



# **(Research) Infrastructures in the Czech Republic**

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# Lecturer



## – Tomáš Rebok

- CERIT-SC Centre @ Institute of Computer Science (ICS), MU  
Head of the *Tom Rebok's Research Group*
- *MetaCentrum @ CESNET z.s.p.o.*
- senior researcher, head of applied-research projects
- long-term activity in the field of computing and data infrastructures  
supporting high-performance computations and data processing
- primary orientation in the field of data infrastructures and analytics  
data infrastructures and analysis  
innovative approaches to specific data-analysis tasks
- interdisciplinary research collaborations with  
security forces & Police of the CR  
environmental research groups

## A bit of theory...



# Supercomputers

- (extremely) powerful computers used for complex calculations and simulations
  - their performance is commonly measured in floating-point operations per second (FLOPS) instead of million instructions per second (MIPS)
- introduced in the 1960s (UNIVAC supercomputer)
- architecture – single, highly integrated systems
  - typically use massive number of specialized processors (up to millions) and high-speed interconnects to achieve their performance
- **pros:** high processing power, used for scientific research, weather forecasting and climate modelling, etc.
- **cons:** very expensive (specialized HW), limited accessibility, and high maintenance costs

# EL CAPITAN – the fastest supercomputer (2025)

**Location:** Lawrence Livermore  
National Laboratory (California, US)

**Performance:** 1,742 petaFLOPS  
(1.742 exaFLOPS)

**First online:** November 2024



# (Computing) Clusters

- consist of multiple interconnected “contemporary” computers (nodes)
  - they work together to perform tasks
- individual nodes may not be as powerful as a supercomputer
  - but the combined power of all the nodes can be significant
- architecture – clusters use standard, off-the-shelf hardware interconnected via a network
  - need for powerful & low-latency interconnection – Infiniband, Asterfusion, etc.
- **pros:** generally, more cost-effective (than supercomputers)
  - because they use standard hardware and can be scaled by adding more nodes (“horizontal scaling”)
- **cons:** powerful, but may not match the peak performance of a supercomputer (reliance on standard hardware and network communication), higher communication latency, more complex to maintain, not as energy-efficient (performance per watt)

# (Computing) Cluster (long days ago 😊)



# (Computing) Cluster (nowadays)





# Supercomputers vs. (Computing) Clusters

**Supercomputers** – single, highly specialized systems designed for maximum performance

**Computing clusters** – collections of standard computers working together to achieve high performance through parallel processing

**Remember: Neither supercomputers nor computing clusters can make your job to run significantly faster if it is not implemented for parallel/distributed processing.**

# (Super)Computing history in the Czech Republic

## Early Developments (1990s):

- **1994: the Supercomputing Center Brno (SCB) was established at Masaryk University**
  - aimed to introduce high-performance computing technologies to the Czech academic community, providing advanced computational resources to researchers and students
  - predecessor of the **Institute of Computer Science MU** and the **CERIT-SC Centre @ MU**



SGI PowerChallenge XL supercomputer with 12 MIPS R10000 processors and 2GB RAM. The first supercomputer at SCB MU. 1994.

# (Super)Computing history in the Czech Republic

## Early Developments cont'd (1990s):

- **1995:** deployment of **five high-performance computers** across major Czech universities
  - Masaryk University and University of Technology in Brno, Charles University and Czech Technical University in Prague, and the University of West Bohemia in Pilsen
- **1996:** the **MetaCentrum project** was launched to integrate these dispersed computing resources into a cohesive national grid.
- **1999:** the MetaCentrum had become a strategic project under the **CESNET association**
  - focuses on creating a unified computational infrastructure to support diverse scientific research across the country
- since then, MetaCentrum operates the National Grid Infrastructure
  - and collaborates with the CERIT-SC and IT4Innovations on the computing/storage services provided to the Czech research community

# (Super)Computing history in the Czech Republic



The core of the **initial supercomputer team** at SCB:

Luděk Matyska (head)

Aleš Křenek

Zdeněk Salvet

Martin Černohorský

Miroslav Ruda

In front of the SGI Origin + Onyx supercomputer (2000):  
40x CPU MIPS, R10000/195MHz, 18 GB RAM, 2x InfiniteReality2 graphics subsystem, 2x raster manager, 160MB frame buffer, 155 GB internal disks, 5x Fast Ethernet, 4x ATM, 270 GB on disk array.

# (Super)Computing (Data)Centers and Infrastructures

To become a **(grid, cloud, container, ...)** infrastructure, the HW and SW components of the (Data)Centers have to be **managed by a solution** that supports distributed computing, resource pooling, and dynamic scalability, tailored to the specific type of the infrastructure.

For example:

- **Grid infrastructure** requires technologies like OpenPBS or UNICORE, which enable resource sharing and task distribution across geographically dispersed systems
- **Cloud infrastructure** relies on platforms such as OpenStack, AWS, or Azure, which provide virtualization, automation, and on-demand resource provisioning
- **Container infrastructure** depends on orchestration tools like Kubernetes or Docker Swarm, which manage containerized applications and ensure efficient deployment, scaling, and networking

**These technologies ensure that the hardware and software components work together, and deliver:**

- the desired infrastructure type
- computing and storage services
- flexibility, efficiency, and scalability

# National Computing Infrastructures supporting research communities



# (Super)Computing Centres in the CR

available in 3 infrastructures (centers) in the Czech Republic:

– Cesnet/MetaCentrum

- grids/PBS
- clouds
- specialized computing

– MUNI/CERIT-SC

- grids/PBS
- clouds and containers
- specialized computing

– VŠB-TUO/IT4Innovations

- grids/PBS
- clouds

**e-INFRA CZ**

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

# MetaCentrum @ CESNET

## – activity of the **CESNET Association**

- CESNET – an association founded (and supported) by Czech universities and Czech Academy of Science provides services to universities + own research

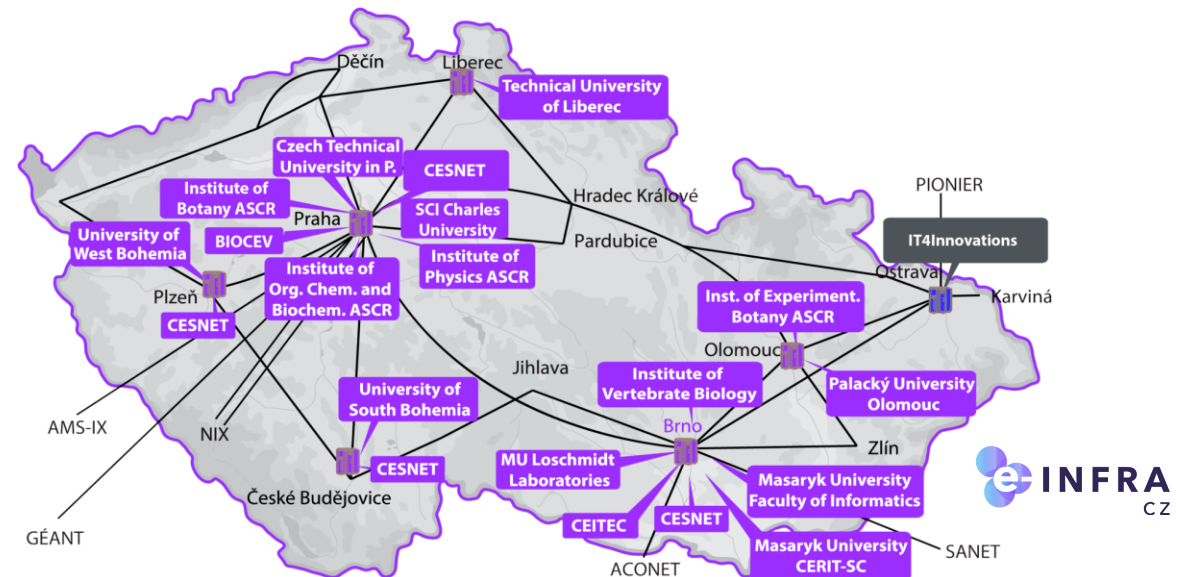
## – since 1996, the **Coordinator of the National Grid Infrastructure (NGI)**

- originally established at MUNI (Supercomputing Centre Brno, SCB, 1994)

## – integrates large/medium-sized HW centers (clusters, powerful servers and storage) of several universities/organizations within the CR

- → provides an environment for (collaborative) computing and data processing

## – Integrated into the European Grid Infrastructure (EGI.eu)





# MetaCentrum NGI

**available to all the employees and students of Czech universities/universities, the Academy of Sciences of the Czech Republic, research institutes, etc.**

- commercial entities for public research only

<http://metavo.metacentrum.cz>

## **offers:**

- Computational resources
- Storage capacities
- Application programs

**After registration available completely free of charge**

**"payment" in the form of publications with acknowledgements**



# NGI – available computing hardware

## computing resources: ca 46750 cores (x86\_64)

- Nodes with a lower number of performance cores:
  - 2x4-8 cores
- Medium core nodes (SMP machines):
  - 32-80 cores
- Up to 10 TB memory per node

## Nodes with a high number of cores: SGI UV 2000

- 504 cores (x86\_64), 10 TB RAM
- 384 cores (x86\_64), 6 TB RAM

## Other "exotic" hardware:

- nodes with GPU accelerators (Nvidia DGX with H100s), etc.



