National Grid Infrastructure (NGI)

for scientific computations, collaborative research & its support services

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National Grid Infrastructure (NGI)

National Grid Infrastructure (NGI)

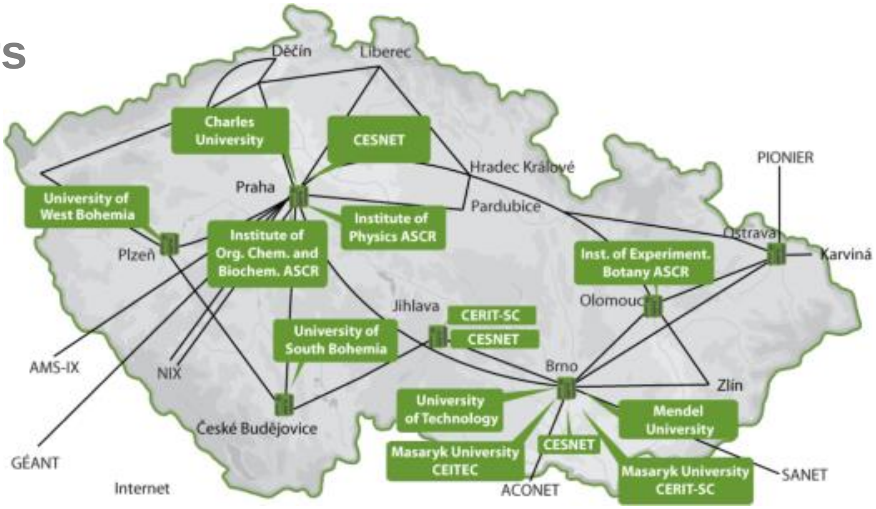
- **operated by MetaCentrum NGI (CESNET) since 1996**
- **MetaCentrum responsible for management and coordination**

Distributed infrastructure

http://www.metacentrum.cz

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

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



Computing clusters

a set of interconnected („common“) computers

(oldschool)

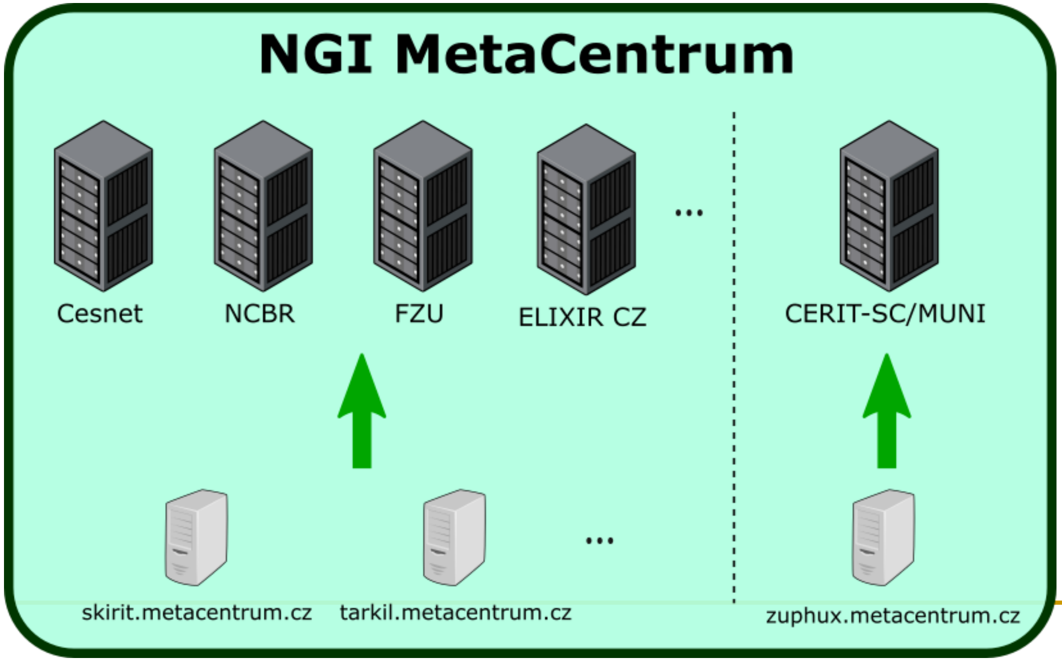
Computing clusters

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


NGI MetaCentrum

+ 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:

http://metavo.metacentrum.cz

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

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 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

Meta NGI – 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

Meta NGI – software available

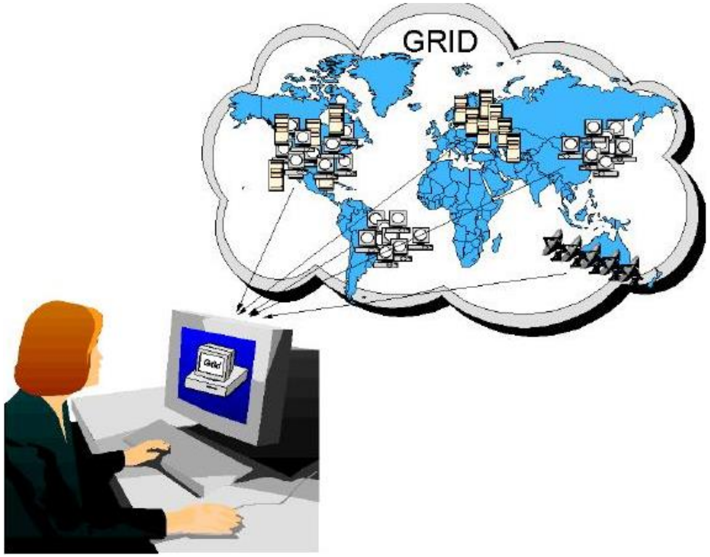
~ 300 different applications (commercial & free/open s.)

- 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, …

Meta NGI – grid environment

- ***batch jobs***
  - the computations described by script files



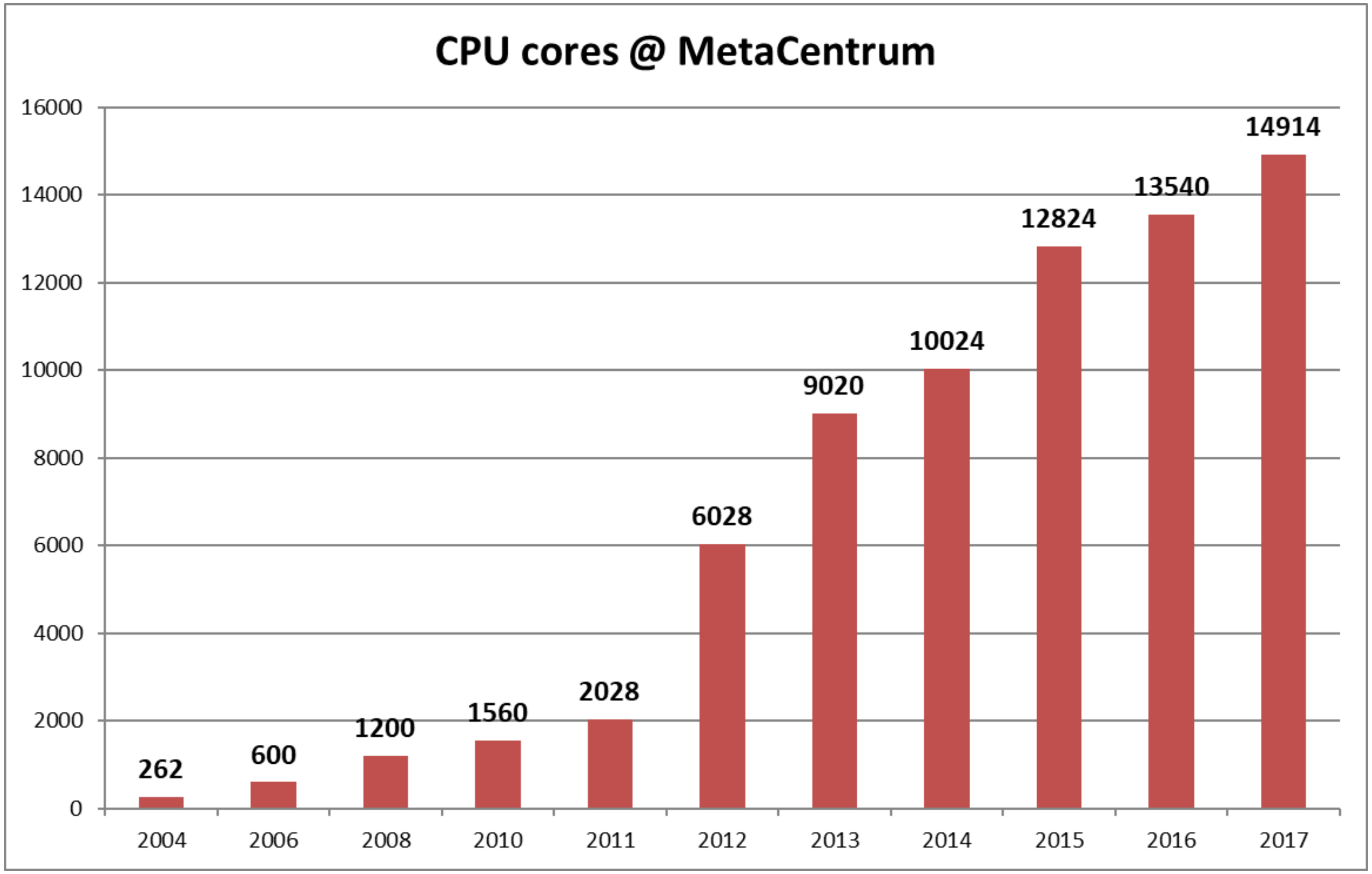
- ***interactive jobs***
  - text & graphical environment
- ***cloud computing***
  - instead of running jobs with computations, users run the whole virtual machines
    - focused on research computations again (not for webhosting)
    - Windows & Linux images provided, user-uploaded images also supported
    - more info later…

Meta VO in numbers…

- *ca 14914 cores, ca 600 server nodes*
- *year 2017:*
  - ***1908 users** (31.12.2017)*
  - ***ca 4,76 mil. of running jobs***
    - *ca 13000 jobs per day*
    - *ca 2500 jobs per user*
  - ***CPU time***

    ca 10,5 thousands of CPUyears

… and graphs


CPU cores @ MetaCentrum
16000
14000
12000
10000
8000
6000
4000
2000
0
262
600
1200
1560
2028
6028
9020
10024
12824
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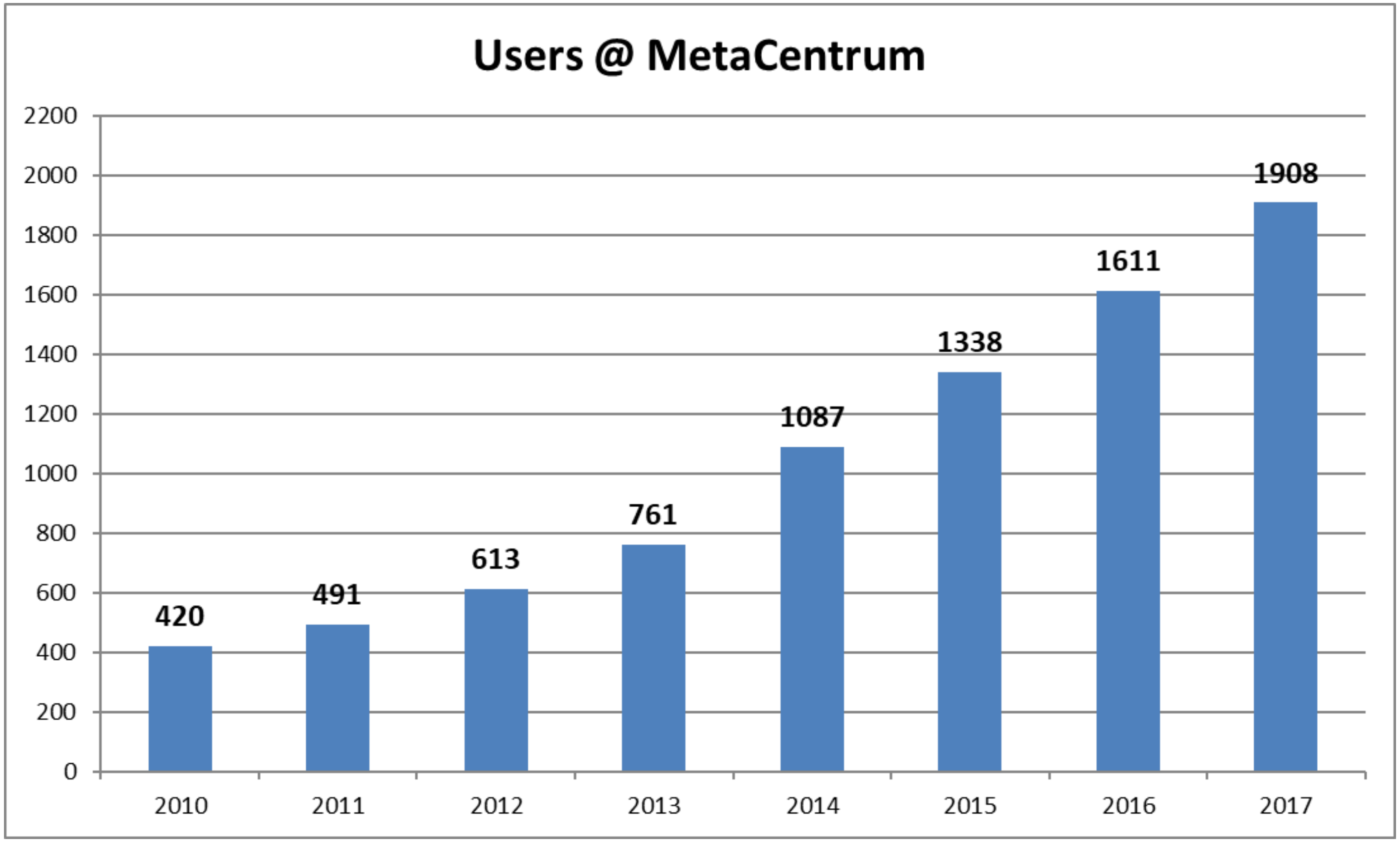
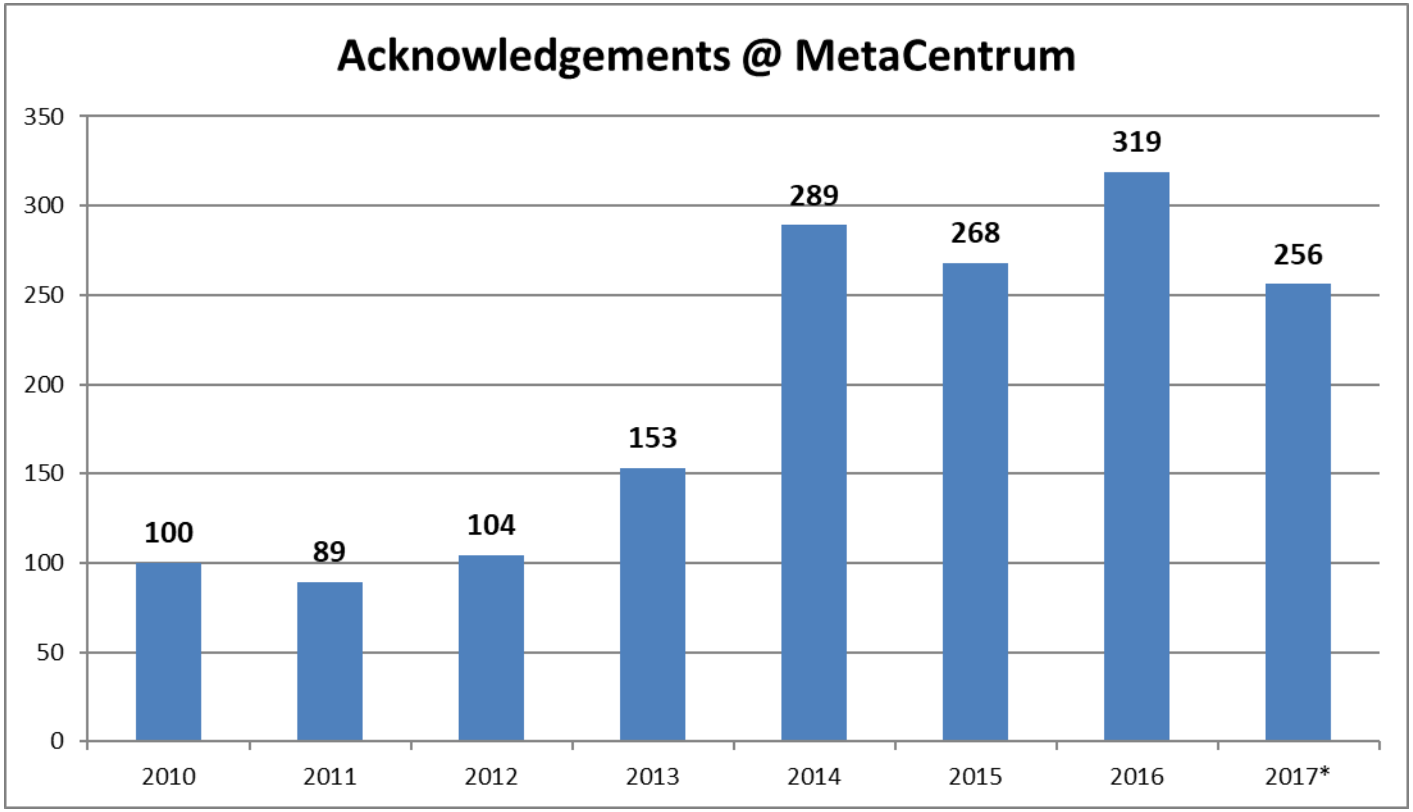
14914
2004
2006
2008
2010
2011
2012
2013
2014
2015
2016
2017

… and graphs


Users @ MetaCentrum
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
420
491
613
761
1087
1338
1611
1908
2010
2011
2012
2013
2014
2015
2016
2017

… and graphs


Acknowledgements @ MetaCentrum
350
300
250
200
150
100
50
0
100
89
104
153
289
268
319
256
2010
2011
2012
2013
2014
2015
2016
2017*

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://www.poznejlinux.cz/linuxbook/xhtml-chunks/ch07.html
- ***compute***

Research Infrastructures in CR I.

- *IT4innovations (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**

Research Infrastructures in CR II.

- ***National Grid Infrastructure (NGI) MetaCentrum***
  - ca **15000 computing cores** (including CERIT-SC resources)
  - attributes:
    - computing time **available free of charge, without formal applications**
    - **heterogeneous resources** available (including „exotic“ ones)
    - **resources shared with competitive users** (sometimes hard to access)
  - purpose:
    - common **smaller to middle –sized computations** (larger computations after agreement)
    - **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 (288 cores, 6 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

What’s the idea?

