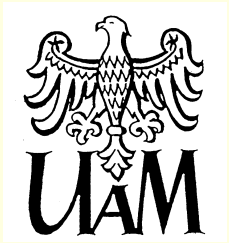

GRID'2008

International Conference on

Distributed computing and Grid technologies in science and education

30 June – 04 July, 2008, Dubna, Russia

VO of EIMM within EGEE GRID: sharing of computing resources

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Outline

1. Motivation
2. NoE MAGMANet $\Rightarrow$ EIMM + ISG
3. Integrated Laboratory Modeling and Computing
4. VO ILMC – sharing of computing resources
5. Conclusions

Motivation

Single-molecule magnets – the basis of the next generation of data storage media or quantum computers.

The aim of this talk is to present sharing of computing resources in the recently founded European Institute of Molecular Magnetism (EIMM).

The computational problems need effective resources shared among the partners involved.

According to this paradigm, a grid-based large-scale computing environment offers such an efficient mutual use of computing resources.

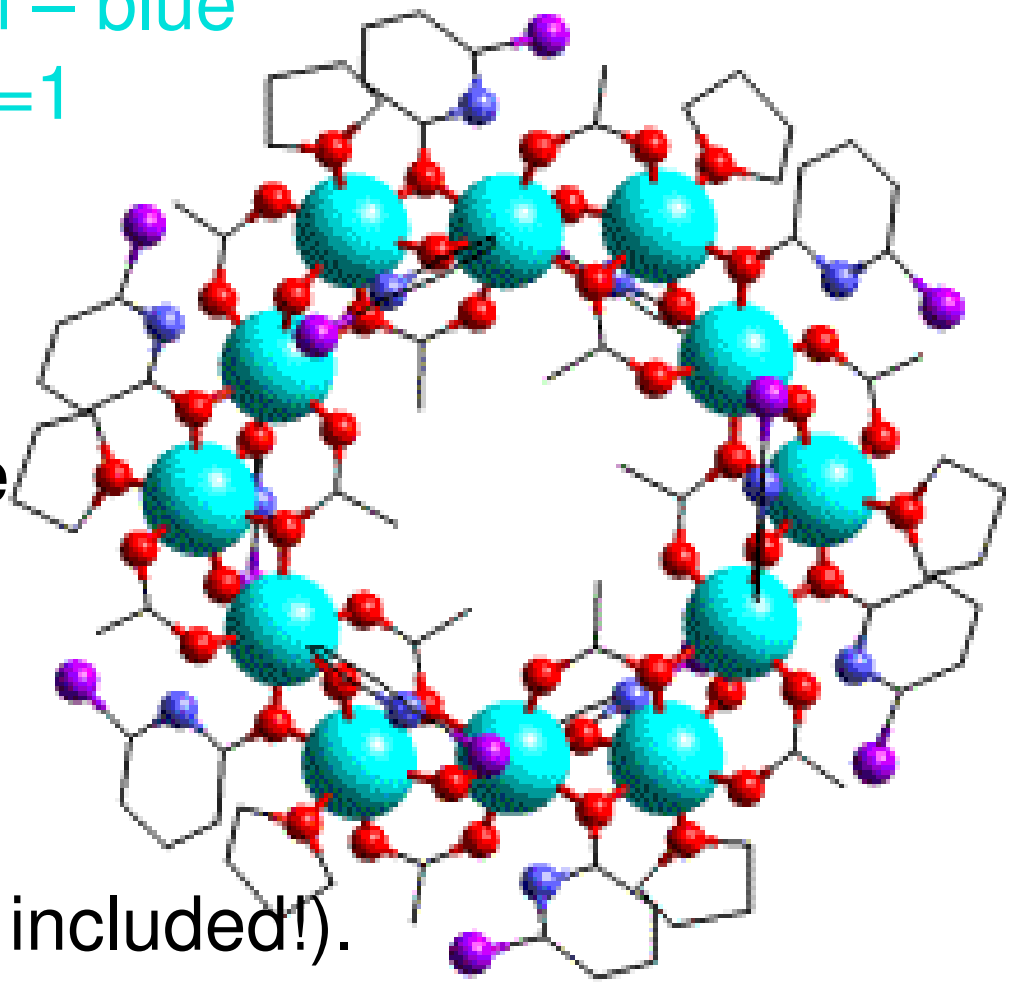
Motivation

Computing of energy spectrum would take more than half of a year on a single CPU.

The higher *S* value or the larger molecule the larger computing problem with diagonalization of a Hamiltonian (S-mixing, anisotropy included!).

