



DigitalWorld
Cancun 1 - 7 February 2009



DEISA

The Evolution of e-Infrastructures in Research, Industry, and Education

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"It's hard to make predictions, especially about the future"

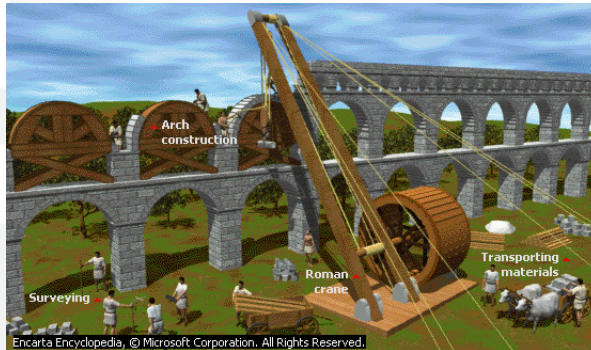
Yogi Berra

Content

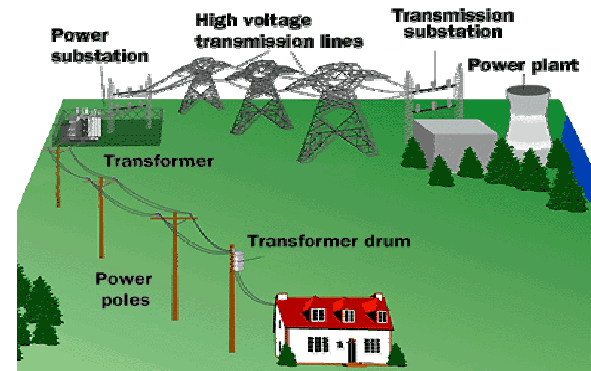
- Service Infrastructures: nothing new
- Building Blocks: Computers, Grids, Clouds
- Example: DEISA Ecosystem for Science Applications
- Next-Generation e-Infrastructures
 - e-Learning on e-Infrastructures = e-Learning 2.0

DEISA

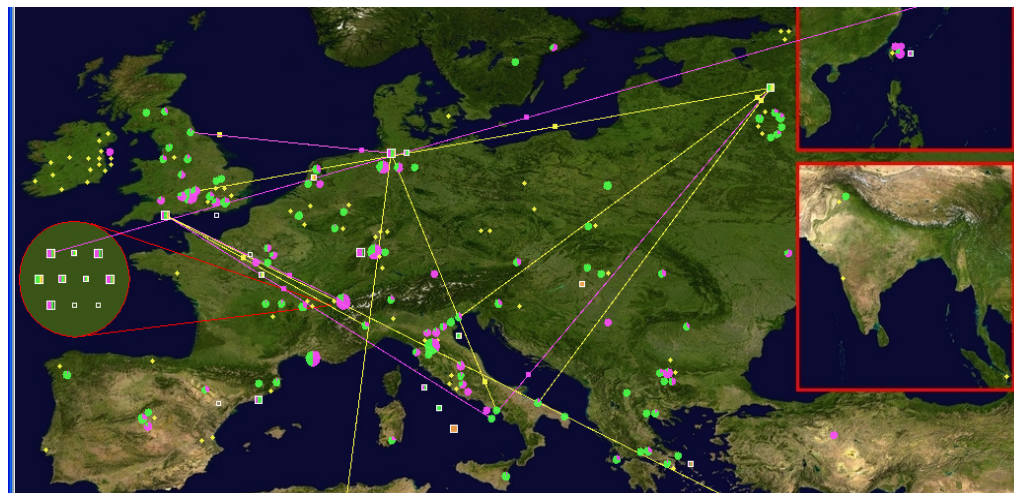
Service Infrastructures



Ancient Rome: ten aqueducts,
some 150,000 m³ of water each day



Electrical Power Grid
Infrastructure



EGEE – Enabling Grids for E-Science

HPC Centers



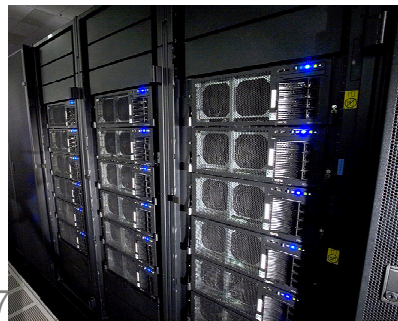
- HPC Centers are **service providers**, for past 35 years
- Computing, storage, applications, data, etc IT services
- Serve (local) research, education, and industry
- Very professional: to end-users, they appear almost as Cloud services (AWS Cloud definition: easy, secure, flexible, on demand, pay per use, self serve)
- But: no virtualization, semi-automatic, static
- They could become a Cloud customer for dynamic scaling and adopting to changing business and user demands

RoadRunner, Today's Fastest SC

- **1986**, Cray-2 breaking the **Gigaflop/s** barrier
- **1997**, Intel ASCI Red, breaking **Teraflop/s** barrier
- **2008**, IBM RoadRunner, breaking **Petaflop/s**
 - At DOE's Los Alamos National Laboratory
 - 1.026 Linpack Petaflop/s solving 2 Mio equations
 - 6912 dual-core Opteron & 12960 IBM Cell
 - #1 on the Top500 list of June 2008



DigitalWorld, Feb 1 - 7



Wolfgang Gentzsch, DEISA



5

Grids



1998: The Grid: Blueprint for a New Computing Infrastructure:

“... hardware and software infrastructure ... dependable, consistent, pervasive, and inexpensive access to high-end computational capabilities.”

2002: The Anatomy of the Grid:

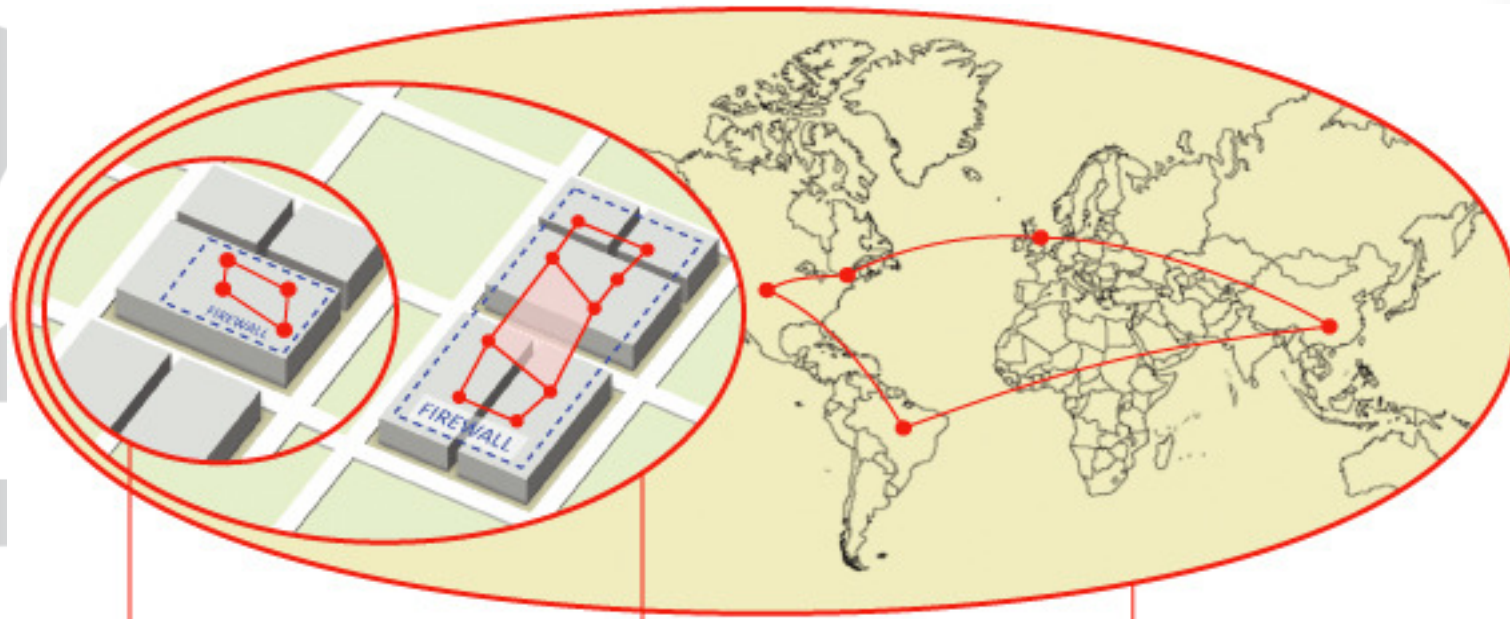
“... coordinated resource sharing and problem solving in dynamic, multi-institutional virtual organizations.”

2002: Grid Checklist:

- 1) *coordinates resources not subject to centralized control ...*
- 2) *... using standard, open protocols and interfaces*
- 3) *... to deliver nontrivial qualities of service.*

Quotes: Ian Foster, Carl Kesselman, Steve Tuecke

Grids



**Departmental
Grids**

**Enterprise
Grids**

**Global
Grids**

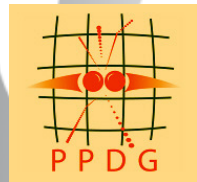
Research is using Grids



Distributed European Infrastructure for



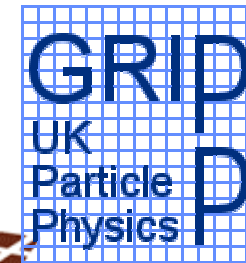
Distributed European Infrastructure for Supercomputing Applications



K*GRID



National Grid SINGAPORE



Grid5000



Versió en Català
English Version
Versión en Castellano

tota la informació sobre el projecte

- presentació
- descripció tècnica dels serveis oferts
- participants
- documentació pública
- com puc participar?

GridCat

grid grid grid grid

dintre del grid

- accés al Portal
- Intranet per a investigadors
- estat dels serveis actius

grid grid grid grid



国立情報学研究所グリッド研究開発推進拠点 NII -The National Institute of Informatics



Industry is using Grids

Distributed
European
Infrastructure for

Schlumberger
Raytheon

Johnson & Johnson

gsk GlaxoSmithKline
Bristol-Myers Squibb

arcelor
Flat Carbon Steel

MERCK

sanofi aventis
Because health matters

Pfizer

COLT

TERRALLIANCE



BEAR STEARNS

Bank of America

NTT WEST
The Abbey National

BNP PARIBAS

ATK

CDC IXIS
Capital Markets



Caboto

ChevronTexaco



CORUS

HSBC

SUNGARD



WACHOVIA



CALYON
CORPORATE AND INVESTMENT BANK



COMMERZBANK

Deutsche Bank

UBS



Fidelity Investments



UniCredit



Hewitt



Algorithmics
Know Your Risk.

Genworth Financial
Built on GE Heritage

BANK ONE



Allstate
You're in good hands.

CREDIT SUISSE | **FIRST BOSTON**

Goldman Sachs



Calypso
technology



Northwestern Mutual
FINANCIAL NETWORK*



Clouds

- IT resources provisioned outside corporate data center
- Resources accessed over the internet
- Variable cost of services
- Service oriented: SaaS, PaaS, IaaS, HaaS
- A virtual computing environment (Vmware, Xen,...)
- Build and deliver, always-on, pay-per-use IT services
- Scaling: computing, storage, database, services, and users, up and down
- Abstraction of the hardware from the service



The Cloud of Cloud Companies

- Amazon
- Google
- Salesforce
- Microsoft
- Sun
- IBM
- Oracle
- EMC
- Cloudera
- Cloudsoft
- Akamai
- Areti Internet
- Enki
- Fortress ITX
- Joyent
- Layered Technologies
- Rackspace
- Terremark
- Xcalibre
-
-

Example of an e-Infrastructure:

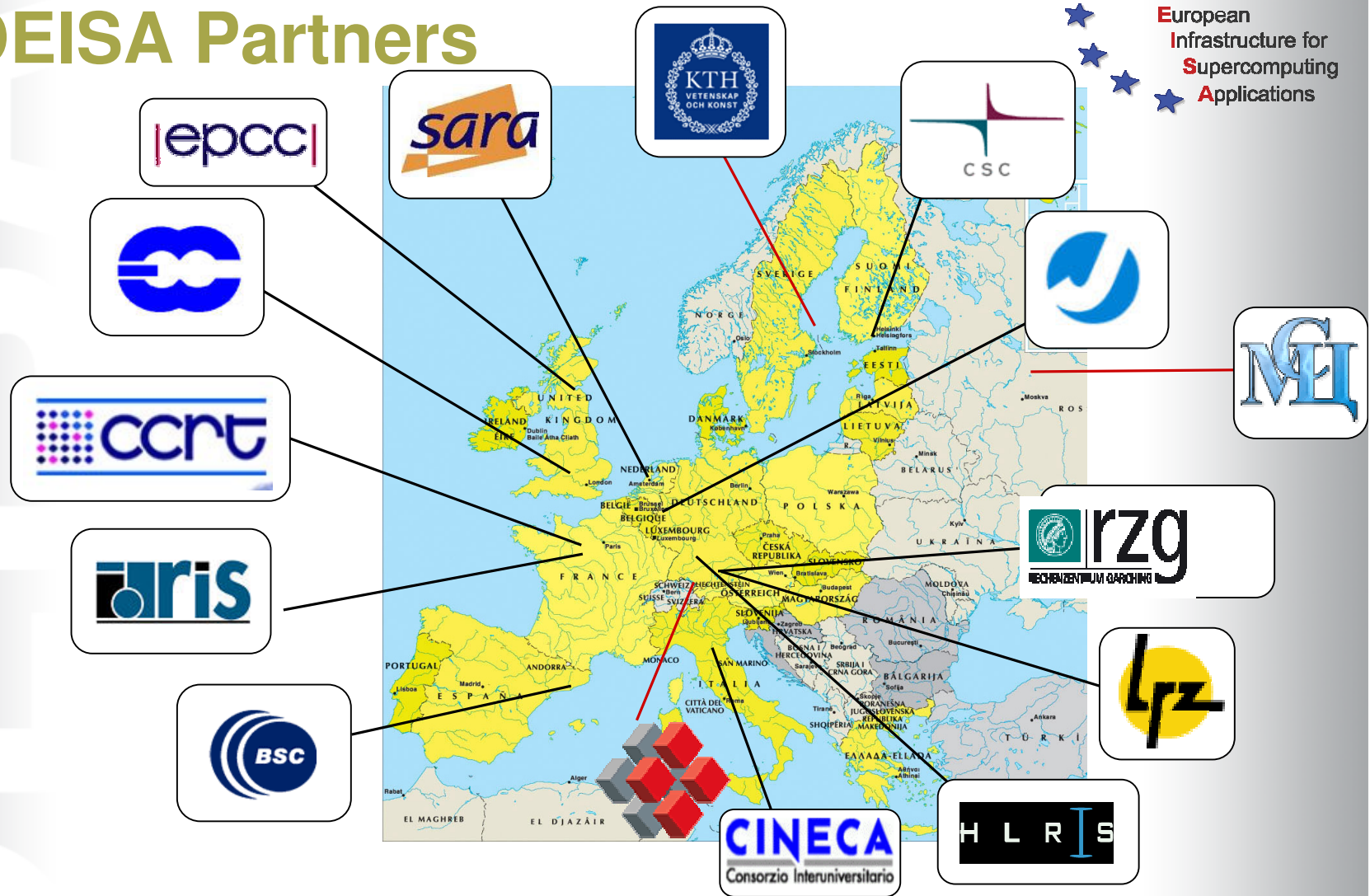
The DEISA Ecosystem for HPC Grand-Challenge Applications

Distributed European Infrastructure for Supercomputing Applications



DEISA Partners

 Distributed
European
Infrastructure for
Supercomputing
Applications



DEISA1: May 1st, 2004 – April 30th, 2008

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



DEISA: Vision - Mission - Strategy



Vision:

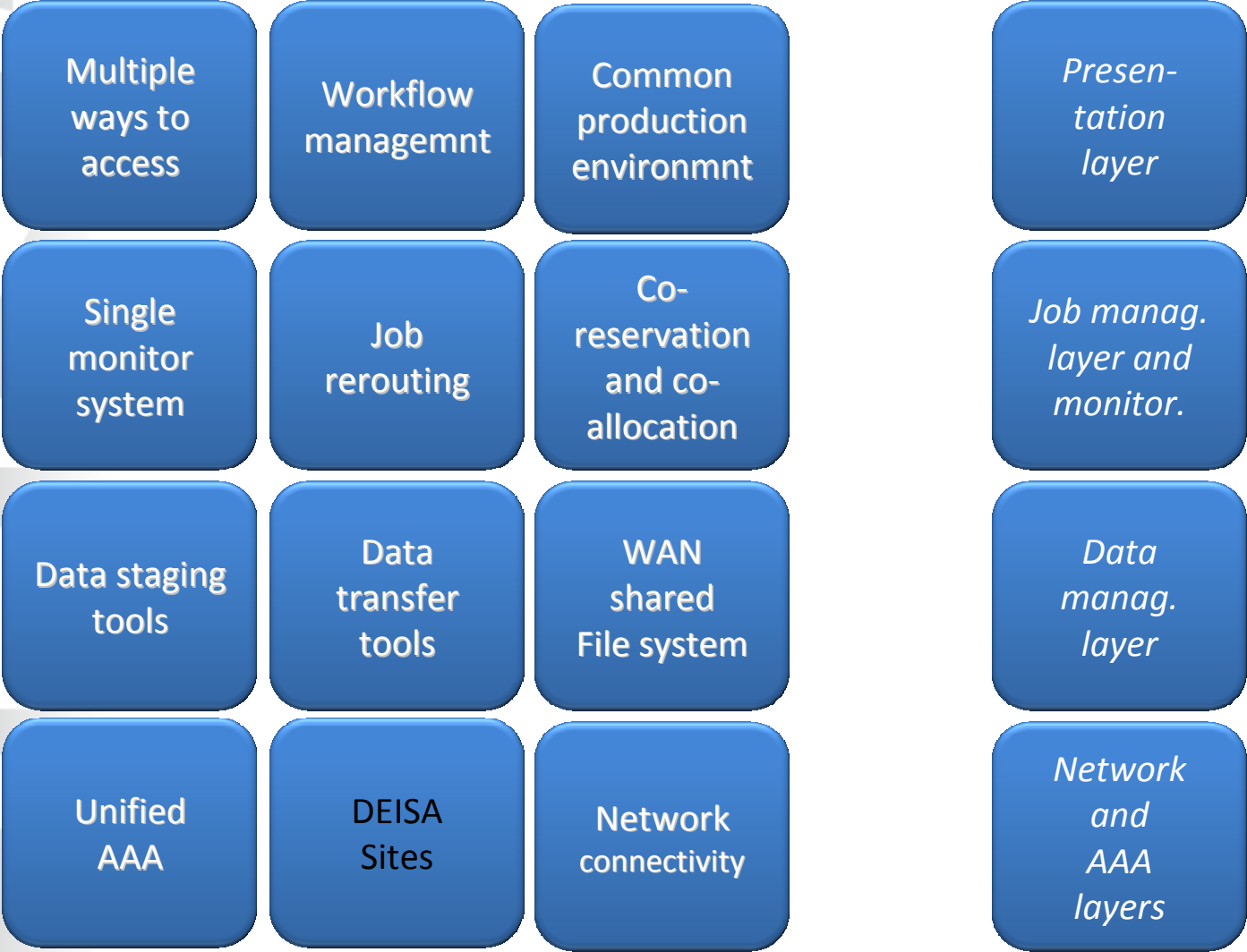
Establishing persistent European **HPC ecosystem** integrating national Tier-1 (Tflop/s) centres and the new European Tier-0 (Pflop/s) centres

Mission:

Enhance Europe's capability in computing and science by **integrating** most powerful **supercomputers** into a European HPC e-infrastructure