We focus on intelligent & novel usage forms of the provided infrastructure

- **the provided HW/SW resources serve just as a tool for research and development**

  → highly-flexible infrastructure (convenient to experiments)

  in comparison with NGI resources, the production computations are at the second-level of interest
- **the centre aims to be equipped with cutting-edge technologies**

  in order to allow top-level research (both internal & collaborative)
- **real research collaboration with our partners**

  the collaborations generate new questions/problems for IT

  the collaborations generate novel opportunities for the science

  (we DON’T want to be a common service organization)

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

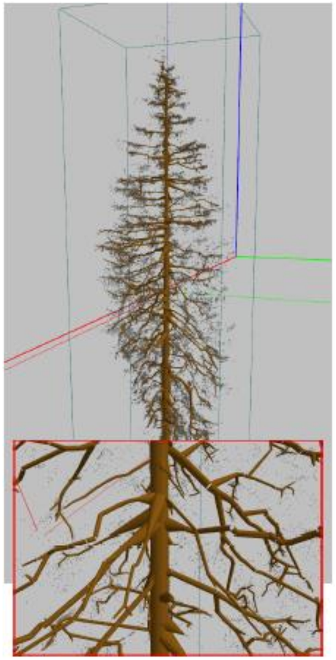
  → consultations with experts in particular areas

Selected research collaborations

Selected (ongoing) collaborations I.

3D tree reconstructions from terrestrial LiDAR scans

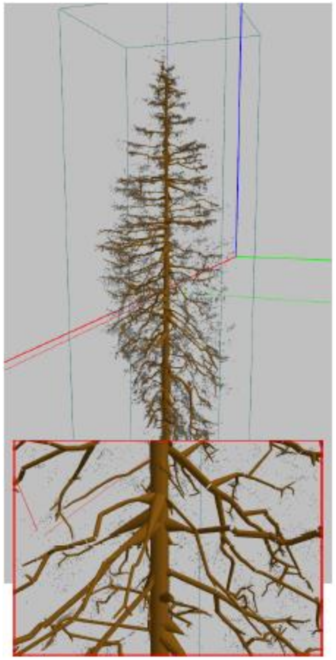
- partner: Global Change Research Centre - Academy of Sciences of the Czech Republic (*CzechGlobe)*
- **the goal: to propose an algorithm able to perform fully-automated reconstruction of tree skeletons (main focus on Norway spruce trees)**
  - from a 3D point cloud
    - scanned by a LiDAR scanner
    - 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

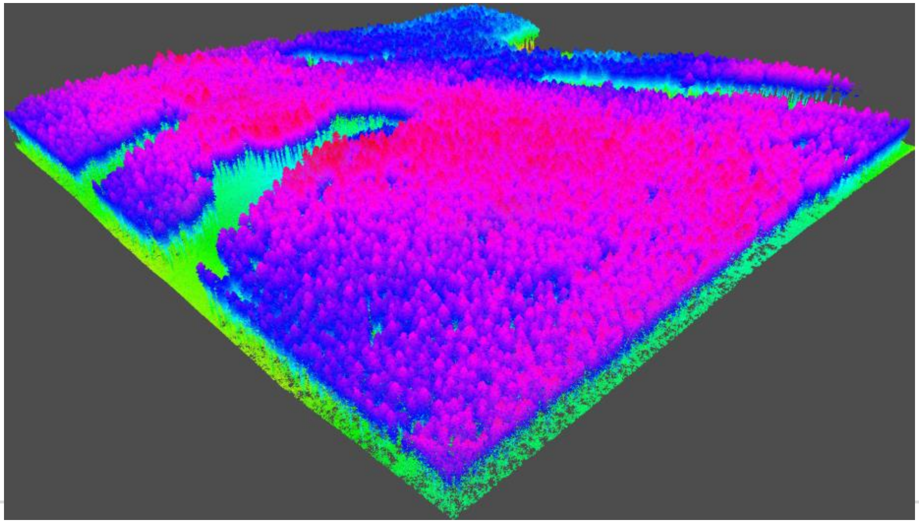
- **the diploma thesis proposed a novel innovative approach to the reconstructions of 3D tree models**
- **the reconstructed models used in subsequent research**
  - **determining a statistical information** about the amount of wood biomass and about basic tree structure
  - **parametric supplementation 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)

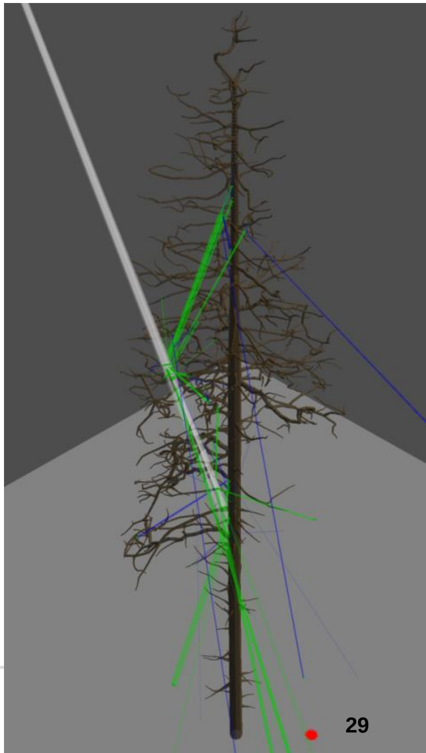


Selected (ongoing) collaborations II.

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

- subsequent PhD thesis, a preparation of joint project
- **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 III.

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*
- **…**

Additional services available
to academic research community

Data services

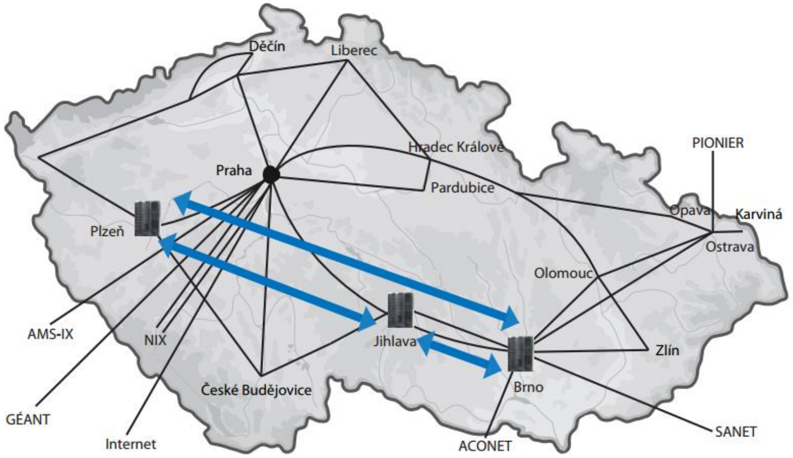
Hierarchical data storages

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

Further end-user services

- FileSender
- OwnCloud

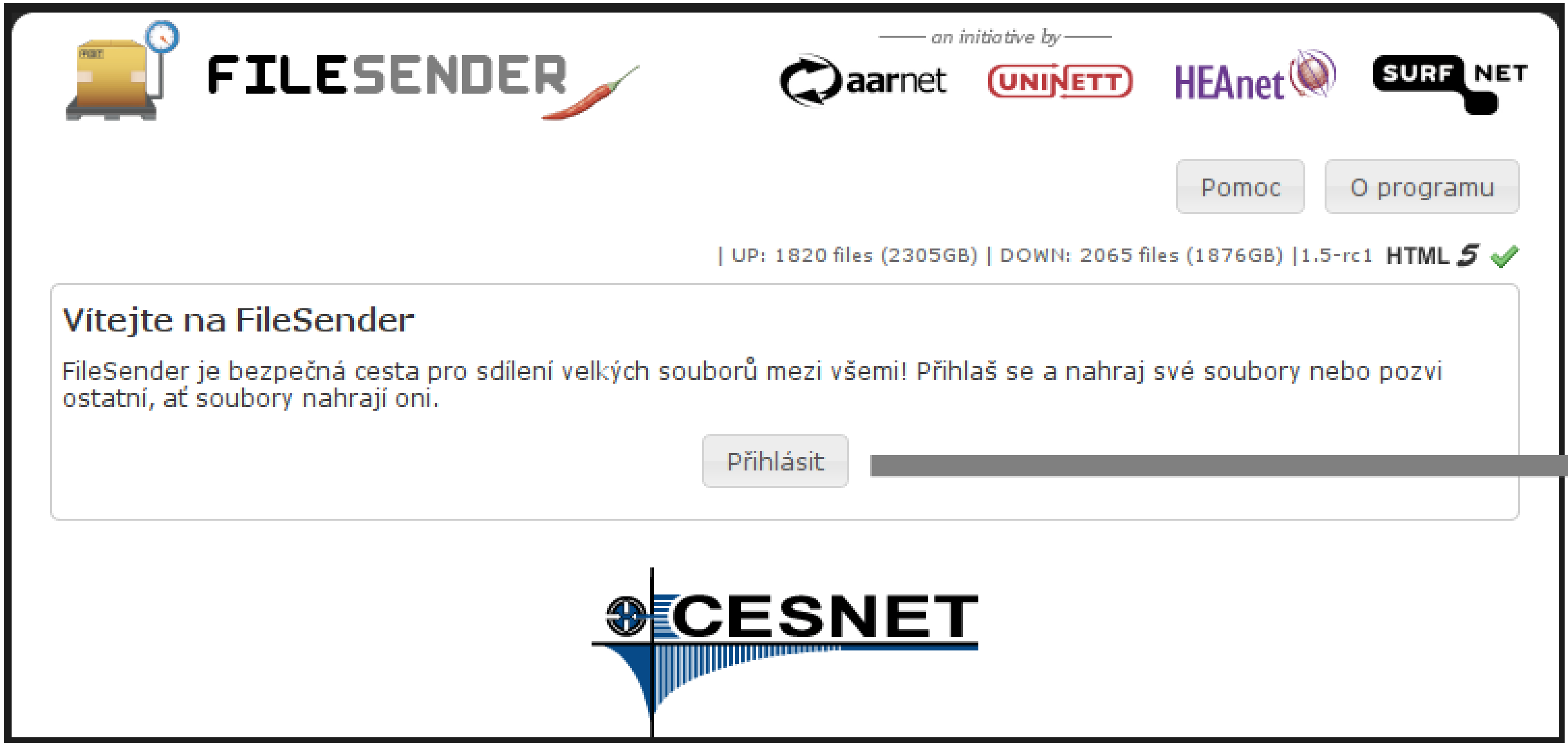
http://du.cesnet.cz



Data Services for end-users

- ***FileSender* – file sharing/transfering 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.

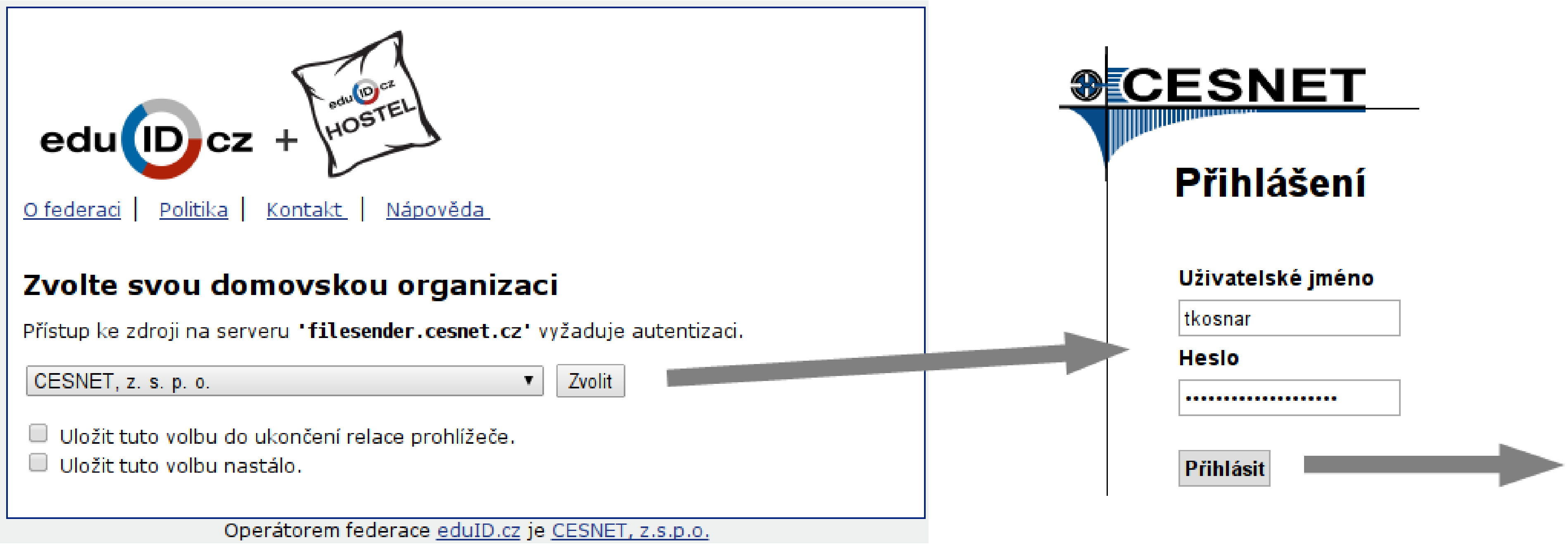


| UP: 1820 files (2305GB) | DOWN: 2065 files (1876GB) |1.5-rc1 HTML 5 ✓

Vítejte na FileSender

FileSender je bezpečná cesta pro sdílení velkých souborů mezi všemi! Přihlaš se a nahraj své soubory nebo pozvi ostatní, ať soubory nahrají oni.

FileSender – example II.



eduID.cz + 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. ▼ Zvolit

□ 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

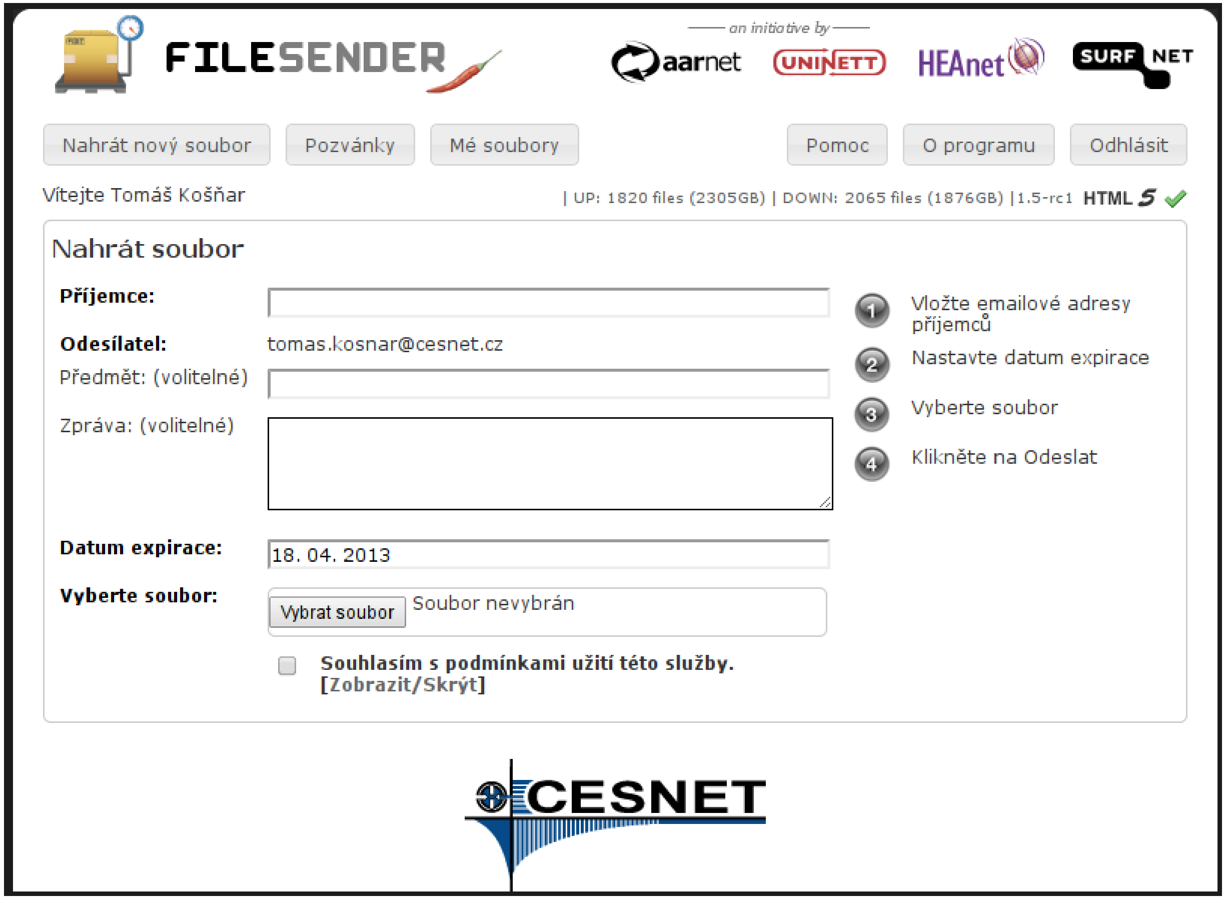
tkosnar

Heslo

••••••••••••••••••••

Přihlásit

FileSender – example III.



Nahrát nový soubor | Pozvánky | Mé soubory | Pomoc | O programu | Odhlásit

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: 18. 04. 2013

Vyberte soubor: Vybrat soubor Soubor nevybrán

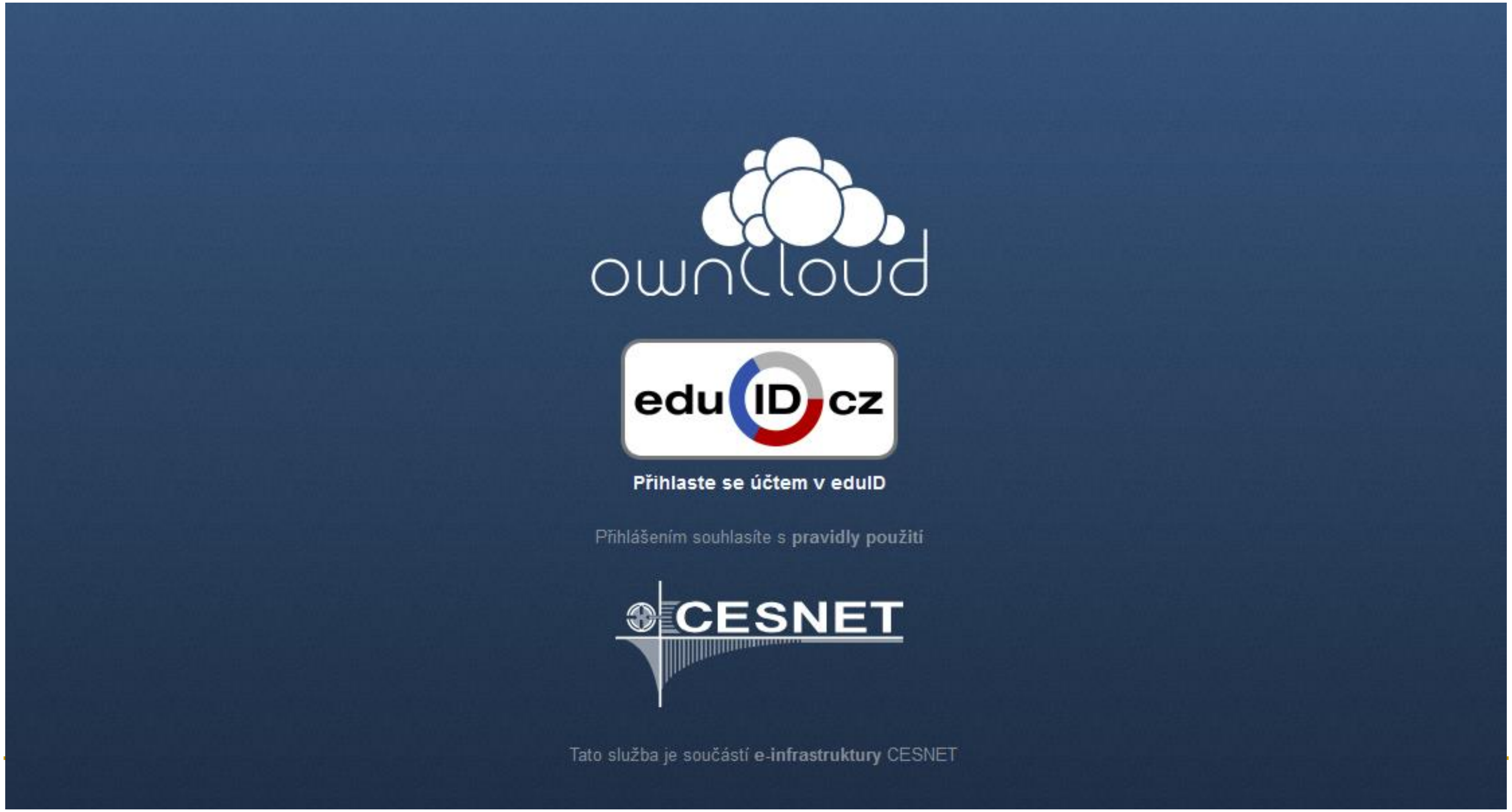
□ **Souhlasím s podmínkami užití této služby. [Zobrazit/Skrýt]**

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.

