MetaCentrum

On the Way from Distributed Computing to e-Infrastructure for Research

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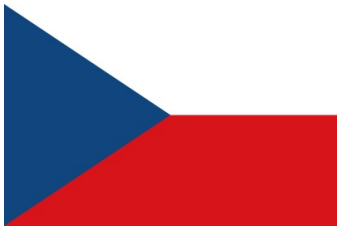
Outline

- MetaCentrum transformation to NGI
- what are EGI, NGI, VO
- MetaCentrum NGI, MetaCentrum VO
- expected new resources in NGI
- NGI and structural biology

MetaCentrum transforms to NGI

- MetaCentrum was originally established as alliance of supercomputing centers of MU, UK and ZČU – hence meta-centrum
- over time other centers joined, became the Czech academic distributed computing infrastructure coordinated by CESNET
- 300 machines, 1560 CPU, 600TB storage
- now is transforming to **National Grid Initiative** (NGI) under **European Grid Initiative** (EGI)
- the era of the European grid begins :-)

EGI, NGI



- three EGEE (Enabling Grids for E-sciencE) projects *created* the world's larges grid infrastructure (267 sites in 55 countries, 150000 CPUs, 69PB,14k users)
- EGI (European Grid Initiative) will maintain *sustainable* infrastructure
- each country will have NGI (National Grid Initiative), the Czech NGI will be CESNET's MetaCentrum

Virtual Organizations

- the grid is organized in VO (Virtual Organizations)
- a VO has users (typically groups from various real organizations) and access to resources (computing and storage)
- resources belong to resource owners

MetaCentrum roles

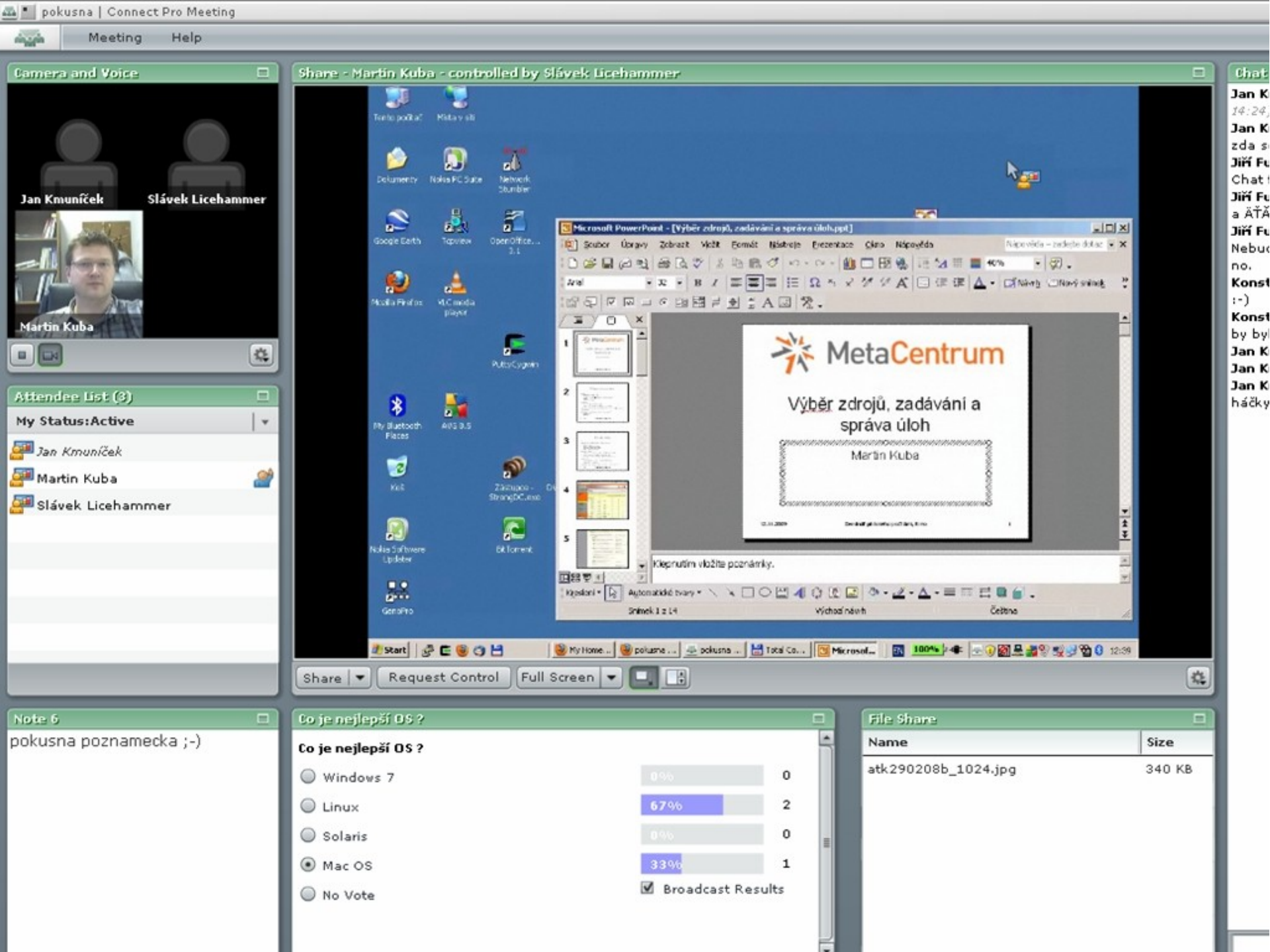
- three better separated roles
  - MetaCentrum NGI – coordinates national VOs and resource owners
  - MetaCentrum VO – free catch-all organization for everybody in the Czech academia
  - MetaCentrum as CESNET resource owner
- other VOs
  - NCBR, LL, AUGER, BELLE, VOCE, ...
- other resource owners
  - NCBR, LL, CERIT, MU, ZČU, UK, VUT, JU, ...