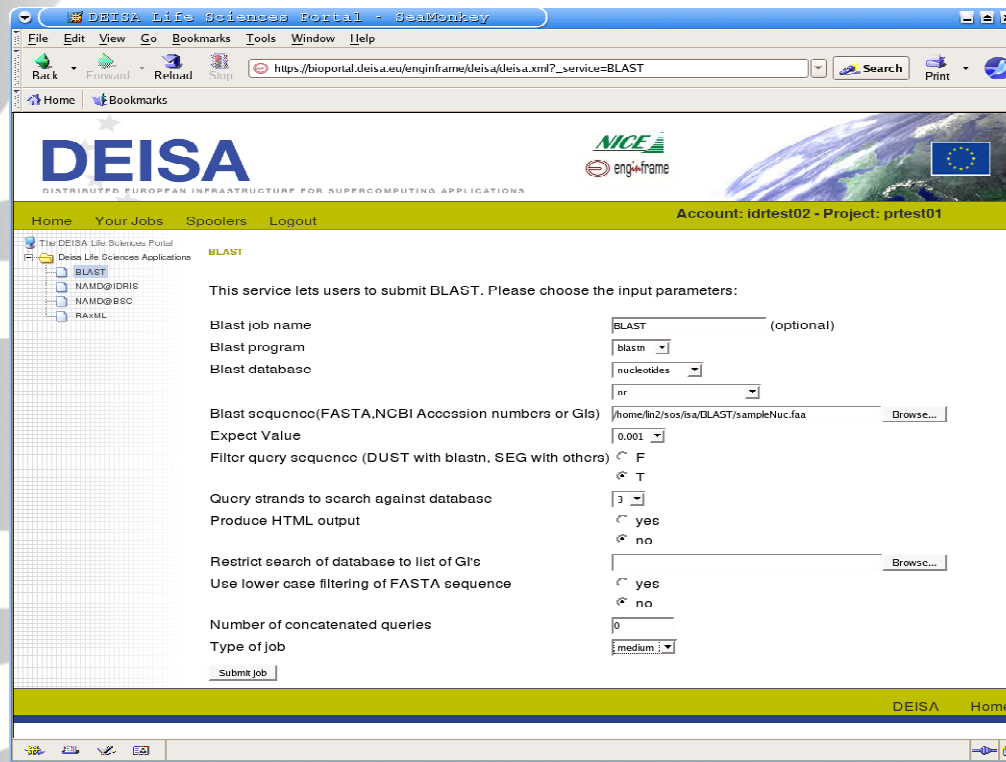
Build European Supercomputing **Service** on top of **existing** national services, based on the deployment and operation of a persistent, **production** quality, distributed supercomputing environment with continental scope

DEISA Service Layers



One Example of Virtual Communities: Joint Research Activity “Life Sciences”

The DEISA Life Science Portal



The screenshot shows a web browser window displaying the DEISA Life Science Portal. The page title is "DEISA Life Science Portal - SeaMonkey". The address bar shows the URL: "https://biportal.deisa.eu/enginframe/deisa/deisa.xml?_service=BLAST". The page features the DEISA logo and the NICE enginframe logo. A navigation menu includes "Home", "Your Jobs", "Spoolers", and "Logout". The main content area is titled "BLAST" and contains a form for submitting BLAST queries. The form includes fields for "Blast job name", "Blast program", "Blast database", "Blast sequence (FASTA, NCBI Accession numbers or GIs)", "Expect Value", "Filter query sequence (DUST with blastn, SEG with others)", "Query strands to search against database", "Produce HTML output", "Restrict search of database to list of GIs", "Use lower case filtering of FASTA sequence", "Number of concatenated queries", and "Type of job". A "Submit job" button is located at the bottom of the form.

Joint Research Activity (JRA)

**Promoting parallel apps in the
life science community**

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

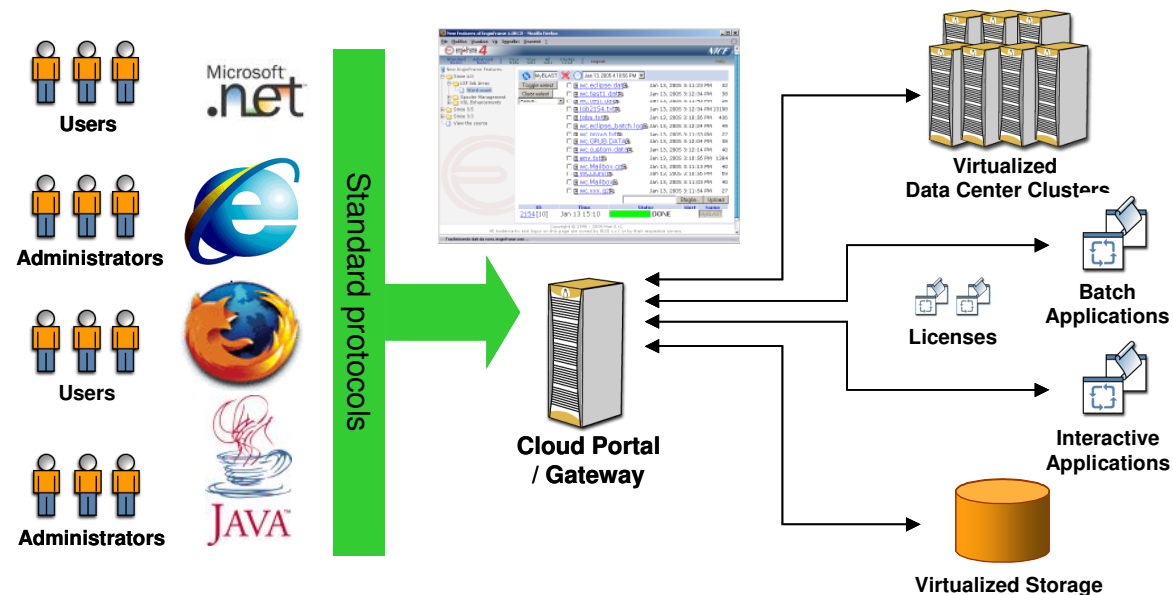
**Providing ease of access to
resources**

**Application support for life
science portal**

Cluster/Grid/Cloud Portal

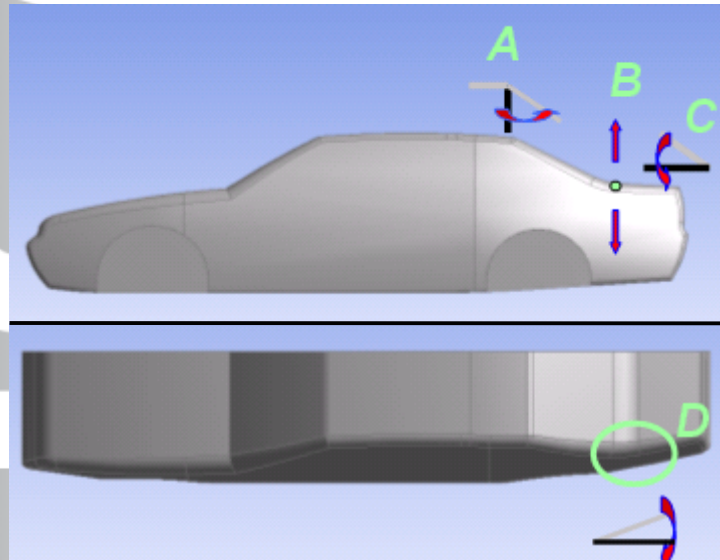
Example: NICE EnginFrame

Provides remote, interactive, transparent, and secure access to applications and data on your corporate Intranet or Internet, or in the Cloud.

