Centre CERIT-SC

scientific computations,

collaborative research &

support services

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Overview

- Centre CERIT-SC – brief introduction
- National Grid Infrastructure (NGI) for research computations
- CERIT-SC & NGI
- Research support by CERIT-SC
- Selected research collaborations
- Additional services available to academic research community

Centre CERIT-SC

A computing and research centre operating at Masaryk University in Brno, Czech Republic

- 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

A long-term experience with:

- operation of large HW/SW & communication infrastructure → High Performance Computing
  - including internal research in e-infrastructures (identity management, security, scheduling algorithms, large data processing – parallel and distributed algorithms, etc.) and computing methods/algorithms
- cooperation in large EU projects and their support
- web portals and projects' back-office
- data back-ups and archiving
- research in collaboration with partners of different science-fields
- additional services for researchers

National Grid Infrastructure (NGI)
for research computations

National Grid Infrastructure (NGI)

CERIT-SC resources integrated into the NGI

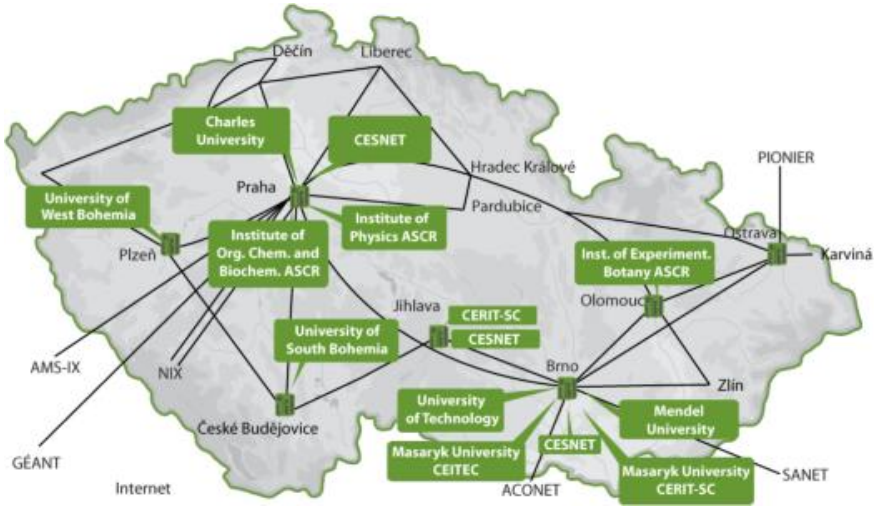
- operated by MetaCentrum NGI (CESNET) since 1996
- MetaCentrum was established by CERIT-SC (previously called SCB)

http://www.metacentrum.cz

National Grid Infrastructure

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

- → **environment for work/collaboration in the area of research computations and data handling**



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

Computing clusters

a group of “common” interconnected computers

(previously)

Computing clusters

a group of “common” interconnected computers

(now)

MetaCentrum Virtual Organization (Meta VO)

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**

- users “pay” via publications with acknowledgements

  → results in user priorities in cases of high load

MetaVO – basic properties

After registration, **the resources are available without any administrative burden**

- → ~ immediately (based on the actual load)
- **no resource applications** have to be provided

User accounts periodically extended every year

- **a proof of continuing user's academic affiliation**
- **publications with acknowledgements simultaneously reported**
  - could help us when asking for funds from public authorities

Best-effort service

Meta VO – computing resources available

Computing resources: ca 10000 cores (x86_64)

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

CERIT-SC: important resource provider **(4512 cores)**

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

Meta VO – storage resources available

ca 1 PB (1063 TB) for operational data

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

ca 19 PB (19000 TB) for archival data

- “unlimited” user quota

CERIT-SC: important resource provider **(5 PB)**

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

Meta VO – software available

~ 250 different applications (commercial & free/open s.)