The dodecanuclear Ni_{12} wheel
$[Ni_{12}(O_2CMe)_{12}(chp)_{12}(H_2O)_6(THF)_6]$

Ni – blue
S=1



Project MAGMANet ⇒ E

The European Commission

↓ 10.7M€ of funding from

Network of centres of Excellence, NoE MAGMANet

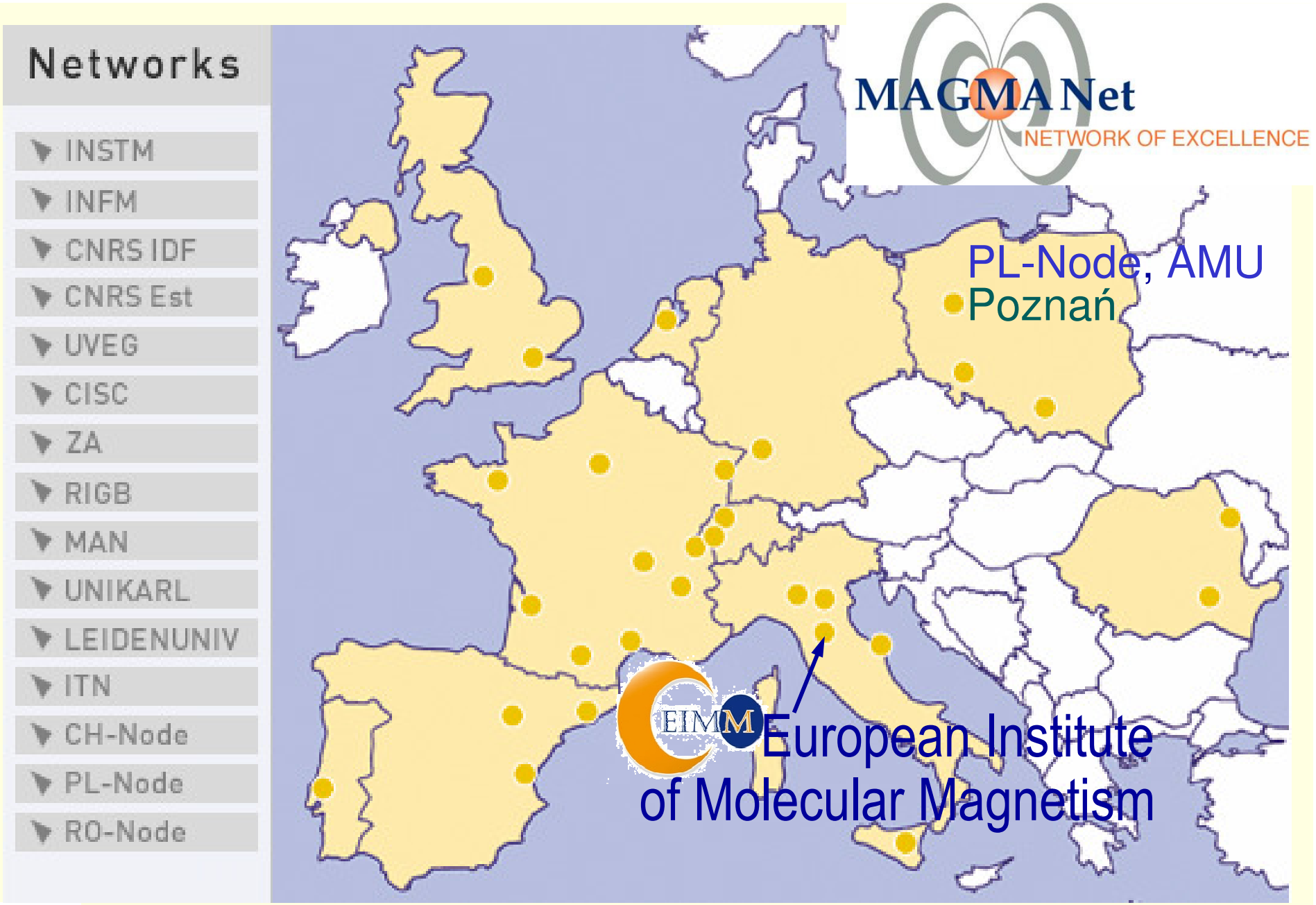
↓ started May 1st, 2005 for 4 years

Project MAGMANet, *Molecular Approach to Nanomagnets and Multifunctional Materials*, coordinated by the Italian INSTM (Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali), Florence, prof. Dante Gatteschi

↓ started April 12th, 2008

European Institute of Molecular Magnetism

located in INSTM in Florence



Researchers from many cities are focused in 15 nodes

Project MAGMANet ⇒ EIMM

Important goals of molecular magnetism in the last two decades to provide examples of novel phenomena like:

– magnetic hysteresis at the molecular level,
– quantum effects in the dynamics of the macroscopic magnetization,
– photoswitchable magnetic materials,
– polyfunctional materials combining conduction and bulk ferromagnetism.

Among others single-molecule magnets should become the basis of the next generation of data storage media or transistors in new generation processors.