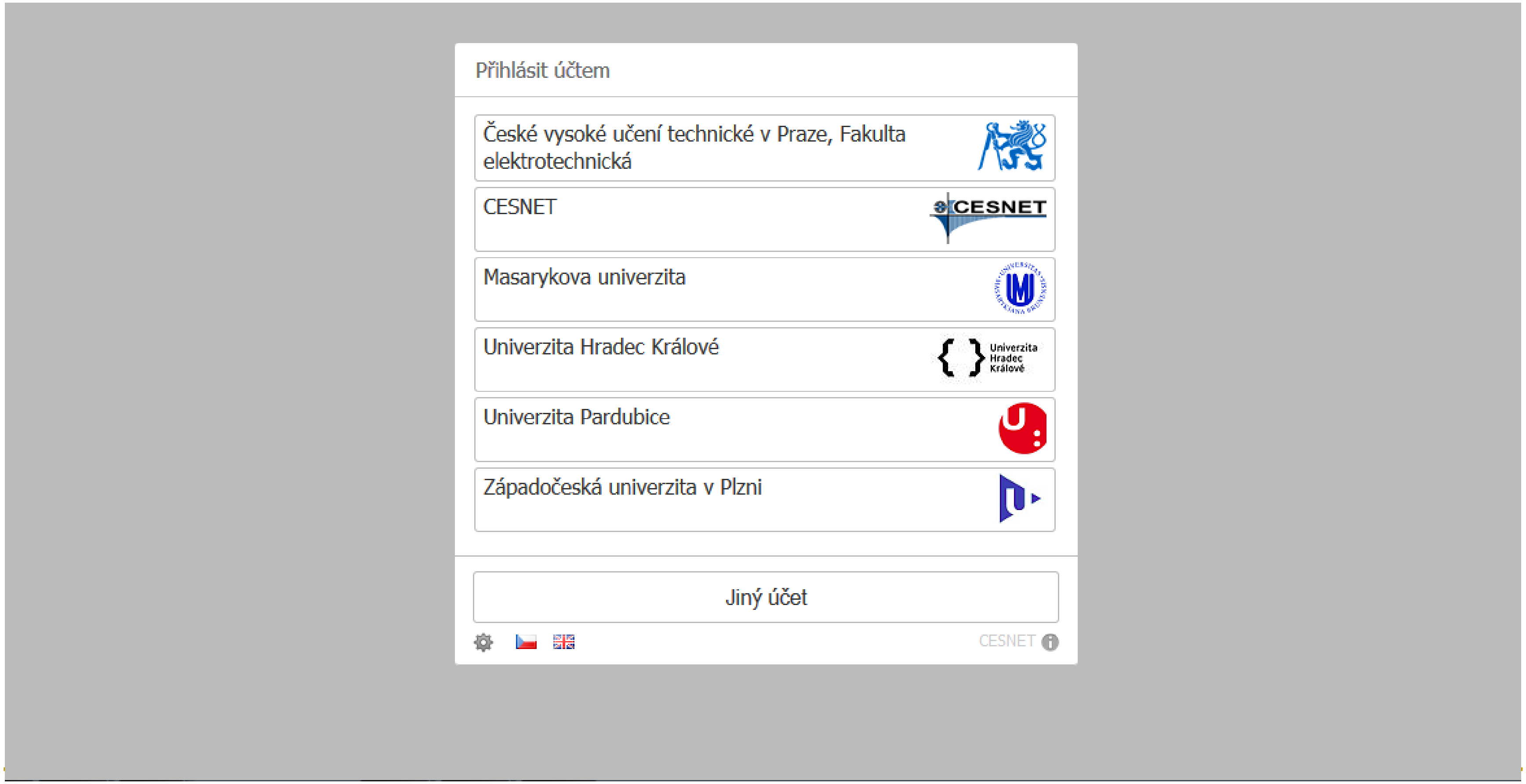


Přihlaste se účtem v eduID

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

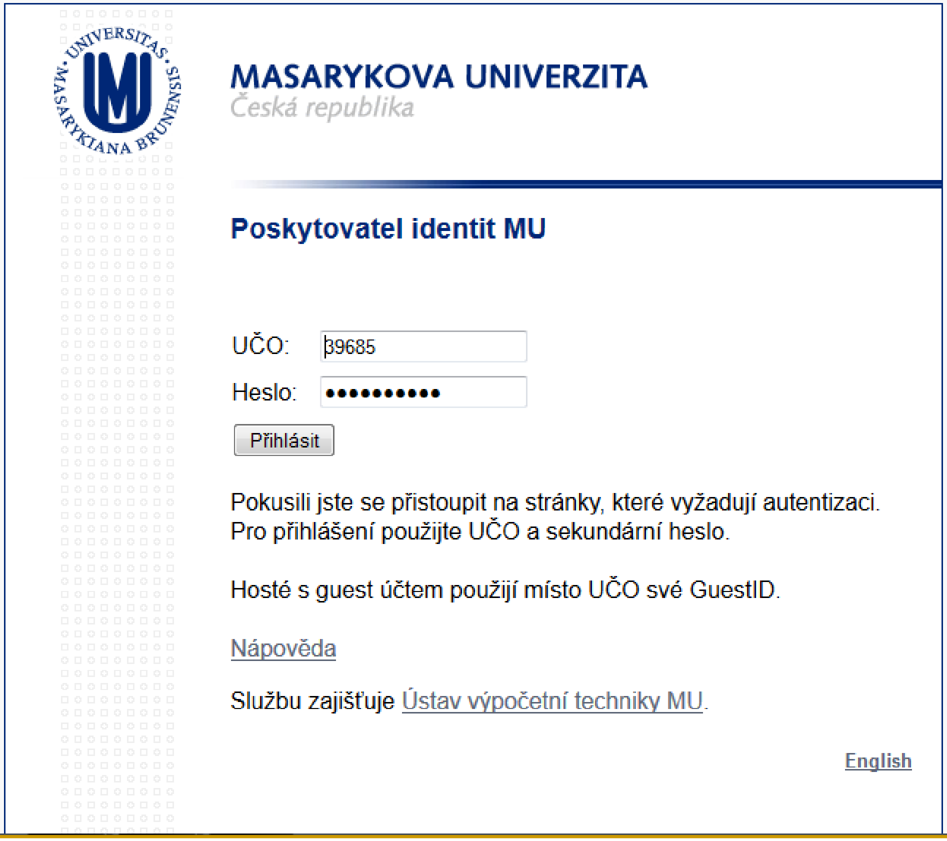
Univerzita Hradec Králové

Univerzita Pardubice

Západočeská univerzita v Plzni

Jiný účet

OwnCloud – example III.



MASARYKOVA UNIVERZITA
Česká republika

Poskytovatel identit MU

UČO: 39685

Heslo: ●●●●●●●●●●●

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

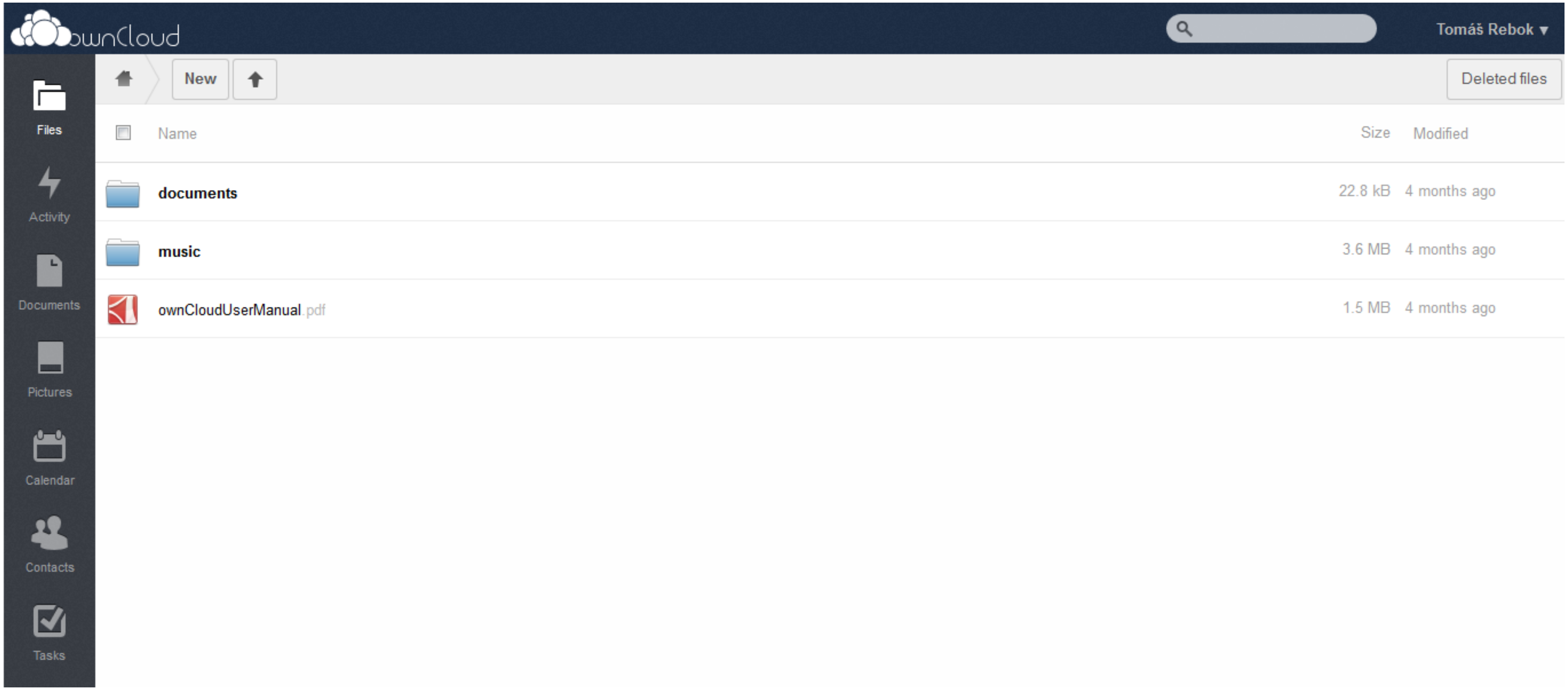
Hosté s guest účtem použijí místo UČO své GuestID.

Nápověda

Službu zajišťuje Ústav výpočetní techniky MU.

English

OwnCloud – example IV.



□ 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

Remote collaboration support

Support for interactive collaborative work in real-time

- **videoconferences**

  HD videoconferencing support via H.323 HW/SW equippment

- **webconferences**

  SD videoconferencing support via Adobe Connect (Adobe Flash)

  http://meetings.cesnet.cz

- **special transmissions**

  HD, UHD, 2K, 4K, 8K with compressed/uncompressed video transmission (UltraGrid tool)

- **IP telephony**

Support for offline content access

- **streaming**
- **video archive**

http://vidcon.cesnet.cz

Security services

Security incidents handling

- detailed monitoring of possible security incidents
- the users/administrators are informed about security incidents, and
- helped to resolve the incident
- additional services:

  seminars, workshops, etc.

Security teams CSIRT-MU and CESNET-CERTS

- several successes:

  e.g., Chuck Norris botnet discovery

http://csirt.cesnet.cz

http://www.muni.cz/ics/services/csirt

Federated identity management

Czech academic identity federation eduID.cz

- provides means for inter-organizational identity management and access control to network services, while respecting the privacy of the users
- users may access multiple applications using just a single password
- service provider administrators do not have to preserve user's credentials and implement authentication
- user authentication is always performed at the home organization, user credenitals are not revealed to the service providers

eduID.cz

http://www.eduid.cz

PKI – users and servers certificates

CESNET CA certification authority

- **provides the users with TERENA (Trans-European Research and Education Networking Association) certificates**
  - usable for electronic signatures as well as for encryption
- **CESNET CA services:**
  - issues personal certificates
  - issues certificates for servers and services
  - certificates registration offices
  - certificates certification offices

Name: “Jane Doe”

Key-Exchange Key:

Signature Key:

Serial #: 29483756

Other Data: 10236283025273

Expires: 6/18/96

Signed: CA’s Signature

public
public

http://pki.cesnet.cz

Mobility and roaming support

Eduroam.cz

– idea to enable transparent usage of (especially wireless) networks of partner (Czech as well as abroad) institutions

http://www.eduroam.cz

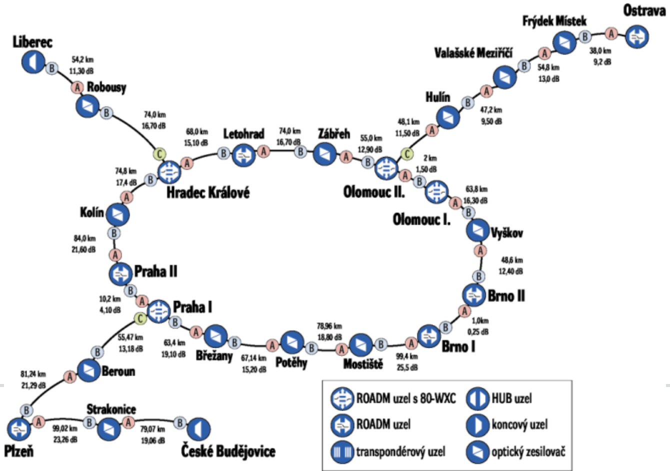
Communication infrastructure and its monitoring

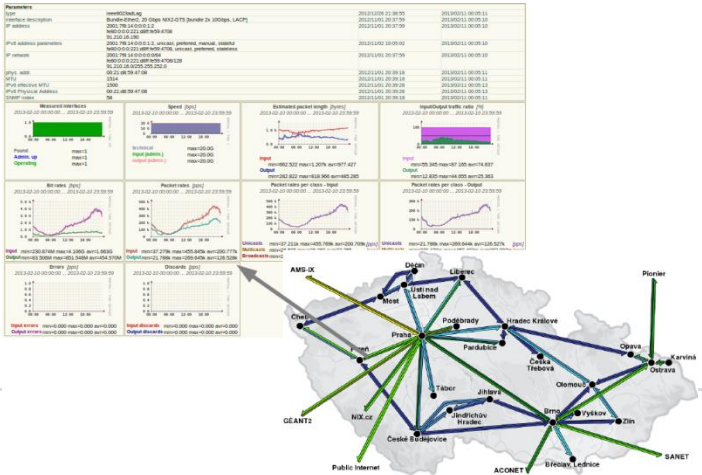
The basis of all the services: high-speed computer network

- 100 Gbps, called CESNET2
- interconnected with pan-european network GÉANT

and its monitoring

- detailed network monitoring (quality issues as well as individual nodes behaviour) available
- automatic detection of various events, anomalies, etc.





Conclusions

Conclusions

- **CESNET infrastructure:**
  - ***computing services* (MetaCentrum NGI & MetaVO)**
  - *data services* (archivals, backups, data sharing and transfers, …)
  - *remote collaborations support servicese* (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…“

EUROPEAN UNION

EUROPEAN REGIONAL
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2007-13
OP Research and
Development for Innovation

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http://metavo.metacentrum.cz http://www.cerit-sc.cz

Hands-on training
for MetaCentrum/CERIT-SC users

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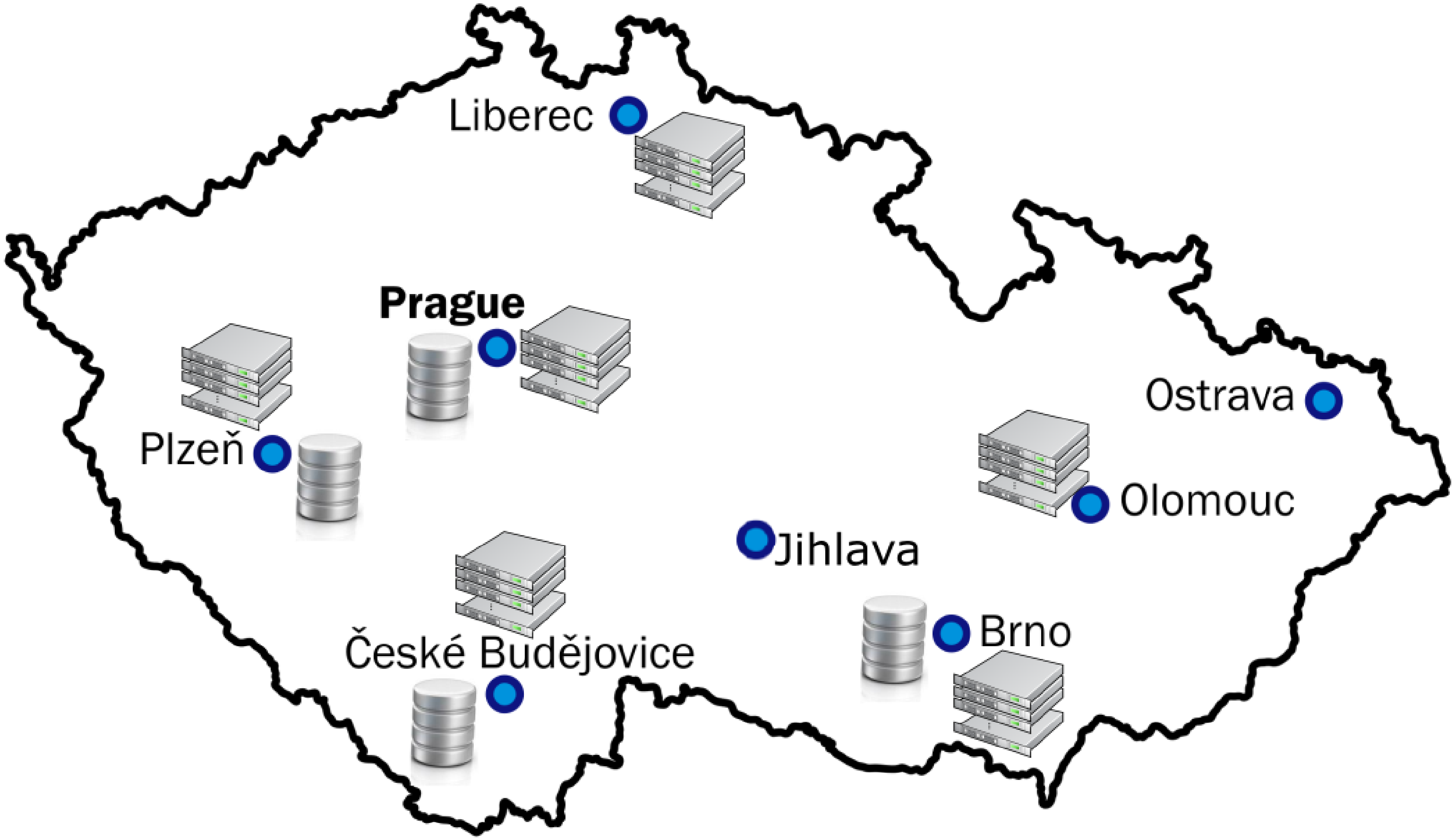
Overview

- Introduction
- **MetaCentrum / CERIT-SC infrastructure overview**
- How to … specify requested resources
- How to … run an interactive job
- How to … use application modules
- How to … run a batch job
- How to … determine a job state
- Another mini-HowTos …
- What to do if something goes wrong?

