

National Grid Infrastructure (NGI)

for scientific computations, collaborative research & its support services

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National Grid Infrastructure (NGI)

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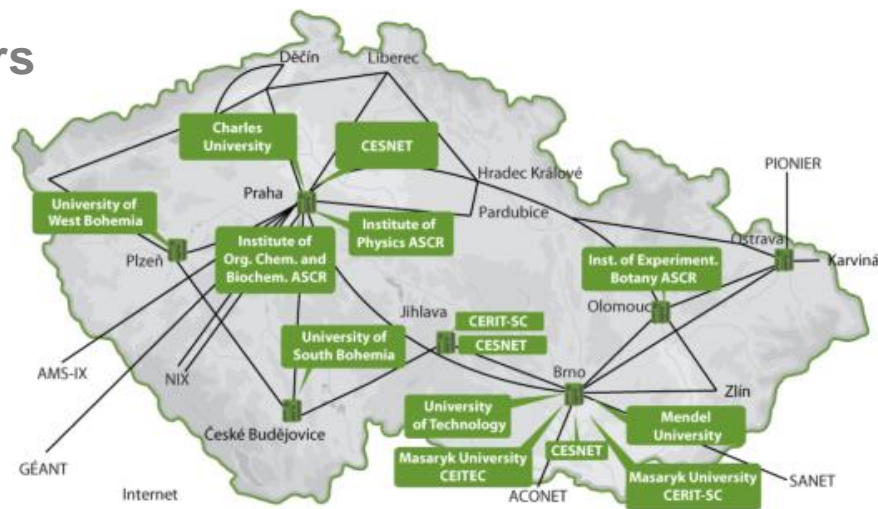
- operated by MetaCentrum NGI (CESNET) since 1996
- MetaCentrum responsible for management and coordination

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)

<http://www.metacentrum.cz>



Computing clusters

a set of interconnected („common“) computers



(oldschool)

Computing clusters

a set of interconnected („common“) computers

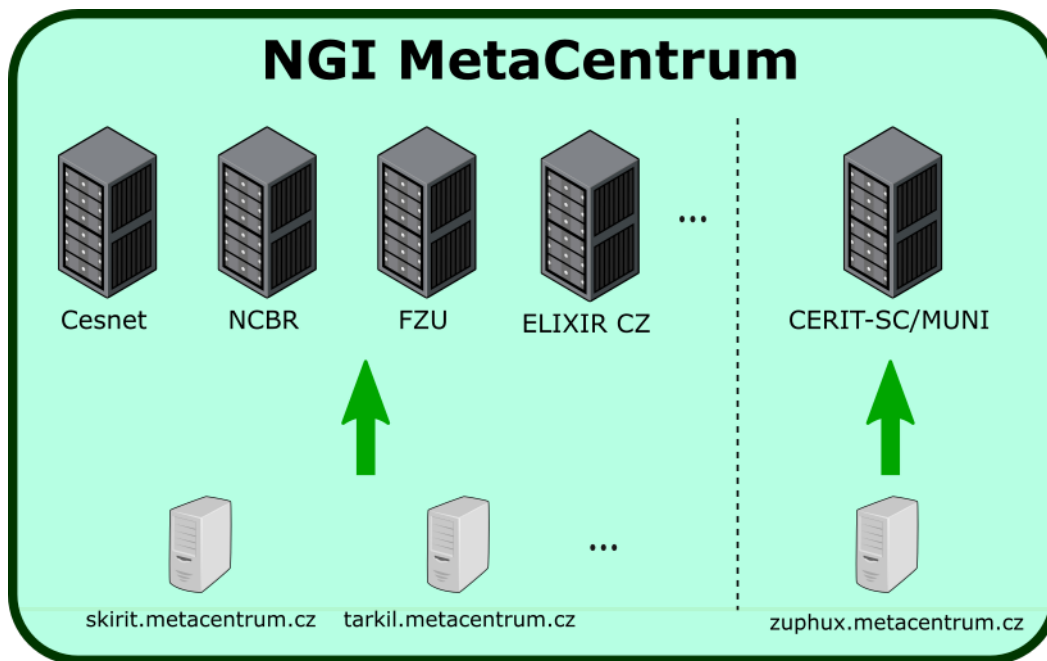


(nowadays)

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

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

- commercial bodies just for public research

Offers:

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

<http://metavo.metacentrum.cz>

After registration, all the resources/services are available free of charge

- without any administrative burden
- users “pay” via publications with acknowledgements
→ results in user priorities in cases of high load



Meta 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**

Meta NGI – computing resources available

Computing resources: ca 22300 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
 - 504 cores (x86_64), 10 TB of RAM
 - 384 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>

Meta NGI – storage resources available

ca 5 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>

Meta NGI – software available

~ **350 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, ...