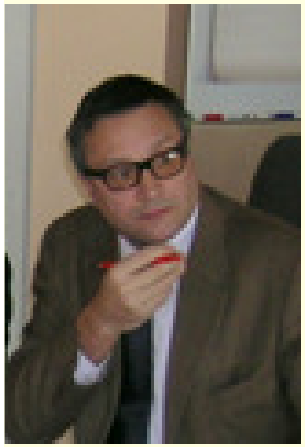
EIMM

The EIMM will continue to integrate European research in Molecular Magnetism by bringing together the scientific excellence of the partners and providing access to world class instrumentation.
We hope we are above „the critical mass” to achieve our goals.

The institute will provide the first European Doctorate in molecular magnetism allowing students access to a range of research facilities within the partner institutions.

EIMM ⇒ Industrial Support Group

Industrial players with an interest in molecular magnetism and a need to maintain their competitive edge may join the EIMM´s Industrial Support Group (ISG) with Pietro Perlo (Centro Ricerche Fiat) the Chairman and Fernando Palacio (Zaragoza University) the executive Secretary.



Pietro

The ISG organizes a range of informative and technology transfer activities providing opportunities for collaborative projects.
It is free of charge and open to all:
http://magmanet.unizar.es/magmanet-isg/

Fernando

EIMM ⇒ ISG

A synergic effort coming from synthetic chemists, experimental physicists and theoreticians to move towards applications and integration with the industrial world.

Everybody is cordially invited.

Apart from world class instrumentation platforms the network defines specialized (virtual) integrated laboratories to achieve integration, research and spreading of excellence objectives.

Integrated Laboratory Modeling and Computing

Two possible meanings of integrated laboratory:

– a virtual existence, with no material existence,

– a set of experimental/theoretical specialized labs sharing expertise on a complementary basis and offering their experience to solve problems for other participants.

10 integrated laboratories is set up within MAGMANet, among others Modeling and Computing, headed by prof. G. Kamieniarz.

This laboratory is of the 1st and of the 2nd type, as sharing the computing basis is natural within grids.

Sharing of computing resources

EGEE project aims at providing researchers in academia and industry with access to major computing resources independent of their geographic location.

To organize sharing of computing resources, we have contacted our partner at the Poznań Supercomputing and Networking Centre involved in the EGEE Grid project, also funded by the EC.

Support for VOs:

ATLAS, ALICE, LHCB, CMS, VOCE, balticgrid, gaussian.

Sharing of computing resources

We have integrated the resources of five partner nodes in EIMM: INSTM, CNR-INFM from Italy, AMU from Poland, UVEG from Spain, UAIC from Romania (together about 5 TFlops) to start the VO ILMC within the EGEE grid.

Our largest computer cluster at the UAIC node, Romania, 130 quad-core CPUs.

We also obtain cross-linking of important EU projects.

Sharing of computing resources

The broad knowledge base provided by this Integrated Laboratory affords transfer of organization skills, access to variety of specialized computational tools and software as well as comprehensive expertise which can address problems
in the following important areas:

- high performance scientific computing
  in materials science,
- grid computing for public and commercial units,
- e-Learning management,
- optimization tasks based on genetic algorithms,
- artificial intelligence in bio-medicine.

