Research e-Infrastructures in Czech Republic (e-INFRA CZ)

for scientific computations, collaborative research & research support

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e-INFRA CZ

Covers three e-infrastructures – MetaCentrum (NGI), IT4I (SuperComputers) and CERIT-SC (NGI & Research Collaborations)

Available to all academic users from Czech universities, Academy of Science, research institutes, etc.

- commercial bodies mainly for public research

Offers:

- **computing resources**
- **storage resources**
- **application programs**

Computing services:

- **grid services**
- **supercomputing services**
- **cloud services**
- **storage services**
- **specialized environments**

https://www.e-infra.cz

Research e-Infrastructures in CR I.

MetaCentrum National Grid Infrastructure (NGI)

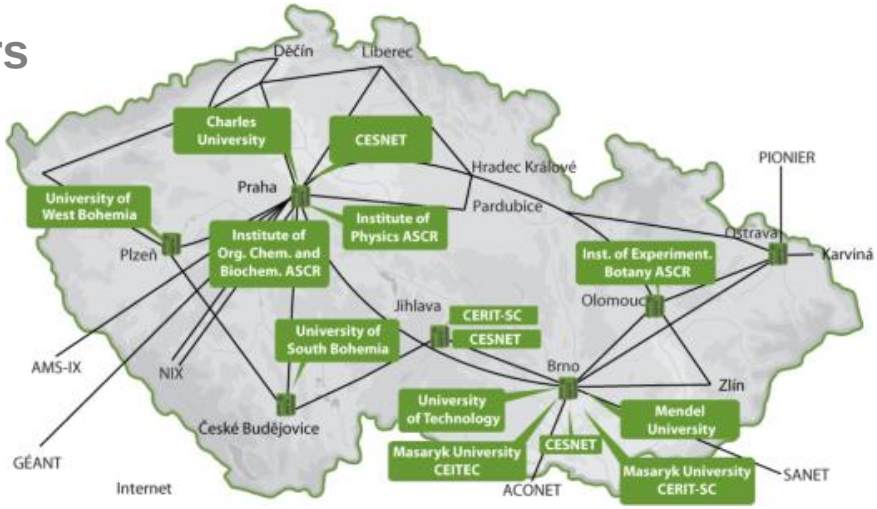
- operated by MetaCentrum NGI (CESNET) since 1996
- MetaCentrum responsible for management and coordination

https://www.metacentrum.cz

Distributed infrastructure

NGI integrates medium/large HW centers (clusters, powerful servers, storages) of several universities/institutions

- further integrated into the European Grid Infrastructure (EGI.eu)



BTW: **Computing clusters**

a set of interconnected („common“) computers

(oldschool)

BTW: **Computing clusters**

a set of interconnected („common“) computers

(nowadays)

Research e-Infrastructures in CR II.

- ***IT4innovations (Supercomputing Centre in Ostrava)***
  - **3344 computing cores** („small“ supercomputer/cluster)
  - **24192 computing cores** („big“ supercomputer/cluster)
  - attributes:
    - computing time assigned to **research projects**
    - **formal application** is necessary (evaluation of research and technical readiness + financial contributions)
    - **public competitions** 2x per year
    - if accepted, easier resource access (low number of competitive users)
  - purpose:
    - **large (proven) computations using homogeneous infrastructure**

https://www.it4i.cz

Research e-Infrastructures in CR III.

Centre CERIT-SC (Masaryk University in Brno)

- **long-term history (→ long-term experience in ICT science)**
  - CERIT-SC evolved from Supercomputing Center Brno (established in 1994), and
  - participates on the operation of National Grid Infrastructure

CERIT-SC mission:

- **production services for computational science**
  - high-performance computing clusters
  - large data storage, back-ups and data archives
  - web portals & projects' back-office
- **an application of top-level ICT in the science**
  - own research in e-infrastructures (know-how)
  - novel forms of infrastructure utilization (experimental usage support)
  - **research collaborations with other science areas**

https://www.cerit-sc.cz

e-INFRA CZ – Basic grid/cloud characteristics

- after registration, **grid and cloud resources** are available **without any administrative burden**
  - → ~ immediately (depending on actual usage)
  - **free of charge**
    - users "pay" via publications with acknowledgements
      - → results in user priorities in cases of high load
  - **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**

e-INFRA CZ – Grid computing resources available

Grid computing resources: ca 14900 cores (x86_64)

