

Mathematica & gridMathematica *in National Grid Infrastructure*

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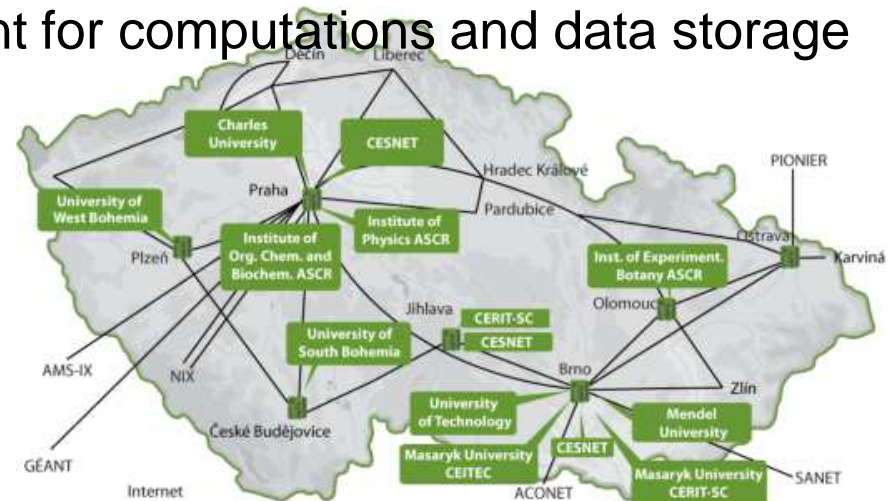
MetaCentrum, CESNET z.s.p.o.

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National Grid Infrastructure

- **MetaCentrum (CESNET) coordinates the national grid infrastructure (NGI) since 1996**
 - **integrates the HW centers (clusters, powerful servers and storages) from several resource providers throughout the CR**
 - → provides uniform environment for computations and data storage
 - **integrated into European Grid Infrastructure (EGI)**
- **users divided into so-called virtual organizations**
 - **e.g., MetaVO**

<http://www.metacentrum.cz>



Meta Virtual Organization (MetaVO)

- ***intended for students and employees of Czech universities, AS CR, research institutes, etc.***
 - ***commercial entities just for public research***
- ***offers:*** <http://metavo.metacentrum.cz>
 - ***computing resources***
 - ***storage resources***
 - ***application programs***
- ***available free of charge (after registration)***
 - ***„payments“ by publications with acknowledgement***
 - → users' priorities when the infrastructure is saturated



MetaVO – available computing HW

- **computing resources: ca 8800 cores (x86_64)**
 - **HD nodes: 2x4-8 cores per node**
 - **SMP nodes: 32-80 cores per node**
 - RAM up to 1 TB per node
 - **SGI UV2000: 288 cores, 6 TB RAM**
 - **specialized hardware:**
 - nodes with GPU cards, ...
- **after registration, the resources are available without additional requests**
 - → ~ **immediately (based on actual load)**
 - **i.e., no resource applications**

MetaVO – available storage HW

- **ca 1 PB (1063 TB) for working data**
 - **storages: 3x in Brno, 1x in Pilsen, 1x in ČB, 1x in Prague, 1x in Jihlava**
 - **user quotas 1-3 TB per storage**
- **ca 3,8 PB (ca 16 PB planned) for permanent/archival data**
 - **user quota 5 TB**

MetaVO – available SW

- **~ 200 distinct applications**
 - see <http://meta.cesnet.cz/wiki/Kategorie:Aplikace>
 - **development tools**
 - GNU, Intel and PGI compilers, debugging and optimization tools (TotalView, Allinea DDT), ...
 - **mathematical software**
 - Matlab, Maple, **Mathematica, gridMathematica**, ...
 - **software for application chemistry**
 - Gaussian 09, Gaussian-Linda, Gamess, Gromacs, ...
 - **material simulations**
 - Wien2k, ANSYS Fluent CFD, Ansys Mechanical...
 - **structural biology, bioinformatics**
 - CLC Genomics Workbench, Geneious, Turbomole, Molpro, ...
 - **etc.**
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MetaVO – Mathematica & gridMathematica

- **Wolfram Mathematica**
 - **10 licenses**
 - **graphical as well as batch use**
 - **available for all registered NGI users**
 - **Wolfram gridMathematica**
 - **extends the parallel processing capabilities of Mathematica**
 - **15 licenses**
 - => up to 240 additional computing kernels available for parallel processing
 - **available for all registered NGI users as well as holders of “Mathematica Site License Agreement”**
-
- requires an explicit authorization by Wolfram Research

MetaVO – How to use Mathematica

- *video*

MetaVO – How to become a user?

- ***submit an application***
 - ***<http://metavo.metacentrum.cz> , section „Application” or “Getting an account“***
 - ***EduID.cz => the verification of your academic identity will be performed using the credentials of your home organization***

- ***become familiar with MetaVO documentation and basics of OS Linux***
 - ***<http://metavo.metacentrum.cz> , section „Documentation“***
 - ***<http://www.poznejlinux.cz/linuxbook/xhtmll-chunks/ch07.html>***
 - ***<http://www.math.muni.cz/~xkuranov/vyuka/tex/p4.html>***

- ***run your computations!***
 - ***a possibility to attend „hands-on“ seminars***

- ***Thank you for your attention***