- Real-world examples
- Appendices

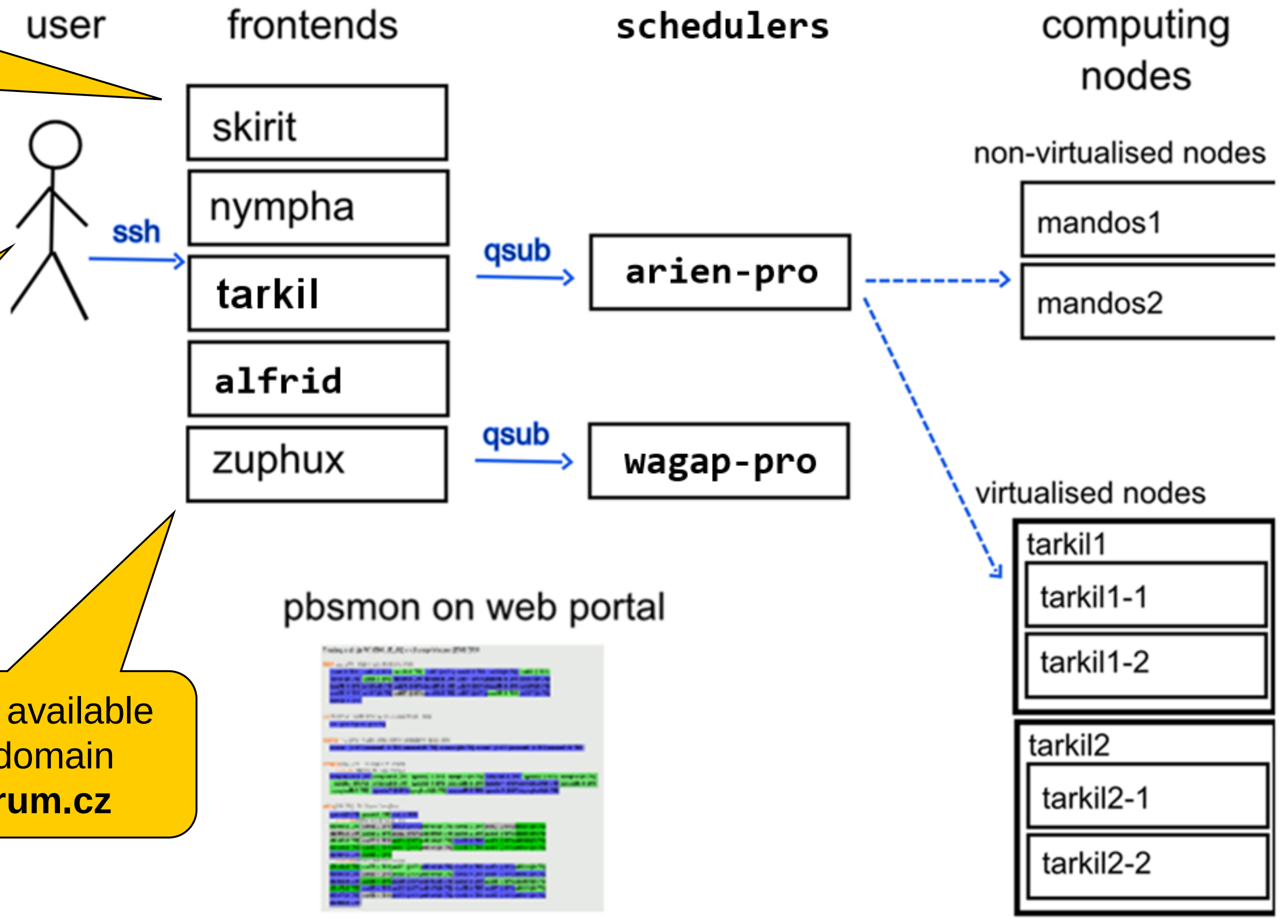
Infrastructure overview



Infrastructure Access

https://wiki.metacentrum.cz/wiki/Frontend

ssh (Linux)
putty (Windows)



user

frontends

schedulers

computing nodes

ssh

skirit

nympha

tarkil

alfrid

zuphux

qsub

qsub

arien-pro

wagap-pro

non-virtualised nodes

mandos1

mandos2

virtualised nodes

tarkil1

tarkil1-1

tarkil1-2

tarkil2

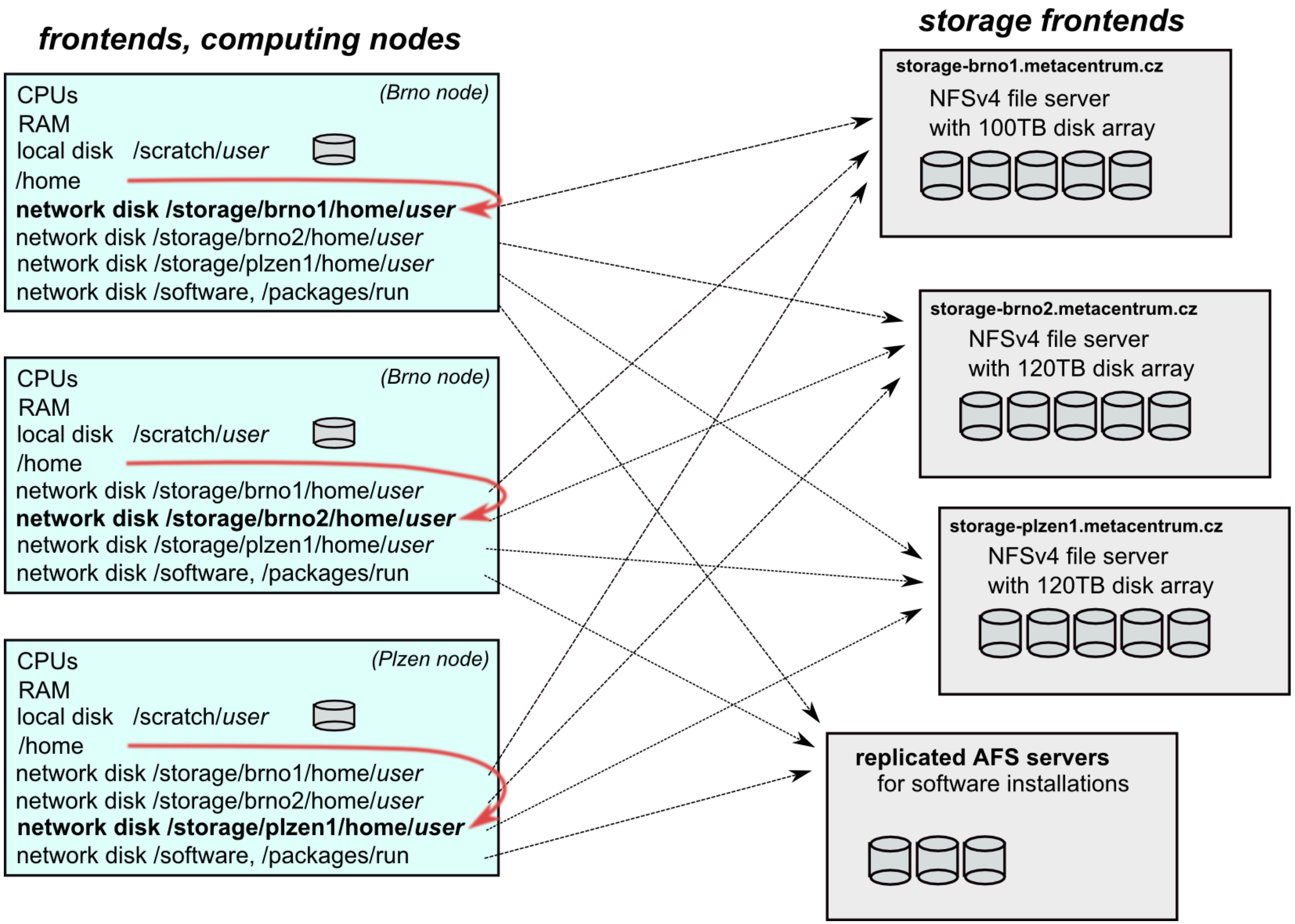
tarkil2-1

tarkil2-2

pbsmon on web portal

all the nodes available under the domain **metacentrum.cz**

Infrastructure System Specifics


frontends, computing nodes
CPUs
(Brno node)
RAM
local disk /scratch/*user*
/home
network disk /storage/brno1/home/*user*
network disk /storage/brno2/home/*user*
network disk /storage/plzen1/home/*user*
network disk /software, /packages/run
CPUs
(Brno node)
RAM
local disk /scratch/*user*
/home
network disk /storage/brno1/home/*user*
network disk /storage/brno2/home/*user*
network disk /storage/plzen1/home/*user*
network disk /software, /packages/run
CPUs
(Plzen node)
RAM
local disk /scratch/*user*
/home
network disk /storage/brno1/home/*user*
network disk /storage/brno2/home/*user*
network disk /storage/plzen1/home/*user*
network disk /software, /packages/run
storage frontends
storage-brno1.metacentrum.cz
NFSv4 file server
with 100TB disk array
storage-brno2.metacentrum.cz
NFSv4 file server
with 120TB disk array
storage-plzen1.metacentrum.cz
NFSv4 file server
with 120TB disk array
replicated AFS servers
for software installations

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How to … specify requested resources I.

- before running a job, one needs to know **what resources the job requires**
  - and how much/many of them
- for example:
  - number of **nodes**
  - number of **CPUs/cores per node**
  - an **upper estimation** of job’s **runtime**
  - amount of **free memory**
  - amount of **scratch space** for temporal data
  - number of requested **software licenses**
  - etc.
- the resource requirements are then **provided to the qsub utility** (when submitting a job)
  - the requested resources are **reserved for the job** by the infrastructure scheduler
    - the computation is allowed to use them

- **details about resources’ specification:** https://wiki.metacentrum.cz/wiki/About_scheduling_system

How to … specify requested resources II.

Graphical way:

- *qsub assembler:* https://metavo.metacentrum.cz/pbsmon2/qsub_pbspro

- allows to:
  - graphically specify the requested resources
  - check, whether such resources are available
  - generate command line options for qsub
  - check the usage of MetaVO resources

Textual way:

- **more powerful** and (once being experienced user) **more convenient**
- see the following slides/examples →

PBS Professional – the infrastructure scheduler

- **a novel scheduling system used in MetaCentrum NGI**
  - see advanced information at https://wiki.metacentrum.cz/wiki/Prostředí_PBS_Professional

New term – CHUNK:

- *chunk* = further indivisible set of resources allocated to a job on a physical node
- contains *resources*, which could be asked from the infrastructure nodes

- for simplicity reasons: ***chunk* = *node***
  - later, we will generalize…

How to … specify requested resources III.

Chunk(s) specification:

- *general format:* `-l` **`select`**`=...`

Examples:

- 2 chunks/nodes:
  - `-l select=2`
- 5 chunks/nodes:
  - `-l select=5`

- by default, allocates just a single core in each chunk
  - → should be used together with **number of CPUs (NCPUs)** specification
- if "`-l select=...`" is not provided, just a single chunk with a single CPU/core is allocated

How to … specify requested resources IV.

Number of CPUs (NCPUs) specification (in each chunk):

- *general format:* `-l select=...:`**`ncpus`**`=...`

- 1 chunk with 4 cores:
  - `-l select=1:ncpus=4`
- 5 chunks, each of them with 2 cores:
  - `-l select=5:ncpus=2`

(Advanced chunks specification:)

- *general format:* `-l select=[chunk_1][+chunk_2]...[+chunk_n]`

- 1 chunk with 4 cores and 2 chunks with 3 cores and 10 chunks with 1 core:
  - `-l select=1:ncpus=4+2:ncpus=3+10:ncpus=1`

How to … specify requested resources V.

Other useful features:

- chunks from just a **single (specified) cluster** (suitable e.g. for MPI jobs):
  - *general format:* `-l select=…:cl_<cluster_name>=true`
  - e.g., `-l select=3:ncpus=1:cl_doom=true`
- chunks located in a **specific location** (suitable when accessing storage in the location)
  - *general format:* `-l select=…:<brno|plzen|praha|...>=true`
  - e.g., `-l select=1:ncpus=4:brno=true`
- **exclusive node(s) assignment** (useful for testing purposes, all resources available):
  - *general format:* `-l select=… -l place=exclhost`
  - e.g., `-l select=1 -l place=exclhost`
- **negative** specification:
  - *general format:* `-l select=…:<feature>=false`
  - e.g., `-l select=1:ncpus=4:hyperthreading=false`
- ...

A list of nodes' features can be found here: http://metavo.metacentrum.cz/pbsmon2/props

How to … specify requested resources VI.

Specifying memory resources (default = 400mb):

- *general format:* `-l select=...:mem=…<suffix>`
  - e.g., `-l select=...:mem=100mb`
  - e.g., `-l select=...:mem=2gb`

Specifying job's maximum runtime (default = 24 hours):

- it is necessary to specify an upper limit on job's runtime:
- *general format:* `-l walltime=[[hh:]mm:]ss`
  - e.g., `-l walltime=13:00`
  - e.g., `-l walltime=2:14:30`

How to … specify requested resources VII.

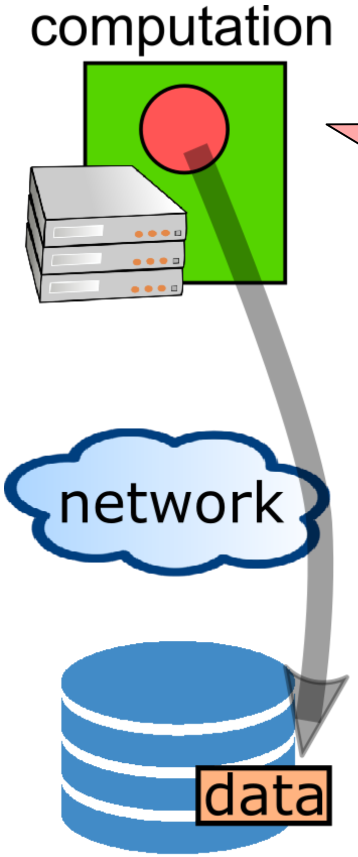
Specifying requested scratch space:

- useful, when the application performs **I/O intensive operations** OR for **long-term computations** (reduces the impact of network failures)
- requesting scratch is **<u>mandatory</u>** (no defaults)
- ***scratch space specification :*** `-l select=...:scratch_type=…<suffix>`
  - `e.g., -l select=...:scratch_local=500mb`

Types of scratches:

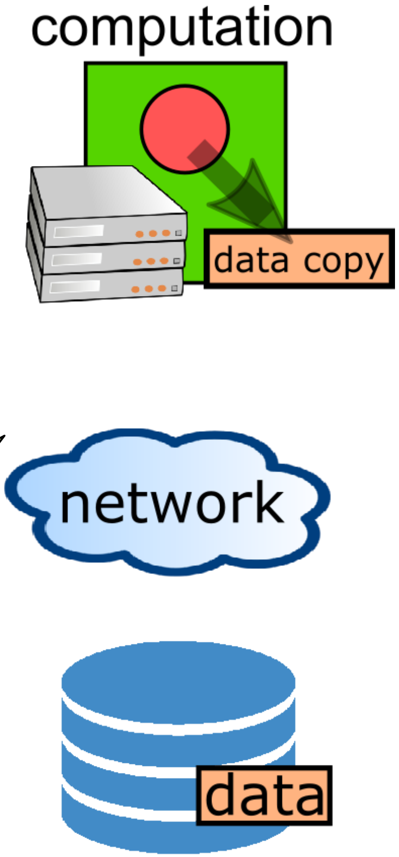
- ***scratch_local***
- ***scratch_ssd***
- ***scratch_shared***

Why to use scratches?



Data processing using central storage
- low computing performance (I/O operations)
- dependency on (functional) network connection
- high load on the central storage

Data processing using scratches
+ highest computing performance
+ resilience to network connection failures
+ minimal load on the central storage



How to use scratches?

- there is a **private scratch directory for particular job**
  - **`/scratch/$USER/job_$PBS_JOBID`** directory for (local) job’s scratch
    - `/scratch.ssd/$USER/job_$PBS_JOBID` for job‘s scratch on SSD
    - `/scratch.shared/$USER/job_$PBS_JOBID` for shared job‘s scratch
  - the master directory `/scratch*/$USER` is not available for writing
- **to make things easier,** there is a **`SCRATCHDIR` environment variable** available in the system
  - (within a job) points to the assigned scratch space/location

Please, clean scratches after your jobs

- there is a “**`clean_scratch`**” **utility to perform safe scratch cleanup**
  - also reports scratch garbage from your previous jobs
  - usage example will be provided later

How to … specify requested resources VIII.