Meta NGI – grid environment

- **batch jobs**

- the computations described by script files

- **interactive jobs**

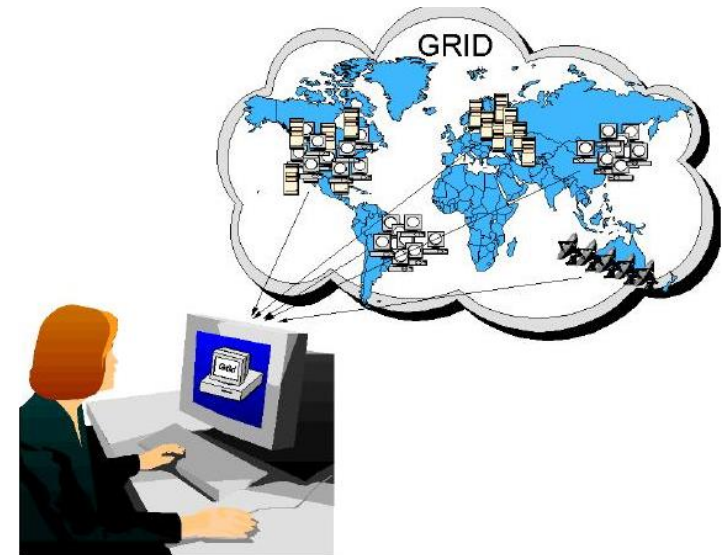
- text & graphical environment

- **cloud computing**

- instead of running jobs with computations, users run the whole virtual machines

focused on research computations again (not for webhosting)

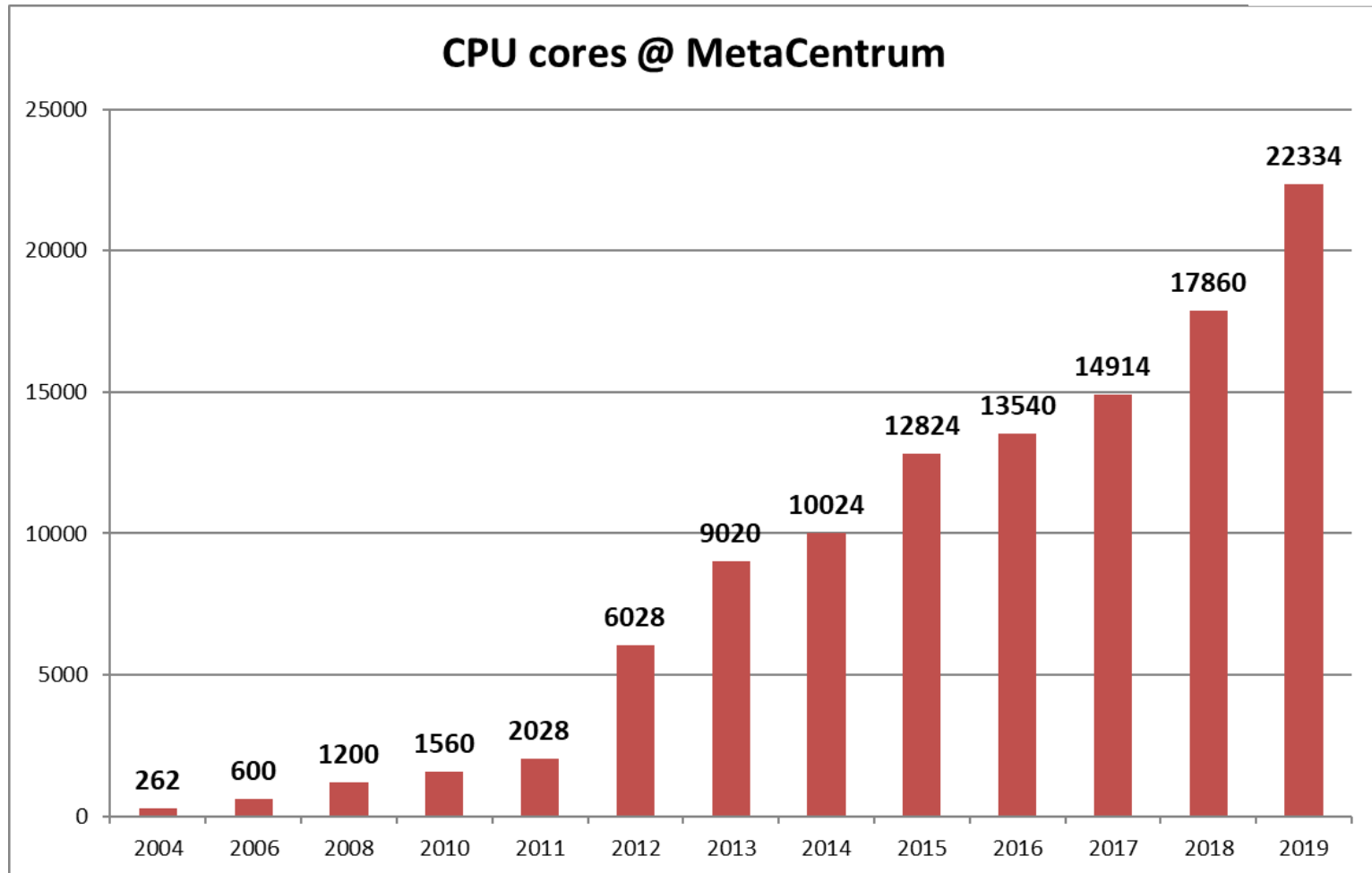
Windows & Linux images provided, user-uploaded images also supported
more info later...



