

DEISA



DEISA European HPC Infrastructure

www.deisa.eu

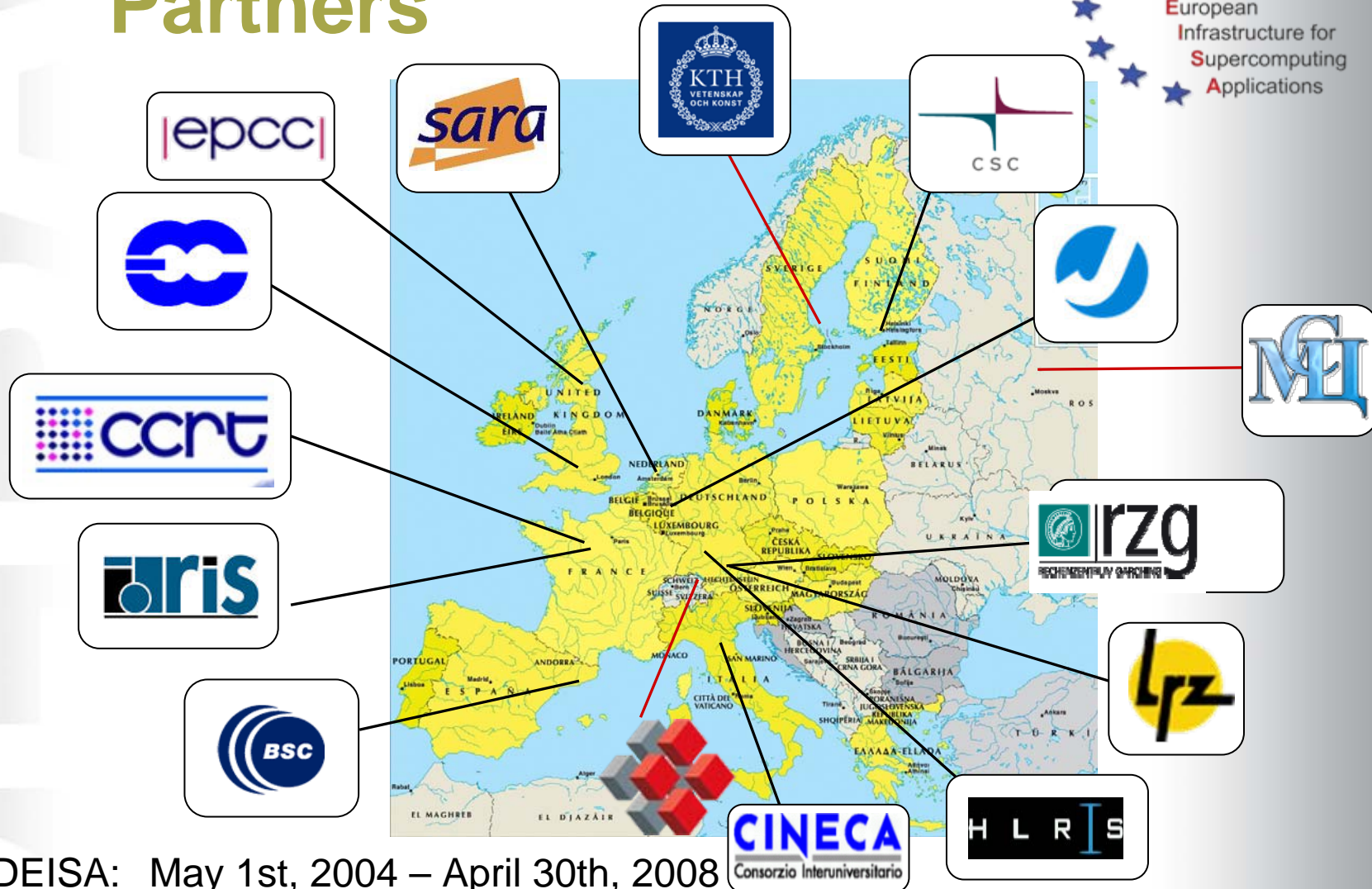
Hermann Lederer
DEISA and RZG, lederer@rzg.mpg.de
Bio ICT 2008
Brussels, Oct 24, 2008