# NGI – available storage hardware

## approx. 33 PB for working data

- repository in Brno, Pilsen, České Budějovice, Liberec, Prague
- user quota of 1-3 TB on each of the storages

## approx. 80+ PB for long-term/archive data

- HSM – tape libraries, MAIDs (massive array of idle drives)
- CEPH object storage (analogy to Amazon S3)

<http://metavo.metacentrum.cz/cs/state/nodes>

# NGI – available software

**~500 different apps / ~3000 modules (installed on request)**

- see <https://docs.metacentrum.cz/software/alphabet/>

**continuously maintained development environment**

- GNU, Intel, PGI, debugging and optimization tools (TotalView, Allinea), ...

**generic math software**

- Matlab, Maple, Mathematica, gridMathematica, ...

**commercial and free software for application chemistry**

- Gaussian 09, Gaussian-Linda, Gamess, Gromacs, Amber, ...

**material simulations**

- ANSYS Fluent CFD, Ansys Mechanical, Ansys HPC...

**structural biology, bioinformatics**

- CLC Genomics Workbench, Geneious, Turbomole, Molpro, ...

**a range of freely available packages**

...

# NGI – basic characteristics

**after registration, all the resources are available without any administrative burden**

- → ~immediately (depending on actual usage)
- no applications for resources

**user accounts extensions every year**

- validates users' relationship to an academic institution
  - federated infrastructure eduID.cz used for minimalization of users' burden
- reports of user publications with acknowledgements to MetaCentrum/CERIT-SC
  - used as a proof of infrastructure benefits for Czech research area

**best-effort service**

- however, still usually 24x7

# NGI – how to compute?

## Batch jobs

- descriptive task script
- job start and end notifications

## Interactive jobs

- text and graphic mode

## Cloud computing

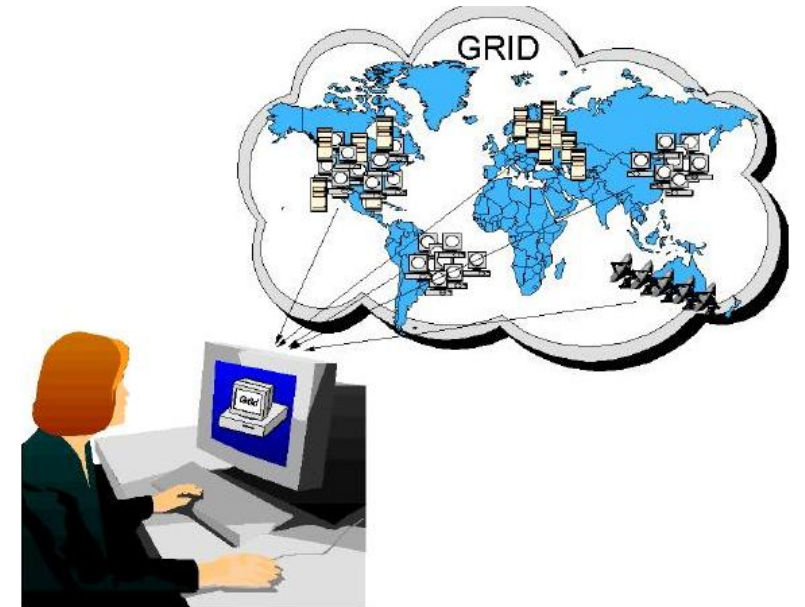
- users don't run jobs, but virtual machines
  - for research only

## graphical applications and virtual desktops in the browser environment

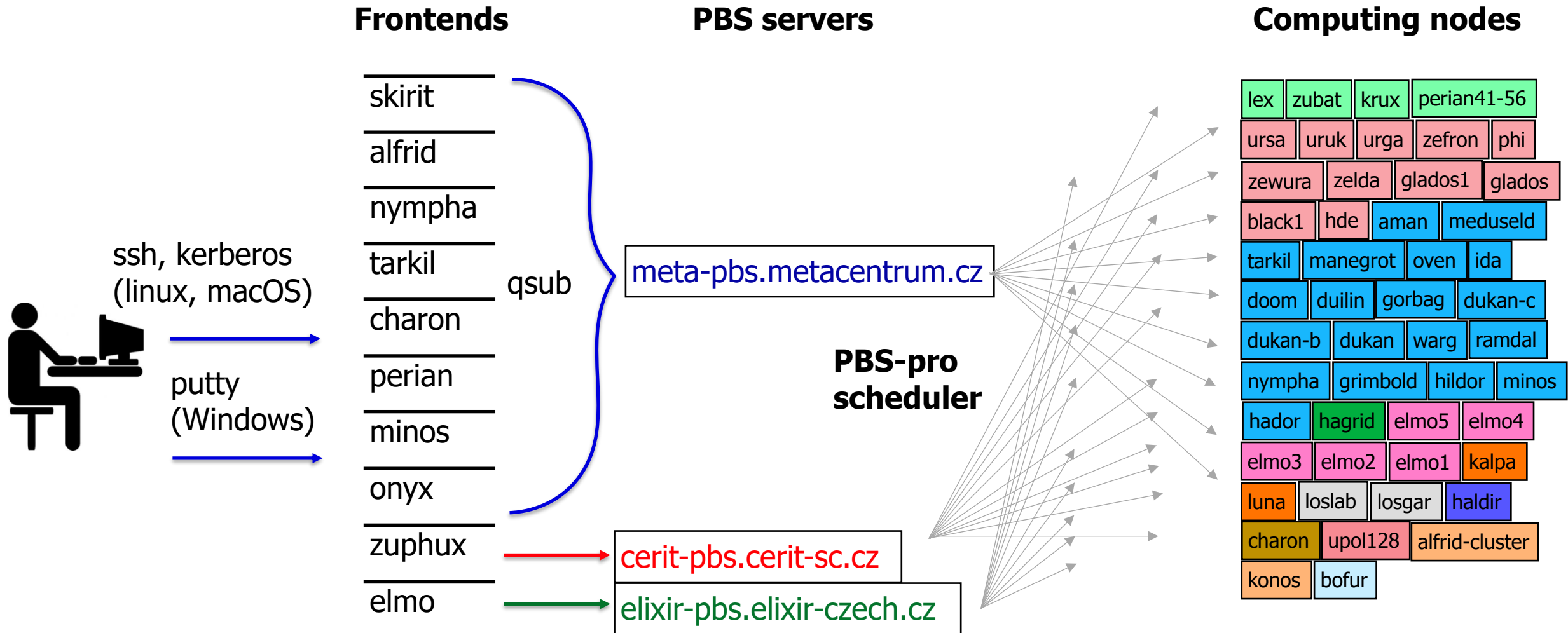
- Open OnDemand, Rancher, JupyterHub, ...

## specialized environments

- Apache Hadoop, Galaxy, ...