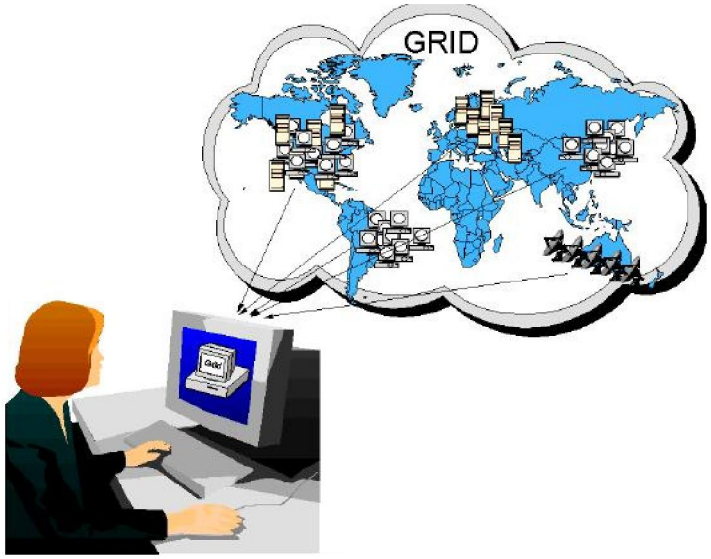
- see http://meta.cesnet.cz/wiki/Kategorie:Aplikace

- **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, …

CERIT-SC: important commercial SW provider

Meta VO – 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** (the whole OS becomes under their control)
    - focused on research computations again (not for webhosting)
    - Windows & Linux images provided, user-uploaded images also supported

CERIT-SC & NGI

Centre CERIT-SC & NGI

CERIT-SC is an important NGI partner

- **HW & SW resources provider**
  - SMP nodes (1600 cores)
  - HD nodes (2624 cores)
  - **SGI UV node (288 cores, 6 TB RAM)**
  - storage capacity (~ 5 PB)

- **significant personal overlaps with NGI exist**

remember, **CERIT-SC (SCB) established MetaCentrum NGI**

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

http://www.cerit-sc.cz

CERIT-SC & NGI – production services

High-performance computing

- parallel/distributed computations

Data back-ups and archiving

- multiple storage systems in geographically distant locations
- advanced hierarchical storage systems

Web portals & projects' back-office

- for *general public & dissemination*
  web pages, RSS feeds, blogs, social media, …
- for *projects' internal needs*
  data & document servers, request tracking, messaging, meeting planners, collaborative environments, …

Authentication and Authorization Infrastructure, Identity Management, Data Security, …

CERIT-SC & NGI – participation in large EU projects

Building European grid research infrastructure:

DataGrid, EGEE, EGEE II, EGEE III, EGI DS, EGI InSPIRE, EMI, EUAsiaGrid, CHAIN, CHAIN-REDS, Thalamos, …

Basic research in grid infrastructures:

GridLab, CoreGrid, Moonshot, …

Other projects' support:

ELIXIR (European life-science infrastructure for biological information)

BBMRI (Biobanking and Biomolecular Resources Research Infrastructure)

ELI (Extreme Light Infrastructure)

Pierre Auger Observatory

Thalassemia

…

CERIT-SC & NGI – services for selected projects being supported I.

EGI.eu (European Grid Infrastructure):

- ***web pages:*** *http://www.egi.eu/*
- ***authentication & authorization infrastructure:*** *http://www.egi.eu/sso/*
- ***blogs:*** *http://www.egi.eu/blog/*
- ***event webs:*** *http://tf2012.egi.eu http://tf2011.egi.eu …*
- ***wiki pages:*** *http://wiki.egi.eu/*
- ***mailinglists:*** *http://mailman.egi.eu/*
- ***document server:*** *http://documents.egi.eu/*
- ***request tracking:*** *http://rt.egi.eu/*
- ***discussion forum:*** *http://forum.egi.eu/*
- ***Indico (meeting planner):*** *http://indico.egi.eu/*
- ***Jabber (no web):*** *jabber.egi.eu*

EGI DS:

- ***web pages:*** *http://web.eu-egi.eu/*

CERIT-SC & NGI – services for selected projects being supported II.