RI-222919



Partners

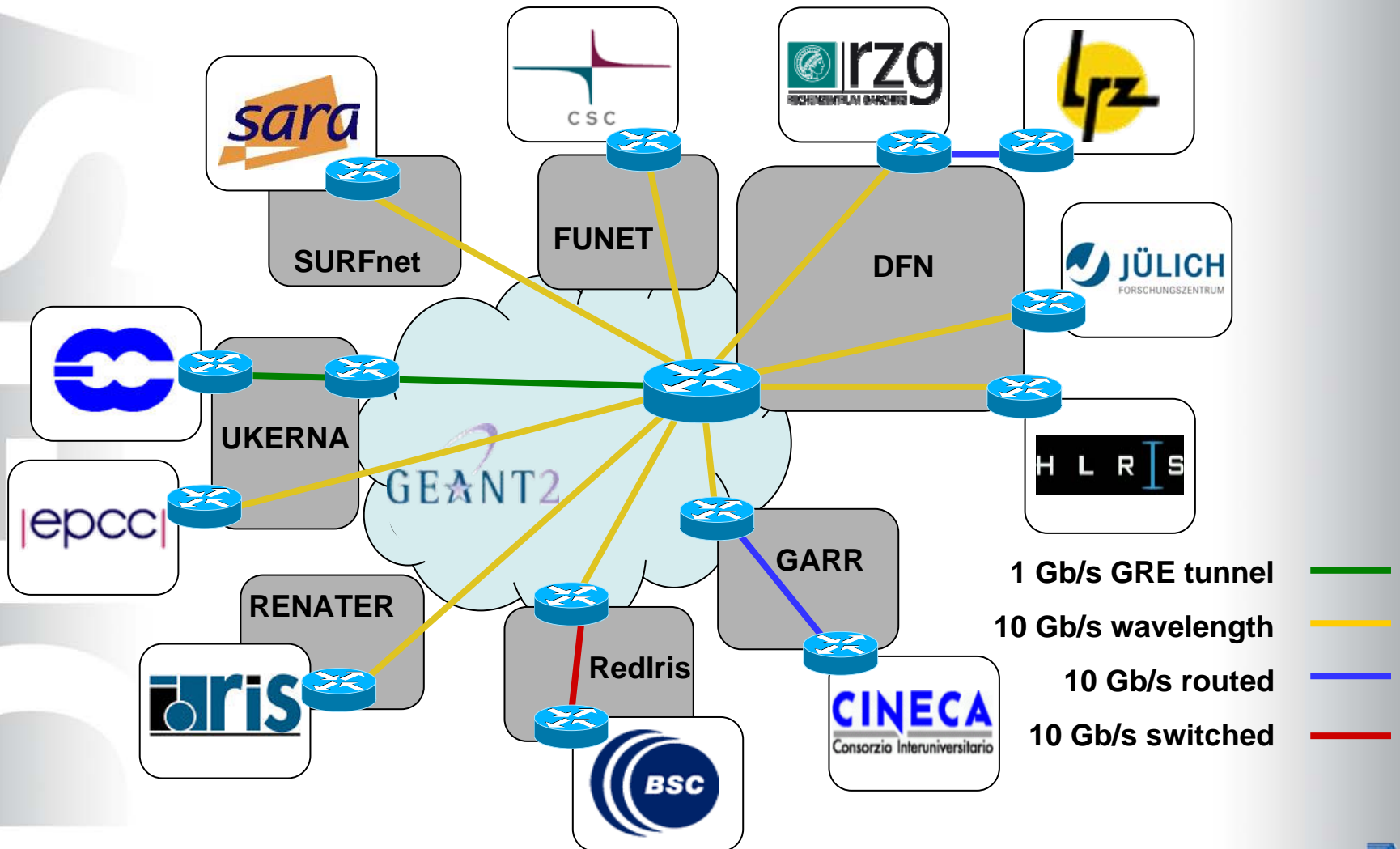


DEISA: May 1st, 2004 – April 30th, 2008

DEISA2: May 1st, 2008 – April 30th, 2011

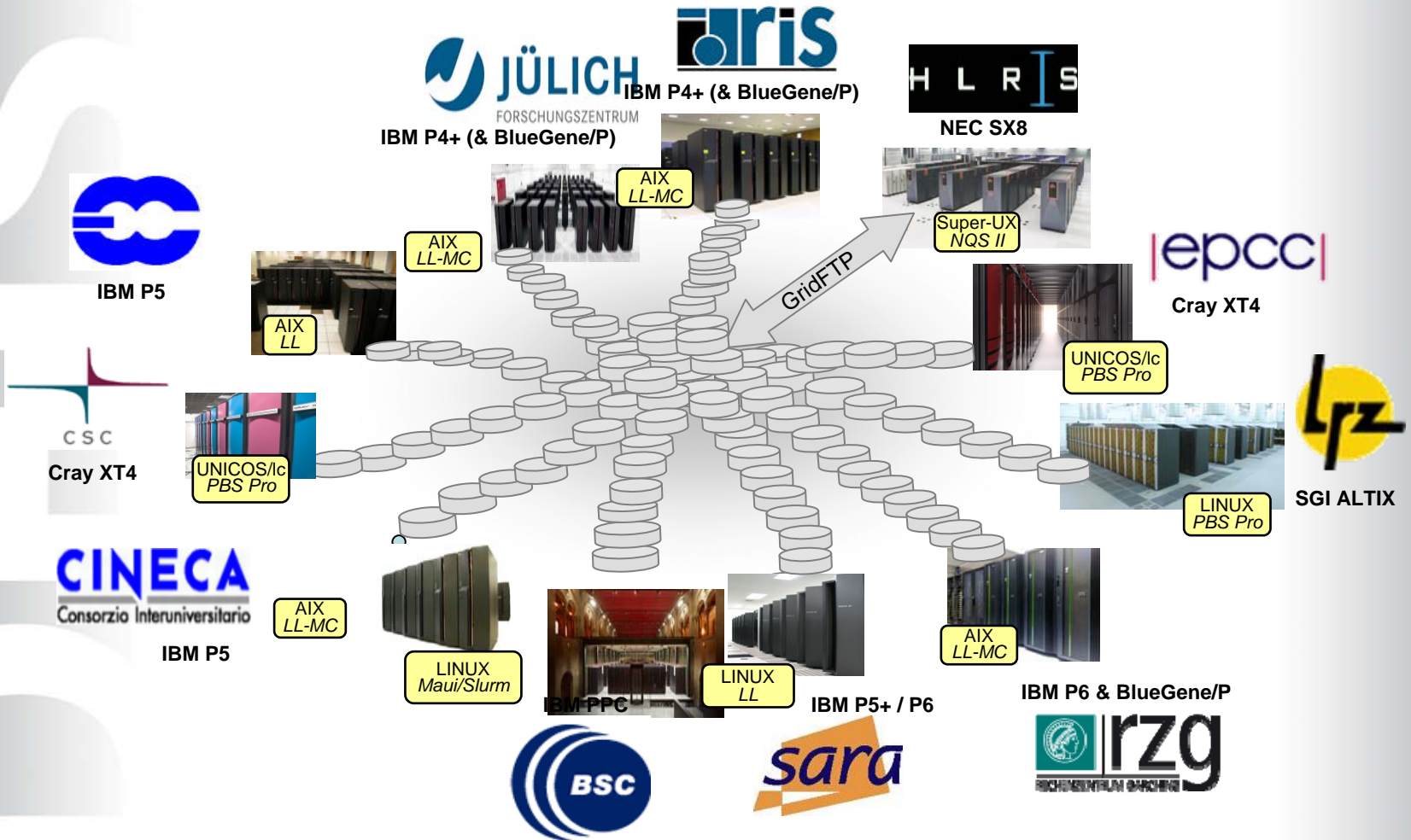
DEISA network 2008

Dedicated high speed network 10 Gb/s



DEISA Global File System 2008

(based on MC-GPFS)



Life Science support in DEISA

- **DEISA Life Science Portal**
- **Single project support:
Regular projects from Life Sciences
in the DEISA Extreme Computing Initiative**
- **Community support:
Support for EU FP6 Life Science
Project VIROLAB in 2008
New options as of 2009**

DEISA Life Science Portal

Promotion of parallel software in the Life Sciences community

The screenshot shows a web browser window with the URL https://bioportal.deisa.eu/engineframe/deisa/deisa.xml?_service=BLAST. The page features the DEISA logo and navigation links: Home, Your Jobs, Spoilers, Logout. The user's account is identified as 'Account: idrttest02 - Project: prtest01'. A sidebar on the left lists 'Deisa Life Sciences Applications' including BLAST, NAMQGIDRW, NAMQDBSC, and RA+ML. The main content area is titled 'BLAST' and contains a form for submitting a BLAST job. The form fields include: 'Blast job name' (text input with 'BLAST' and '(optional)'); 'Blast program' (dropdown menu with 'blastn'); 'Blast database' (dropdown menu with 'nucleotides'); 'Blast sequence (FASTA, NCBI Accession numbers or GIs)' (text input with 'nr' and a 'Browse...' button); 'Expect Value' (text input with '0.001'); 'Filter query sequence (DUST with blastn, SEG with others)' (radio buttons for 'F' and 'T', with 'F' selected); 'Query strands to search against database' (dropdown menu with '1'); 'Produce HTML output' (radio buttons for 'yes' and 'no', with 'no' selected); 'Restrict search of database to list of GIs' (text input with a 'Browse...' button); 'Use lower case filtering of FASTA sequence' (radio buttons for 'yes' and 'no', with 'no' selected); 'Number of concatenated queries' (text input with '0'); and 'Type of job' (dropdown menu with 'medium'). A 'Submit job' button is located at the bottom of the form.

