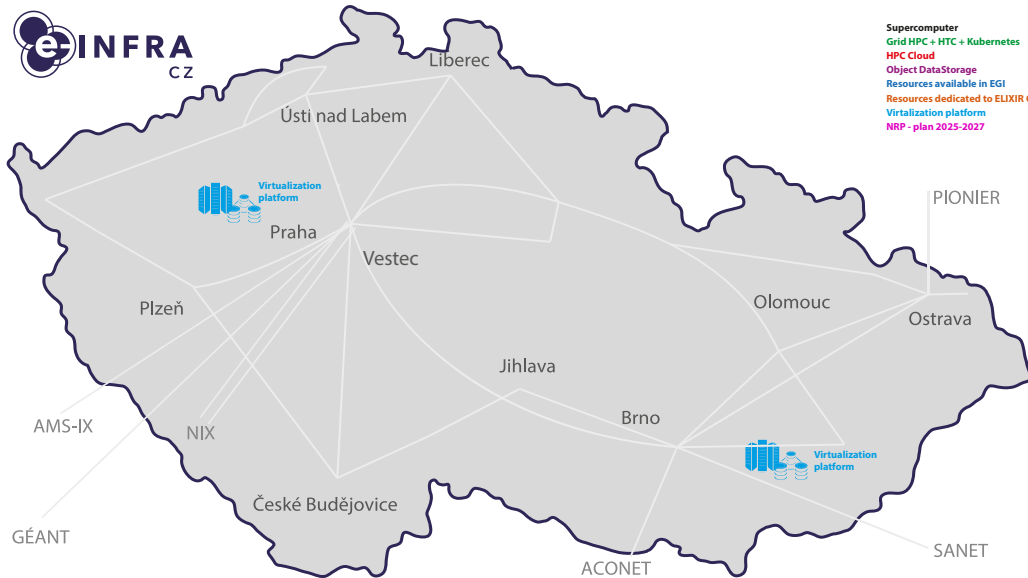




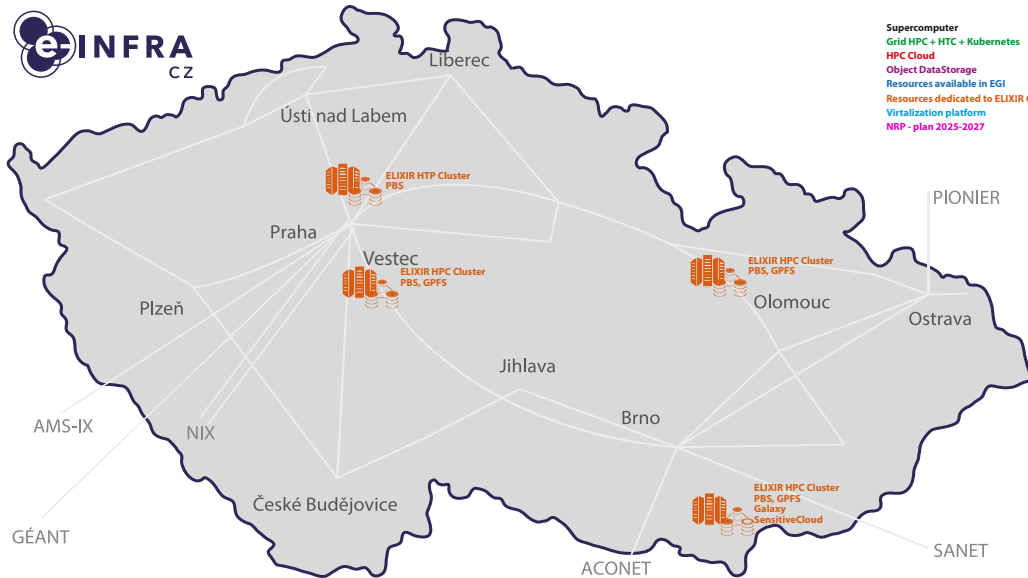




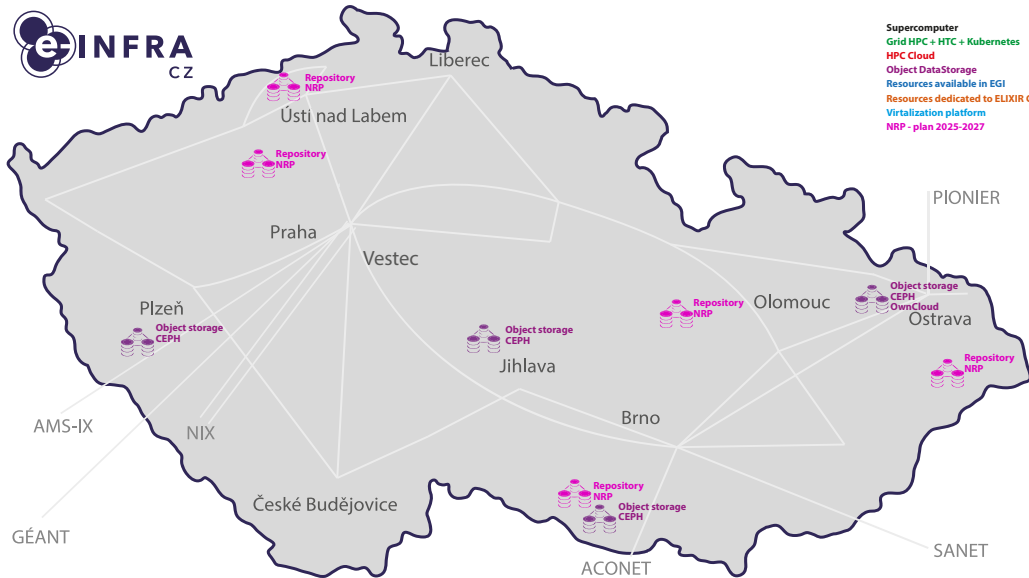
- Supercomputer
- Grid HPC + HTC + Kubernetes
- HPC Cloud
- Object DataStorage
- Resources available in EGI
- Resources dedicated to ELIXIR CZ
- Virtualization platform
- NRP - plan 2025-2027