MetaCentrum NGI + VO:

- ***web pages:*** *http://www.metacentrum.cz , http://metavo.metacentrum.cz/*
- ***authentication & authorization infrastr.:*** *http://perun.metacentrum.cz/*
- ***mailinglists:*** *https://www.metacentrum.cz/mailman/admin/*

MediGrid:

- ***web pages:*** *http://www.medigrid.cz/cs/*
- ***application for searching drug interactions:*** *http://www.medigrid.cz/interakce/*

Pathological atlases:

- ***web pages, data storage & archive:*** *http://atlases.muni.cz/*

EEF - European E-infrastructure Forum

- ***web pages:*** *http://www.einfrastructure-forum.eu/*

Research support by CERIT-SC

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

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 diploma/doctoral 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
- **in an ideal case, once the thesis become offended, the collaboration continues via an externally funded project**

Strong ICT expert knowledge available:

- **long-term collaboration with Faculty of Informatics MU**
- **long-term collaboration with CESNET**

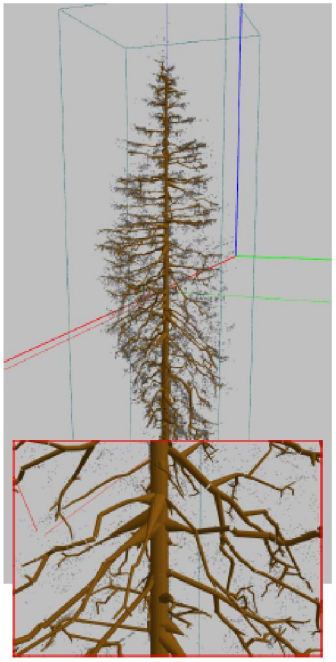
  → consultations with experts in the particular areas

Selected research collaborations

Selected (ongoing) collaborations I.

3D tree reconstructions from terrestrial LiDAR scans

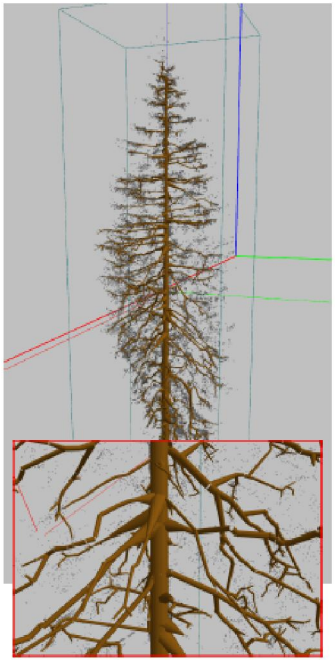
- partner: Global Change Research Centre - Academy of Sciences of the Czech Republic (*CzechGlobe)*
- **the goal: to propose an algorithm able to perform fully-automated reconstruction of tree skeletons (main focus on Norway spruce trees)**
  - from a 3D point cloud
    - scanned by a LiDAR scanner
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