Running big simulations on the DEISA infrastructure that couldn't be done locally

Providing ease of access to resources

Application support for life science portal (BLAST, RAXML, NAMD)

DEISA Extreme Computing Initiative (DECI)



- DECI launched in early 2005 to enhance DEISA's impact on science and technology
- Identification, enabling, deploying and operation of “flagship” applications in selected areas of science and technology
- Complex, demanding, innovative simulations requiring the exceptional capabilities of DEISA
- Multi-national proposals especially encourage
- Proposals reviewed by national evaluation committees
- Projects chosen on the basis of innovation potential, scientific excellence, relevance criteria, and national priorities
- Most powerful HPC architectures in Europe for the most challenging projects
- Most appropriate supercomputer architecture selected for each project
- Mitigation of the rapid performance decay of a single national supercomputer within its short lifetime cycle of typically about 5 years, as implied by Moore's law

DEISA Extreme Computing Initiative



Calls for Proposals for challenging supercomputing projects from all areas of Science

DECI call 2005

51 proposals, 12 European countries involved, co-investigator from US)
30 mio cpu-h requested
29 proposals accepted, 12 mio cpu-h awarded (normalized to IBM P4+)

DECI call 2006

41 proposals, 12 European countries involved
co-investigators from N + S America, Asia (US, CA, AR, ISRAEL)
28 mio cpu-h requested
23 proposals accepted, 12 mio cpu-h awarded (normalized to IBM P4+)