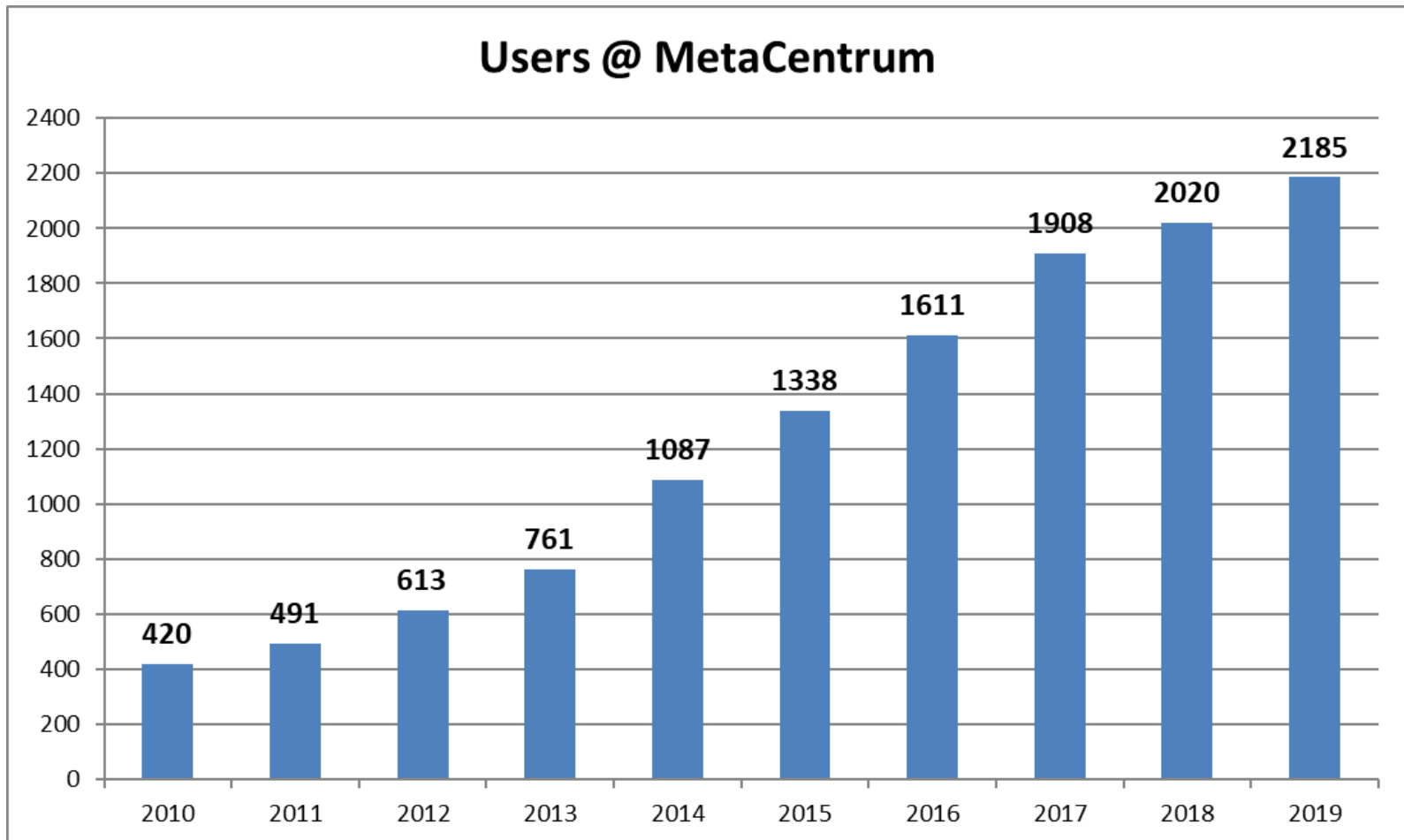
Meta VO in numbers...