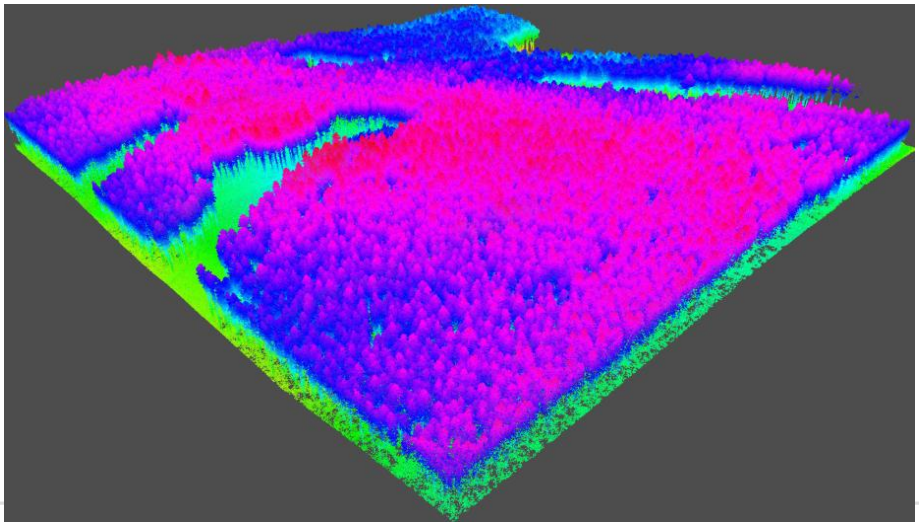
- **the diploma thesis proposed a novel innovative approach to the reconstructions of 3D tree models**
- **the reconstructed models used in subsequent research**
  - **determining a statistical information** about the amount of wood biomass and about basic tree structure
  - **parametric supplementation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

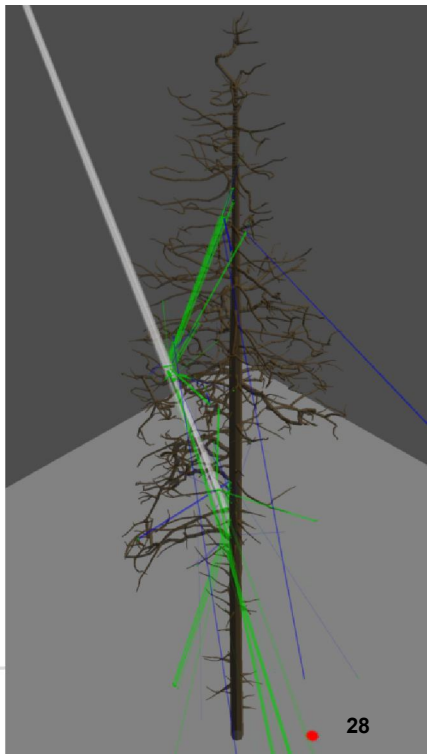


Selected (ongoing) collaborations II.

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, …

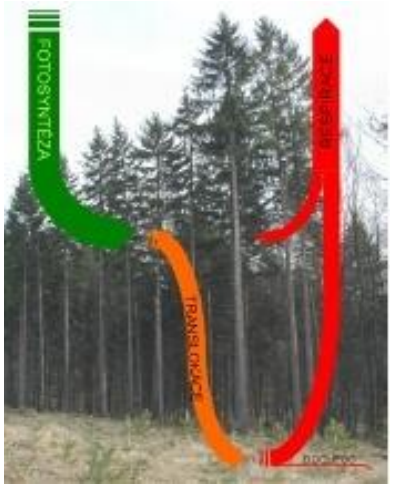




Selected (ongoing) collaborations III.

An application of neural networks for filling in the gaps in eddy-covariance measurements

- partner: Global Change Research Centre - Academy of Sciences of the Czech Republic (*CzechGlobe)*
- **the goal: to propose a novel fully-automated method for gap-filling of eddy-covariance data**
  - based on historical measurements and self-learning
    - *accompanying characteristics* – temperature, pressure, humidity, …
- **main issues:**
  - historical data have to be taken into account
  - the forest evolves (grows)



Selected (ongoing) collaborations IV.