# NGI under the hood – how to connect?



# NGI under the hood – in numbers ...

**approx. 46750 computing cores, approx. 700 nodes**

– and 462 of GPU accelerators

**year 2024:**

– 3490 users (31.12.2024)

– ca 15 million of jobs running

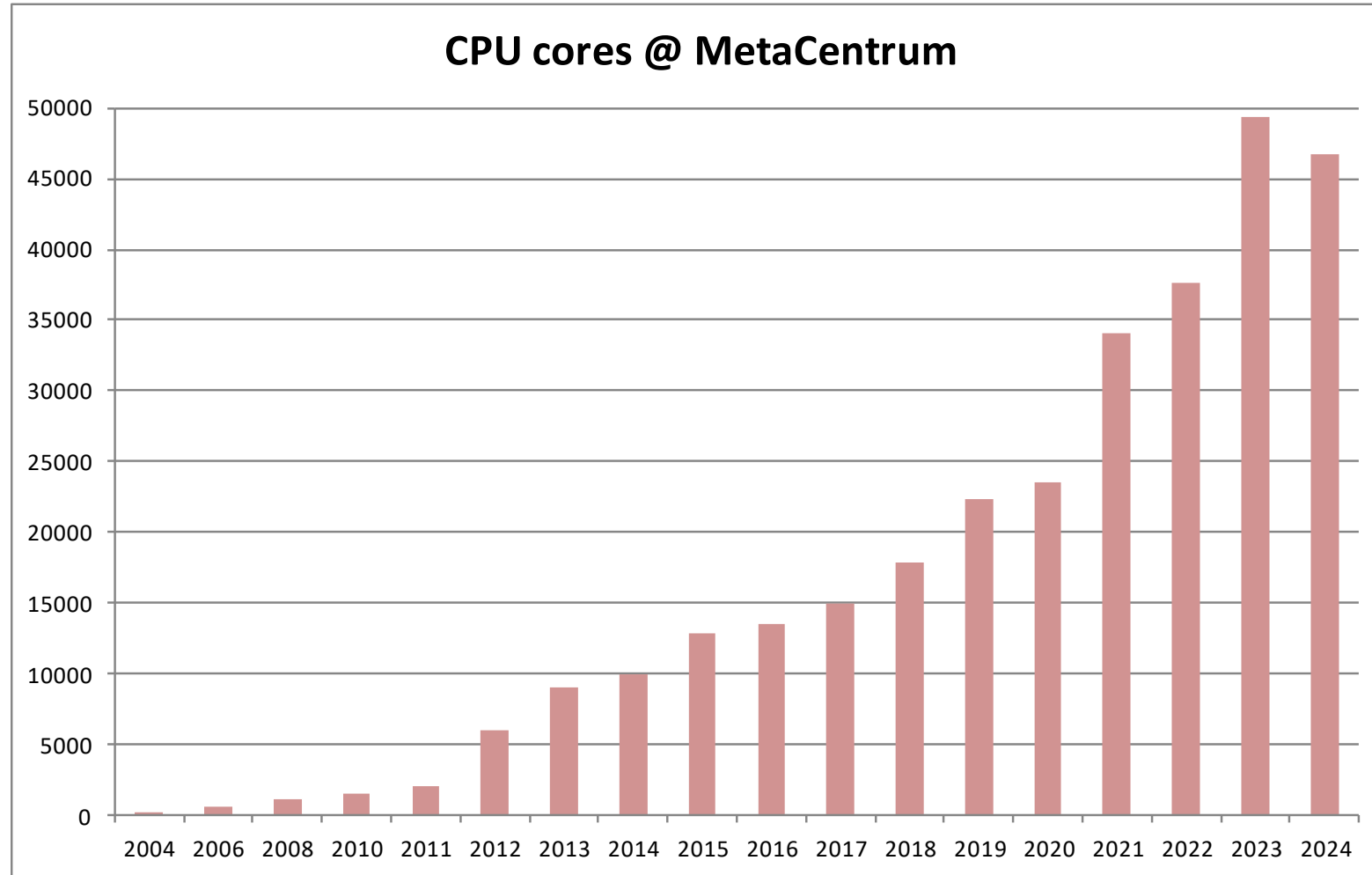
- ca 41100 jobs per day
- ca 4300 jobs per user