- *ca 22300 cores, ca 700 server nodes*
- *year 2019:*
 - *2185 users (31.12.2019)*
 - *ca 8,7 mil. of running jobs*
 - *ca 23700 jobs per day*
 - *ca 4000 jobs per user*
 - *CPU time*
ca 13,1 thousands of CPUyears

... and graphs

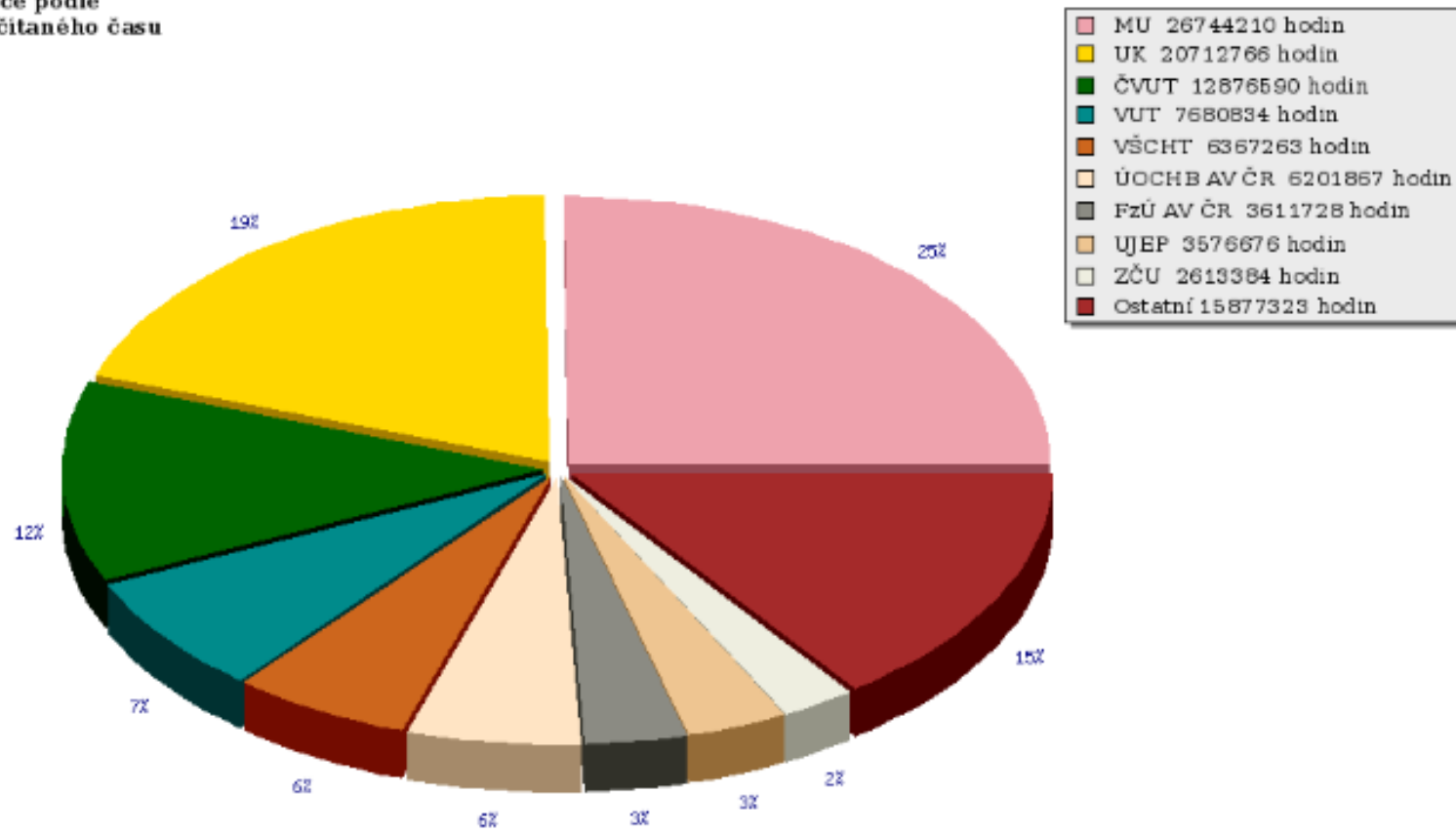


... and graphs



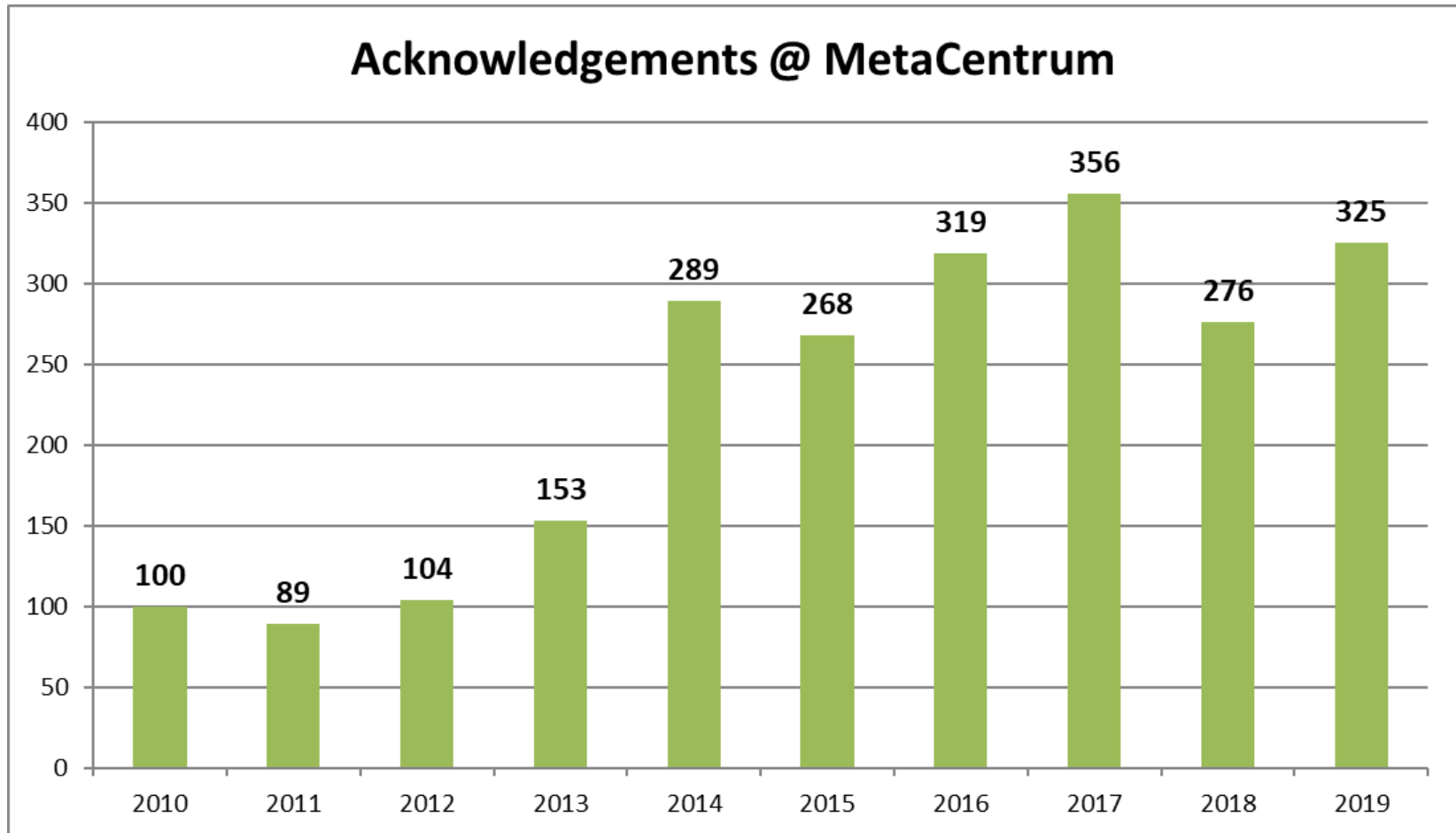
... and graphs

Instituce podle
propočítaného času



1.1.2019 -- 1.1.2020

... and graphs