Sharing of computing resources

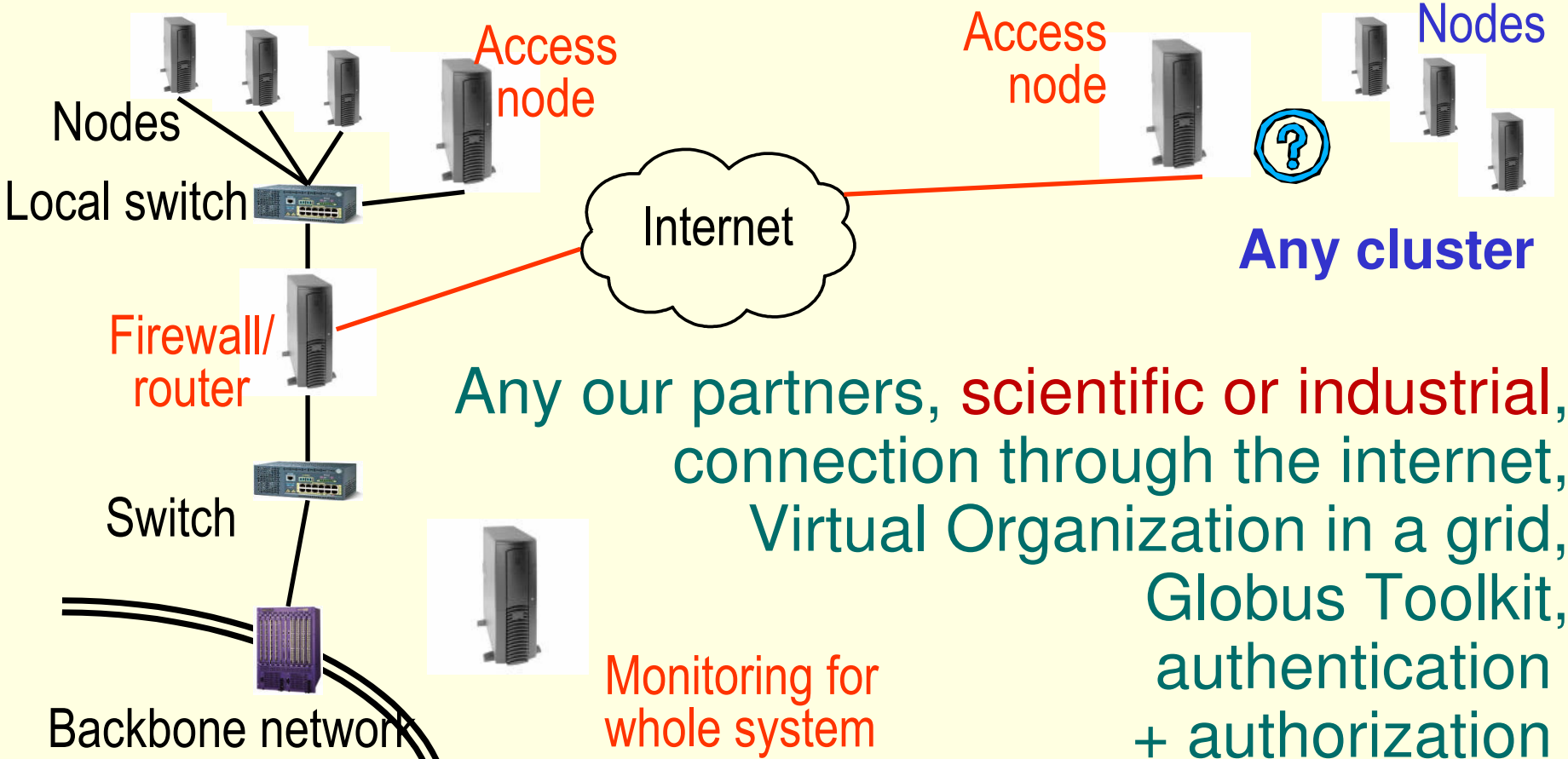
To make the decisions easier we argue:
sharing means not loosing control of own resources,
as one can offer only some percent
of computing power for a grid, instead of it,
one can run much bigger jobs.

For example: one of our Italian partners concluded that it would be worth to join our VO if they obtain access to the cluster with nodes having 64 GB RAM. What is the answer?

Our VO obtained the access to some resources within Baltic Grid where there are nodes of 64 GB RAM!

Sharing of computing resources

Offering only some percent of computing power for a grid, one obtains the access to the specialized computational resources and software.



Any our partners, scientific or industrial, connection through the internet, Virtual Organization in a grid, Globus Toolkit, authentication + authorization

Monitoring for whole system

PL-Grid – Polish Grid Initiative

The Polish Grid Consortium (2007) – a response to the needs of Polish scientists, compatible with ongoing grid activities in other European countries (within EGI) and all over the world, made up of 5 largest Polish supercomputing & networking centers (to be financed by national funds for 2008-2010).

The main aim of the PL-Grid Project is to create and to develop a stable Polish Grid infrastructure, fully compatible and interoperable with European and worldwide Grids. The Project should provide scientific communities in Poland with Grid services, enabling realization of the e-Science model in various scientific fields.

Thanks to prof. H.F. Hoffmann

Conclusions

Organization and software problems for sharing of computing resources are solved already, there are only the problems to transfer the knowledge how to get and to run parallel applications, the political will and of a mentality of (wo)men.

Most of calculations within molecular magnetism scale very well with efficiency about 0.9. Many of the simulations can be run with hundreds or even thousands of parallel processes.

Not only parallel processing but grid computing opens a new scale of modeling in molecular magnets.

Conclusions

Scalability of simulations is better and better at larger and larger molecules.

This makes possible to consider much larger systems. The larger the systems considered the better the analysis the more reliable the results.

The candidates for the next generation of data storage media or transistors in new generation processors are rather large molecules for which we utilize self-assembling and self-organizing when putting them on the surface. Thus, modeling them needs a huge number of CPUs available at grid computing.

Acknowledgements

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Some cluster and grid organization details
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and Networking Center

http://www.man.poznan.pl/

Thanks for your attention and patience!!!

E-mail: gmusial@amu.edu.pl

EIMM: http://www.eimm.org/

ISG: http://magmanet.unizar.es/magmanet-isg/