– approx. 37.5 thousands of CPUyears computed in total

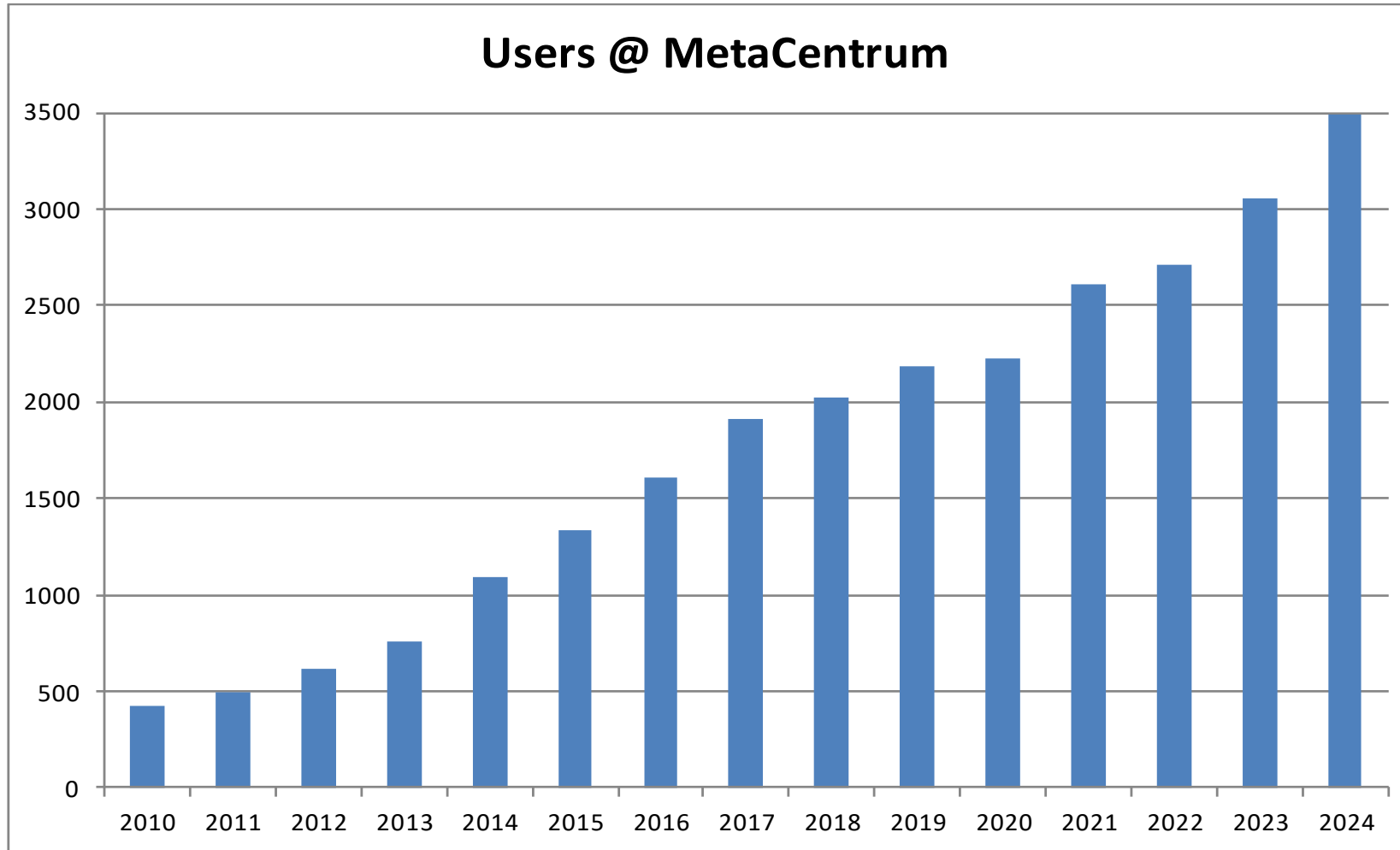
- and 357 of GPUyears



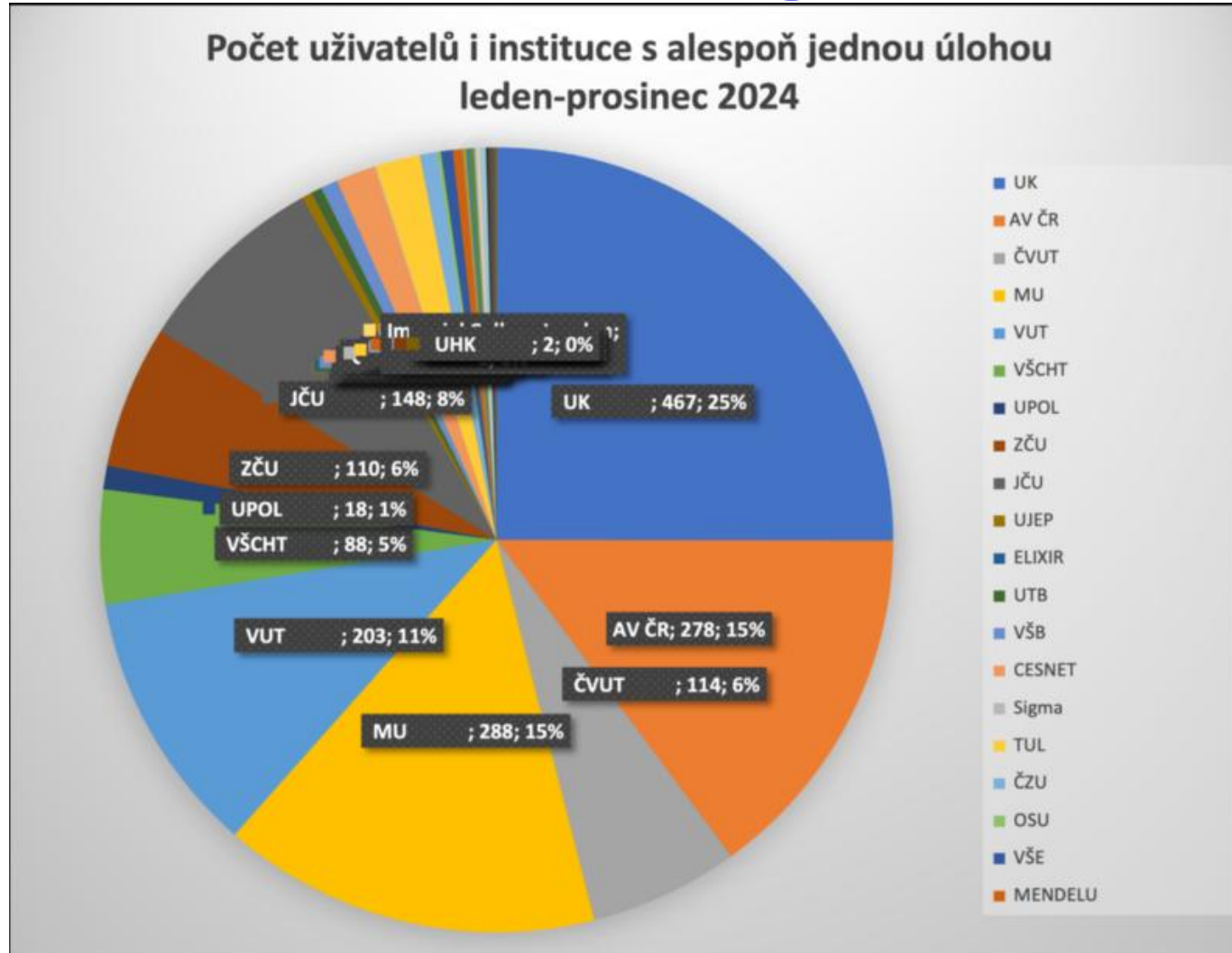
# NGI under the hood – and graphs ...



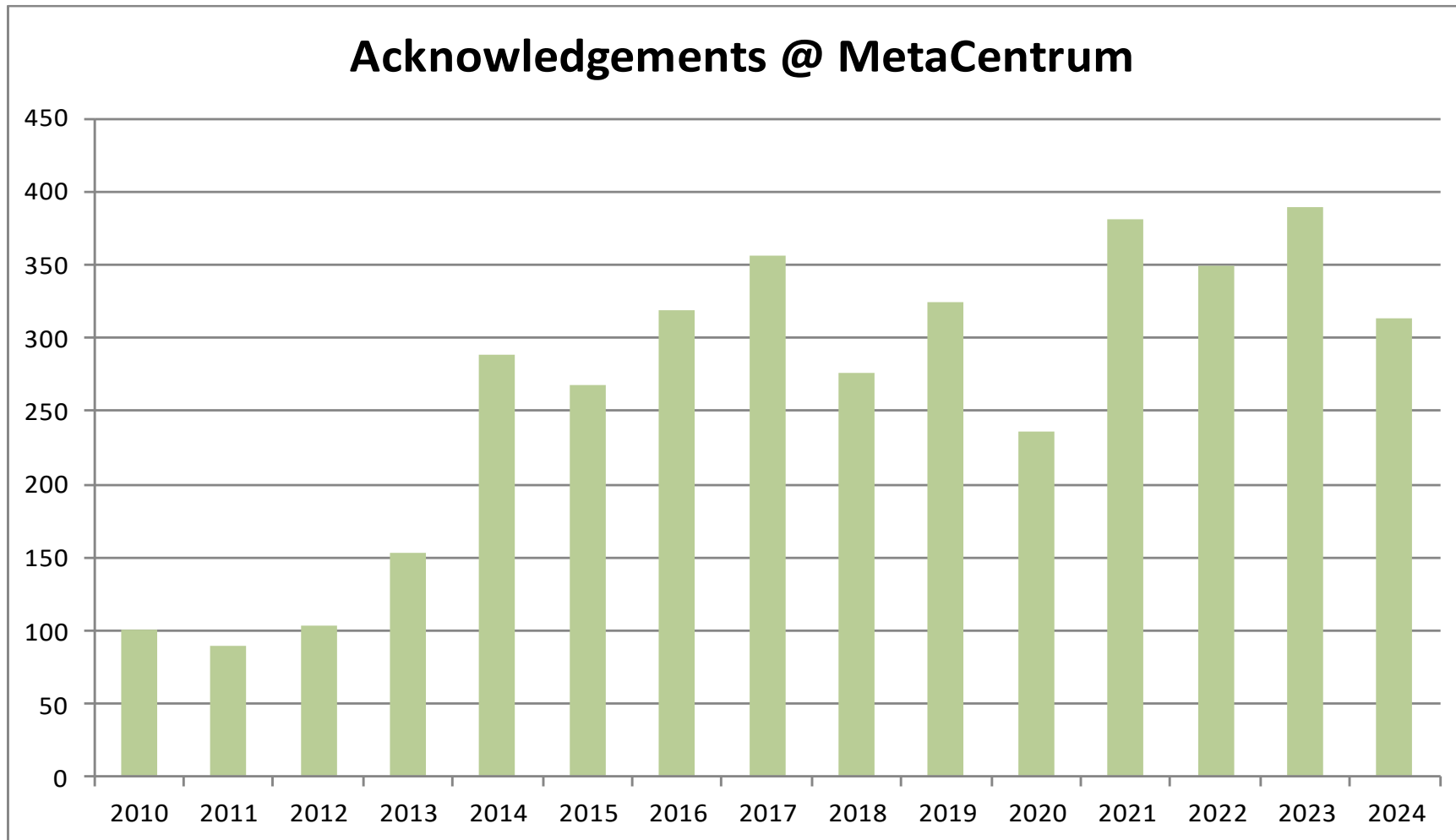
# NGI under the hood – and graphs ...