DECI call 2007

63 proposals, 14 European countries involved, co-investigators from
N + S America, Asia, Australia (US, CA, BR, AR, ISRAEL, AUS)
70 mio cpu-h requested
45 proposals accepted, ~30 mio cpu-h awarded (normalized to IBM P4+)

DECI call 2008 (ending June 30, 2008)

66 proposals, 15 European countries involved, co-investigators from
N + S America, Asia, Australia
134 mio cpu-h requested (normalized to IBM P4+)
Evaluation in progress

DEISA Extreme Computing Initiative

Involvements in projects from DECI calls 2005, 2006, 2007:

157 research institutes and universities

from

15 European countries

Austria
Italy
Russia

Finland
Netherlands
Spain

France
Poland
Sweden

Germany
Portugal
Switzerland

Hungary
Romania
UK

with collaborators from

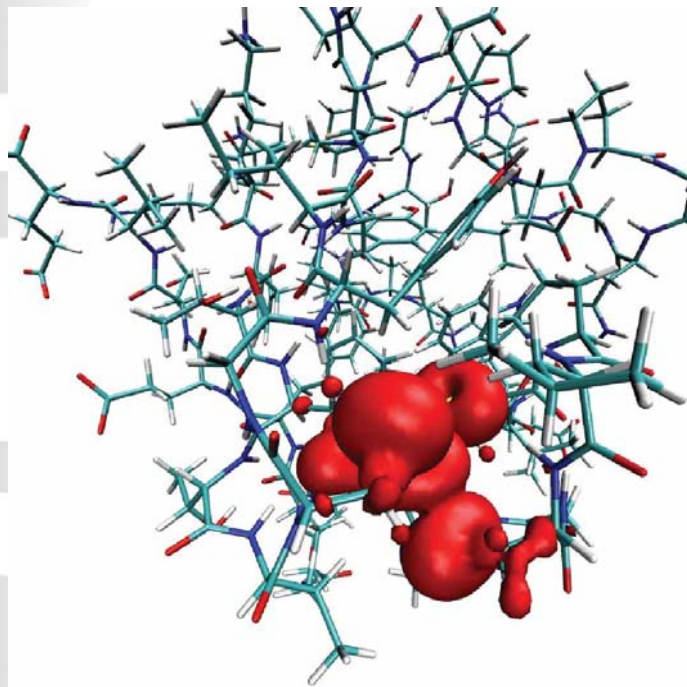
four other continents

North America, South America, Asia, Australia

Biological electron transfer simulated

A RESEARCHER GROUP HAS USED FIRST-PRINCIPLES TECHNIQUES TO INVESTIGATE ELECTRON TRANSFER IN THE CONTEXT OF IRON- AND COPPER-BASED PROTEINS.

FOR THE FIRST TIME AB INITIO INVESTIGATION OF ENTIRE ELECTRON-TRANSFER PROTEINS IN AQUEOUS SOLUTION WAS PERFORMED.



Isosurface enclosing 95 per cent of the total spin density (difference of the up and down electron densities) in the oxidized form of the rubredoxin from *Clostridium pasteurianum*.

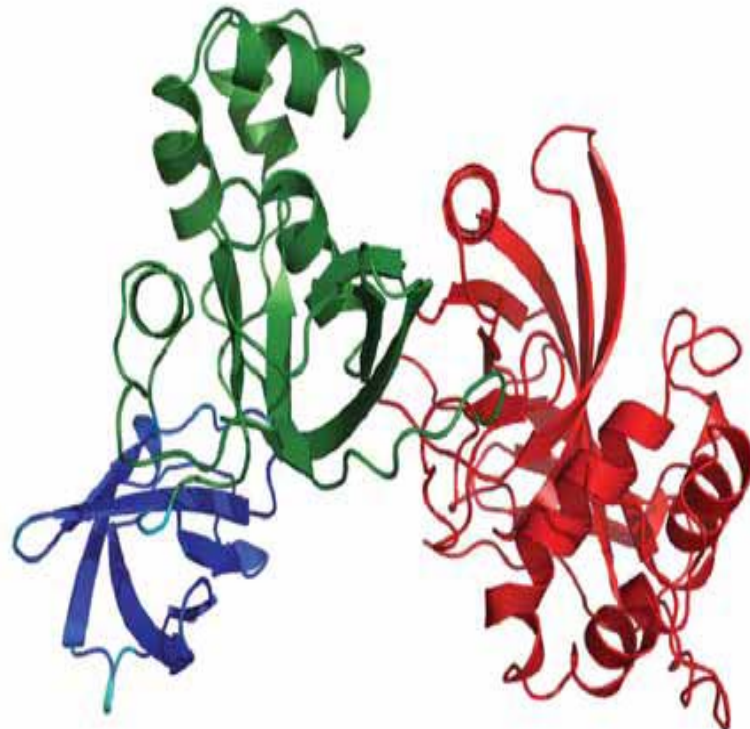
All of the atoms were explicitly taken into account at ab initio (DFT) level.