Meta VO – 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)

- **make yourself familiar with basics of OS Linux**

- <http://metavo.metacentrum.cz> , section „Documentation“
- <http://lb.poznejlinux.cz/xhtml/linuxbook.html#id2571419>

- **compute**

CESNET – Data services

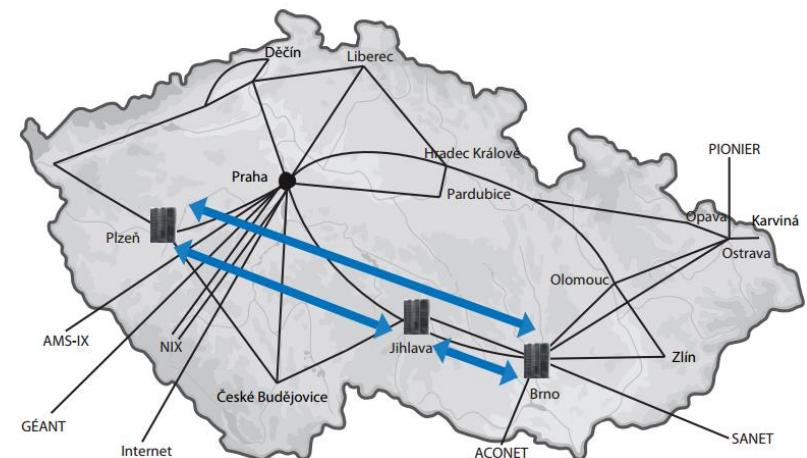
Hierarchical data storages

- 22+ PB of physical capacity
- useful for data archivals, backups, etc.
- various access protocols available