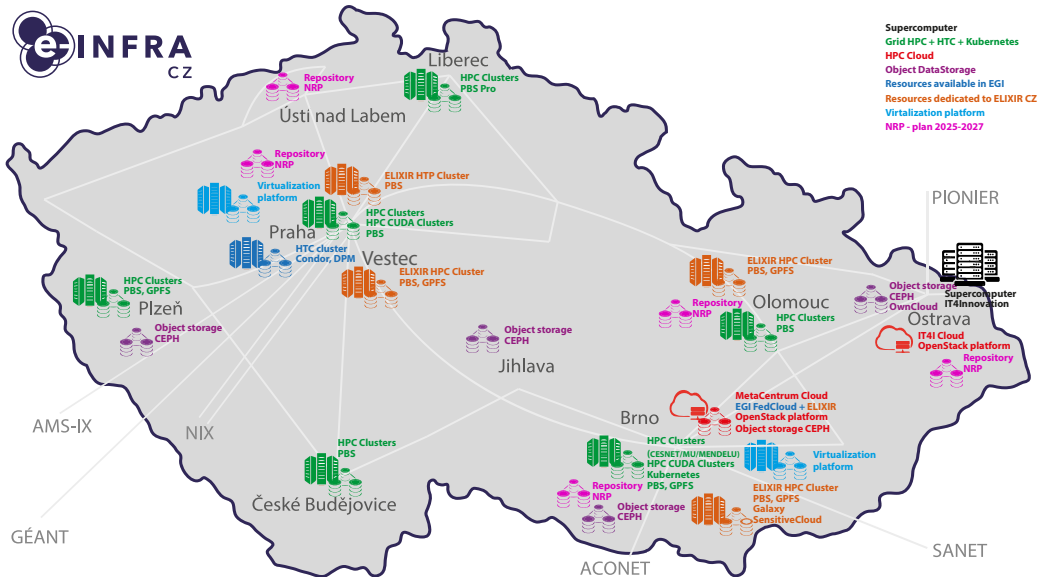








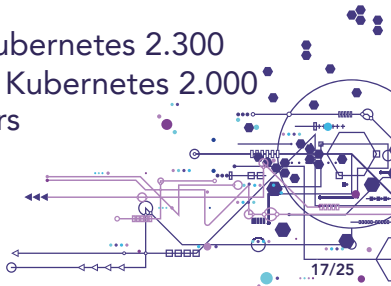




# Metacentrum in numbers, April 2024

48.000 CPU cores, 15 PB storage, 460 GPU cards, 3.000 users, 300+ WoS

- HD nodes - 32-128 CPU cores (x86\_64), 256-1024 GB RAM
- SMP servers - 2-3 TB RAM
  - specialized servers with 6/10 TB RAM
- GP-GPU cards - 160 nodes, 460 cards
  - latest NVIDIA DGX2 with 8xH100 GPU cards
  - NVIDIA T4, 1080 Ti, 2080 Ti, A100, A40, H100
- CPU cores: grid - 32.500 + 6.500, IaaS 6.500, Kubernetes 2.300
- CPU years: grid - 22.000 + 13.000, IaaS 10.000, Kubernetes 2.000
- clusters provided by growing number of partners
  - CESNET 23.000 and CERIT-SC 8.000
  - VI ELIXIR 5.500
  - FZU 5.400 for LHC/EGI
  - ZČU, MU, UK, TUL, AV ČR



	2012	2014	2016	2018	2019	2020	2021	2022	2023
Number of MC users	613	1112	1611	2020	2185	2225	2606	2710	<b>3055</b>
New users coming	312	605	742	713	762	774	792	767	<b>850</b>
Jobs [millions] Meta/EGI	1,1/ n/a	3,9/ n/a	3,6/ 6	5/ 6,7	8,6/ 6,8	13,1/ 10	12,1/ 9,3	11,1/ 14,2	<b>11,7/ 5,4</b>
CPU time [CPU years] Meta/EGI	2500/ n/a	6403/ n/a	9475/ 5963	11357/ 4074	13129/ 4531	16630/ 9160	22647/ 9581	27547/ 9218	<b>31858/ 14770</b>
CPU cores incl. EGI	6028	14164	17234	21344	26602	29874	34084	44088	<b>47748</b>
GPU cards					255	322	434	455	<b>462</b>

# Latest achievements, future plans I

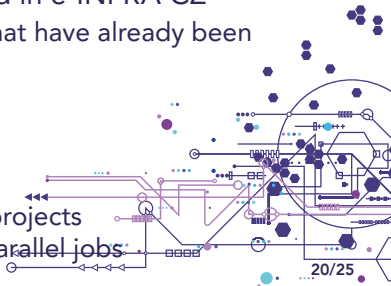