Molecular simulation to accelerate vaccine development

A LARGE THREE-YEAR PROJECT INVOLVING PHARMACEUTICAL AND BIOINFORMATICS COMPANIES AND UNIVERSITIES HAS EXPLOITED THE DEISA RESOURCES TO RENDER VACCINE DEVELOPMENT SIMPLER, FASTER AND THEREFORE LESS EXPENSIVE FOR PHARMACEUTICAL COMPANIES.

To study protein dynamics, classical molecular dynamics simulation in combination with empirical biomolecular force fields have been used.

High throughput cloning and expression of large sets of genomic ORFs has become a preferred industrial strategy for genome-wide searches of new vaccine candidates. For invasive infections in particular, the aim is to find proteins eliciting antibodies capable of binding to the bacterial cell surface and, through interaction with the complement system, effectively kill the bacteria.

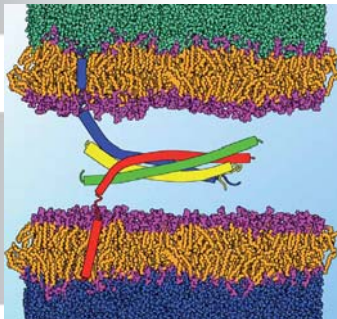


Membranes under tension

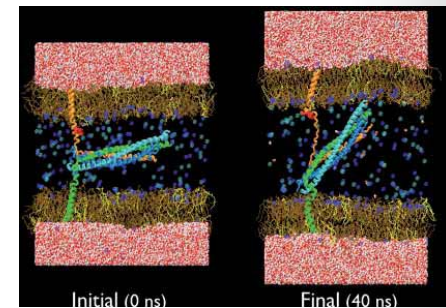
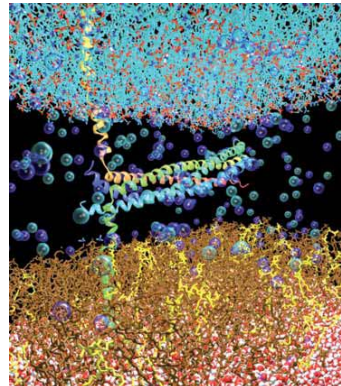
MODELLING OF A PROTEIN COMPLEX THAT ACTS AS A CATALYST IN THE FUSION OF TWO CELL MEMBRANES.

UNDERSTANDING THE GUIDING PRINCIPLES OF MEMBRANE FUSION WILL OPEN NEW OPPORTUNITIES FOR PHARMACEUTICAL DEVELOPMENT.

Perspective view on the membrane embedded SNARE system, highlighting the counterions Na^+ and Cl^- as bubbles. They are required to neutralize the high charge density of the mixed POPC (brown) / POPS (yellow) membrane.



Schematic view of the SNARE complex embedded in two membranes. The upper membrane represents the vesicle, the lower membrane is the target with which fusion occurs.

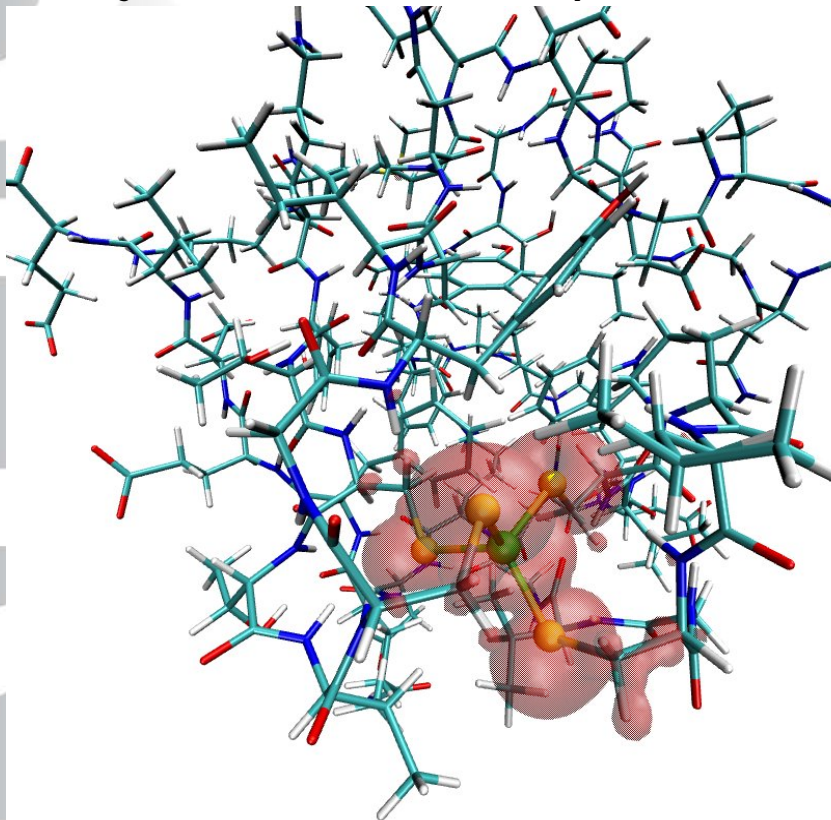


Initial and final structures of simulations on the membrane embedded SNARE complex. Tryptophanes 89 and 90 of synaptobrevin (orange) are highlighted in red. The composition of the membranes is visible with neutral POPC in brown and charged POPS in yellow.