Further end-user services

- FileSender
- OwnCloud

<http://du.cesnet.cz>



Data Services for end-users

FileSender – file sharing/transferring service

- web service intended for sending big data files
 - big = current limit is 500 GB
 - <http://filesender.cesnet.cz>
- at least one user has to be an authorized infrastructure user
 - federated authentication through eduID.cz

Authorized user is allowed to upload a file (and send a notification to the receiver)

If an authorized user needs to receive data from a non-authorized user, she sends him an invitation link

- (so he is allowed to use it for uploading the file)

FileSender – example I.



The screenshot shows the FileSender website interface. At the top left is the FileSender logo, which includes a yellow truck icon and the text "FILESENDER" with a red chili pepper. To the right of the logo, it says "an initiative by" followed by logos for aarnet, UNINETT, HEAnet, and SURF NET. Below these logos are two buttons: "Pomoc" and "O programu". In the center, there is a status bar: "| UP: 1820 files (2305GB) | DOWN: 2065 files (1876GB) | 1.5-rc1 HTML5 ✓". Below this is a white box with the heading "Vítejte na FileSender" and the text "FileSender je bezpečná cesta pro sdílení velkých souborů mezi všemi! Přihlaš se a nahraj své soubory nebo pozvi ostatní, ať soubory nahrají oni." Below the text is a "Přihlásit" button. A large grey arrow points from the right side of the page towards the "Přihlásit" button. At the bottom center is the CESNET logo.

FileSender – example II.

eduID.cz + HOSTEL

[O federaci](#) | [Politika](#) | [Kontakt](#) | [Nápověda](#)

Zvolte svou domovskou organizaci

Přístup ke zdroji na serveru '**filesender.cesnet.cz**' vyžaduje autentizaci.

CESNET, z. s. p. o.

Uložit tuto volbu do ukončení relace prohlížeče.
 Uložit tuto volbu nastálo.

Operátorem federace [eduID.cz](#) je [CESNET, z.s.p.o.](#)


CESNET



Přihlášení



Uživatelské jméno
tkosnar


Heslo
.....

FileSender – example III.




FILESENDER


— an initiative by —






Vítejte Tomáš Košňar | UP: 1820 files (2305GB) | DOWN: 2065 files (1876GB) | 1.5-rc1 **HTML 5** ✓

Nahrát soubor

Příjemce:
Odesílatel: tomas.kosnar@cesnet.cz
Předmět: (volitelné)
Zpráva: (volitelné)
Datum expirace:
Vyberte soubor: Soubor nevybrán
 Souhlasím s podmínkami užití této služby.
 [Zobrazit/Skrýt]

1 Vložte emailové adresy příjemců
 2 Nastavte datum expirace
 3 Vyberte soubor
 4 Klikněte na Odeslat



OwnCloud

- **cloud storage „like Dropbox“**
 - quota: 100 GB / user
 - available through web interface
 - <https://owncloud.cesnet.cz/>
 - clients for Windows, Linux, OS X
 - clients for smartphones and tablets
 - allows sharing among a group of users
 - data backups every day
 - document versioning
 - calendars and contacts sharing
 - etc.



OwnCloud – example I.



Přihlaste se účtem v eduID







Přihlášením souhlasíte s pravidly použití







Tato služba je součástí e-Infrastruktury CESNET


OwnCloud – example II.

Přihlásit účtem

České vysoké učení technické v Praze, Fakulta elektrotechnická	
CESNET	
Masarykova univerzita	
Univerzita Hradec Králové	
Univerzita Pardubice	
Západočeská univerzita v Plzni	
Jiný účet	

   CESNET 

OwnCloud – example III.

 **MASARYKOVA UNIVERZITA**
Česká republika

Poskytovatel identit MU

UČO:

Heslo:

Pokusili jste se přistoupit na stránky, které vyžadují autentizaci.
Pro přihlášení použijte UČO a sekundární heslo.

Hosté s guest účtem použijí místo UČO své GuestID.

[Nápověda](#)

Službu zajišťuje [Ústav výpočetní techniky MU](#).

[English](#)

OwnCloud – example IV.

The screenshot displays the OwnCloud web interface. At the top left is the OwnCloud logo. The top right features a search bar and the user name 'Tomáš Rebok'. Below the header is a navigation bar with a home icon, a 'New' button, and an upload icon. A 'Deleted files' button is also present. The main content area shows a table of files and folders:

	Name	Size	Modified
	documents	22.8 kB	4 months ago
	music	3.6 MB	4 months ago
	ownCloudUserManual.pdf	1.5 MB	4 months ago

A vertical sidebar on the left contains icons for 'Files', 'Activity', 'Documents', 'Pictures', 'Calendar', 'Contacts', and 'Tasks'.