## OP JAK projects, e-infrastructure e-INFRA CZ and RI ELIXIR CZ

- in total, in 2024-2026 approx. 220 mil. Kč (170+50, without VAT)/ 10 mil. \$ for clusters and semi-permanent data storages
  - modernization of infrastructure -> upgrade of resources, support for current trends (GPU, AI, big data)
- 2024: new license for Matlab - 200 licenses, all toolboxes
- 2024: running tender for new versions of Ansys, Gaussian, MolPro
- 2024: network connection 100Gb in Brno, Mendel a Plzen, in progress in UMG/Biocev
- planned: new approaches in user-support
  - ideas as Campus Champion/Ambassador for a large scientific group



# Latest achievements, future plans II

- mentors for small groups, 2 weeks of focused work with new user group
- planned: medium size projects
  - MetaCentrum – access to all scientific users, no need for projects
    - fair-share access policy - citations/acknowledgement instead of payments
  - IT4Innovations – standard projects, 3 rounds per year, scientific review
  - plan for lightweight project - capacity dedicated in e-INFRA CZ
    - policy taking into account accepted projects that have already been successfully evaluated (GACR, TACR, EU)
- planned: medium sized computational clusters
  - two larger installations in Brno and Pilsen
    - better support for mid-size projects
    - possibility to dedicate non-trivial capacity for projects
    - Lustre/BeeGFS based scratch filesystems for parallel jobs