Specifying requested software licenses:

- necessary when an application requires a SW licence
  - the job becomes started once the requested licences are available
  - the information about a licence necessity is **provided within the application description** (see later)
- *general format:* `-l <lic_name>=<amount>`
  - e.g., `-l matlab=2`
  - e.g., `-l gridmath8=20`

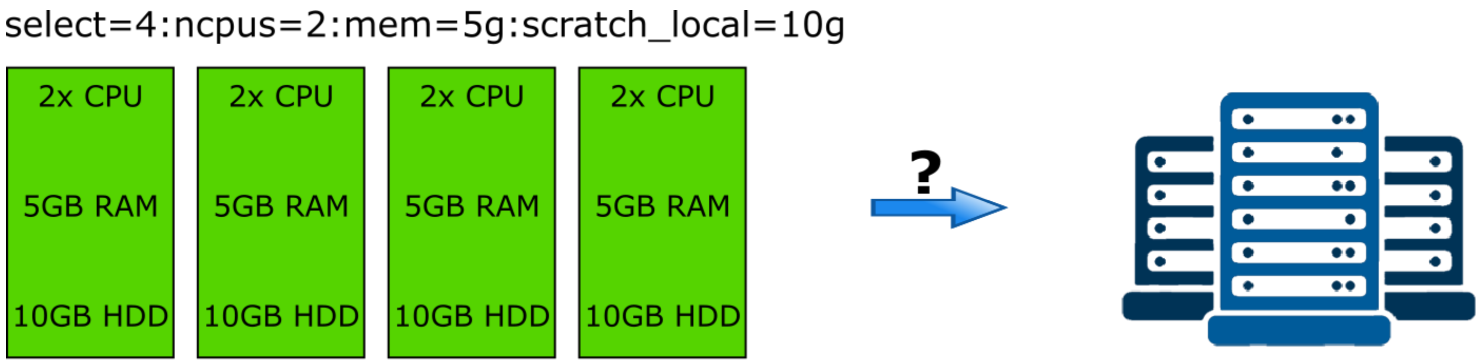
(advanced) Dependencies among jobs

- allows to create a workflow
  - e.g., to start a job once another one successfully finishes, breaks, etc.
- see qsub’s “**`–W`**” option (`man qsub`)
  - e.g., `$ qsub ... -W depend=afterok:12345.arien-pro.ics.muni.cz`

Resource chunks vs. nodes

How do chunks correspond to nodes?

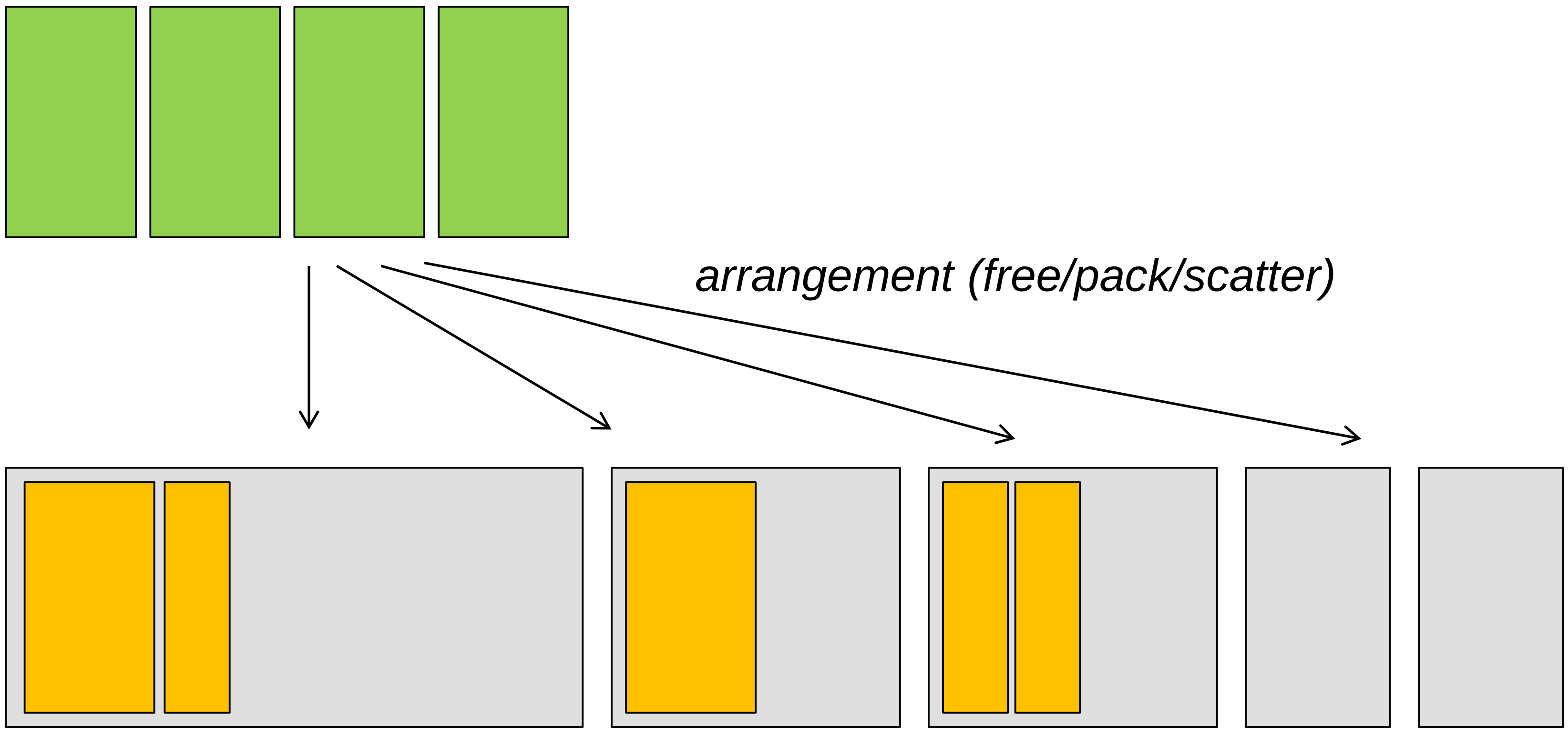
- chunks arrangement – option „`-l place=...`“
  - `-l place=free`: chunks are **free to spread** over available nodes
    - default behaviour
  - `-l place=pack`: all chunks will be allocated **on the same node**
    - the node has to have enough resources available
  - `-l place=scatter`: each chunk will be allocated **on a different node**