Planned new resources in NGI

- CERIT Center of Education, Research and Innovation in ICT in Brno
  - Supercomputer Center with about 10000 CPU and 15-20 petabytes of storage
- CESNET storage infrastructure
  - large storage services in Internet points of presence (8-12 PB)
- integrated resources from large infrastructures

NGI and structural biology

- NGI provides
  - data storage for backup and archiving
  - common infrastructure for cooperation with foreign partners
  - collaboration environment for geographically dispersed teams and individuals (next slide)
  - computational resources (second next slide)


pokusna | Connect Pro Meeting
Meeting
Help
Camera and Voice
Jan Kmuníček
Slávek Licehammer
Martin Kuba
Share - Martin Kuba - controlled by Slávek Licehammer
MetaCentrum
Výběr zdrojů, zadávání a správa úloh
Martin Kuba
Share
Request Control
Full Screen
Attendee List (3)
My Status:Active
Jan Kmuníček
Martin Kuba
Slávek Licehammer
Note 6
pokusna poznamecka ;-)
Co je nejlepší OS ?
Co je nejlepší OS ?
Windows 7 0%
Linux 67% 2
Solaris 0%
Mac OS 33% 1
No Vote
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Name
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atk290208b_1024.jpg
340 KB
Chat

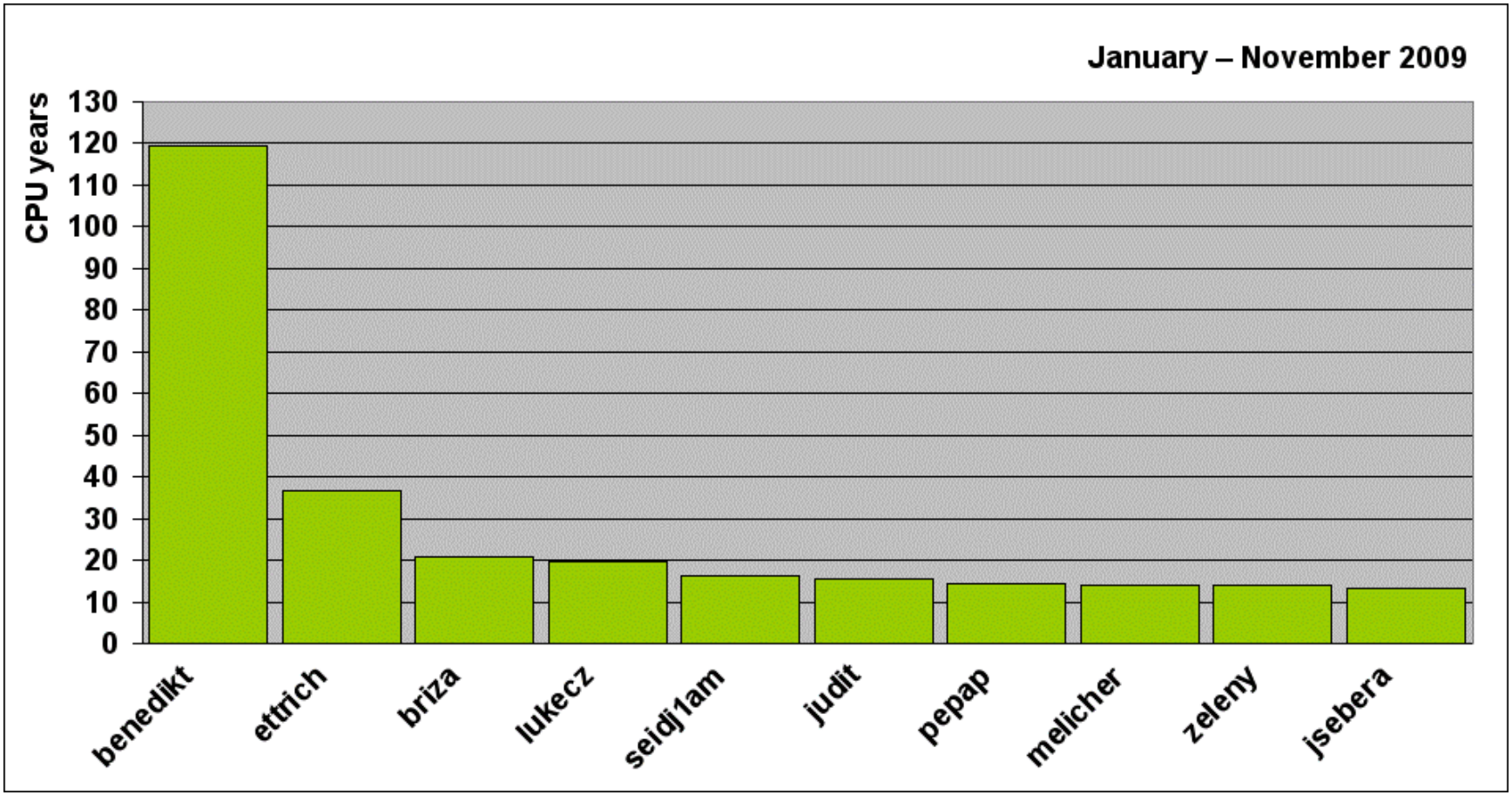
Computational resources for

- long term (bio)molecular simulations
- protein engineering of enzymatic structures
- QM/MM studies of catalytic reactions
- QM calculations of interaction energies and NMR parameters
- free energy calculations of intermolecular interactions and conformational changes of biomolecules
- detailed exploration of binding sites and processes in biomolecules
- prediction of 3D structure of macromolecules (proteins and nucleic acids)
- biostatistics analysis and multidimensional parametric studies
- analysis of genome and its evolution
- bioinformatics methods of virtual screening of biologically active compounds
- quantitative structure activity / function relationships studies
- ...

MetaCentrum VO

- free membership in MetaCentrum VO for everybody in academia
- demand for resources is prioritized by scientific results
- new resources are welcome
- we offer maintenance of computing resources for IT non-experts
- international cooperation through user groups within EGI

Top users' time



Summary

- MetaCentrum evolves from SC alliance to NGI in the upcoming EGI
- the “free access” part will become MetaCentrum VO
- the “restricted” parts will be other VOs
- collaboration tools and storage will be in the NGI, available to all VOs

Thank you