# NGI under the hood – and graphs ...



# NGI under the hood – and graphs ...

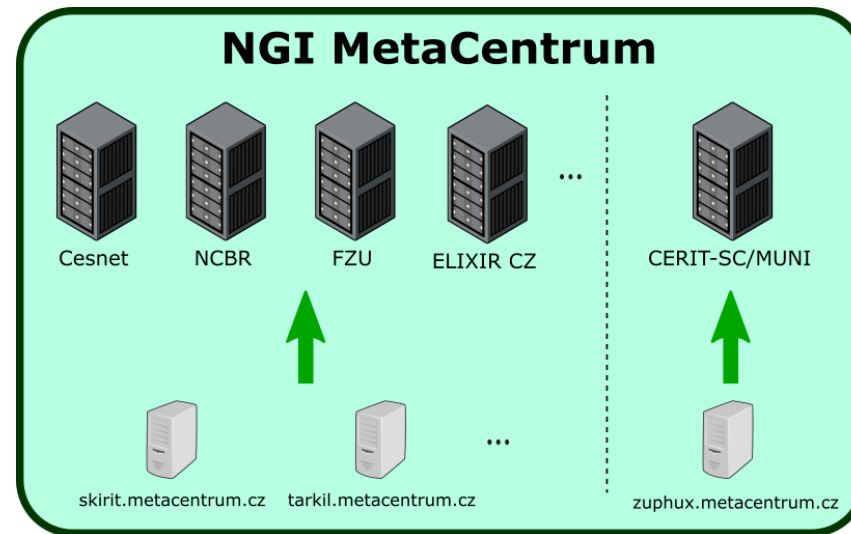


# MetaCentrum NGI & Resource integration I.

## MetaCentrum and CERIT-SC

– MetaCentrum provides own HW resources (CESNET) and integrates resources of external providers

- CERIT-SC/MUNI is one of them
- others are CEITEC/NCBR, FZU, ČVUT, JČU, ZČU, UPOL, MU, TUL, etc.  
as well as global projects like ELIXIR CZ



**+ shared storages  
and shared SW apps**

# MetaCentrum NGI & Resource integration II.

**resource owners (usually) have priority access to their HW resources**

- under agreed conditions
- technically accomplished using specific scheduler queues
  - more details later

# MetaCentrum NGI & Support of external partners

## Assistance with:

- purchase and integration computational resources into NGI
- selection, installation and maintenance of the clusters
- software maintenance
- maintenance of user accounts
- priority/exclusive access to owned clusters

# CERIT-SC Centre

## CERIT-SC Centre – a research centre built at ICS MU

- originally Supercomputing Centre Brno (SCB)

### 1. provider of HW and SW resources

- esp. the special ones (DGX, UV 2000)
- part of the MetaCentrum NGI

### 2. services beyond the scope of a “common” HW centre

- **interdisciplinary research**
  - cooperation of IT researchers and partners from other fields





# CERIT-SC Centre

## main objectives of the CERIT-SC @ MUNI Centre:

- flexible infrastructure, own research in infrastructure areas
- three main **research pillars**:
  - *High-performance computing* – acceleration of calculations, GPU computing, ...
  - *Artificial Intelligence* – application of artificial intelligence and machine learning methods (esp. in biology)
  - *Data Infrastructures and Big Data analytics* – design and implementation of data analytics infrastructures and

*Tom Rebok's Research Group*

# CERIT-SC Centre – key research activities

**High-Performance Computing (HPC)** – accelerating research by providing powerful computing resources

- supporting a wide range of scientific fields including artificial intelligence, data science, and computational biology
- including sensitive data processing and GPU acceleration support

**Data Science** – unified analysis of vast, heterogeneous data (data collection, processing, analysis, storage, and sharing)

- development of (both national and international) data and analysis infrastructures

**Artificial Intelligence (AI)** – application of AI / ML techniques in various applied solutions (biology, crime & security, data management, etc.)

**EOSC / FAIR Data** – promoting Findable, Accessible, Interoperable, and Reusable (FAIR) data principles (see later)

**Digital Identity and Access Management** – management of digital identities and controlled access to services (Perun AAI ecosystem)

# CERIT-SC Centre – research collaborations

## How are the research collaborations performed?

- the work is carried via a doctoral/diploma thesis of a FI MU student
- the CERIT-SC staff supervises/consults the student and regularly meets with the research partners
  - the partners provide the expert knowledge from the particular area

## Collaborations through (international) projects

- CERIT-SC participates on several projects, usually developing IT infrastructure supporting the particular research area
  - ELIXIR-CZ, BBMRI, Thalamoss, SDI4Apps, Onco-Steer, CzeCOS/ICOS, ...
  - KYPO, 3M SmartMeters in cloud, MeteoPredictions, ...

## Strong ICT expert knowledge available

- long-term collaboration with Faculty of Informatics MU
- long-term collaboration with CESNET
  - → consultations with experts in particular areas

# IT4Innovations

## IT4Innovations – national supercomputing centre at VSB TUO in Ostrava

- established in 2012
- provides cutting-edge computational resources and support for research and innovation in HPC, artificial intelligence, big data analytics, and related fields
  - one of the leading supercomputing centers in Europe
- currently available supercomputers
  - Karolina, Barbora, LUMI, NVIDIA DGX-2
- available to academic staff as well as the commercial bodies

### **services: HW provider and interdisciplinary research**

- own research laboratories
- research cooperation with the centre's users

### **computing time has to be officially requested**

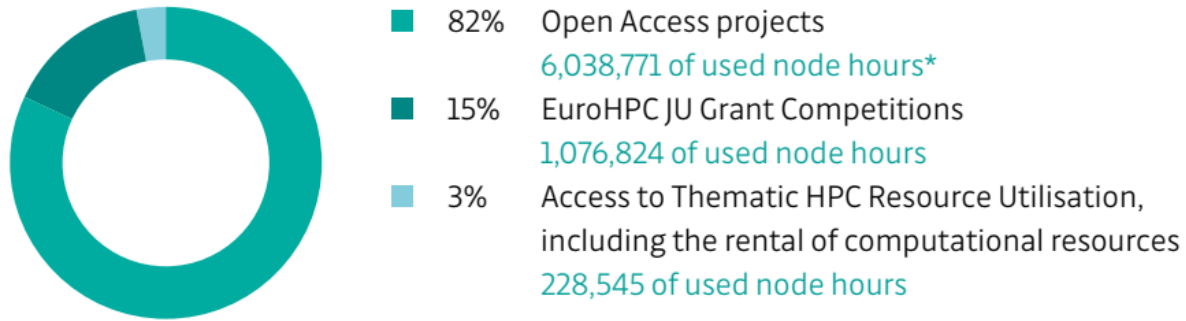
- so-called grant competitions (every 6 months)
  - subsequently, dedicated computing time
  - (might require financial participation)