Study of electron-transfer proteins

P. Carloni:

First ab initio investigation of entire electron-transfer proteins in aqueous solution: studies of a copper protein (azurin for *Pseudomonas Aeruginosa*) and two iron-sulfur proteins (rubredoxin from *Clostridium Pasteurianum* and from *Pyrococcus Furiosus*).



Isosurface enclosing the 95% of the total spin density (difference of the up and down electron densities) in the oxidized form of the **rubredoxin from *Clostridium Pasteurianum***.

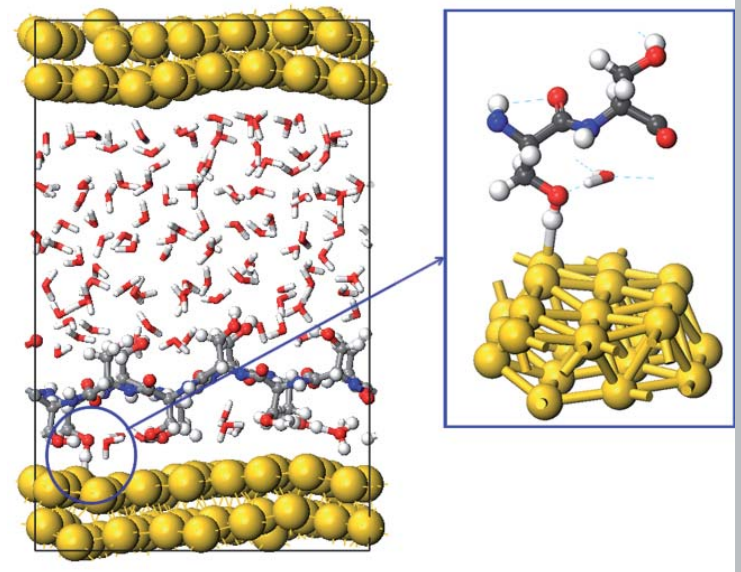
Optimization of the simulation for big biological systems.

Protein–surface interactions mediated by water

THE MOLECULAR RECOGNITION CAPABILITY OF PROTEINS CAN BE SPECIFICALLY ORIENTED TOWARD INORGANIC SURFACES. THIS PROJECT AIMS TO ELUCIDATE THE MECHANISMS OF INTERACTION BETWEEN A SURFACE AND A PROTEIN, INCLUDING THE ROLE PLAYED BY WATER.

Snapshot from ab initio molecular dynamics of protein–gold–water system.

The atoms represented (left) are repeated by 3D periodic boundary conditions, creating an infinite gold slab and an infinite poly-Serine β -sheet. The right highlights the instantaneous interaction between the Serine side-chain and the gold surface, which takes place via the hydrogen atom of the hydroxyl group.



The dynamics of gold atoms are important for explaining the interaction with the protein and with water.

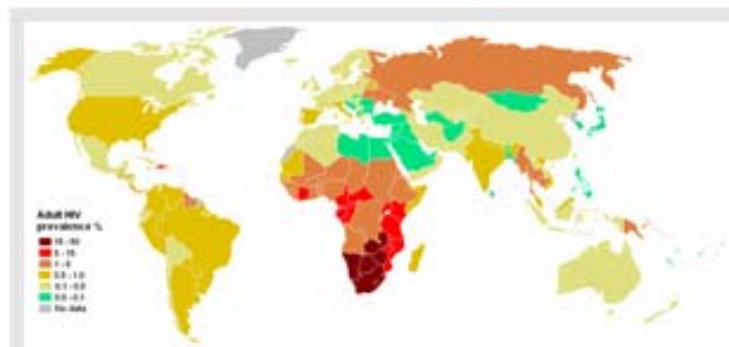


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Announcement - DEISA and GridAustralia demo HIV drug simulations over grids

[DEISA](#), the Distributed European Infrastructure for Supercomputing Applications, and [GridAustralia-APAC](#), joined by [Monash University](#), have demonstrated the interoperation of their HPC infrastructures with distributed simulations in both continents on the effectiveness of drugs against mutants of the Human Immunodeficiency Virus.

Both DEISA and GridAustralia-APAC use different, incompatible underlying main middleware



Prevalence of HIV among adults per country at the end of 2005.
Images courtesy of Wikipedia

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LHC and the grid

21 October 2008

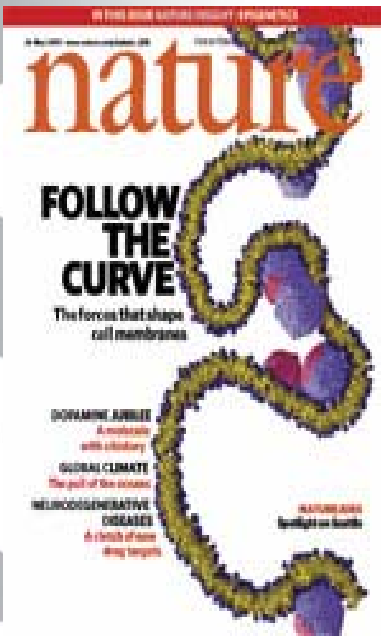
LHC INAUGURATION

[LHC coverage in iSGTW](#)

iSGTW 15 October 2008

[Feature - Opportunistic storage increases grid success rate](#)