select=4:ncpus=2:mem=5g:scratch_local=10g

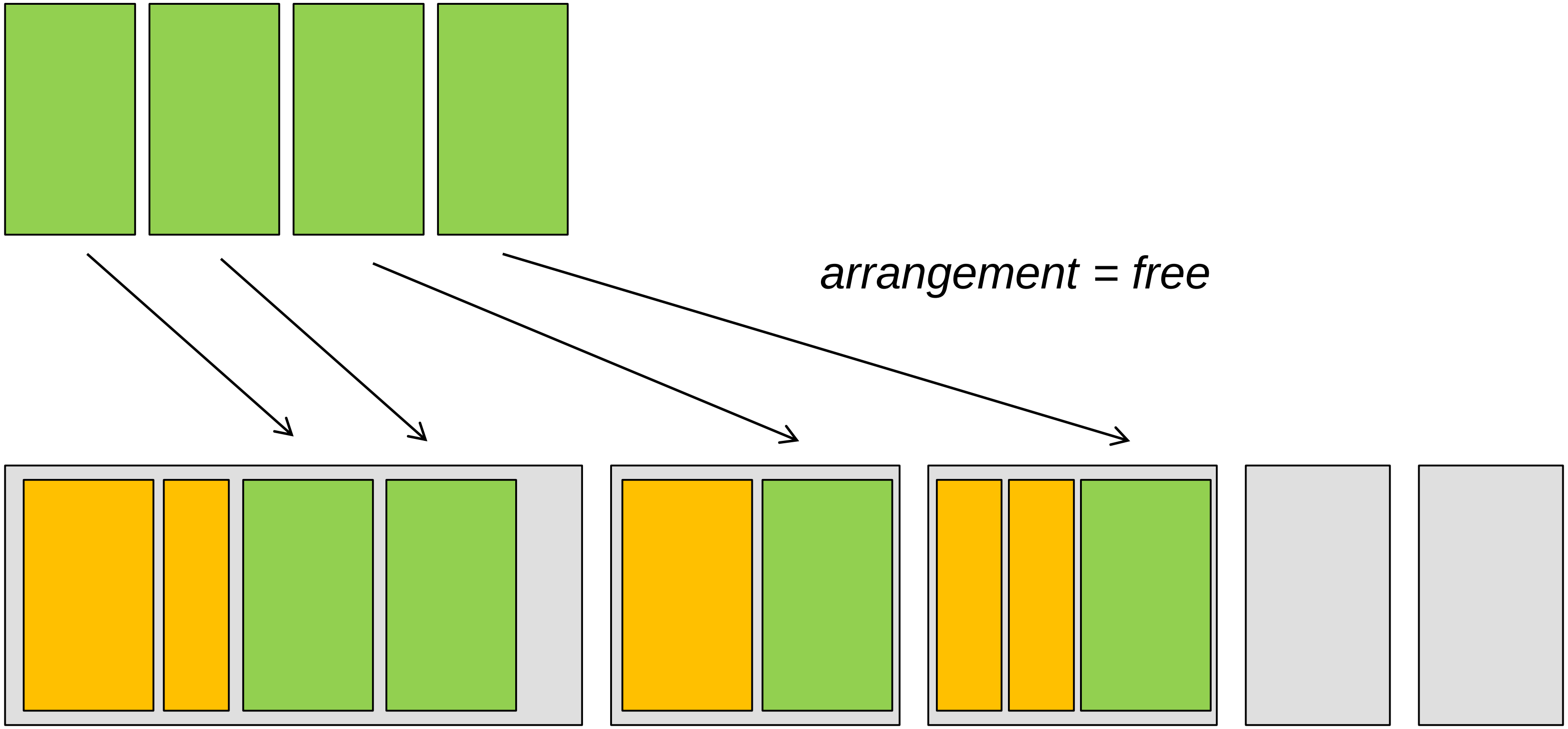
Chunks arrangement

- free vs. pack vs. scatter



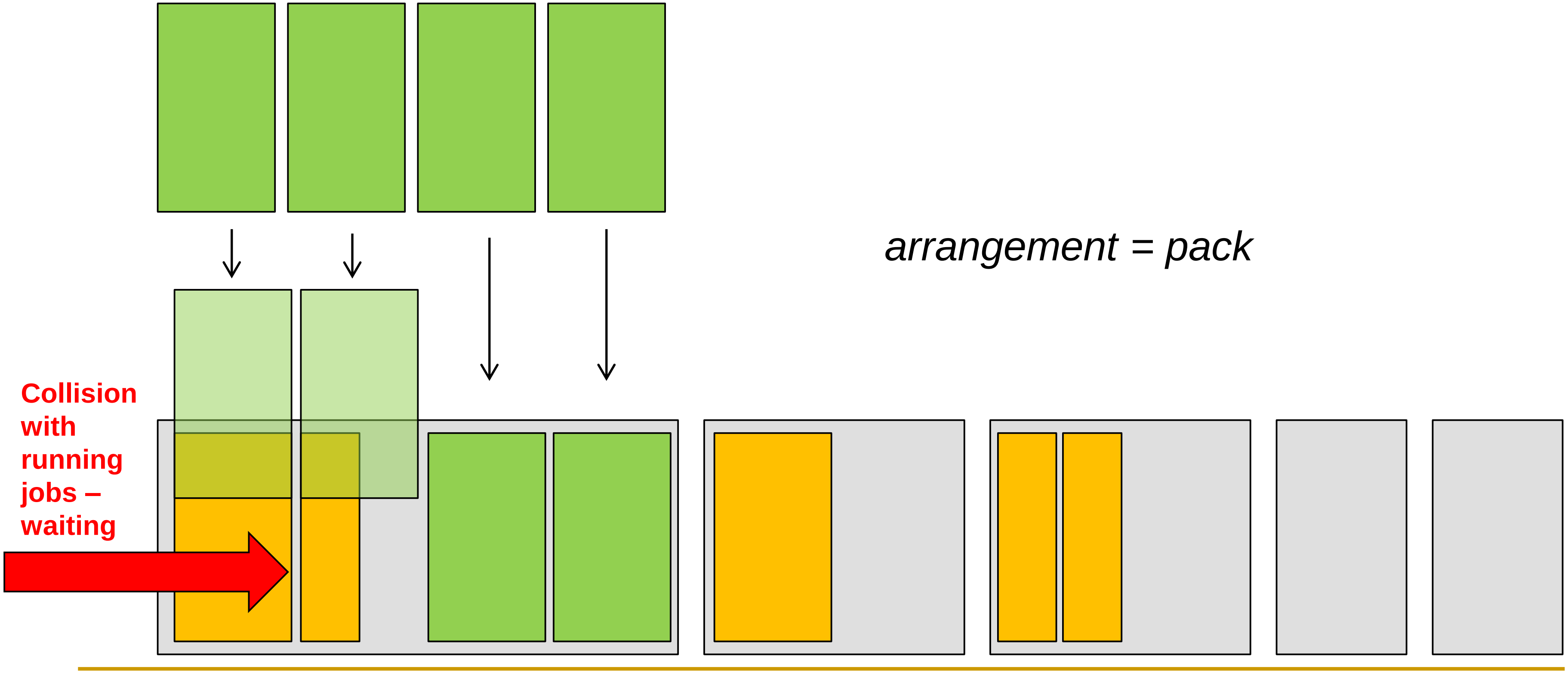
Chunks arrangement

- **free** vs. pack vs. scatter



Chunks arrangement

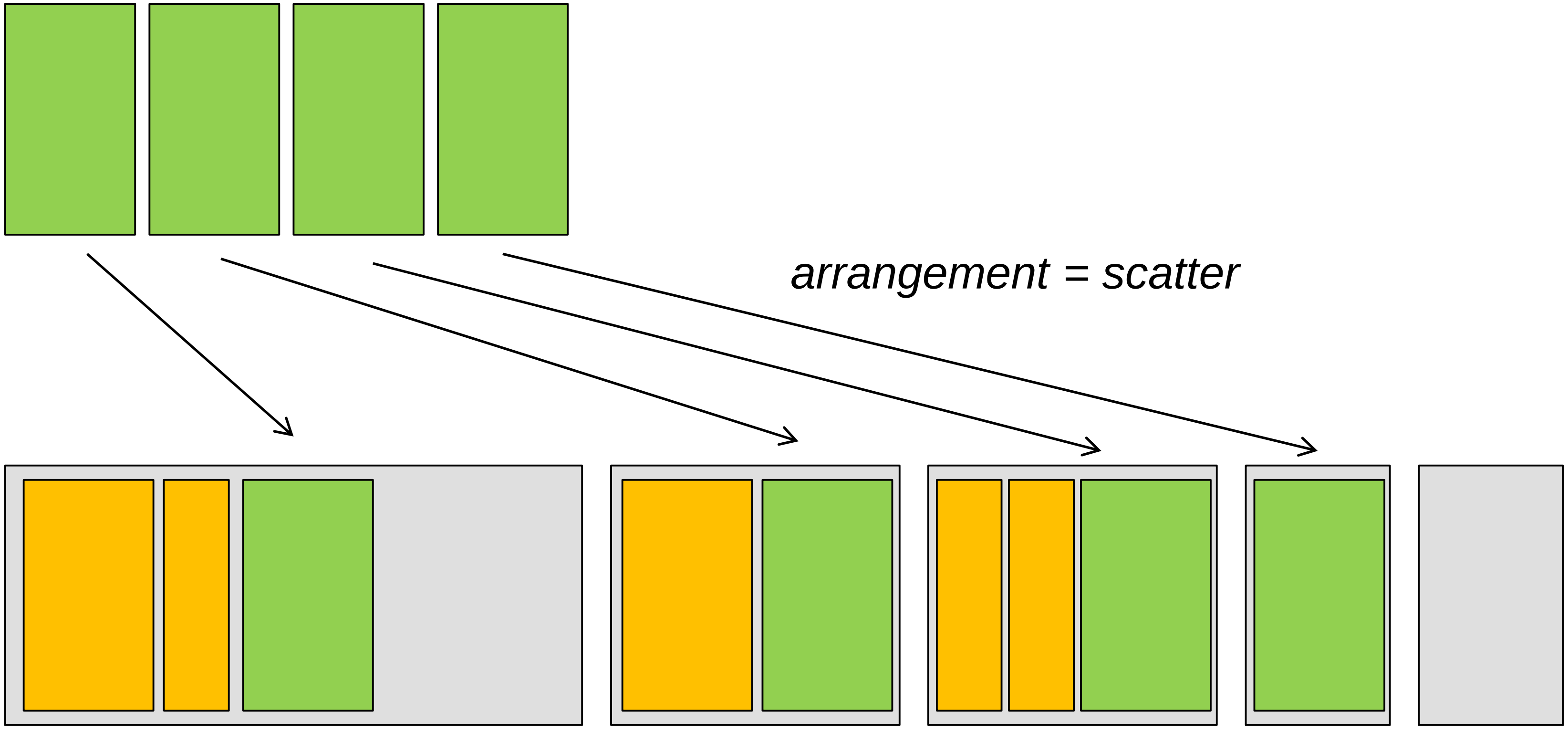
- free vs. **pack** vs. scatter



arrangement = pack

Chunks arrangement

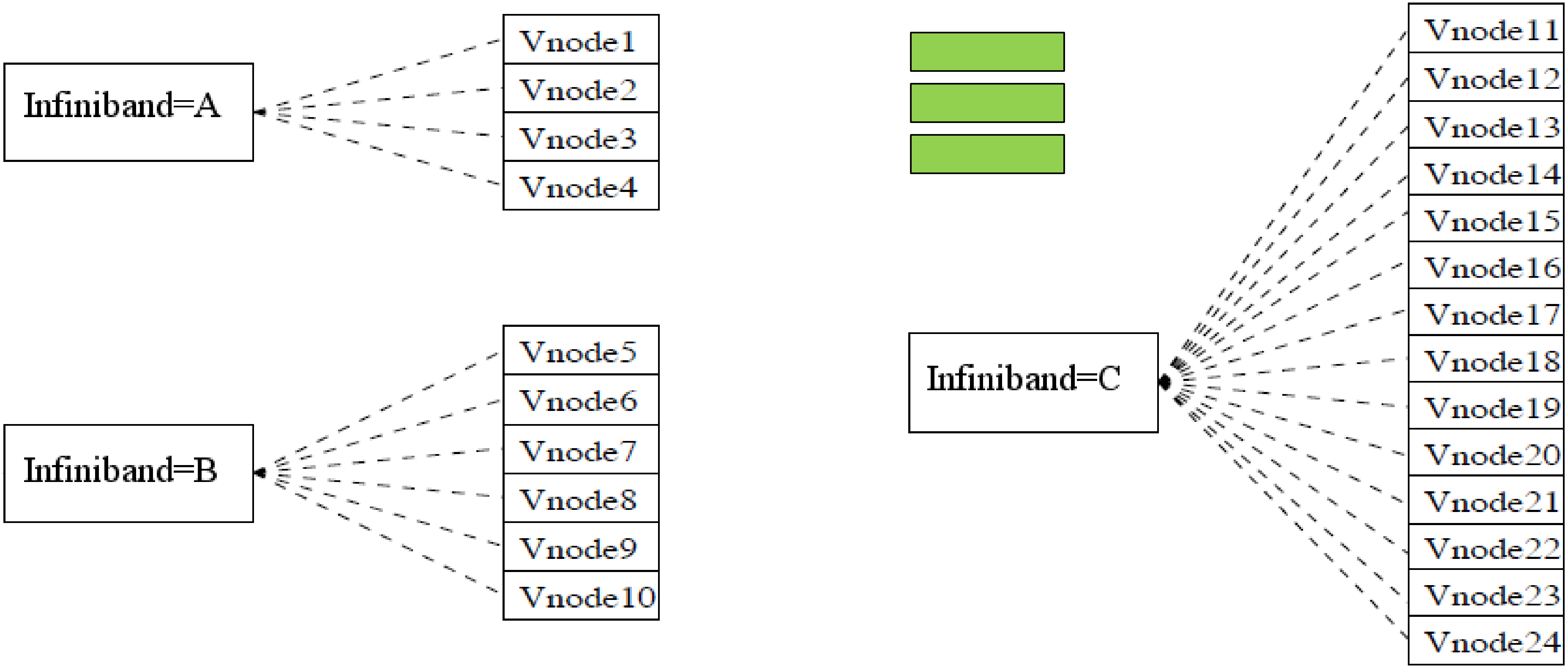
- free vs. pack vs. **scatter**



arrangement = scatter

Chunks grouping

- useful for distributed jobs
- `-l place=group=infiniband`



Infiniband=A

Vnode1
Vnode2
Vnode3
Vnode4

Infiniband=B

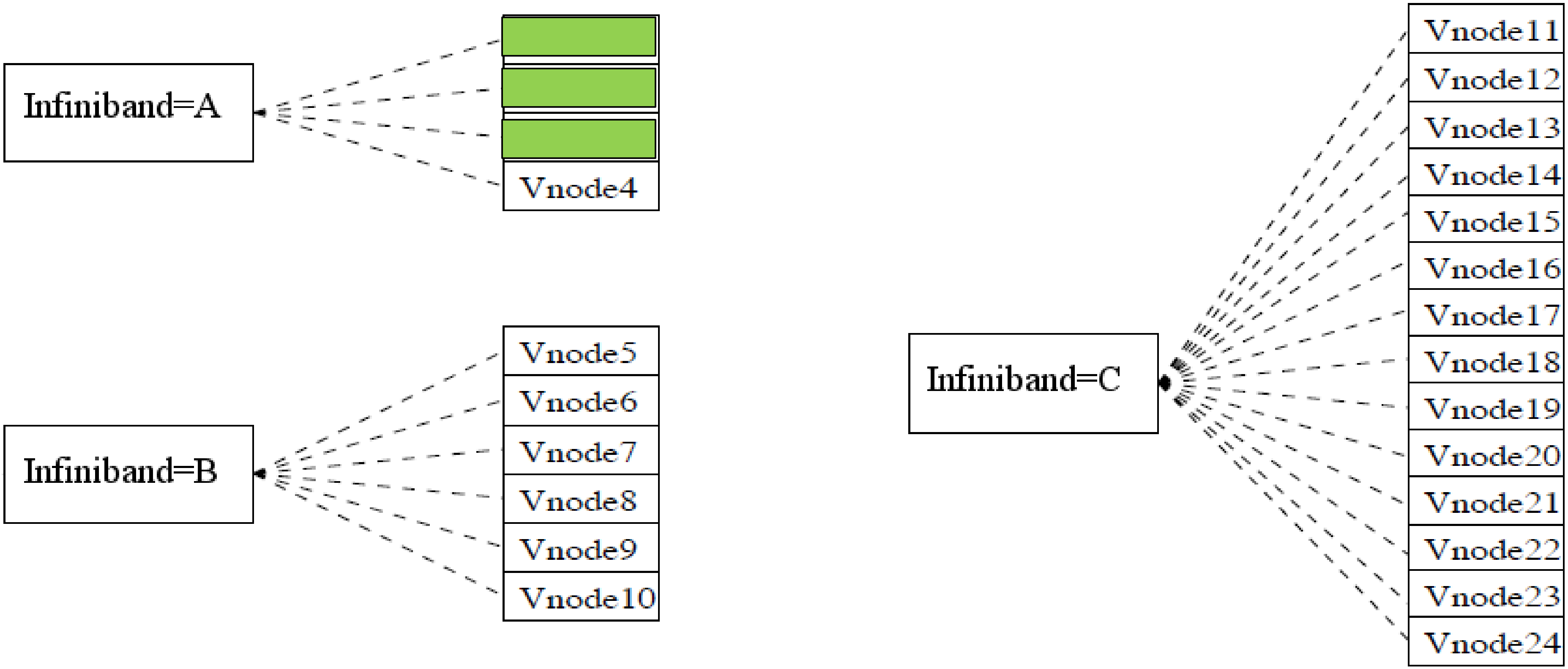
Vnode5
Vnode6
Vnode7
Vnode8
Vnode9
Vnode10

Infiniband=C

Vnode11
Vnode12
Vnode13
Vnode14
Vnode15
Vnode16
Vnode17
Vnode18
Vnode19
Vnode20
Vnode21
Vnode22
Vnode23
Vnode24

Chunks grouping

- useful for distributed jobs
- `-l place=group=infiniband`



Chunks grouping

- useful for distributed jobs
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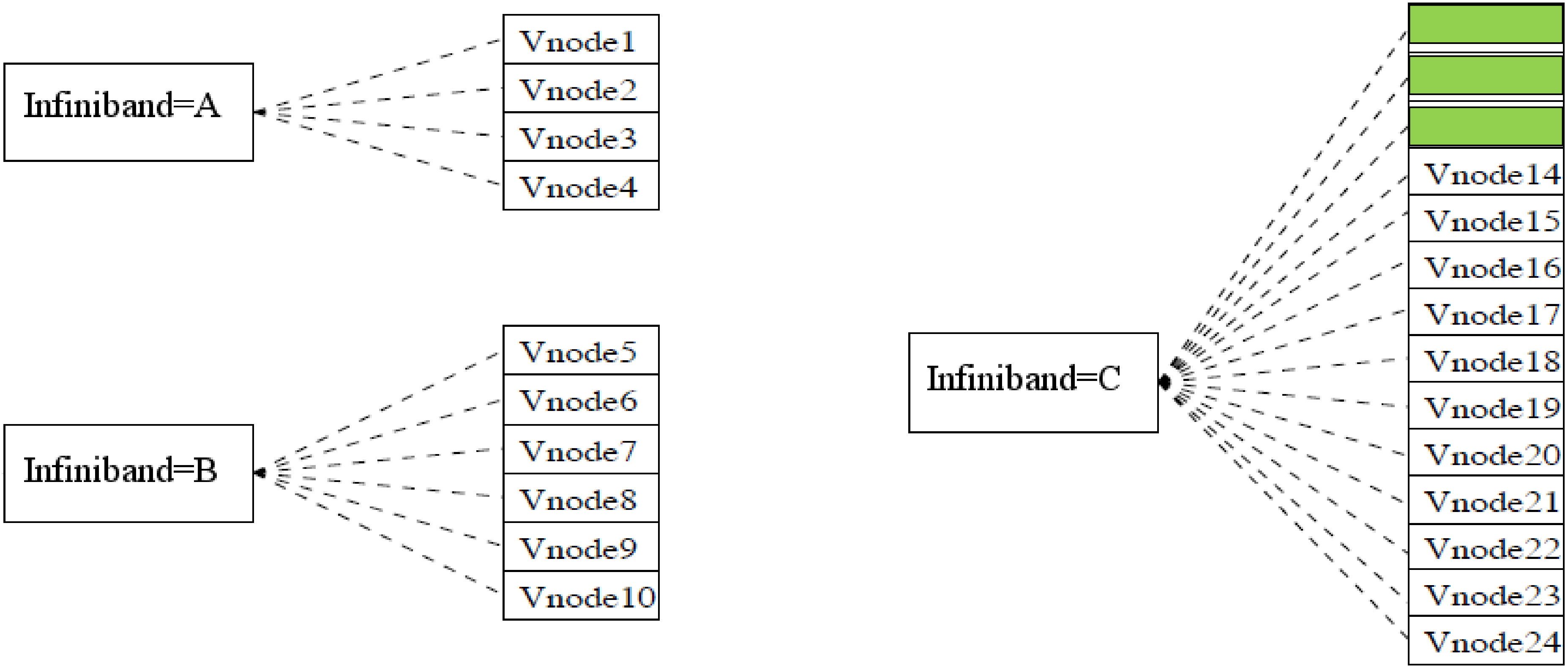
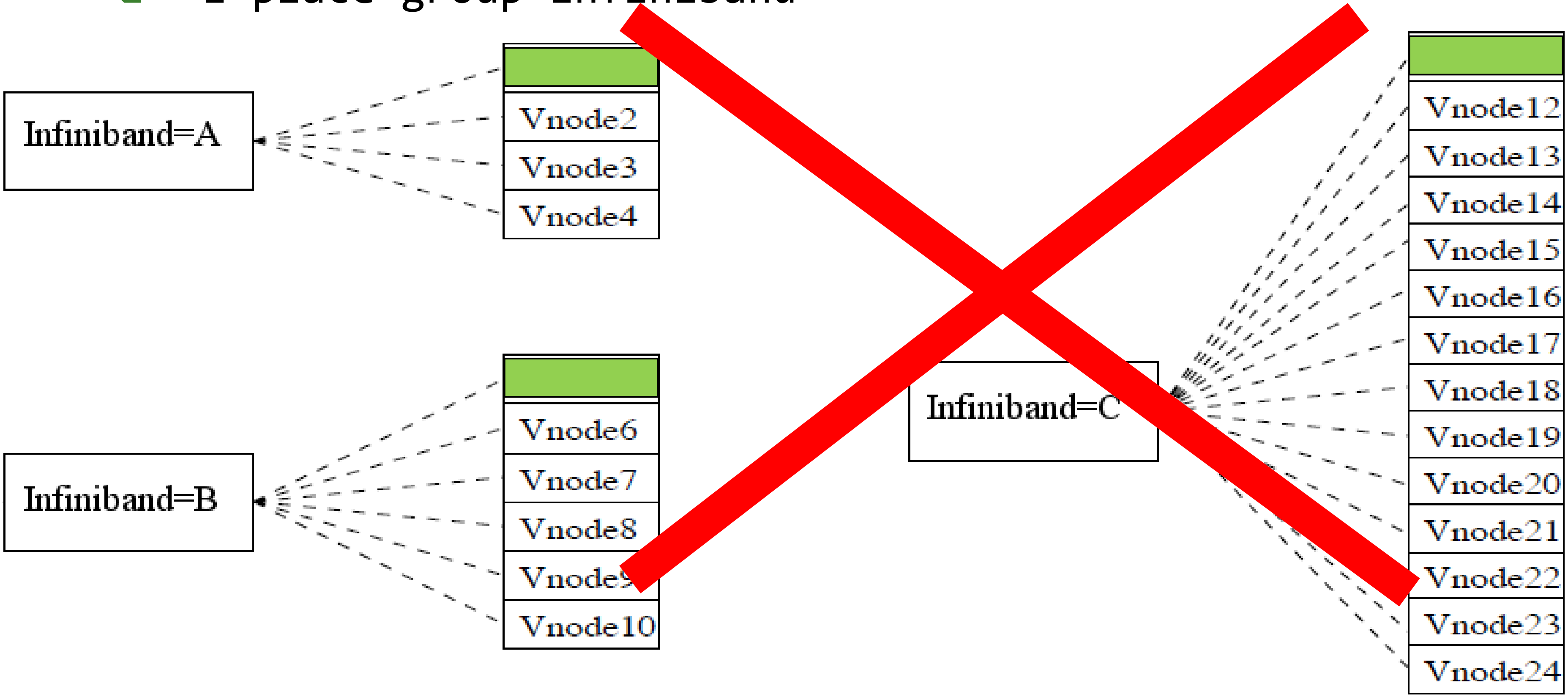


Chunks grouping

- useful for distributed jobs
- `-l place=group=infiniband`



How to … specify requested resources IX.

Questions and Answers:

- *Why is it necessary to specify the resources in a proper number/amount?*
  - because when a job consumes more resources than announced, it will be **killed** by us (you'll be informed)
    - otherwise it may influence other processes running on the node
- *Why is it necessary not to ask for excessive number/amount of resources?*
  - the jobs having smaller resource requirements are started (i.e., get the time slot) **faster**

- *Any other questions?*

How to … specify requested resources IX.

Questions and Answers:

- *Why is it necessary to specify the resources in a proper number/amount?*
  - because when a job consumes more resources than announced, it will be **killed** by us (you'll be informed)
    - otherwise it may influence other processes running on the node
- *Why is it necessary not to ask for excessive number/amount of resources?*
  - the jobs having smaller resource requirements are started

See more details about PBSpro scheduler:

https://metavo.metacentrum.cz/cs/seminars/seminar2017/presentation-Klusacek.pptx

SHORT guide:

https://metavo.metacentrum.cz/export/sites/meta/cs/seminars/seminar2017/tahak-pbs-pro-small.pdf

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How to … run an interactive job I.

Interactive jobs:

- result in getting a prompt on a single **(master) node**
  - one may perform interactive computations
  - the other nodes, if requested, remain allocated and accessible (see later)

- How to **ask for** an **interactive job**?
  - add the option "`-I`" to the qsub command
  - e.g., `qsub -I -l select=1:ncpus=4`

- **Example** (valid just for this demo session):
  - `qsub -I -q MetaSeminar     # ( -l select=1:ncpus=1)`

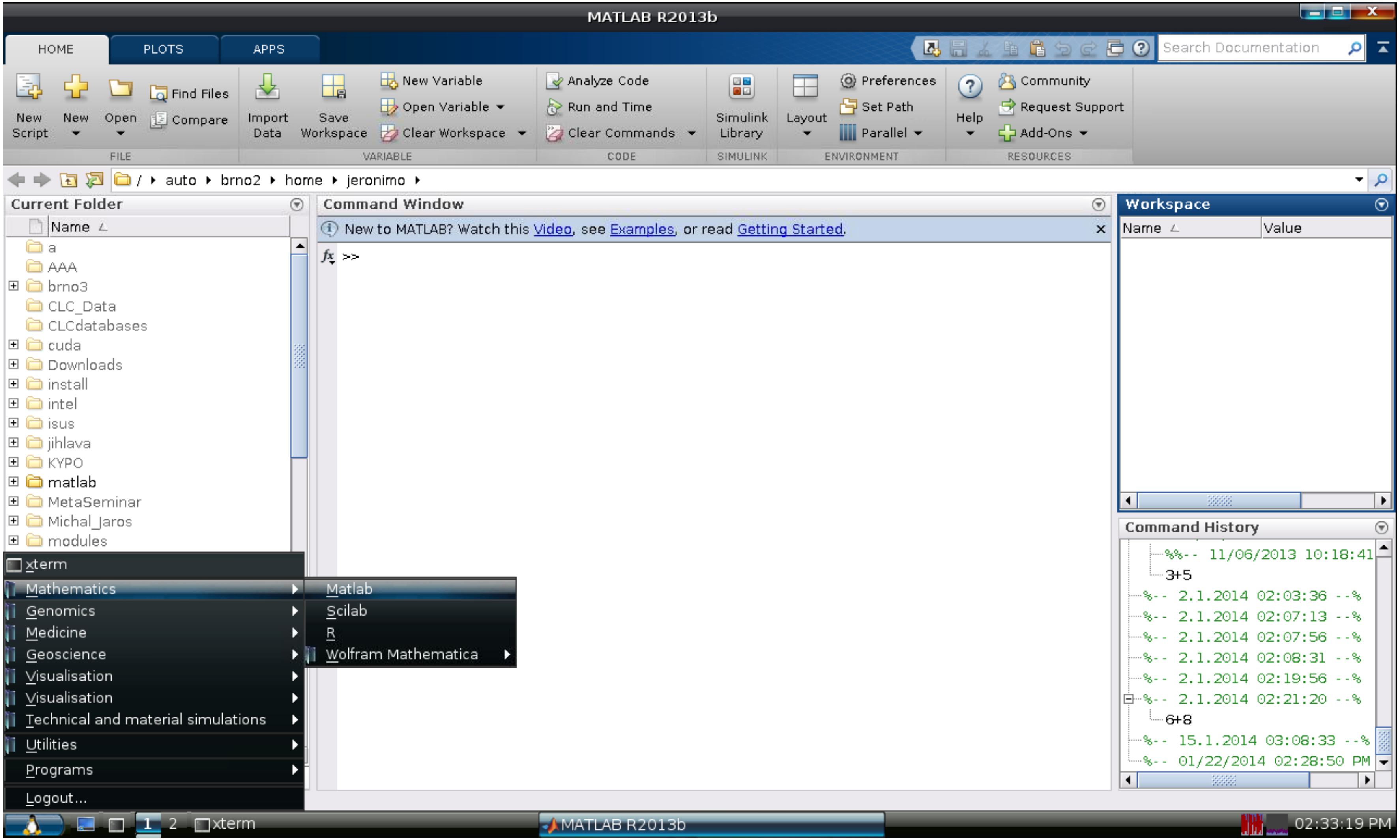
How to … run an interactive job II.

Textual mode: simple

Graphical mode:

- *(preffered)* **remote desktops based on VNC servers (pilot run):**
- available from frontends as well as computing nodes (interactive jobs)
  - `module add gui`
  - `gui start [-s] [-g GEOMETRY] [-c COLORS]`
    - uses one-time passwords
    - allows to access the VNC via a supported **TigerVNC client**
    - **allows SSH tunnels** to be able to connect with a wide-range of clients
    - allows to specify several parameters (e.g., **desktop resolution, color depth**)
    - `gui info [-p]` ... displays active sessions (optionally with login password)
      - gui traverse [-p] … display all the sessions throughout the infrastructure
    - `gui stop [sessionID]` ... allows to stop/kill an active session
- see more info at https://wiki.metacentrum.cz/wiki/Remote_desktop

How to … run an interactive job II.



```
/ ▸ auto ▸ brno2 ▸ home ▸ jeronimo ▸
```

New to MATLAB? Watch this Video, see Examples, or read Getting Started.

```
fx >>
```

```
%%-- 11/06/2013 10:18:41
  3+5
%-- 2.1.2014 02:03:36 --%
%-- 2.1.2014 02:07:13 --%
%-- 2.1.2014 02:07:56 --%
%-- 2.1.2014 02:08:31 --%
%-- 2.1.2014 02:19:56 --%
%-- 2.1.2014 02:21:20 --%
  6+8
%-- 15.1.2014 03:08:33 --%
%-- 01/22/2014 02:28:50 PM
```

How to … run an interactive job II.

Graphical mode (further options):

- *(fallback)* **tunnelling a display through `ssh`** (Windows/Linux)**:**
  - connect to the frontend node having SSH forwarding/tunneling enabled:
    - Linux: `ssh –X skirit.metacentrum.cz`
    - Windows:
      - install an XServer (e.g., Xming)
      - set Putty appropriately to enable X11 forwarding when connecting to the frontend node
        - Connection → SSH → X11 → Enable X11 forwarding
  - ask for an interactive job, **adding "`–X`" option** to the qsub command
    - e.g., `qsub –I` **`–X`** `–l select=... ...`

- *(tech. gurus)* **exporting a display** from the master node to a Linux box:
  - `export DISPLAY=mycomputer.mydomain.cz:0.0`
  - on a Linux box, run "`xhost +`" to allow all the remote clients to connect
    - be sure that your display manager allows remote connections

How to … run an interactive job III.