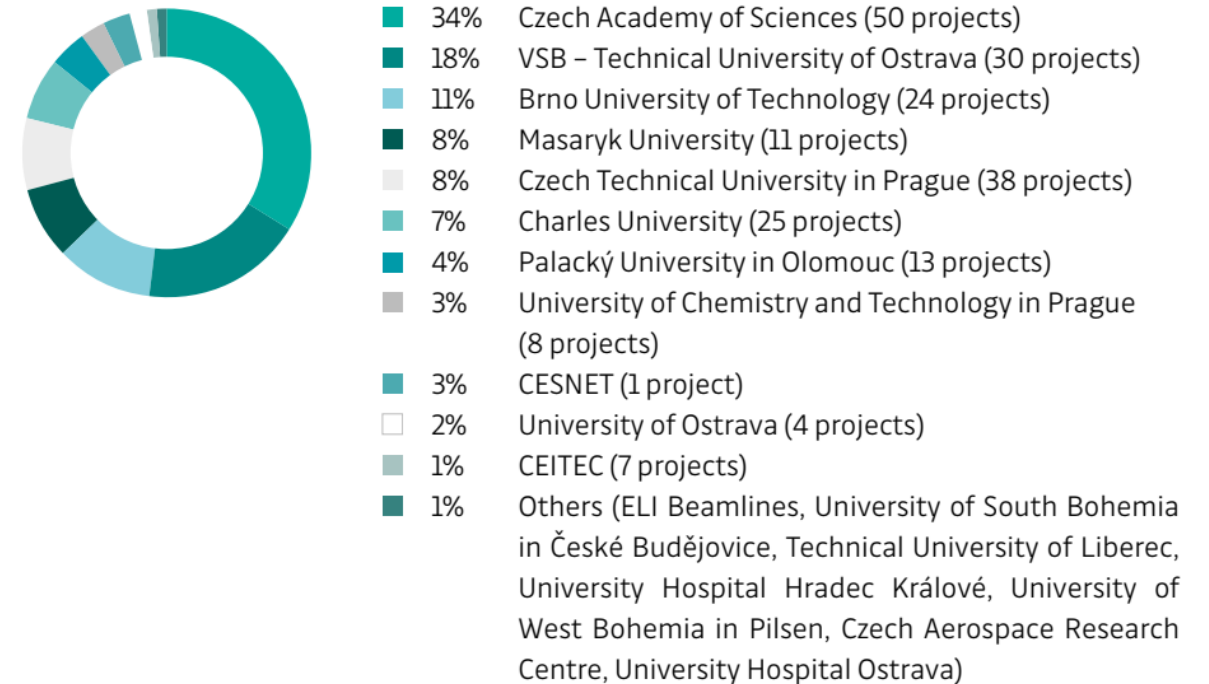
	NVIDIA DGX-2	Barbora	Karolina	LUMI
Put into operation	Spring 2019	Autumn 2019	Summer 2021	Winter 2023
Theoretical peak performance	130 TFlop/s	849 TFlop/s	15.7 PFlop/s	531.5 PFlop/s
Operating system	CentOS 7	RHEL 8	Rocky Linux 8.x	HPE Cray OS
Compute nodes	1	201	831	5,042
Types of compute nodes	<p><b>1 GPU node</b> 2x Intel Xeon Platinum 8168, 24 cores, 2.7 GHz, 1.5 TB RAM, 16x NVIDIA Tesla V100, 32 GB HBM2</p>	<p><b>192 CPU nodes</b> 2x Intel Cascade Lake 6240, 18 cores, 2.6 GHz, 192 GB RAM</p> <p><b>8 GPU nodes</b> 2x Intel Skylake 6126, 12 cores, 2.6 GHz, 192 GB RAM, 4x NVIDIA Tesla V100, 16 GB HBM2</p> <p><b>1 SMP node</b> 8x Intel Xeon 8153, 16 cores, 2.0 GHz, 6 TB RAM</p>	<p><b>756 CPU nodes</b> 2x AMD EPYC 7h12, 64 cores, 2.6 GHz, 256 GB RAM (of which 36 nodes used for Cloud services)</p> <p><b>72 GPU nodes</b> 2x AMD EPYC 7763, 64 cores, 2.45 GHz, 1 TB RAM, 8x NVIDIA A100, 40 GB HBM2</p> <p><b>1 data analytics node</b> 32x Intel Xeon-SC 8628, 24 cores, 2.9 GHz, 24 TB RAM</p> <p><b>2 visualisation nodes</b> 2x AMD EPYC 7452, 32 cores, 2.35 GHz, 256 GB RAM, 1x NVIDIA RTX 6000 GPU</p>	<p><b>2,048 CPU nodes</b> 2x AMD EPYC 7763, 64 cores, 2.45 GHz, 256 – 1,024 GB RAM</p> <p><b>2,978 GPU nodes</b> 1x AMD EPYC 7A53, 64 cores, 2.45 GHz, 512 GB RAM, 4x AMD Instinct MI250X GPUs, 128 GB HBM2e</p> <p><b>8 data analytics nodes</b> 2x AMD EPYC 7742, 64 cores, 2.25 GHz, 4 TB RAM</p> <p><b>8 visualisation nodes</b> 2x AMD EPYC 7742, 64 cores, 2.25 GHz, 2 TB RAM, 8x NVIDIA A40 GPU</p>
Accelerators in total	16x NVIDIA Tesla V100	32x NVIDIA Tesla V100	576x NVIDIA Tesla A100, 2x NVIDIA RTX 6000	11,912x AMD Instinct MI250X, 8x NVIDIA A40
CPU cores in total	48	7,232	106,880	454,784
Storage	30 TB NVMe	29 TB / home 310 TB / scratch (28 GB/s)	30 TB / home 1,275 TB / scratch (NVMe, 730 GB/s SWP, 1,198 GB/s SRP)	81 PB / (home + project + scratch) (240 GB/s)
Interconnection	Infiniband EDR 100 Gb/s	Infiniband HDR 200 Gb/s	Infiniband HDR 200 Gb/s	200 Gb/s Slingshot-11

# IT4Innovations – statistics

## Distribution of computational resources in 2023



## Computational resources allocated within the Open Access Grant Competitions in 2023 by institutions



# e-INFRA CZ – how to become a user?

## submit an application

- <https://docs.e-infra.cz/cs/account/> , section „Account creation“
- EduID.cz => verification of your academic identity will be made using your home institution

## learn about the documentation and basics of Linux OS

- <http://metavo.metacentrum.cz> , section „Documentation“
- practical seminars: <https://metavo.metacentrum.cz/cs/seminars/index.html>
- <https://www.abclinuxu.cz/ucebnice/zaklady>

## compute

- *NGI and CERIT-SC*: no need for submitting any requests for computing time
- *IT4Innovation*: participate in the grant competitions

# e-INFRA CZ – selected services for end users

## FileSender – web service for sending large files

- current limit: 2 TB (~2000 GB)
- expiration time: up to 1 month

<http://filesender.cesnet.cz>



## Either the sender or recipient must be an authorized academic staff member

- an authorized user can **send data files to any user**
  - may include email notifications about the data lifecycle
- an authorized user can **send an invitation to receive data files from any user**



# FileSender – how to use



Preferred language English

[Help](#) [About](#) [Login](#)

## Welcome to Filesender.Cesnet.cz

Filesender.Cesnet.cz is a secure way to share large files with anyone!

Login to upload your files or invite people to send you a file.

If you have received an invitation to access this site as a guest then the email will contain the information you will need to access this site and upload files.

By logging in, you confirm that you have been informed of the [terms of service](#) and of the information about the [processing of personal data](#).

Login



# FileSender – how to use

Přihlásit účtem

Masarykova univerzita

MUNI

Jiný účet

MUNI Jednotné přihlášení

English  Українська



Učo

39685j

Primární heslo

••••••••

Zapamatovat si mě

PŘIHLÁSIT

> [Mám problém s přihlášením](#)

# FileSender – how to use

vouchers/invitations

The screenshot shows the FileSender web interface. At the top, there is a navigation bar with 'Upload', 'Guests', 'My Transfers', 'My profile', 'Help', 'About', 'Privacy', and 'Log-off'. The 'Preferred language' is set to 'English'. The main area features a large dashed box with the text 'drag & drop your files here'. Below this are 'Clear all' and 'Select files' buttons. A red arrow points to the 'Select files' button. To the right of the 'Select files' button is a green callout box containing the text 'advanced notifications, reference links, etc.' and a link to 'Advanced settings'. Below the main area are 'From : rebok@ics.muni.cz', a 'File Encryption' checkbox, an 'Expiry date: 27/02/2025' field, and a 'Send me daily statistics' checkbox. A 'Send' button is located below these options. At the bottom, there is a line chart titled 'Globální průměrná rychlost nahrávání souborů 1 GB' showing upload speeds in MB/s from Jan 18 to Feb 17. The chart has two series: 'Šifrování při přenosu & rest' (green) and 'Šifrování při přenosu' (orange). The green series shows significant peaks around Jan 28 and Feb 17, reaching approximately 110 MB/s.

advanced notifications, reference links, etc.

## e-INFRA CZ – selected services for end users

### OwnCloud – cloud storage a la Google Drive or Dropbox

- current quota: 100 GB / user

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

### Synchronization and availability of data between devices

- clients available for OS Windows, Linux, OS X
- available for smartphones and tablets as well
- enables data sharing among users
- provides backups
- etc.



# OwnCloud – how to use

datacare

Uživatelská dokumentace FAQ Kontakt [Přihlásit se](#)

## ownCloud @ CESNET

Sync, Share & Backup all of your academic data.

PŘIHLÁSIT SE

Přihlášením potvrzujete, že jste byl/a seznámen/a s [podmínkami služby](#) a s [informacemi o zpracování osobních údajů](#).