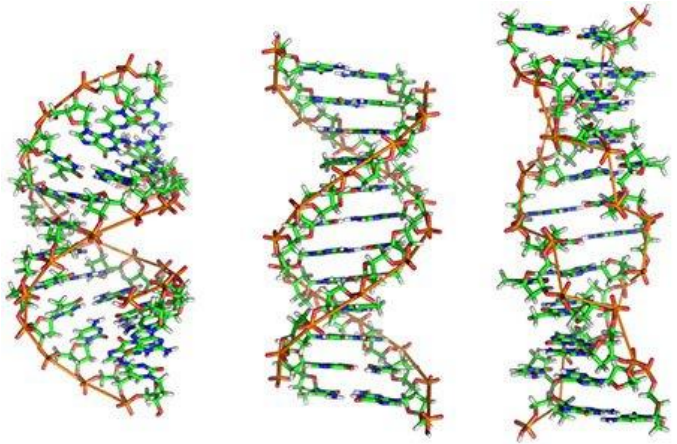
Identification of areas affected by geometric distortions in aerial landscape scans

- partner: Global Change Research Centre - Academy of Sciences of the Czech Republic (*CzechGlobe)*
- **the goal: to propose a novel, fully-automated method for an identification of regions within the scans, where the airplane suddenly deviated**
  - and thus introduce distortions in the scanned data
  - → *image processing*
  - current approaches are suitable for determining distortions in the scans of regular objects (like buildings in the city scans) rather than their determination in the diverse vegetable
- **main issue: diverse tree structure**

Selected (ongoing) collaborations V.

De-novo sequencing *Trifolium pratense*

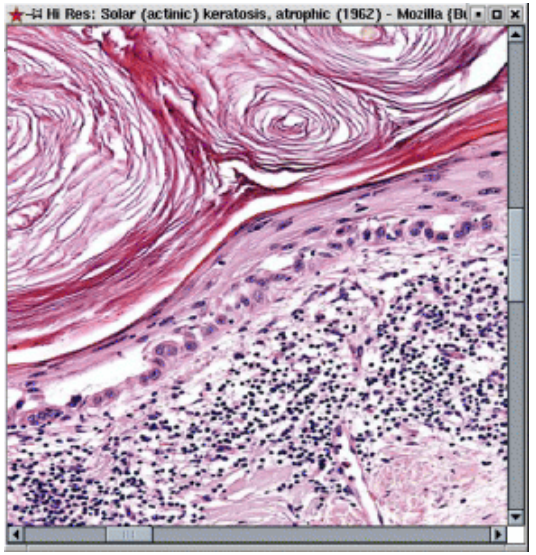
- **partner: *Institute of Experimental Biology SCI MU***
- **the goal: evaluation and optimization of available tools for DNA reads corrections and assembly**
  - ***Trifolium pratense* analysis results in large computations**
    - **~ 500 GB of memory**
    - **computations take weeks/months**
- **main issue: computation demands**



Selected (ongoing) collaborations VI.

Virtual microscope, pathologic atlasses

- partner: *Faculty of Medicine MU*
- **the goal: an implementation of virtual microscope for dermatology atlas (web application)**
  - shows the tissue scans
    - resolution up to 170000x140000 pixels
    - composed from tiles (up to 30000 of tiles)
  - allows to „focus“ like real microscope
- **main issues:**
  - optimization of scans processing (GPU)