Research Infrastructures in CR I.

- *IT4innovations (Ostrava)*

- **3344 computing cores** („small“ supercomputer/cluster)
- **7232 computing cores** („medium“ 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 + socio-economic factors)
 - **public competitions** 2x per year
 - if accepted, easier resource access (low number of competitive users)
- purpose:
 - **large (proven) computations** using homogeneous infrastructure

Research Infrastructures in CR II.

- **National Grid Infrastructure (NGI) MetaCentrum**

- ca **22300 computing cores** (including CERIT-SC resources)

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MetaCentrum NGI, IT4I a CERIT-SC
currently integrating themselves into

e-INFRA CZ

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

- preparation of computations/projects for computations at IT4innovations (~ technical readiness)

- **CERIT-SC @ ICS MU**

- *HW and SW provider (resources available through NGI)*

- *main emphasis on **services supporting user research***

CERIT-SC & NGI

Centre CERIT-SC

A computing and research centre operating at Masaryk University

- 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

Our mission:

<http://www.cerit-sc.cz>

- 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

Centre CERIT-SC & NGI

CERIT-SC is an important NGI partner

- **HW & SW resources provider**

 - SMP nodes (2592 cores)

 - HD nodes (2624 cores)

 - SGI UV node (504 cores, 10 TB RAM)

 - SGI UV node (384 cores, 6 TB RAM)

 - storage capacity (~ 3,5 PB)

- **significant personal overlaps
with NGI exist**

CERIT-SC (SCB) established MetaCentrum NGI

- → **much research/work is performed in collaboration**

<http://www.cerit-sc.cz>



Research support by CERIT-SC

Fact I. Common HW centers provide just a “dumb” power without any support how to effectively use it

Fact II. Common HW centers do not participate on the users’ research aiming to help them with ICT problems

CERIT-SC collaborates with its users:

- to help them effectively use the provided resources
- to help them to cope with their ICT research problems focusing on an application of top-level ICT in the science smaller as well as bigger (= funded) projects

Main research areas of interest

High performance computing

- GPU computing, fine-tuning of computing algorithms, ...

(Big) Data processing

- high volumes of data, heterogeneous data, real-time data, ...

Artificial Intelligence

- neural networks and their application in real-life, deep neural networks, ...

but also many others interesting projects...

How do we fulfill the idea?

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

Selected research collaborations

Selected (ongoing) collaborations I.

3D tree reconstructions from terrestrial LiDAR scans

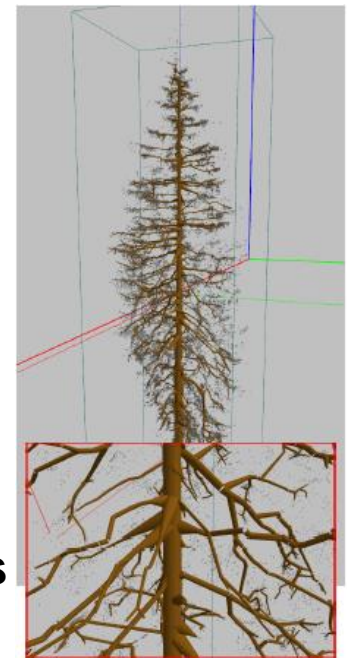
- partner: Global Change Research Centre - Academy of Sciences of the Czech Republic (*CzechGlobe*)
- **the goal: to propose an algorithm able to perform fully-automated reconstruction of tree skeletons (main focus on Norway spruce trees)**
 - from a 3D point cloud
 - scanned by a LiDAR scanner
 - the points provide information about XYZ coordinates + reflection intensity
 - *the expected output: 3D tree skeleton*
- **the main issue:** overlaps (→ gaps in the input data)



Selected (ongoing) collaborations I.