# OwnCloud – how to use

The screenshot displays the OwnCloud web interface. At the top, a blue header bar contains the text "Soubory" on the left, the "ownCloud@CESNET DataCare" logo in the center, and search, notification, and user profile icons on the right. The user profile is identified as "RNDr. Tomáš Rebok Ph.D.". Below the header, a navigation breadcrumb shows "Všechny soubory" > "Shared" > "+". A left sidebar lists navigation options: "Všechny soubory", "Oblíbené", "Sdíleno s vámi", "Sdíleno s ostatními", "Sdíleno pomocí odkazu", and "Značky". The main content area shows a table of shared files:

<input type="checkbox"/>	Název		Velikost	Upraveno
<input checked="" type="checkbox"/>	MetaCentrum	Mgr. Miroslav Ruda	4.7 MB	před 5 měsíci
<input checked="" type="checkbox"/>	prezentace-tabor	Jan Růžička	281 KB	před 3 měsíci
2 adresáře			5 MB	

# e-INFRA CZ – selected services for end users

## Open OnDemand – a user-friendly UI interface to interactive computing

- simplifies interaction with supercomputing systems

<https://ondemand.metacentrum.cz>

### Key Features:

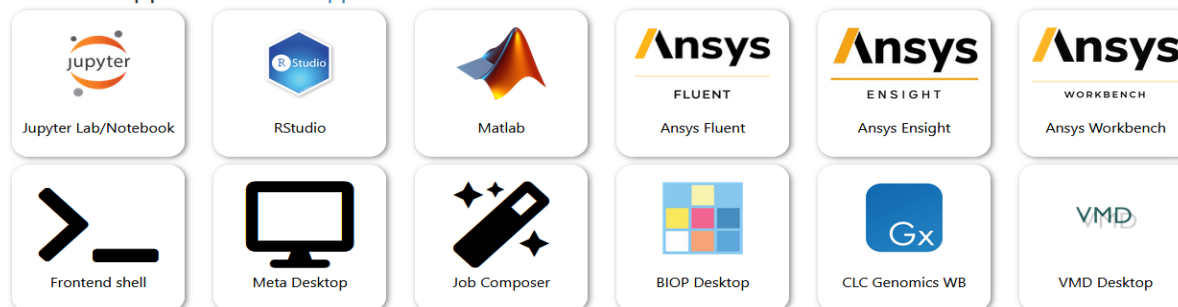
- **User-Friendly Interface** – no command-line expertise required
- **File Management** – easily upload, download, and manage files
- **Job Submission** – submit, monitor, and manage HPC jobs via a web browser
- **Interactive Apps** – run GUI-based applications (e.g., Jupyter Notebook, MATLAB, RStudio)
- **Remote Visualization** – visualize data and results directly in the browser

# OnDemand – how to use (after federated login)



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

OnDemand has been upgraded to the major version 3.





# OnDemand – how to use

The screenshot shows the OnDemand web interface. At the top, there is a navigation bar with the 'metacentrum' logo and menu items: Files, Jobs, Clusters, Interactive Apps, and My Interactive Sessions. On the right side of the navigation bar, there are links for Help, 'Logged in as jeronimo', and Log Out.

Below the navigation bar, a breadcrumb trail reads: Home / My Interactive Sessions / RStudio Server.

The main content area is divided into two columns. The left column, titled 'Interactive Apps', contains a list of application categories and specific apps. Under 'Desktops', there are: Ansys/Ensignt, Ansys/Fluent, Ansys/Workbench, BIOP Desktop, CLCgenomicsWB, Matlab, MetaCentrum Desktop, and VMD Desktop. Under 'Servers', there are: Jupyter Notebook/Lab, Matlab webapp (beta), and RStudio Server (which is highlighted in blue).

The right column, titled 'RStudio Server', contains the following information and configuration options:

- Description: 'This app will launch an RStudio server on one or more nodes. Geospatial and Tensorflow packages are preinstalled.'
- Number of hours: A dropdown menu set to '1'.
- Number of CPUs on single node: A dropdown menu set to '1'.
- Memory (GB): A dropdown menu set to '2'.
- GPUs: A dropdown menu set to '0'.
- Scratch local (GB): A dropdown menu set to '1'.
- RStudio Image version: A dropdown menu set to 'RStudio-geospatial-4.4.1'.
- RStudio working directory location: A dropdown menu set to '/storage/brno2'.
- A blue 'Launch' button.
- A note: '\* The RStudio Server session data for this session can be accessed under the [data](#) root directory.'

A large red arrow points from the bottom right towards the 'Launch' button.

# OnDemand – how to use

The screenshot displays the OnDemand web interface. At the top, a navigation bar includes the 'metacentrum' logo, a search bar, and menu items for 'Files', 'Jobs', 'Clusters', 'Interactive Apps', and 'My Interactive Sessions'. On the right side of the navigation bar, there are links for 'Help', 'Logged in as jeronimo', and 'Log Out'. A green notification banner at the top of the main content area states 'Session was successfully created.' Below this, a breadcrumb trail shows 'Home / My Interactive Sessions'. On the left, a sidebar titled 'Interactive Apps' lists various desktop and server environments under 'Desktops' and 'Servers' categories. The 'RStudio Server' option is selected. The main content area shows details for the 'RStudio Server (8886350.pbs-m1.metacentrum.cz)' session, which is currently 'Running' with '1 node' and '1 core'. It includes the host name 'nympha53.meta.zcu.cz', a 'Delete' button, the creation time '2025-02-17 09:23:01 CET', a 'Time Remaining' of '59 minutes', and a 'Session ID'. A blue button labeled 'Connect to RStudio Server' is visible, with a red arrow pointing to it.

## e-INFRA CZ – selected services for end users

**Rancher (Kubernetes)** – open-source platform for managing Kubernetes clusters

- simplifies deployment, scaling, and management of containerized applications

<https://rancher.cloud.e-infra.cz>

### **Key Feature:**

- reduces complexity of Kubernetes management as well as container deployment

# Rancher – how to use (after federated login)

The screenshot shows the Rancher dashboard interface. At the top, there is a navigation bar with the 'INFRA' logo and a user profile icon. Below the navigation bar is a large banner with the text 'Welcome to Rancher' and a landscape illustration. A blue notification bar below the banner contains the text 'Learn more about the improvements and new capabilities in this version and read about the UI framework migration in 2.10' and a link 'What's new in 2.10'. The main content area is titled 'Clusters' and shows a table with one cluster entry. A red arrow points to the 'kuba-cluster' entry. To the right of the table is a 'Links' sidebar with links for 'File an Issue', 'Documentation', and 'Commercial Support'.

State	Name	Provider Distro	Kubernetes Version Architecture	CPU	Memory	Pods
Active	kuba-cluster	Imported RKE2	v1.31.4+rke2r1 -	3072 cores	30 TiB	2972/7040

# Rancher – how to use (Apps menu)

The screenshot displays the Rancher web interface. On the left, a navigation sidebar is visible with the 'KA' namespace selected. A red arrow points to the 'Charts' option in the sidebar. The main content area shows the 'Charts' page for the 'certif-sc' namespace. At the top right, there are buttons for 'Browse' and 'Featured'. Below the featured charts, a message states: 'All charts have at least one version that is installable on clusters with Linux and Windows nodes unless otherwise indicated.' Below this message, there are filters for 'certif-sc' and 'All Categories'. A checkbox for 'Show deprecated apps' is present. The main area contains a grid of 20 chart cards, each with a logo, name, and version. The cards are: ansys (ANSYS 2021R1), bibs, blender (Blender), code-server (VSCode Code-server), cplex (IBM ILOG CPLEX Studio), desktop (Remote Desktop), knime (Knime over VNC), matlab (Matlab 9.11), maxquant (MaxQuant), minio (Minio personal server), moodle (Moodle Server), mpijob (OPEN MPI), neo4j (neo4j server), owncloud (ownCloud Client), paraview (ParaView Server), and personal-monitoring (Personal Monitoring v0.0.4). Each card has a 'Linux only' label in the bottom right corner.