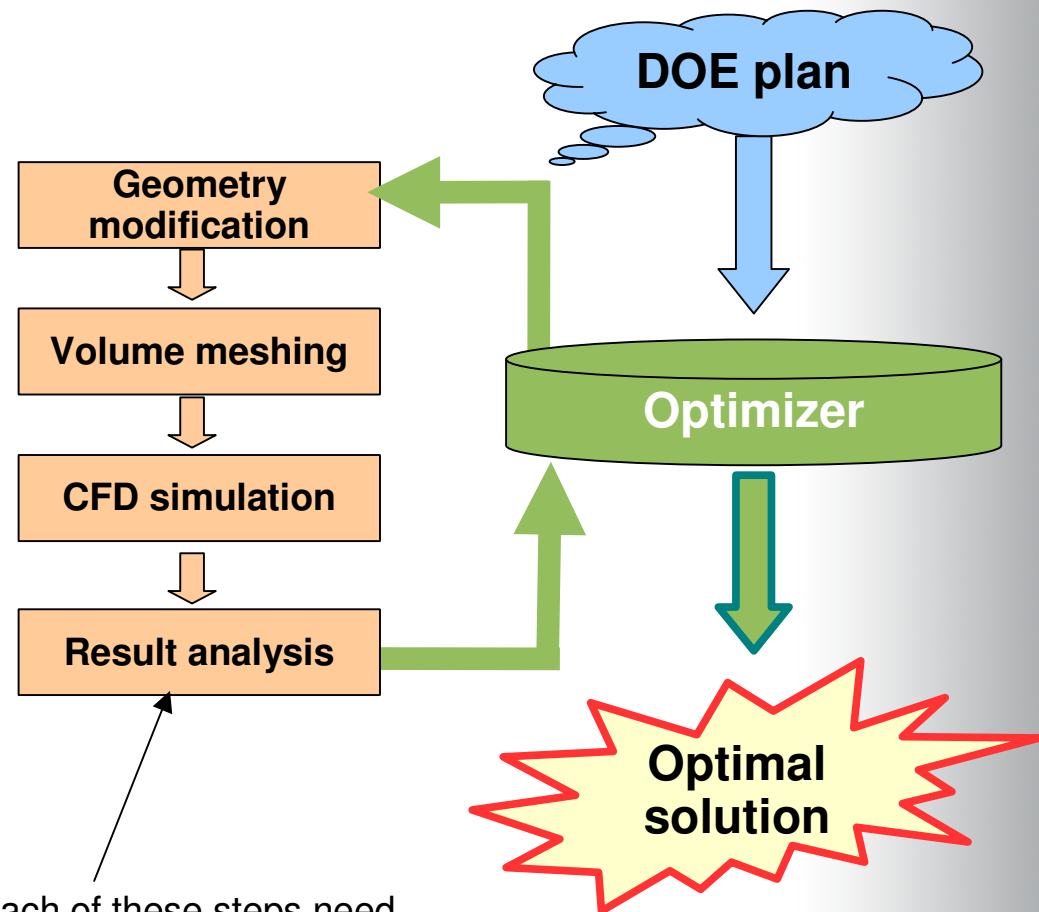


Users and administrators can access and control computing resources via an intuitive and standard Web interface virtually anywhere using a standard Web browser.

Aerodynamic Shape Optimization



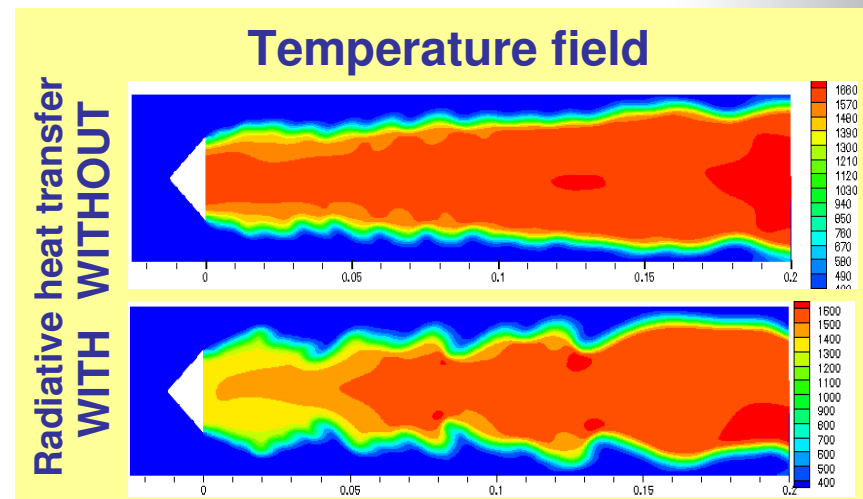
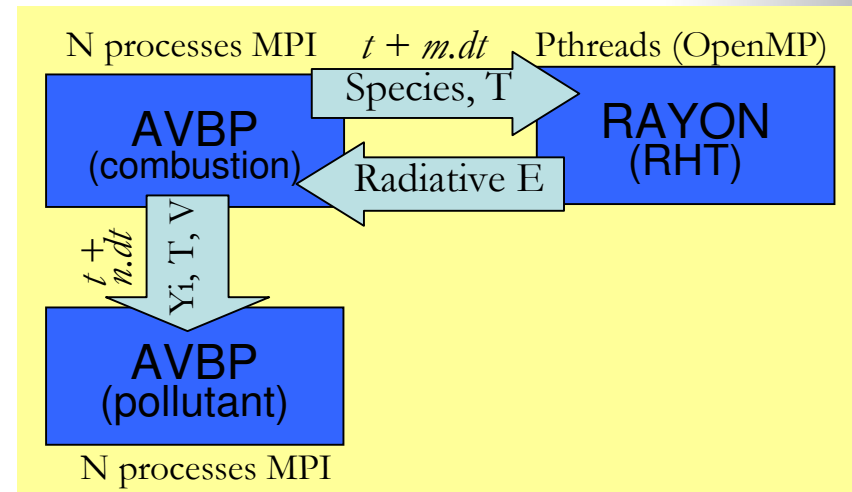
- 4 parameters to be optimized
- cubic face centered DOE
- 25 cases+16 extra cases for error estim.
- polynomial response function
- 70 hours wall clock time on 64 cpus