- nodes **with lower number of computing cores**: 2x4-8 cores
- nodes **with medium number of comp. cores (SMP nodes)**: 32-80 cores
- memory (RAM) up to **1 TB per node**
- nodes with **high number of computing cores: SGI UV2000**
  - **384 cores (x86_64), 6 TB of RAM**
  - **288 cores (x86_64), 6 TB of RAM**
- other **„exotic“ hardware:**
  - **nodes with GPU cards, SSD discs, Xeon Phi, etc.**

http://metavo.metacentrum.cz/cs/state/hardware.html

e-INFRA CZ – Storage resources available

ca 3 PB for operational data

- centralized storage arrays distributed through various cities in the CR
- user quota 1-3 TB on each storage array

ca 22 PB for archival data

- (HSM – MAID, tapes)
- “unlimited” user quota

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

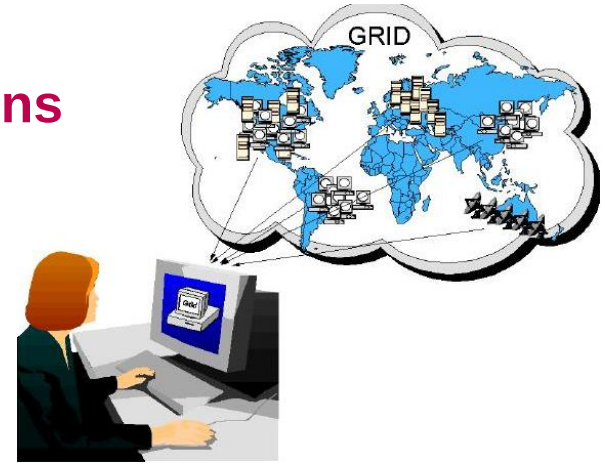
e-INFRA CZ – Software available

~ 300 different applications (commercial & free/open s.)

- see http://meta.cesnet.cz/wiki/Kategorie:Aplikace

- **development tools**
  - GNU, Intel, and PGI compilers, profiling and debugging tools (TotalView, Allinea), …
- **mathematical software**
  - Matlab, Maple, Mathematica, gridMathematica, …
- **application chemistry**
  - Gaussian 09, Gaussian-Linda, Gamess, Gromacs, …
- **material simulations**
  - Wien2k, ANSYS Fluent CFD, Ansys Mechanical, Ansys HPC…
- **structural biology, bioinformatics**
  - CLC Genomics Workbench, Geneious, Turbomole, Molpro, …

e-INFRA CZ – Grid computing services



Suitable for:

- **long-term and/or large-scale computations**
  - **(primarily batch processing)**
- **applications not requiring special OSs (features)**
  - **pre-installed or users' ones**

How to compute?

- ***batch jobs***
  - **the work described by job scripts and managed by scheduler(s)**
  - **sets of many jobs, long-running jobs, …**
- ***interactive jobs***
  - **text interface**
  - **graphical user interface (VNC)**

e-INFRA CZ – Cloud computing services

Suitable for:

- applications requiring special environment (OS) and/or features
  - one can run various operating systems (incl. Windows OS) and/or application equipment
  - administrator/root access is provided
  - still focused on research computations (not for webhosting)
    - Windows & Linux images provided, user-uploaded images also supported

How to compute?

- OpenNebula GUI for deployed nodes management
  - nodes simply created based on predefined templates
  - new version being built on OpenStack
- interact via:
  - cloud/VM console
  - internal OS services (SSH, VNC, Rdesktop, …)

e-INFRA CZ – Hadoop computing services

Hadoop:

- an open-source framework for distributed storage and distributed processing of large volumes of data
  - large data blocks splitted and distributed amongst nodes
  - a MapReduce-based algorithm (= data processing code) is distributed over the distributed blocks and processed in parallel

Suitable for:

- huge datasets to be processed
  - but NOT suitable for arbitrary data processing one can imagine
  - just for the processing meeting the MapReduce programming model
    - e.g., counting the number of times words occur in a corpus

e-INFRA CZ – Specialized frontends/environments

Suitable for:

- user communities with well-defined processing needs
  - workload & computing pipeline orchestrators available via GUI
  - usually adapted to user needs and/or because of interoperability with our infrastructure
    - in background, the proper computing method is used (grid, cloud, etc.)

How to compute?

- Galaxy, Chipster, etc.

e-INFRA CZ – How to become our user?

- ***register***
  - http://metavo.metacentrum.cz , section *„Application“*
  - EduID.cz => **proves your academic identity** using your home institution services (and credentials)
    - foreign users (researchers) have to be somehow related to a research group in CR
- ***make yourself familiar with basics of OS Linux***
  - http://metavo.metacentrum.cz , section *„Documentation“*
  - http://www.poznejlinux.cz/linuxbook/xhtml-chunks/ch07.html
- ***compute***

Conclusions

- **Research e-infrastructures in CR – e-INFRA CZ**
  - **comprises of MetaCentrum (CESNET), IT4I (Ostrava) and CERIT-SC (MUNI) infrastructures**
    - *ongoing tight integration*
  - *computing services* (grid, cloud, Hadoop/specialized and supercomputing services)
  - *data services* (archivals, backups, data sharing and transfers, …)
  - *services supporting collaborative research* (research collaboration with partners, project partners supporting projects‘ IT part, etc.)
  - further supporting services (remote collaborations support services, etc.…)

- *The message:* „If you cannot find a solution to your specific needs in the provided services, let us know – we will try to find the solution together with you…“

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OP Research and Development for Innovation

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