## e-INFRA CZ – selected services for end users

**Foldify** – a web application based on **AlphaFold** tools

- predicting **protein structures** with high accuracy

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

**AlphaFind** – a web-based search engine that allows for structure-based search of the entire AlphaFold Protein Structure Database

- developed by FI MUNI in cooperation with CERIT-SC

<https://alphafind.fi.muni.cz/>

# European Computing & Data Research Infrastructures



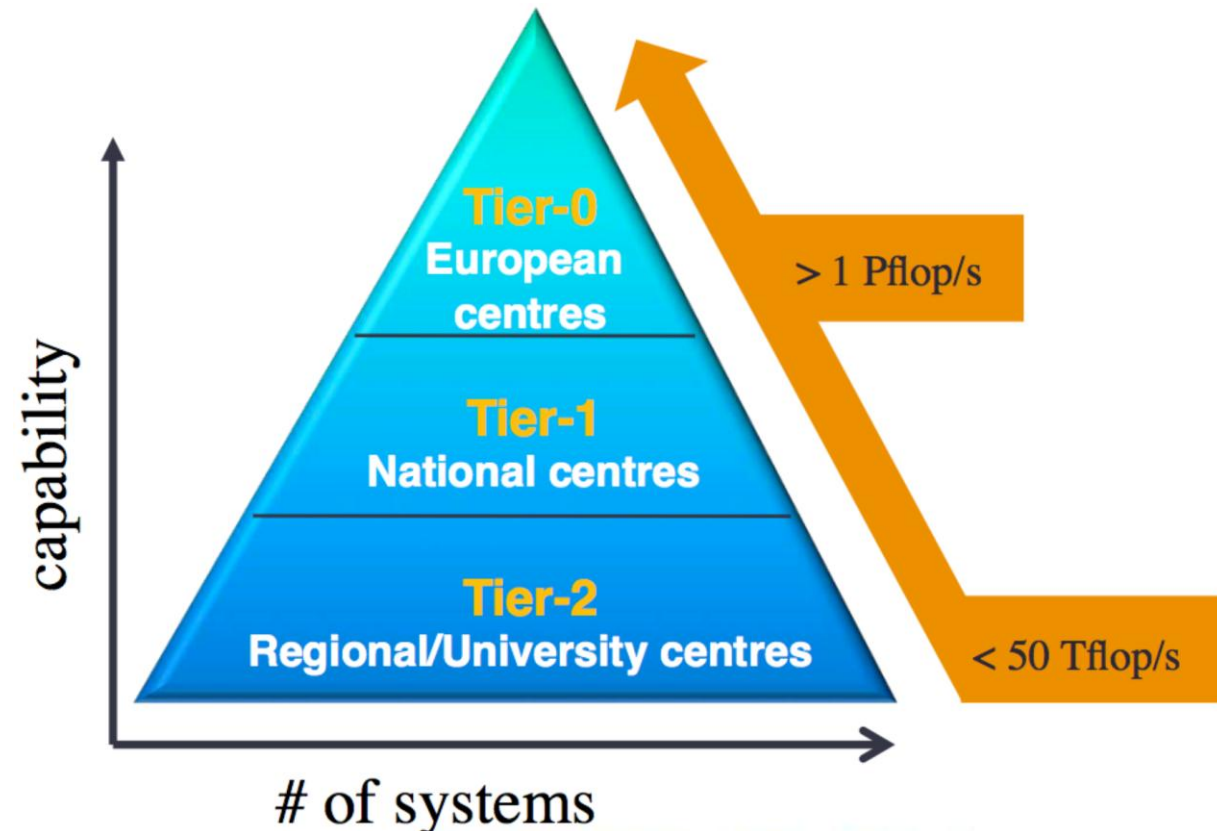
# European HPC Infrastructures

## Structured provision of European HPC facilities:

- Tier-0: European Centres (> petaflop machines)
- Tier-1: National Centres
- Tier-2: Regional/University Centres

## Tiers planned as part of an EU Research Infrastructure Roadmap

This is coordinated through “PRACE” – <http://prace-ri.eu>





# PRACE

## Partnership foR Advanced Computing in Europe

- international non-profit association (HQ office in Brussels)
- established in 2010 following ESFRI roadmap to create a persistent pan-European Research Infrastructure (RI) of world-class supercomputers
  - ESFRI = European Strategy Forum on Research Infrastructures

**Mission:** enable high-impact scientific discovery and engineering research and development across all disciplines to enhance European competitiveness for the benefit of society

- provide access to leading-edge computing and data management resources and services for large-scale scientific and engineering applications at the highest performance level

# PRACE members

Currently 25 members:

- Austria
- Belgium
- Bulgaria
- Cyprus
- Czech Republic
- Denmark
- Finland
- France
- Germany
- Greece
- Hungary
- Ireland
- Israel
- Italy
- The Netherlands
- Norway
- Poland
- Portugal
- Slovakia
- Slovenia
- Spain
- Sweden
- Switzerland
- Turkey
- UK

**CR participates through IT4Innovations.**



# EGL.eu (European Grid Infrastructure)

## EGL.eu

- a federation of computing and storage resource providers united by a mission to support data-intensive research with a wide range of advanced computing services
- established to create a persistent pan-European Research Infrastructure (RI) that facilitates scientific discovery and innovation

## Key Features:

- **Federated e-Infrastructure:** comprises national computing and data centers
- **Technologies:** Grid/PBS computing, cloud computing, containers
- **Services:** HPC, cloud computing platforms, data management, and analytics
- **Community Support:** engages with diverse user communities to identify needs, provide support, and drive innovation

**CR participates through MetaCentrum NGI.**

# EUDAT (European Data Infrastructure)

## EUDAT

- a comprehensive set of research data services, expertise, and technology solutions to all European scientists and researchers
- established to create a persistent pan-European Research Infrastructure (RI) that supports data stewardship and management

## Key Features:

- **Federated Data Infrastructure:** distributed across 15 European nations, integrating data storage with some of Europe's most powerful supercomputers
- **Technologies Used:** data management tools, cloud storage, federated identity management
- **Services:** solutions for finding, sharing, storing, replicating, and computing with research data, including the B2 Service Suite (B2SAFE, B2SHARE, B2DROP, etc.)
- **Community Support:** engages with diverse research communities to provide tailored data services and support

# European Open Science Cloud (EOSC) – core ideas

## 1. Research data are valuable

- And large part is lost after initial processing

## 2. Only properly annotated data are valuable (even in mid term)

- The value goes beyond groups that create the (primary) data

## 3. The data are critical for the research reproducibility

## 4. Not only data, but the processing tools and environments must be maintained

- ie., the other digital artefacts

⇒ besides the HPC infrastructures, **data infrastructures are also of high importance**

# European Open Science Cloud (EOSC)

## What is EOSC?

- a pan-European initiative to create a virtual environment for open science
- aims to provide seamless access to research data and services
- supports European researchers and innovation through data sharing

**Key Goal: Build a federated and interoperable ecosystem for research data and services.**

- EU started with EOSC around 2016

# European Open Science Cloud (EOSC) – main principles

**Open Science:** promotes transparency, accessibility, and collaboration

**Federation:** connects national and international data repositories

**Interoperability:** ensures seamless integration across disciplines and services

**Trust and Security:** provides reliable access to research data with ethical considerations

## FAIR Data Principles

- **Findable:** Data should have unique identifiers and metadata.
- **Accessible:** Data should be retrievable via standard communication protocols.
- **Interoperable:** Data should use standard formats and vocabularies.
- **Reusable:** Data should have clear licensing and provenance information.

# European Open Science Cloud (EOSC) – FAIR data

## Why FAIR data?

- Findable, Accessible, Interoperable, Reusable

## Benefits:

- You don't lose your data (Findable)
- You will know where they are and how to get them (Accessible)
- You have your data properly described/annotated (Interoperable)
- You will be able to use them again (Reusable)

## Additional benefits

- You can share such data without (much) work on your side
- You can (easily) combine such data with data from other sources
- And you can publish your data



# European Open Science Cloud (EOSC) – basic components

**Metadata Repositories:** store and manage metadata for research data

- metadata? key-value information associated with the data files

**Data Storage & Management:** secure and scalable storage solutions for research data

- place for storing the data

**Computational Services:** cloud computing and HPC resources

- close interconnection with HPC infrastructures

**Identity and Access Management (IAM):** ensures secure access control for researchers

- AAI – authentication, authorization, identities

**Collaboration Platforms:** virtual research environments and shared workspaces

- place to analyze the data (and place to cooperate)

# European Open Science Cloud (EOSC) – summary

- EOSC aims to transform European research through open science and data sharing
- FAIR principles ensure accessibility and reuse of research data
- cooperation with HPC infrastructures enhances computational capabilities
- EOSC is considered as a key driver for the future of scientific innovation in Europe

## Czech EOSC node: <https://www.eosc.cz/>

- designed, managed and operated by the e-INFRA CZ
  - close cooperation of CERIT-SC and CESNET