Questions and Answers:

- *How to **get an information** about the **other nodes/chunks allocated** (if requested)?*
  - `master_node$ cat $PBS_NODEFILE`
  - works for batch jobs as well
- *How to **use the other nodes/chunks**? (holds for batch jobs as well)*
  - MPI jobs use them automatically
  - otherwise, use the **pbsdsh** utility (see `"man pbsdsh"` for details) to run a remote command
  - if the pbsdsh does not work for you, use the **ssh** to run the remote command
- *Any other questions?*

How to … run an interactive job III.

Questions and Answers:

- *How to* ***get an information*** *about the other* ***nodes/chunks allocated***

un a

Hint:

- there are several useful environment variables one may use
  - `$ set | grep PBS`
- e.g.:
  - PBS_JOBID … job's identificator
  - PBS_NUM_NODES, PBS_NUM_PPN … allocated number of nodes/processors
  - PBS_O_WORKDIR … submit directory
  - …

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How to … use application modules I.

Application modules:

- the **modullar subsystem** provides a user interface to modifications of user environment, which are necessary for running the requested applications
- allows to “add” an application to a user environment

- **getting a list** of available application modules:
  - `$ module avail`
  - `$ module avail matl`
  - https://wiki.metacentrum.cz/wiki/Kategorie:Applications
    - provides the documentation about modules’ usage
    - besides others, includes:
      - information whether it is necessary to ask the scheduler for an available licence
      - information whether it is necessary to express consent with their licence agreement

How to … use application modules II.

Application modules:

- **loading** an application into the environment:
  - `$ module add <modulename>`
  - e.g., `module add maple`
- **listing** the already loaded modules:
  - `$ module list`
- **unloading** an application from the environment:
  - `$ module del <modulename>`
  - e.g., `module del openmpi`

- ***Note:** An application may require to express consent with its licence agreement before it may be used (see the application's description). To provide the aggreement, visit the following webpage:* https://metavo.metacentrum.cz/cs/myaccount/licence.html

- for more information about application modules, see https://wiki.metacentrum.cz/wiki/Application_modules

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How to … run a batch job I.

Batch jobs:

- perform the computation as described in their **startup script**
  - the submission results in getting **a job identifier**, which further serves for getting more information about the job (see later)

- How to **submit** a **batch job**?
  - add the reference to the startup script to the qsub command
  - e.g., `qsub -l select=3:ncpus=4` **`<myscript.sh>`**

- **Example** (valid for this demo session):
  - `qsub` **`-q MetaSeminar`** `-l select=1:ncpus=1` **`myscript.sh`**
  - results in getting something like "`12345.arien-pro.ics.muni.cz`"

How to … run a batch job I.

B

for

Hint:

- create the file `myscript.sh` with the following content:
  - `$ vim myscript.sh`

```
#!/bin/bash

# my first batch job
uname -a
```

- see the standard output file (`myscript.sh.o<JOBID>`)
  - `$ cat myscript.sh.o<JOBID>`

❑ `qsub -q MetaSeminar -l select=1:ncpus=1 myscript.sh`

❑ results in getting something like “`12345.arien-pro.ics.muni.cz`”

How to … run a batch job II.

Startup script skelet: (non IO-intensive computations)

- use just when you know, what you are doing…

```
#!/bin/bash

DATADIR="/storage/brno2/home/$USER/"    # shared via NFSv4
cd $DATADIR

# ... load modules & perform the computation ...
```

- **further details** – see https://wiki.metacentrum.cz/wiki/How_to_compute/Requesting_resources

How to … run a batch job III.

Recommended startup script skelet: (IO-intensive computations or long-term jobs)

```
#!/bin/bash

# set a handler to clean the SCRATCHDIR once finished
trap ‘clean_scratch’ TERM EXIT
# if temporal results are important/useful
# trap 'cp -r $SCRATCHDIR/neuplna.data $DATADIR && clean_scratch' TERM

# set the location of input/output data
# DATADIR="/storage/brno2/home/$USER/“
DATADIR=“$PBS_O_WORKDIR”

# prepare the input data
cp $DATADIR/input.txt $SCRATCHDIR

# go to the working directory and perform the computation
cd $SCRATCHDIR

# ... load modules & perform the computation ...

# copy out the output data
# if the copying fails, let the data in SCRATCHDIR and inform the user
cp $SCRATCHDIR/output.txt $DATADIR || export CLEAN_SCRATCH=false
```

How to … run a batch job IV.

Using the application modules within the batch script:

- `module add SW`
  - e.g., „module add maple“
- include the initialization line (“`source` …”) if necessary:
  - i.e., if you experience problems like “`module: command not found`”, then add `source /software/modules/init` before *„module add“* sections

Getting the job’s standard output and standard error output:

- once finished, there appear **two files** in the directory, which the job has been started from:
  - *`<job_name>.o<jobID>`* ... standard output
  - *`<job_name>.e<jobID>`* ... standard error output
  - the `<job_name>` can be modified via the “`-N`” qsub option

How to … run a batch job V.

Job attributes specification:

in the case of batch jobs, the requested resources and further job information (*job attributes* in short) may be specified either on the command line (see "`man qsub`") or directly within the script:

- by adding the "`#PBS`" directives (see "`man qsub`"):

```
#PBS -N Job_name
#PBS -l select=2:ncpus=1:mem=320kb:scratch_local=100m
#PBS -m abe
#
< … commands … >
```

- the submission may be then simply performed by:
  - `$ qsub myscript.sh`
    - if options are provided both in the script and on the command-line, the **command-line arguments override the script ones**

How to … run a batch job VI. (complex example)

```
 #!/bin/bash
 #PBS -l select=1:ncpus=2:mem=500mb:scratch_local=100m
 #PBS -m abe

# set a handler to clean the SCRATCHDIR once finished
trap “clean_scratch” TERM EXIT

# set the location of input/output data
DATADIR=“$PBS_O_WORKDIR"

# prepare the input data
cp $DATADIR/input.mpl $SCRATCHDIR

# go to the working directory and perform the computation
cd $SCRATCHDIR

# load the appropriate module
module add maple

# run the computation
maple input.mpl

# copy out the output data (if it fails, let the data in SCRATCHDIR and inform the user)
cp $SCRATCHDIR/output.gif $DATADIR || export CLEAN_SCRATCH=false
```

How to … run a batch job VII.

Questions and Answers:

- *Should you prefer batch or interactive jobs?*
    - definitely the **batch ones** – they use the computing resources **more effectively**
    - use the interactive ones just for testing your startup script, GUI apps, or data preparation

- *Any other questions?*

How to … run a batch job VIII.

Example:

- Create and submit a batch script, which performs a simple Maple computation, described in a file:

```
plotsetup(gif, plotoutput=`myplot.gif`,
    plotoptions=`height=1024,width=768`);
plot3d( x*y, x=-1..1, y=-1..1, axes = BOXED, style =
    PATCH);
```

  - process the file using Maple (from a batch script):
    - hint: `$ maple <filename>`

How to … run a batch job VIII.

Example:

- Create and submit a batch script, which performs a simple Maple computation, described in a file:

```
plotsetup(gif, plotoutput=`myplot.gif`,
    plotoptions=`height=1024,width=768`);
plot3d( x*y, x=-1..1, y=-1..1, axes = BOXED, style =
    PATCH);
```

  - process the file using Maple (from a batch script):
    - hint: `$ maple <filename>`

Hint:

- see the solution at `/storage/brno2/home/jeronimo/MetaSeminar/latest/Maple`

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- **How to … determine a job state**
- Another mini-HowTos …
- What to do if something goes wrong?

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How to … determine a job state I.

Job identifiers

- every job (no matter whether interactive or batch) is **uniquely identified** by its identifier (JOBID)
  - e.g., `12345.arien-pro.ics.muni.cz`
- to obtain any information about a job, the **knowledge of its identifier is necessary**
  - how to list all the recent jobs?
    - graphical way – PBSMON: http://metavo.metacentrum.cz/pbsmon2/jobs/allJobs
    - `frontend$ qstat` (run on any frontend)
      - **to include finished ones, run `$ qstat -x`**
  - how to list all the recent jobs of a specific user?
    - graphical way – PBSMON: https://metavo.metacentrum.cz/pbsmon2/jobs/my
    - `frontend$ qstat -u <username>` (again, any frontend)
      - **to include finished ones, run `$ qstat -x -u <username>`**

How to … determine a job state II.

How to determine a job state?

- graphical way – see PBSMON
  - list all your jobs and click on the particular job's identifier
  - http://metavo.metacentrum.cz/pbsmon2/jobs/my
- textual way – `qstat` command (see `man qstat`)
  - brief information about a job: `$ qstat JOBID`
    - informs about: job's state (*Q=queued*, *R=running*, *E=exiting*, *F=finished*, …), job's runtime, …
  - complex information about a job: `$ qstat -f JOBID`
    - shows all the available information about a job
    - useful properties:
      - *exec_host* -- the nodes, where the job did really run
      - *resources_used, start/completion time, exit status, …*
  - necessary to add **„-x“ option** when examining already finished job(s)

How to … determine a job state III.

Hell, when my jobs will really start?

- nobody can tell you ☺
  - the **God/scheduler decides** (based on the other job's finish)
  - we're working on an estimation method to inform you about its probable startup

- check the **queues' fulfilment**: http://metavo.metacentrum.cz/cs/state/jobsQueued
  - the higher fairshare (queue's AND job's) is, the earlier the job will be started
- **stay informed** about job's startup / finish / abort (via email)
  - by default, just an information about job's abortation is sent
  - → when submitting a job, add "`-m abe`" option to the `qsub` command to be informed about all the job's states
    - or "`#PBS -m abe`" directive to the startup script

How to … determine a job state IV.

Monitoring running job's stdout, stderr, working/temporal files

1. via ssh, log in directly to the execution node(s)
   - how to get the job's execution node(s)?

- to examine the working/temporal files, navigate directly to them
  - logging to the execution node(s) is necessary -- even though the files are on a shared storage, their content propagation takes some time
- to examine the stdout/stderr of a running job:
  - navigate to the `/var/spool/pbs/spool/` directory and examine the files:
    - `$PBS_JOBID.OU` for standard output (stdout – e.g., "`1234.arien-pro.ics.muni.cz.OU`")
    - `$PBS_JOBID.ER` for standard error output (stderr – e.g., "`1234.arien-pro.ics.muni.cz.ER`")

Job's forcible termination

- `$ qdel JOBID` (the job may be terminated in any previous state)
- during termination, the job turns to *E (exiting)* and finally to *F (finished)* state

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Another mini-HowTos …

- **how to use privileged resources?**
  - if your institution/project integrates HW resources, a defined group of users may have priority access to them
    - technically accomplished using scheduler queues
    - a job has to be **submitted to the particular queue**
      - `qsub –l select=… -l walltime=… -q PRIORITY_QUEUE script.sh`
    - e.g., ELIXIR CZ project integrates a set of resources
      - priority queue „**`elixir_2w`**“ available for ELIXIR CZ users
  - moving jobs between scheduler queues
    - from priority queue **to default queue**
      - `qmove default JOBID`
    - from default queue(s) **to a priority queue**
      - `qmove elixir_2w JOBID`

Another mini-HowTos …

- **how to make your SW tool available within MetaVO?**
  - *commercial apps:*
    - ***assumption:*** you **own a license**, and the **license allows the application to be run on our infrastructure** (nodes not owned by you, located elsewhere, etc.)
    - once installed, we can **restrict its usage** just for you (or for your group)
  - *open-source/freeware apps:*
    - you can compile/install the app in your HOME directory
    - **OR** you can install/compile the app on your own and ask us to make it available in the software repository
      - compile the application in your HOME directory
      - **prepare a modulefile** setting the application environment
        - inspire yourself by modules located at `/packages/run/modules-2.0/modulefiles`
      - **test the app/modulefile**
        - `$ export MODULEPATH=$MODULEPATH:$HOME/myapps`
      - see https://wiki.metacentrum.cz/wiki/How_to_install_an_application
    - **OR** you can ask us for preparing the application for you

Another mini-HowTos …

- **how to ask for nodes equipped by GPU cards?**
  - determine, **how many GPUs** your application will need (`-l ngpus=X`)
    - consult the HW information page: http://metavo.metacentrum.cz/cs/state/hardware.html
  - determine, **how long** the application will run (if you need more, let us know)
    - `gpu` queue … maximum runtime 1 day
    - `gpu_long` queue … maximum runtime 1 week
  - make the submission:
    - $ qsub -l select=1:ncpus=4:mem=10g:**ngpus=1 -q gpu_long** –l walltime=4d …
    - specific GPU cards by restricting the cluster:
      `qsub -l select=...:cl_doom=true ...`
  - **do not change** the CUDA_VISIBLE_DEVICES environment variable
    - it's automatically set in order to determine the GPU card(s) that has/have been reserved for your application
  - details about GPU cards performance within MetaVO:
    - see http://metavo.metacentrum.cz/export/sites/meta/cs/seminars/seminar5/gpu_fila.pdf
  - general information: https://wiki.metacentrum.cz/wiki/GPU_clusters

Another mini-HowTos …

How to ask for nodes equipped with Xeon Phi?

phi[1-6].cerit-sc.cz

- new cluster purchased by CERIT-SC
  - available through “`phi`” queue (PBS Pro) on zuphux.cerit-sc.cz frontend

    `zuphux$ qsub -q phi -l select=…`
- **the newest generation of Xeon Phi** (7210 Knights Landing)
  - currently, the only installation in the CR
- see more details at https://metavo.metacentrum.cz/export/sites/meta/cs/seminars/seminar2017/meta-xeonphi-17.pdf

Installation specifics:

- **/storage/brno3-cerit** is the only central storage **directly mounted**
  - all the rest storages available through SCP only

Central storages of phi.cerit-sc.cz cluster

Central storages not available through NFS

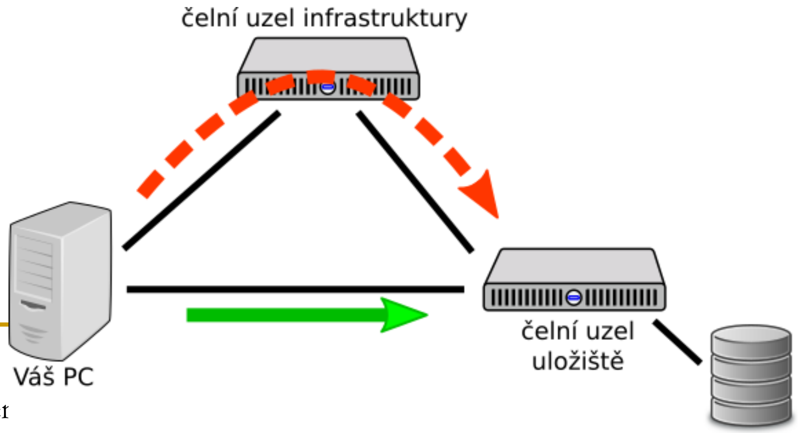
i.e. /storage/XXX/home/<username>

- technical reasons
- data storages available through SCP
  - besides `brno3-cerit`, which is mounted directly
  - in most cases, just a minor change in your scripts

NFS sharing (most clusters)	SCP sharing (phi[1-6].cerit-sc.cz)
DATADIR=“**/storage/brno2/home/<username>/example**” **cp** –R $DATADIR/mydata $SCRATCHDIR	DATADIR=“**storage-brno2.metacentrum.cz:~/example**” **scp** –R $DATADIR/mydata $SCRATCHDIR

Another mini-HowTos …

- **how to transfer large amount of data to computing nodes?**
  - copying through the frontends/computing nodes may not be efficient (hostnames are *`storage-XXX.metacentrum.cz`*)
    - XXX = brno2, brno3-cerit, plzen1, budejovice1, praha1, ...
  - → connect directly to the storage frontends (via **SCP** or **SFTP**)
    - `$ sftp storage-brno2.metacentrum.cz`
    - `$ scp <files> storage-plzen1.metacentrum.cz:<dir>`
    - etc.
    - use FTP only together with the Kerberos authentication
      - otherwise insecure



Another mini-HowTos …

- **how to get information about your quotas?**
  - by default, all the users have quotas on the storage arrays (per array)
    - may be different on every array
  - to get an information about your quotas and/or free space on the storage arrays
    - **textual way:** log-in to a MetaCentrum frontend and see the *"motd"* (information displayed when logged-in)
    - **graphical way:**
      - *your quotas:* https://metavo.metacentrum.cz/cs/myaccount/kvoty
      - *free space:* http://metavo.metacentrum.cz/pbsmon2/nodes/physical
- **how to restore accidentally erased data**
  - the storage arrays (⇒ including homes) are regularly backed-up
    - several times a week
  - → write an email to meta@cesnet.cz specifying what to restore

Another mini-HowTos …

- **how to secure private data?**
  - by default, all the data are readable by everyone
  - → use **common Linux/Unix mechanisms/tools** to make the data private
    - `r`,`w`,`x` rights for *user*, *group*, *other*
    - e.g., `chmod go= <filename>`
      - see `man chmod`
      - use “`–R`” option for recursive traversal (applicable to directories)

- **how to share data among working group?**
  - ask us for creating a **common unix user group**
    - user administration will be up to you (GUI frontend is provided)
  - **use common unix mechanisms** for sharing data among a group
    - see “`man chmod`” and “`man chgrp`”
  - see https://wiki.metacentrum.cz/wikiold/Sdílení_dat_ve_skupině

Another mini-HowTos …

- **how to use SGI UV2000 nodes? (`ungu,urga .cerit-sc.cz`)**
  - because of their nature, these nodes **are not** – by default – **used by common jobs**
    - to be available for jobs that really need them
  - to use these nodes, one has to **submit the job to a specific queue** called **"uv"**

    -
      ```
      $ qsub -l select=1:ncpus=X:mem=Yg -q uv
          -l walltime=Zd ...
      ```
      - to use a specific UV node, submit e.g. with

        ```
        $ qsub -q uv -l select=1:ncpus=X:cl_urga=true ...
        ```
  - for convenience, **submit from `zuphux.cerit-sc.cz` frontend**

Another mini-HowTos …

- **how to run a set of (managed) jobs?**
  - some computations consist of a set of (managed) sub-computations
  - optional cases:
    - the computing workflow **is known when submitting**
      - specify dependencies among jobs
        - qsub’s “**–W**” option (`man qsub`)
      - in case of many parallel subjobs, use „job arrays“ (qsub‘s **„-J“** option)
    - the computing workflow **depends on result(s) of subcomputations**
      - run a master job, which analyzes results of subjobs and submits new ones
        - the master job should be submitted to a node dedicated for low-performance (controlling/re-submitting) tasks
          - available through the „oven“ queue
          - `qsub -q oven –l select=1:ncpus=… control_script.sh`

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What to do if something goes wrong?

1. check the MetaVO/CERIT-SC documentation, application module documentation
    - whether you use the things correctly
2. check, whether there haven’t been any infrastructure updates performed
    - visit the webpage http://metavo.metacentrum.cz/cs/news/news.jsp
        - one may stay informed via an RSS feed
3. write an email to meta@cesnet.cz, resp. support@cerit-sc.cz
    - your email will create a ticket in our Request Tracking system
        - identified by a unique number → one can easily monitor the problem solving process
    - please, include **as good problem description as possible**
        - problematic job’s JOBID, startup script, problem symptoms, etc.