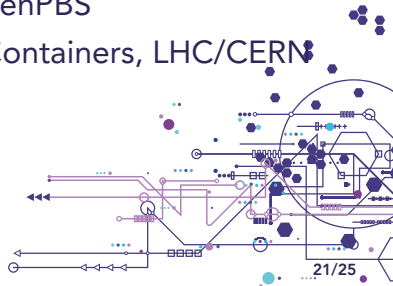




# Latest achievements, future plans III

## Grid infrastructure

- 2023: Spack for software compilation, 5.000 packages in modules
- 2023: NVIDIA DGX2, 8xH100 GPU cards
- 2024: on-going migration to Debian 12 and OpenPBS
- Singularity - Debian/Centos, NVIDIA GPU, BioContainers, LHC/CERN
- conda/mamba for tools installed by users
- planned: BeeGFS/Lustre scratch in Pilsen



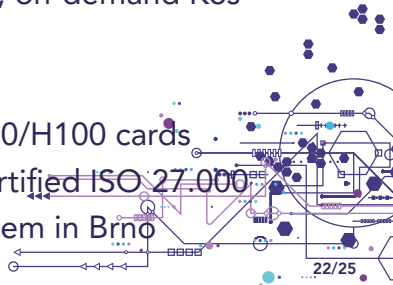
# Latest achievements, future plans IV

## IaaS OpenStack cloud

- 2023: next generation OpenStack distribution Bescar Cloud
- 2023: second cloud instance in Ostrava/IT4Innovations
- 2024: migration to new generation in Brno
- planned: HPC cloud installation, HA installation, on-demand K8s

## PaaS Kubernetes

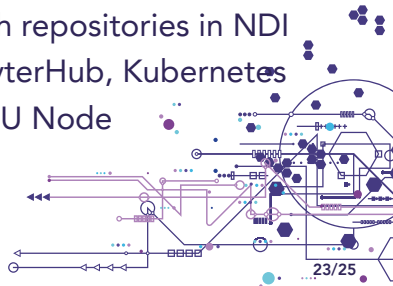
- 2023: Rancher UI and Kubernetes in production
- 2023: improved support for GPU, available A100/H100 cards
- 2024: Sensitive Cloud based on Kubernetes, certified ISO 27.000
- planned: new setup with parallel scratch filesystem in Brno



# Latest achievements, future plans V

Interactive GUIs – OnDemand, Galaxy, Jupyter Notebooks, Rancher

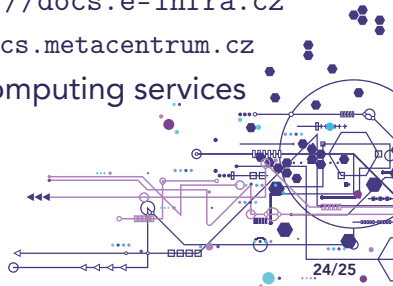
- 2023: OnDemand interactive jobs (Matlab, RStudio, Fluent, desktop)
- planned: OnDemand also for cloud applications, Kubernetes
- 2023: usegalaxy.cz in production
- 2024: two Galaxy instances provided for Recetox and Repeat Explorer
- planned: Galaxy in NRP project: integration with repositories in NDI
- 2023: Jupyter in production – OnDemand, JupyterHub, Kubernetes
- 2024: CESNET+EGI Notebooks part of EOSC EU Node
- planned: Jupyter Notebooks in EU projects
  - EOSC Beyond, ENVRI-Hub Next
- 2024: Rancher UI supports e-INFRA AAI



# Latest achievements, future plans VI

## e-INFRA CZ integration

- 2023: unified AAI across e-INFRA CZ
  - one account in MetaCentrum and IT4I
- 2023 - 2024: common documentation at <https://docs.e-infra.cz>
  - still work in progress, currently also <https://docs.metacentrum.cz>
- 2023-2024: questionnaire of satisfaction with computing services
  - many thanks for all responses!





**Thanks for your attention**

`support@metacentrum.cz`

`https://www.metacentrum.cz`

`https://metavo.metacentrum.cz/en/state/`

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

A circular logo consisting of two concentric circles. The text 'e-infra.cz' is centered between the two circles.

`e-infra.cz`