[Feature - Tracking malaria vaccines](#)



Polymer Research

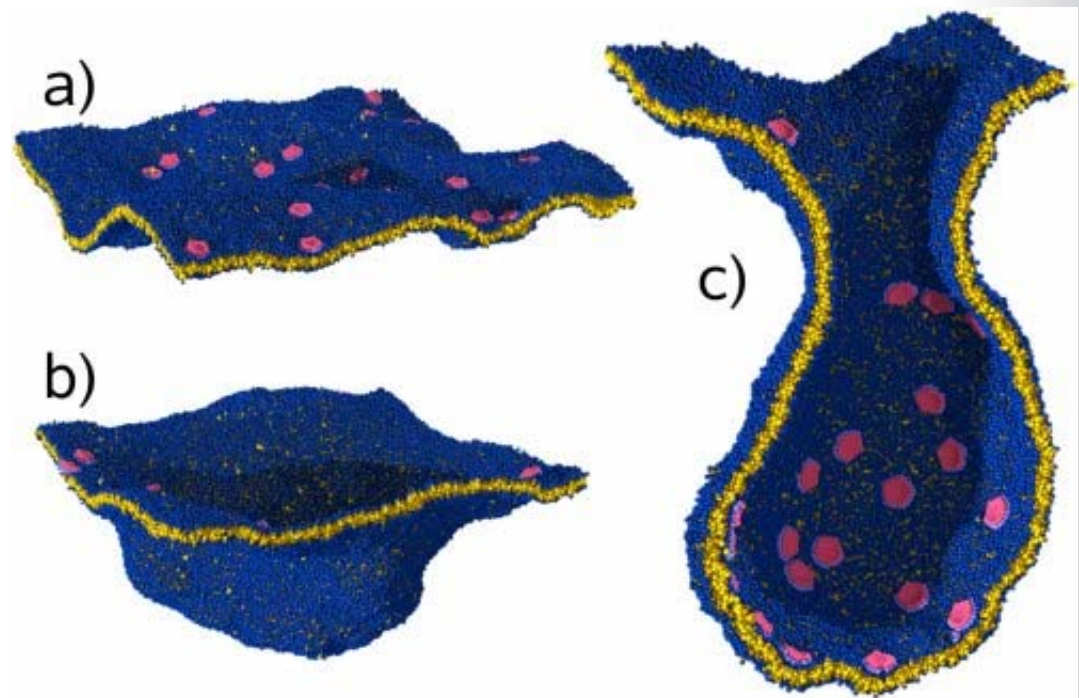
Cover story of Nature - May 24, 2007

Curvy membranes make proteins attractive

For almost two decades, physicists have been on the track of membrane mediated interactions. Simulations in DEISA have now revealed that curvy membranes make proteins attractive

Nature 447 (2007), 461-464

- proteins (red) adhere on a membrane (blue/yellow) and locally bend it;
- this triggers a growing invagination.
- cross-section through an almost complete vesicle



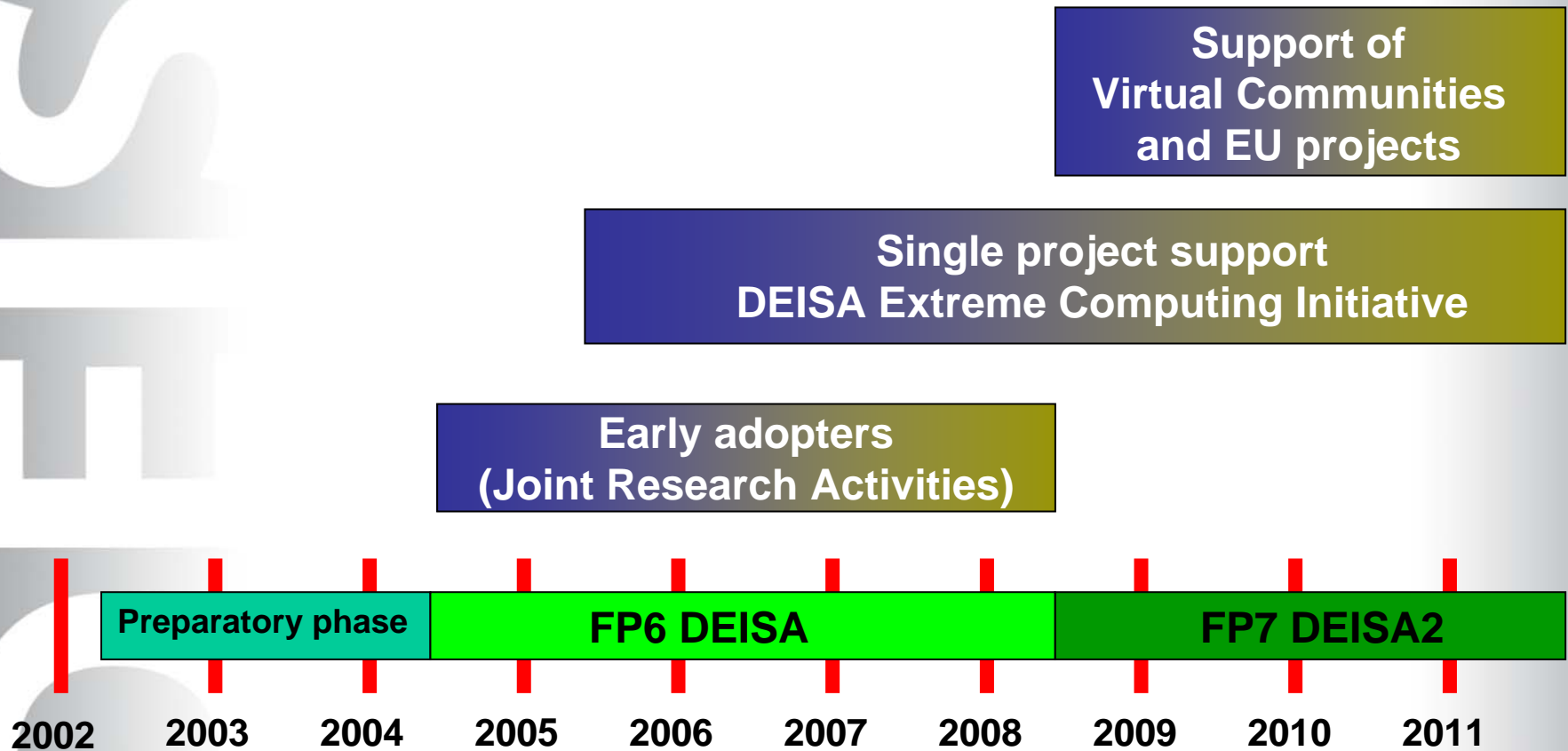
B. J. Reynwar et al.: **Aggregation and vesiculation of membrane proteins by curvature mediated interactions**, NATURE Vol 447|24 May 2007| doi:10.1038/nature05840