Each of these steps need to be fully automated and controlled by the optimizer

Combustion / Radiation

- Study the impact of radiative heat transfer (RHT) on the combustion process (2D)
- Couple combustion (AVBP), the RHT (Rayon) codes and the pollutant formation (AVBP)
- Parallelization of the Rayon code and improvement of the coupling part
- Load balancing issue
- 3D extension proposed to DECI and accepted

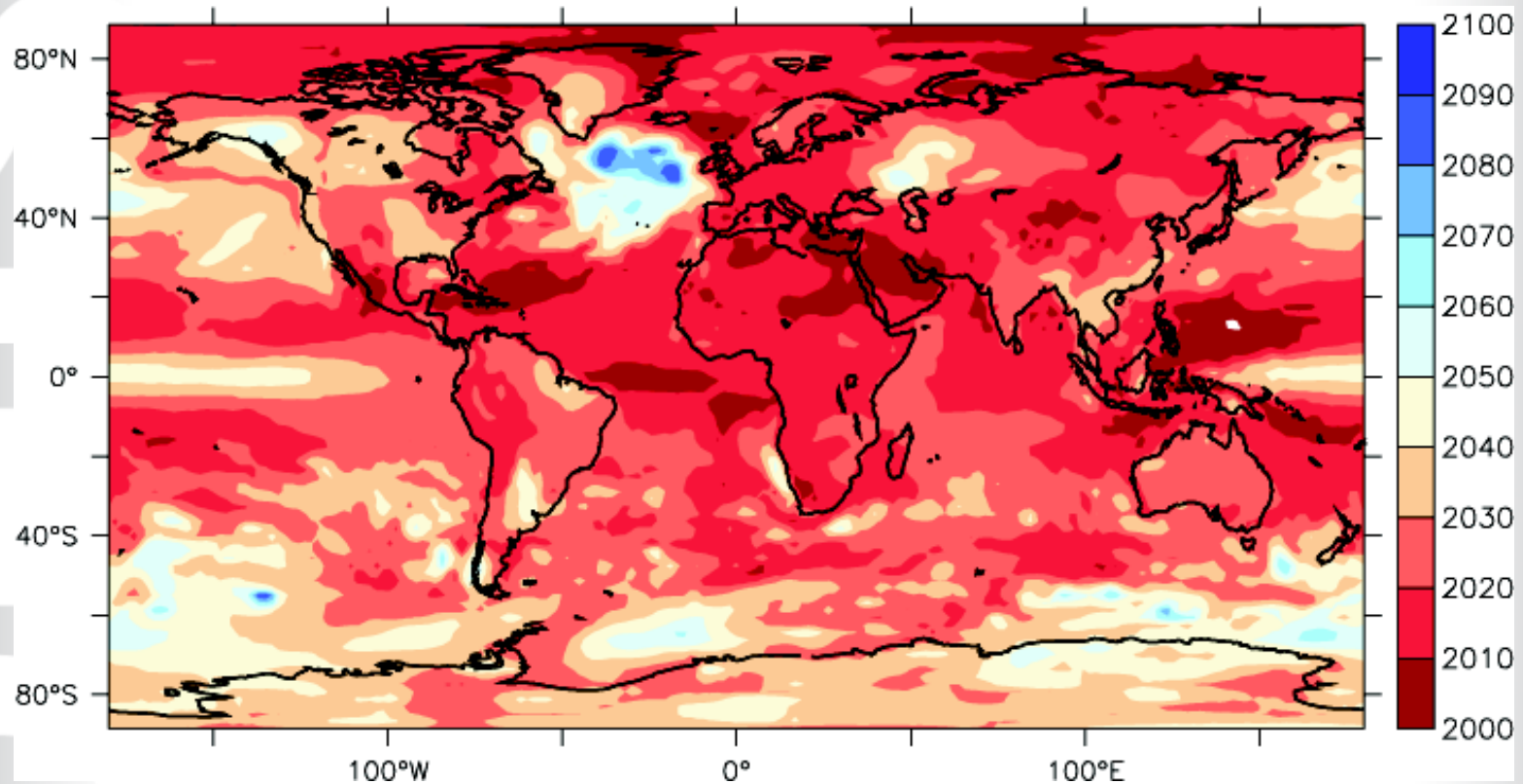


Climate Research

Statistics of Climate Variability



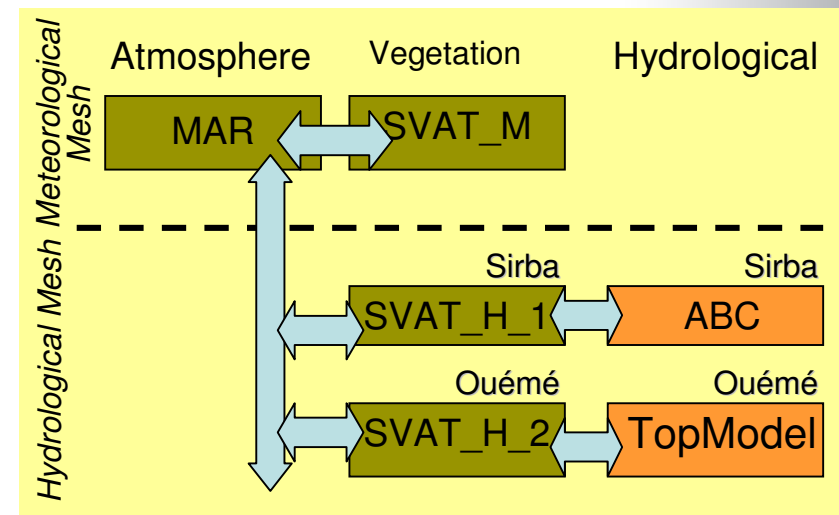
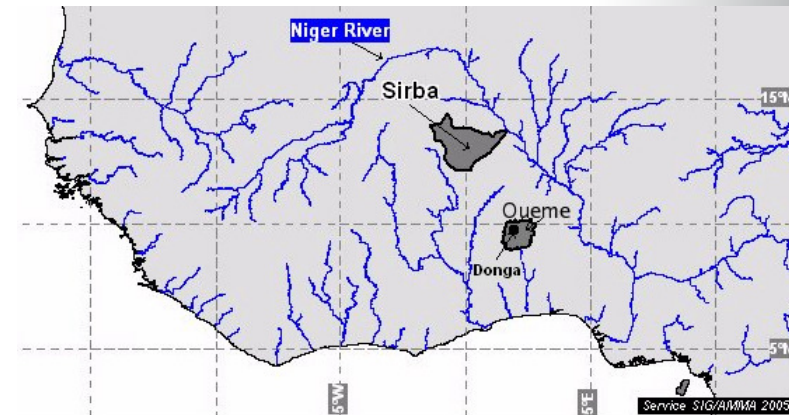
Project to study climate trends, each 50 TB output data