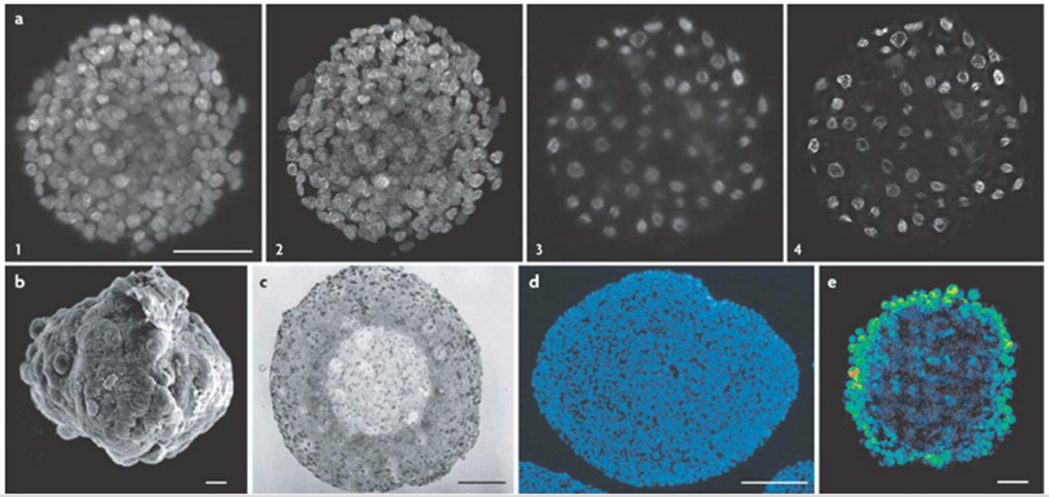


- **the result is available at http://atlases.muni.cz**

Selected (ongoing) collaborations VII.

Segmentation of live cell cultures in microscope images

- partner: *University of South Bohemia*
- **the goal: to determine interesting/important objects in the images of live cell cultures, filtering the noise out of attention**
  - implemented in C and CUDA
  - achieved acceleration: 10x – 1000x



Selected (ongoing) collaborations VIII.

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 IX.

- **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

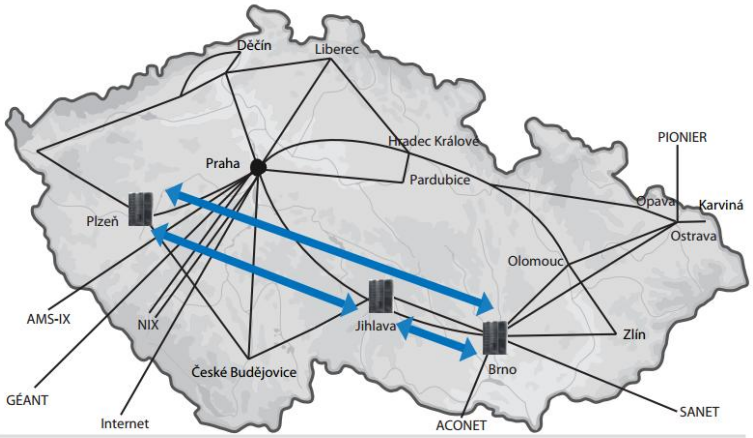
Storage and archival services

The need to archive long-term scientific data increases

- **e.g., archival of data used in experiments**
  in order to allow further usage or results revision

Centralized storage infrastructure:

- **3 hierarchical storage systems available**
  located in Pilsen, Jihlava (CERIT-SC) and Brno
  the total capacity available: ca 19 PB
- **suitable for backups, archival, and data sharing**
- **additional services:**
  FileSender
  OwnCloud



http://du.cesnet.cz

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)
- **special transmissions**
  HD, UHD, 2K, 4K, 8K with compressed/uncompressed video transmission (UltraGrid tool)
- **IP telephony**

Support for offline content access

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

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

CSIRT-MU

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

http://csirt.cesnet.cz

CESNET CERTS

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

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

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

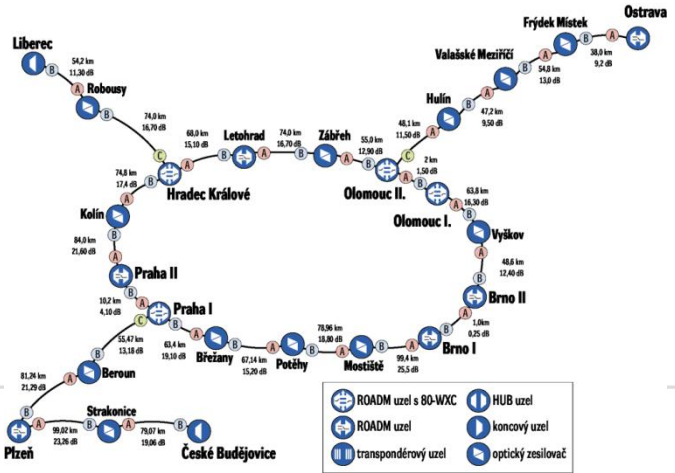
Communication infrastructure and its monitoring