3D tree reconstructions from terrestrial LiDAR scans – cont'd

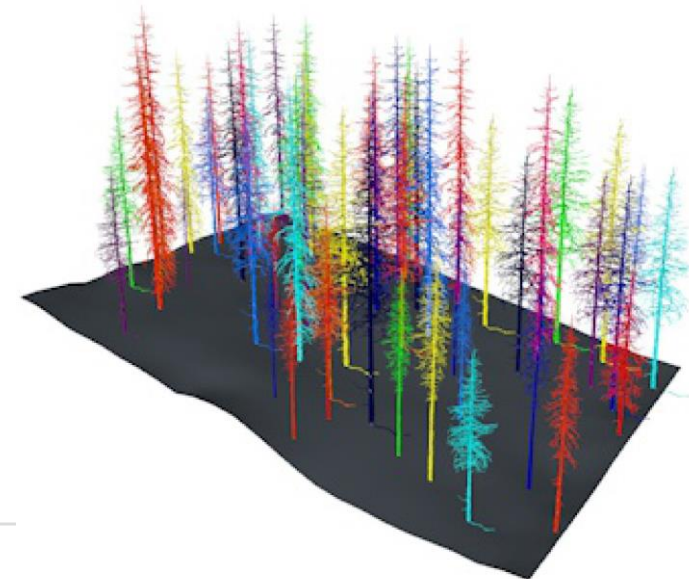
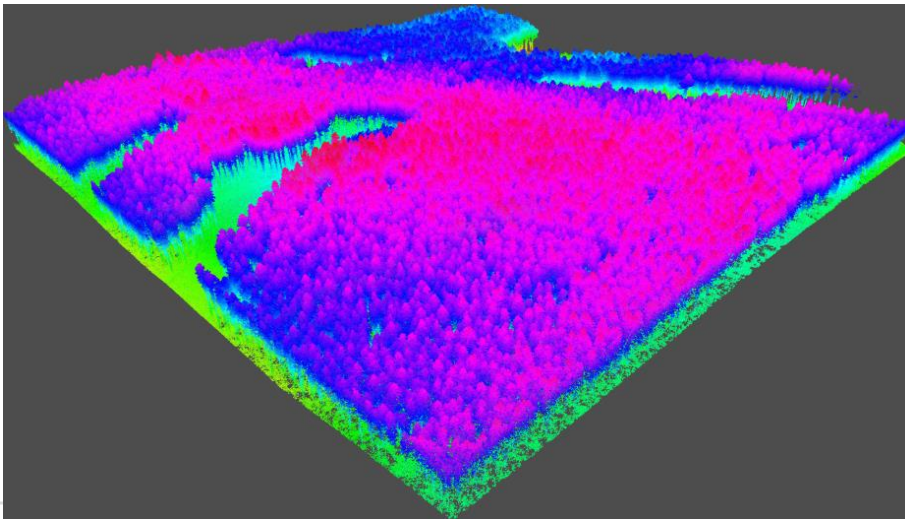
- the diploma thesis proposed a novel innovative approach to the reconstructions of 3D tree models
- the reconstructed models used in subsequent research
 - **determining a statistical information** about the amount of wood biomass and about basic tree structure
 - **parametric supplementation of green biomass** (young branches+ needles) – a part of the PhD work
 - **importing the 3D models into tools performing various analysis** (e.g., DART radiative transfer model)



Selected (ongoing) collaborations II.

3D reconstruction of tree forests from full-wave LiDAR scans

- subsequent work
- **the goal: an accurate 3D reconstruction of tree forests scanned by aerial full-waveform LiDAR scans**
 - possibly supplemented by hyperspectral or thermal scans, in-situ measurements,...



Selected (ongoing) collaborations II.

An algorithm for determination of problematic closures in a road network

- partner: *Transport Research Centre, Olomouc*
- **the goal: to find a robust algorithm able to identify all the road network break-ups and evaluate their impacts**
- **main issue: computation demands**
 - the brute-force algorithms fail because of large state space
 - 2 algorithms proposed able to cope with multiple road closures

Selected (ongoing) collaborations IV.

- **An application of neural networks for filling in the gaps in eddy-covariance measurements**
 - *partner: CzechGlobe*
- **Biobanking research infrastructure (BBMRI_CZ)**
 - *partner: Masaryk Memorial Cancer Institute, Recamo*
- **Propagation models of epilepsy and other processes in the brain**
 - *partner: MED MU, ÚPT AV, CEITEC*
- **Photometric archive of astronomical images**
- **Extraction of photometric data on the objects of astronomical images**
 - *2x partner: partner: Institute of theoretical physics and astrophysics SCI MU*
- **Bioinformatic analysis of data from the mass spectrometer**
 - *partner: Institute of experimental biology SCI MU*
- **Synchronizing timestamps in aerial landscape scans**
 - *partner: CzechGlobe*
- **Optimization of Ansys computation for flow determination around a large two-shaft gas turbine**
 - *partner: SVS FEM*
- **3.5 Million smartmeters in the cloud**
 - *partner: CEZ group, MycroftMind*
- ...

Conclusions

Conclusions

- **CESNET infrastructure:**
 - *computing services (MetaCentrum NGI & MetaVO)*
 - *data services (archivals, backups, data sharing and transfers, ...)*
 - *remote collaborations support services (videoconferences, webconferences, streaming, ...)*
 - *further supporting services (...)*
 - **Centrum CERIT-SC:**
 - *computing services (flexible infrastructure for production and research)*
 - *services supporting collaborative research*
 - *user identities/accounts shared with the CESNET infrastructure*
 - *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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<http://metavo.metacentrum.cz>

<http://www.cerit-sc.cz>