H. Dijkstra, U Utrecht, and W. Hazeleger, KNMI

Environmental Application

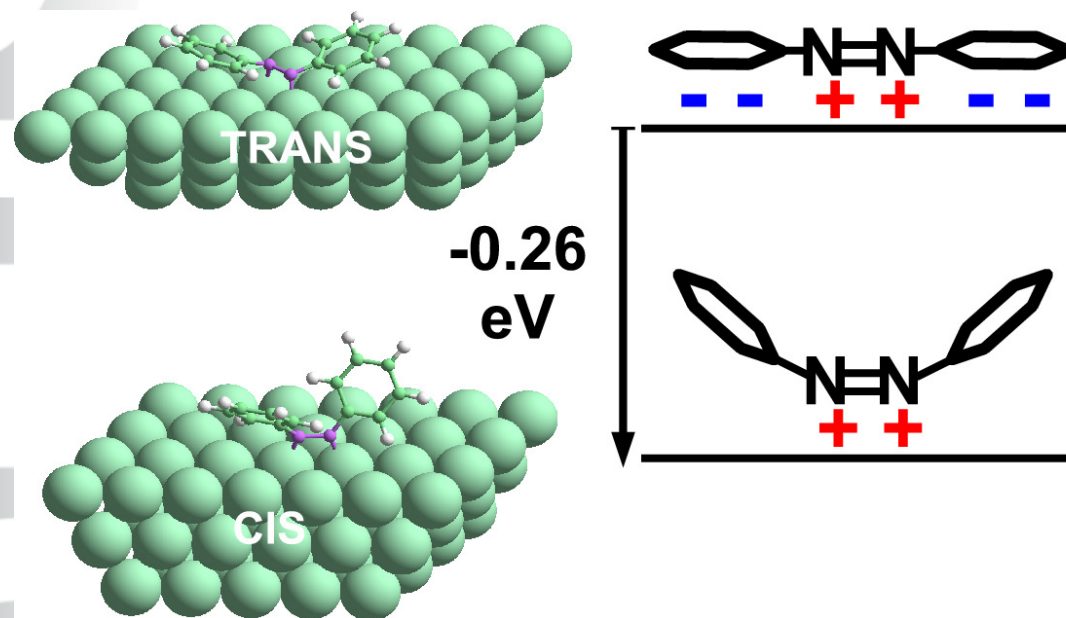
- Study the impact of water cycles of the hydrological and vegetation models on climate models
- Coupling area in West Africa
- Best performances with a vector and scalar platform
- Improve extensibility of the architecture and the coupling part
- AMMA project, PhD thesis, 2 publ. and 2 comms.



Materials Science

First-principles statistical mechanics for molecular switches at surfaces (MolSwitch)

Azobenzene on copper, silver and gold surfaces



Controlled reversible switching should be possible on Ag surfaces

Courtesy: K. Reuter, FHI



Polymer Research

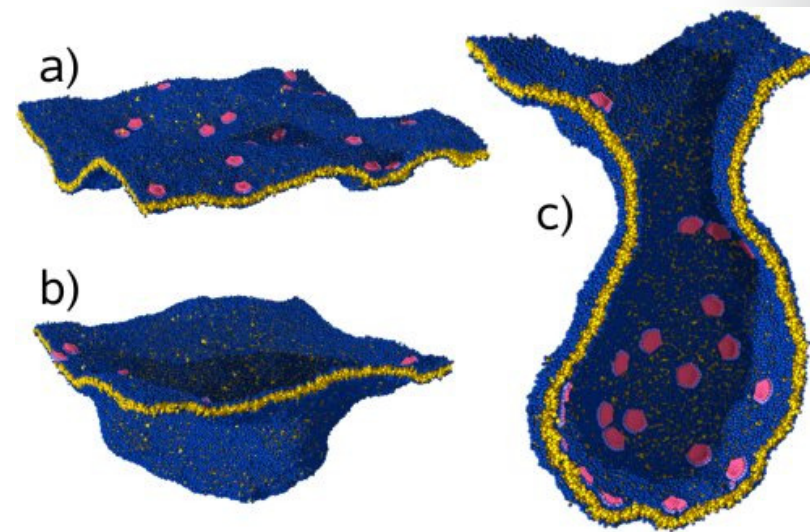
Cover story of Nature - May 24, 2007

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

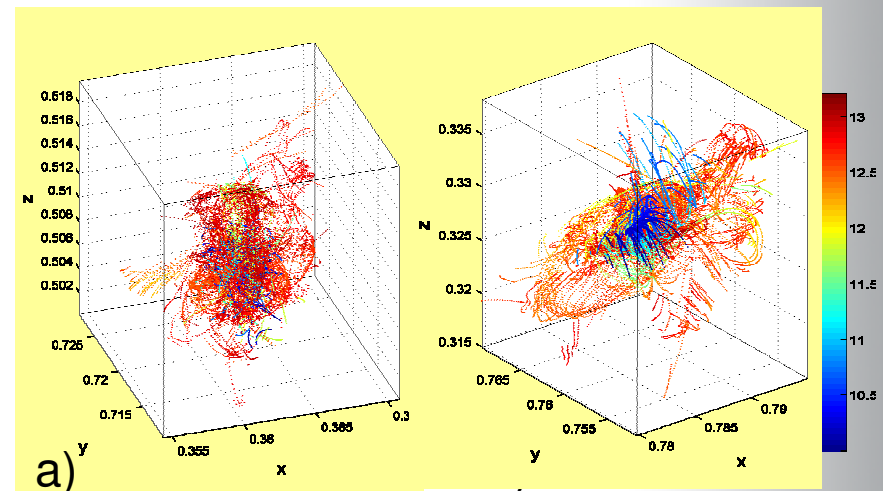
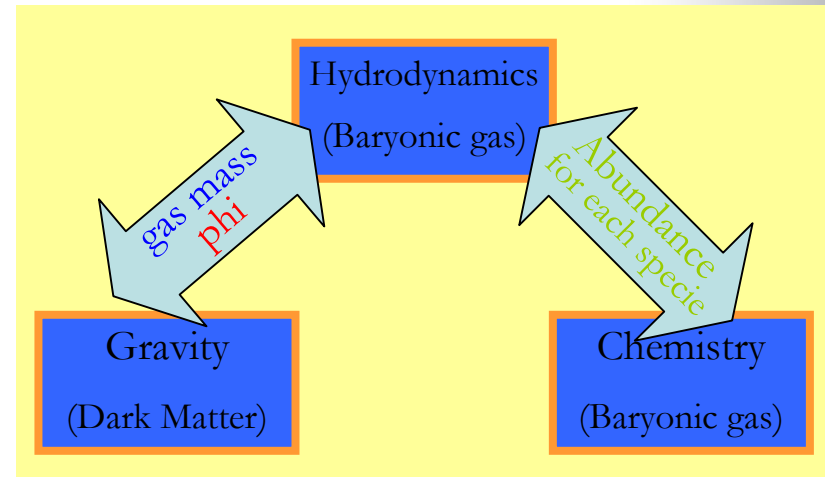
- proteins (red) adhere on a membrane (blue/yellow) and locally bend it;
- this triggers a growing invagination.
- cross-section through an almost complete vesicle