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Real-world examples

Examples:

- Maple
- Gaussian + Gaussian Linda
- Gromacs (CPU + GPU)
- Matlab (parallel & GPU)
- Ansys CFX
- OpenFoam
- Echo
- R – Rmpi

- demo sources:

`/storage/brno2/home/jeronimo/MetaSeminar/latest`

command: `cp -rH /storage/brno2/home/jeronimo/MetaSeminar/latest $HOME`

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Projekt CERIT Scientific Cloud (reg. no. CZ.1.05/3.2.00/08.0144) byl podporován operačním programem *Výzkum a vývoj pro inovace*, 3 prioritní osy, podoblasti 2.3 *Informační infrastruktura pro výzkum a vývoj.*

www.cesnet.cz www.metacentrum.cz www.cerit-sc.cz

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Appendices

- **Common mistakes in computations**
- **How to deal with parallel/distributed computations?**
- **Other computing possibilities**
  - MetaCloud
  - Hadoop (MapReduce)
  - Specialized frontends – Galaxy, Chipster, …

Common mistakes in computations

Common mistakes in computations

Feel free to use the infrastructure – if something crashes, it‘s our fault. ☺

Big data transfers

Do not copy higher amounts of data through frontends

- slower transfer
- frontends load

Big data transfers

Do not copy higher amounts of data through frontends

- slower transfer
- frontends load

Data could be copied directly through storage frontends

- SCP, WinSCP

  /storage/brno2 -> storage-brno2.metacentrum.cz

  /storage/brno3-cerit -> storage-brno3-cerit.metacentrum.cz

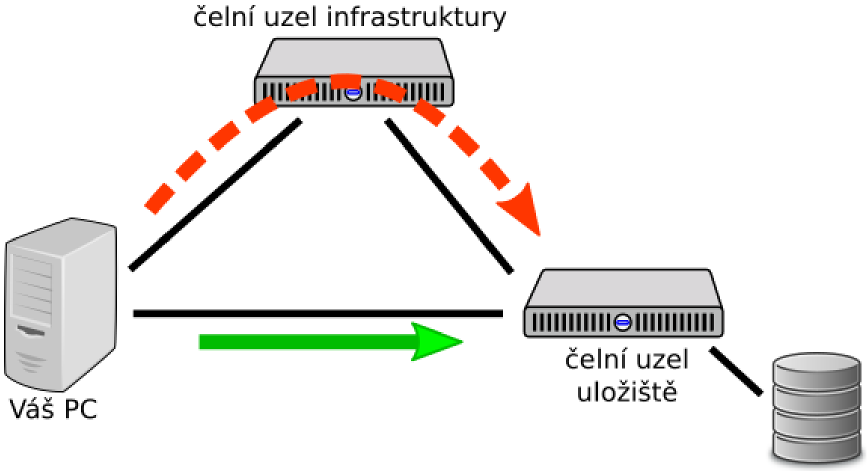
  …

  - https://wiki.metacentrum.cz/wiki/Working_with_data/Direct_access_to_data_storages

Big data transfers

Do not copy higher amounts of data through frontends

- slower transfer
- frontends load



Data could be copied directly through storage frontends

- SCP, WinSCP

  /storage/brno2 -> storage-brno2.metacentrum.cz

  /storage/brno3-cerit -> storage-brno3-cerit.metacentrum.cz

  …

  - https://wiki.metacentrum.cz/wiki/Working_with_data/Direct_access_to_data_storages

Computations and central storages

Do not run computations that compute over data located at central storages

- especially the I/O-intensive ones
  - increses central storage load and makes the computation slower

Compute over local copies in scratch directories

- *benefits:*
  - faster computations
  - computations do not rely on the availability of the central storage
- usage:
  - $ qsub –l select=1:ncpus=4:**scratch_local=1gb** …
    cp /storage/…/home/<username>/mydata $SCRATCHDIR/mydata
    cd $SCRATCHDIR
    <compute>
    cp $SCRATCHDIR/results /storage/…/home/<username>/results
  - …:scratch_shared=Xgb … *shared scratch (distributed computations)*
  - …:scratch_ssd=Xgb … *local scratch – SSD disks*

Data in scratches

Clean the scratches once computations finish

- scratch data could be seen similarly as data in RAM memory
  - once a computation finishes, the data should be cleaned
- scratches are automatically cleaned by us
  - usually after 2 weeks a computation finishes

Clean scratch after your computations

- „`clean_scratch`" utility
- usage (in script file):

```
trap 'clean_scratch' TERM EXIT
…
cp results /storage/…  || export CLEAN_SCRATCH=false
```

  - if the central storage is not available (the results could not be copied out), the data will remain in the particular scratch directory
    - user is informed about (non-)useful scratch cleanup
    - user is informed about scratches not correctly cleaned after previous computations

Central storages overused

Central (working) storages are not infinitely large ☹

/storage/<CITY>

Clean/move currently unnecessary data

- *possibilities:*
  - delete unnecessary data
  - move actually unnecessary data to archival storages
    see https://wiki.metacentrum.cz/wiki/Archival_data_handling

Huge jobs‘ outputs and data in `/tmp`

Computing nodes restrict the amount of data a user is able to store to local disks (outside the scratch space) = 1 GB quota

– influences the `/tmp` direktory (temporal files)

– influences the huge job‘s outputs (stdout, stderr)

Store bigger amounts of data to scratches

– forwarding the temporal directory

many applications follow the system variable TMPDIR

- usage: `export TMPDIR=$SCRATCHDIR`

– forwarding the stdout/stderr of an application

- `myapp … 1>$SCRATCHDIR/stdout 2>$SCRATCHDIR/stderr`

– checking the status of your local quota and a list of files occupying it (once being informed by email)

- utility `$ check-local-quota`
  has to be run on the particular node (with exhausted local quota)

Non-effective computations

Be aware of the resource usage effectivity of your jobs

- a request for multiple CPUs/cores will not make a single-processor (single-thread) computation parallel (= it won‘t be faster)
  - just a single CPU will be used
- many applications significantly vary between the number of CPUs used throughout a computation
  - higher number of CPUs might be used just for a short time of the computation

Observing the computation usage of (not only) CPUs:

- *during a computation:*
  - log-in to the computation node (SSH) and use standard Linux tools (`top`, `htop`, …)
- *after a computation:*
  - see the list of jobs at the MetaCentrum portal (https://metavo.metacentrum.cz/cs/myaccount/myjobs.html)
    the non-effective jobs have red background color

Infiniband

Distributed jobs might run ineffectively because of slow communication channel

- the inter-process communication using standard network services (Ethernet) is slow
- **Infiniband** – specialized low-latency interconnect for fast inter-process communication in distributed computations

Most of our clusters are equipeed with Infiniband

- considerably accelerates the performance of distributed (MPI) computations
  - the Infiniband availability is automatically detected
    computations started always in the same way: `mpirun myapp`
  - if the Infiniband is not available, Ethernet is used as a fallback
- *request:*
  - $ qsub –l select=… **–l place=group=infiniband** script.sh

Many short-term jobs processing

Group/gather short-term jobs

- e.g., the ones running less than few minutes
  - startup overhead may be a significant part of the whole processing time
    results in wasting resources

Run more computations within a single job

- *possibilities:*
  - serial computations run inside a single job
    process data1
    process data2
    …
  - parallel computations run inside a single job (necessary to ask for enough CPUs)
    - `pbsdsh`
    - `parallel`

Computations on frontends

Do not run computations on frontends

- neither for computations nor for complex results analyses
  - increased frontend load results in limitation of its services (and usually frontend crash)
- frontend's primary job is jobs' preparation and very simple and short-term computations

Use interactive jobs

- *request:*
  - `$ qsub -I -l select=…`
- *usage possibilities:*
  - textual mode
  - graphical mode – VNC access
    $ module add gui
    $ gui start
    - see https://wiki.metacentrum.cz/wiki/Remote_desktop

Interactive jobs

Minimize the time lags in interactive jobs

- especially the time between job startup and your work (starting computations)
  - -> in the time lag, the resources are wasted

Stay informed about your job‘s startup

- *request:*
  - `$ qsub` **`-m ab`** `-I -l select=…` will send you an email once the job begins
    - („`-m abe`” also in the case of job‘s finish)
- these options could be also used in batch jobs **but be aware of running too many jobs with this option set!**
  - overloads your mailbox
  - may blacklist our mailservers at external mail providers ☺

Cloud nodes

Be aware about your VMs running

– even the unused VMs/nodes (but running) consume infrastructure resources

  - -> results in wasting resources, which somebody could use

Terminate/Suspend unused VMs

– we‘ll regularly inform you about your VMs running

in case of no response (= time extension), the VMs are terminated

How to deal with parallel/distributed computations?

How to … run a parallel/distributed computation I.

Parallel jobs (OpenMP):

- if your application is able to use multiple threads via a shared memory, **ask for a single node with multiple processors**

```
$ qsub -l select=1:ncpus=...
```

- **make sure**, that before running your application, the **OMP_NUM_THREADS** environment variable **is appropriately set**
  - otherwise, your application will use all the cores available on the node
    - → and influence other jobs…
  - usually, setting it to **NCPUs** is OK

```
$ export OMP_NUM_THREADS=$PBS_NUM_PPN
```

How to … run a parallel/distributed computation II.

Distributed jobs (MPI):

- if your application consists of multiple processes communicating via a message passing interface, **ask for a set of nodes** (with arbitrary number of processors)

```
$ qsub –l select=...:ncpus=...
```

- **make sure**, that before running your application, the appropriate **openmpi/mpich2/mpich3/lam** module is loaded into the environment

```
$ module add openmpi
```

  - then, you can use the `mpirun/mpiexec` routines

```
$ mpirun myMPIapp
```

    - it’s **not necessary** to provide these routines neither with the number of nodes to use ("`-np`" option) nor with the nodes itself ("`--hostfile`" option)
      - the computing nodes are **automatically detected** by the openmpi/mpich/lam

How to … run a parallel/distributed computation III.

Distributed jobs (MPI): accelerating their speed I.

- to accelerate the speed of MPI computations, ask just for the nodes interconnected by a **low-latency Infiniband interconnection**
  - all the nodes of a cluster are interconnected by Infiniband
  - there are several clusters having an Infiniband interconnection
    - mandos, minos, hildor, skirit, tarkil, nympha, gram, luna, manwe (MetaCentrum)
    - zewura, zegox, zigur, zapat (CERIT-SC)

- *submission example:*

```
$ qsub -l select=4:ncpus=2 -l place=group=infiniband MPIscript.sh
```

- *starting an MPI computation using an Infiniband interconnection:*
  - in a common way: `$ mpirun myMPIapp`
    - the Infiniband will be automatically detected
  - is the Infiniband available for a job? **check using** `$ check-IB`

How to … run a parallel/distributed computation IV.

Questions and Answers:

- *Is it possible to simultaneously use both OpenMP and MPI?*
  - Yes, it is. But be sure, how many processors your job is using
    - appropriately set the “-np” option (MPI) and the OMP_NUM_THREADS variable (OpenMP)
      - **OpenMPI:** a single process on each machine (`mpirun -pernode …`) being threaded based on the number of processors (`export OMP_NUM_THREADS=$PBS_NUM_PPN`)

- Any other questions?

Other computing possibilities

Cloud computing – MetaCloud

Grid vs. Cloud computing

Grid computing suitable for:

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

Cloud computing suitable for:

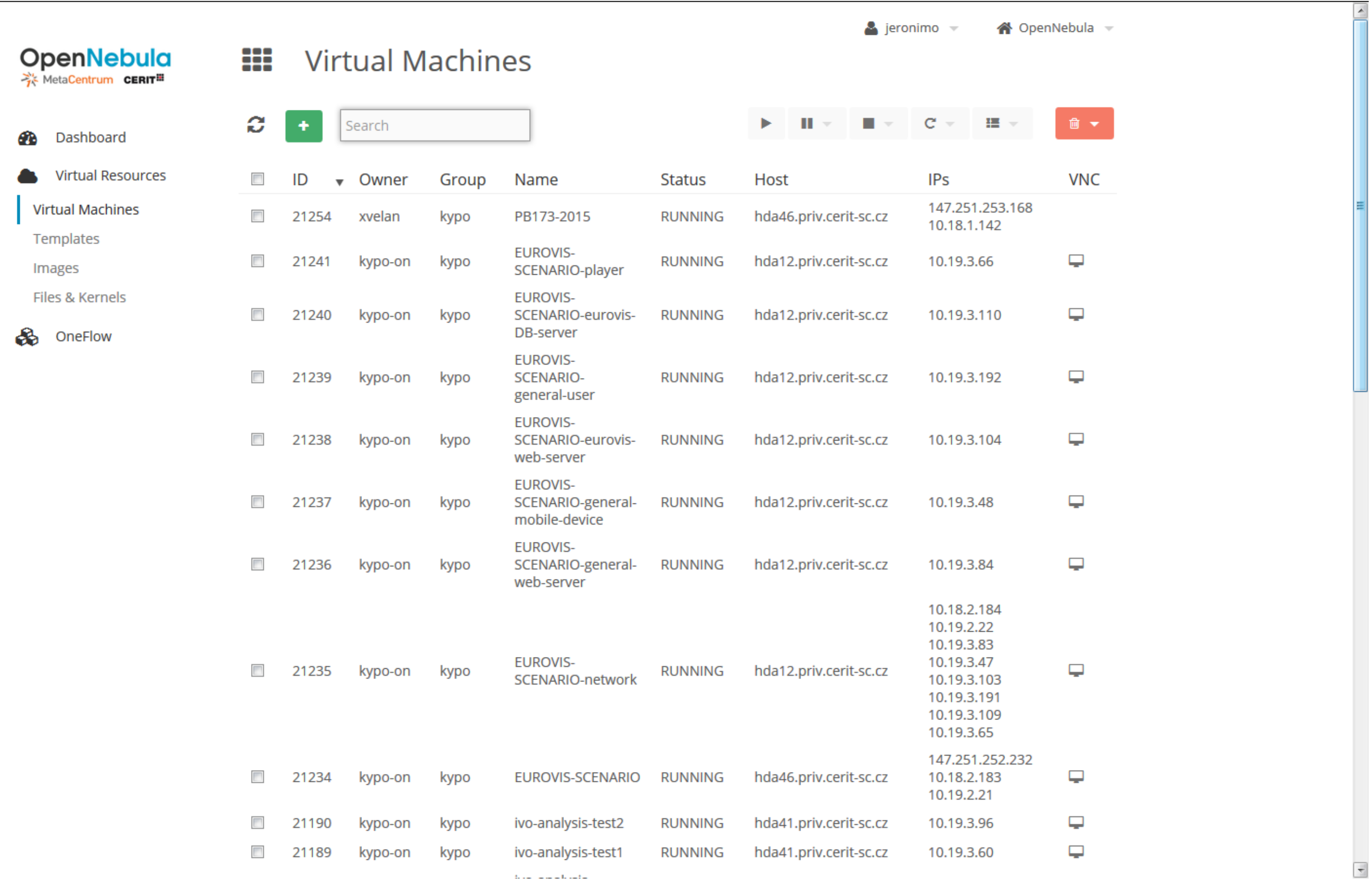
- applications requiring special environment (OS) and/or features
  - one can run various operating systems (incl. Windows OS) and/or application equipment
  - administrator/root access is provided

Cloud computing

How to compute?

- **additional registration to MetaCloud** group required
  - your SSH key is needed to access the VMs
  - https://perun.metacentrum.cz/fed/registrar/?vo=meta&group=metacloud
- OpenNebula GUI for deployed nodes management
  - https://cloud.metacentrum.cz/
- interact via:
  - cloud/VM console
  - internal OS services (SSH, VNC, Rdesktop, …)

Cloud computing



Virtual Machines

ID	Owner	Group	Name	Status	Host	IPs	VNC
21254	xvelan	kypo	PB173-2015	RUNNING	hda46.priv.cerit-sc.cz	147.251.253.168 10.18.1.142	
21241	kypo-on	kypo	EUROVIS-SCENARIO-player	RUNNING	hda12.priv.cerit-sc.cz	10.19.3.66	🖵
21240	kypo-on	kypo	EUROVIS-SCENARIO-eurovis-DB-server	RUNNING	hda12.priv.cerit-sc.cz	10.19.3.110	🖵
21239	kypo-on	kypo	EUROVIS-SCENARIO-general-user	RUNNING	hda12.priv.cerit-sc.cz	10.19.3.192	🖵
21238	kypo-on	kypo	EUROVIS-SCENARIO-eurovis-web-server	RUNNING	hda12.priv.cerit-sc.cz	10.19.3.104	🖵
21237	kypo-on	kypo	EUROVIS-SCENARIO-general-mobile-device	RUNNING	hda12.priv.cerit-sc.cz	10.19.3.48	🖵
21236	kypo-on	kypo	EUROVIS-SCENARIO-general-web-server	RUNNING	hda12.priv.cerit-sc.cz	10.19.3.84	🖵
21235	kypo-on	kypo	EUROVIS-SCENARIO-network	RUNNING	hda12.priv.cerit-sc.cz	10.18.2.184 10.19.2.22 10.19.3.83 10.19.3.47 10.19.3.103 10.19.3.191 10.19.3.109 10.19.3.65	🖵
21234	kypo-on	kypo	EUROVIS-SCENARIO	RUNNING	hda46.priv.cerit-sc.cz	147.251.252.232 10.18.2.183 10.19.2.21	🖵
21190	kypo-on	kypo	ivo-analysis-test2	RUNNING	hda41.priv.cerit-sc.cz	10.19.3.96	🖵
21189	kypo-on	kypo	ivo-analysis-test1	RUNNING	hda41.priv.cerit-sc.cz	10.19.3.60	🖵

Basic terminology

- **template –** a description of the node („computer“) you are asking from the cloud
  - speficies requested CPUs, memory, disk storage, network interfaces, etc.
  - predefined ones & own ones
- **image –** a storage space („HDD“)
  - equipped with an OS or not
  - *persistent* & *non-persistent* (default; data are lost when destroying the VM)
- **network security group –** a set of firewall rules
  - restricts the access to the VM
- **instance –** a running node/computer created based on some template receipt
- **VM console –** a VNC connection to the VM („computer screen“)

Common usage

Common operations with MetaCloud:

- see video tutorial
- for advanced use, see MetaCloud documentation
  - e.g., creating your own template (duplicate existing one) or disk image

Warning: Please, be aware of the VMs you are running.

And if not used, suspend or terminate them…

- every 3 months, we‘ll recommend you your running VMs
  - if not explicitly renewed/extended in the defined time period, **the VMs will be terminated**

Other computing possibilities

Hadoop computing

Hadoop / MapReduce computing

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

https://wiki.metacentrum.cz/wiki/Kategorie:Hadoop

Other computing possibilities

Specialized frontends – Galaxy, Chipster, …

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** (docs https://wiki.metacentrum.cz/wiki/Galaxy)
  - *ELIXIR RepeatExplorer Galaxy* – https://repeatexplorer-elixir.cerit-sc.cz
  - *MetaCentrum Galaxy* – https://galaxy.metacentrum.cz
- **Chipster** (docs https://wiki.metacentrum.cz/wiki/Chipster)
  - http://chipster.metacentrum.cz:8081
- basic details are provided in the leaflet