Fighting AIDS with supercomputers

Joint DEISA Australian Simulations of HIV drugs

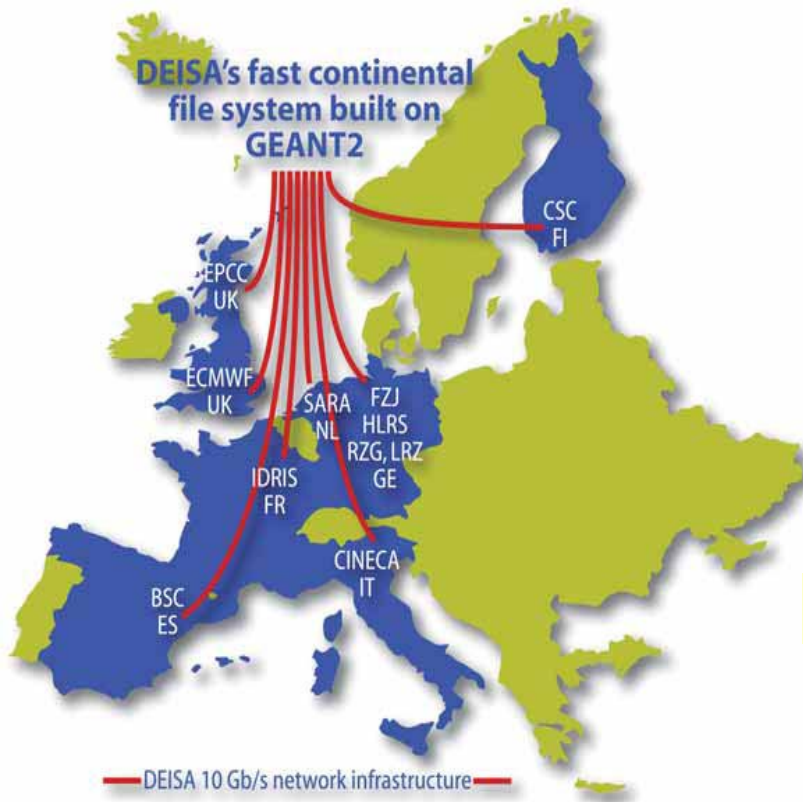
- Simulations have been designed to gather drug binding interaction energies of anti-HIV drugs bound to the active site of HIV protease, including drug-resistant versions of the protein.
- To assess the drug binding interactions, each drug and respective HIV mutant enzyme is run as a short molecular dynamics simulation to try and get an averaged energy of interaction between the drug and the HIV protease strain.
- Huge number of calculations required:
 - well suited for distributed processing
 - time-to-solution can be significantly reduced by employing at the same time several supercomputers in a suitable HPC grid
 - Given a certain level of interoperability, the compute tasks can even be spread over different grids.
- Effort successfully undertaken by DEISA and GridAustralia, joined by Monash University, during SC07 in Reno
- Successful interoperation of both infrastructures

Evolution of user categories



DEISA

Contributing to advancing European sciences in the HPC area



Most powerful European super-computers for most challenging projects

~1 PetaFlop/s
Aggregated peak performance

Grand Challenge projects performed on a regular basis

Virtual Community Support

Top-level Europe-wide application enabling