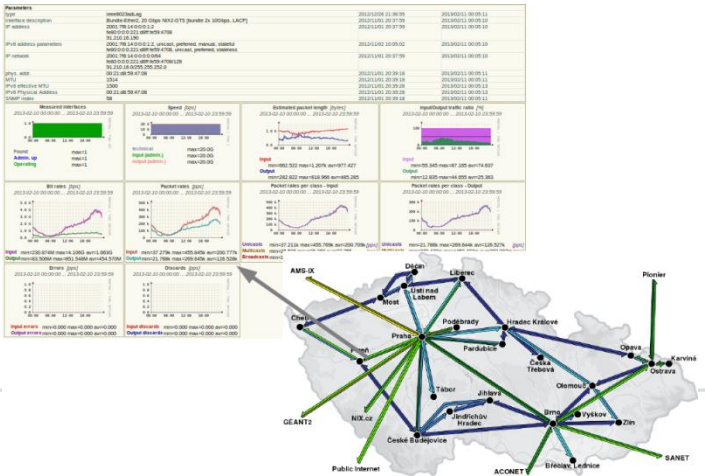
The basis of all the services: high-speed computer network

- 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 I.

There're three computing e-infrastructures being established in the Czech Republic

IT4Innovations (VŠB-Technical University of Ostrava)

- **currently ca 3300 cores (around 30000 cores planned)**
- **intended for large production academic/commercial computations** (more resources available thanks to integration into PRACE) **on more or less homogeneous infrastructure**
  - formal applications (research project proposals) required
  - financial participation required (highly welcomed)

National Grid Infrastructure + CERIT-SC

- **currently ca 10000 cores, available for public research only**
- **free of charge, heterogeneous resources (exotic HW available)**
- **intended for common small-to-medium scientific computations or IT4I projects preparation**

Conclusions II.

CERIT-SC aims to provide additional services beyond the scope of common HW centers

an environment for collaborative research

- **not only HW/SW provider, but**
- **→ a real collaboration of IT experts and users**

we focus on novel and beneficial approaches to e-infrastructure usage

- **big focus on internal research in e-infrastructure services**

we collaborate with several EU projects, including the ESFRI ones

- **participation in the preparation of EU H2020 projects**

however, we're also interested in collaboration with smaller groups/individuals

- **currently, the interest exceeds our (personal) capacities (we have to choose among the collaboration proposals)**

Conclusions III.

CERIT-SC didn't grow on a green meadow …

… and doesn't operate on an isolated island

- long-term history & experience (SCB established in 1994)
- strong interconnection with European infrastructures
  - 10 Gbps connection to NREN academic network (core 100 Gbps)
  - NREN directly connected to European 10 Gbps GÉANT network

Centre location in Brno, CZ is highly beneficial:

- Brno city provides a strong academic & IT background
  - 5 universities (→ intellectual background, sustainability)
- many worldwide IT companies reside in Brno:
  - we cooperate with Red Hat, IBM, Microsoft, NetSuite, …
  - further companies in Brno: Honeywell, AVG, Avast, Solarwinds, GoodData, 2K, …
- *"Brno ~ Mekka IT in the CR"*

EUROPEAN UNION

EUROPEAN REGIONAL DEVELOPMENT FUND
INVESTING IN YOUR FUTURE

OP Research and Development for Innovation

The CERIT Scientific Cloud project (reg. no. CZ.1.05/3.2.00/08.0144) is supported by the *Operational Program Research and Development for Innovations*, priority axis 3, subarea 2.3 *Information Infrastructure for Research and Development.*

http://metavo.metacentrum.cz

http://www.cerit-sc.cz