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

Cosmology Project

- Study galaxy formation in cosmology
- Physics / modules: Gravitation, Hydrodynamics, Chemistry
- Best performance on heterogeneous platforms
- Load balancing issue and improvement of the coupling part
- Proposed to DECI



Next-Generation e-Infrastructures for

ACHI: Advances in Computer-Human Interactions

eKNOW: Information, Process, and Knowledge Management

eL & mL: Mobile, Hybrid, and On-line Learning

eTELEMED: Health, Telemedicine, and Social Medicine

GEOWS: Advanced Geographic Information Systems & Web Services

ICDS: Digital Society

ICQNM: Quantum, Nano, and Micro Technologies

Connected: anyone, anywhere, anytime, any device



- Integration of new devices, data and information sources
- Cell phones, PDAs, smart sensors, sensor arrays, health monitors
- Devices embedded in cars, engines, roads, bridges, clothes,...
- Huge amount of data for real-time analysis
- Policies, grid economy, to maintain stability and efficiency
- Support organizational and societal structures, to bridge political and social boundaries . . .

Example: e-Learning on e-Infrastructures



The Challenges:

World-wide data and knowledge explosion

We need more scientists and engineers, but not enough students are interested in science

Schools and teachers are not prepared

The Solution:

New ways of teaching and learning for our digital natives

e-Infrastructures for enriched learning

Working with didactic and pedagogic experts

The Prototype:

e-School, interactive science laboratory, the digital sand-box for life-long learning in the sciences

Today's Education Challenges

- **Information** & knowledge growing exponentially
- **Teaching** methods + materials do not keep pace
- **Learning** is too passive and static, life is highly active and dynamic

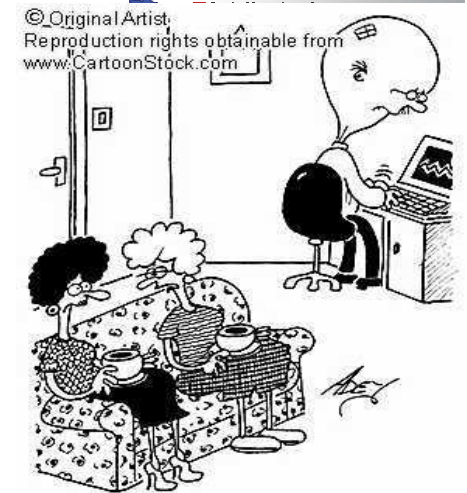
Prof. Srivathsan, India: „...education today is not learning centric, it is exams centric.“

- **Students** become de-motivated and lack creativity
- **e-Learning** environments just scratching the surface

We need 100Ks of new jobs in science and engineering



We have to focus on K-12 students and their teachers



I've tried to tell Bill he's overloading himself with too much information

e-School Prototype

A **Virtual Laboratory** based on an e-Infrastructure and a distributed digital repository for science and engineering applications for students and educators

Bridging the Chasm between

Education



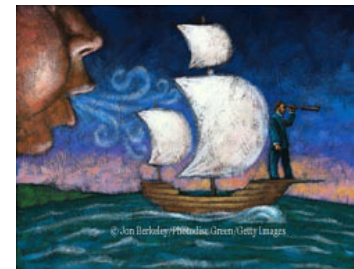
Science

Vision: e-School Science Collaboratory for a better learning experience

- **Inter-active** learning tools for creative students (edutainment)...
- ...**same tools** engineers & scientists are using in the 21st century
- Edu portal provides seamless access to **virtual laboratory**
- 100s of real-world computer simulations available for all ages
- On dynamic, shared, remote resources, **at your finger tip**

e-School: empowering education

- **Learning by doing** -



e-School Prototype Website

<http://eschool.gridwisetech.pl>



Distributed
European
Infrastructure for
Supercomputing

Prototype developed by Wolfgang Gentsch and: "e-School" partner



Logout
Welcome, admin

[e-School Grid](#) [Applications](#) [e-School Administration](#) [User Settings](#) [Administration](#)

[Welcome](#) [What is e-School](#) [Downloads](#) [Wiki](#) [Virtual Classroom](#) [Schoolbooks](#)

Welcome

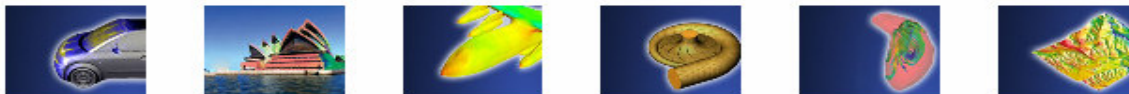
Welcome to the e-School Digital Laboratory !

This is a prototype of e-School which will demonstrate how you can easily and interactively build, modify and run physics applications on remote computers in the Internet.

Therefore, after some initial reading, the most important action for YOU is to go to the Application section and run at least one application.

PLEASE TRY IT, IT'S EASY !

In the future, here, you will find a wealth of digital experiments in areas such as math, physics, chemistry, biology, weather, climate, environment, bioinformatics, biophysics, medicine, aero and fluid mechanics, economy, finance, and even music, arts and humanities, especially prepared for your specific interest, school grade and curriculum.



You are now in your personal and secure e-School website. You can personalize this site further by adding your favorite links on the right side of this page, or by sharing information with others, in the Wiki, or by including in the application library your own digital examples which you have designed and developed yourself.

Next, you want to configure your system for the e-School prototype in an optimal way. For that, we recommend to follow the 'Configuration' steps on the 'Downloads' section.

Next, you want to learn how to use this e-School prototype. For this, we have included a so-called "e-School Primer" which you get from the "Downloads" page. From the same place you can get e-School's newsletter.

Now, you are ready to go! Click on the red "Applications" tab, and let you take through the world of digital virtual laboratory experiments !

Thank you very much for visiting us. We appreciate any comment! Please send to wgentsch@d-grid.de.

My Favorite Links

	Name	Type
<input type="checkbox"/>	Vitalsource	Public
<input type="checkbox"/>	CEI	Public
<input type="checkbox"/>	Friday Institute	Public
<input type="checkbox"/>	TryScience	Public
<input type="checkbox"/>	Ansys	Public
<input type="checkbox"/>	CAD-FEM	Public

Delete Selected

To include a new favorite link, please give it a name, type its URL, and mark as public if you want the link to be seen to all users (otherwise, it's just seen by you as the creator):

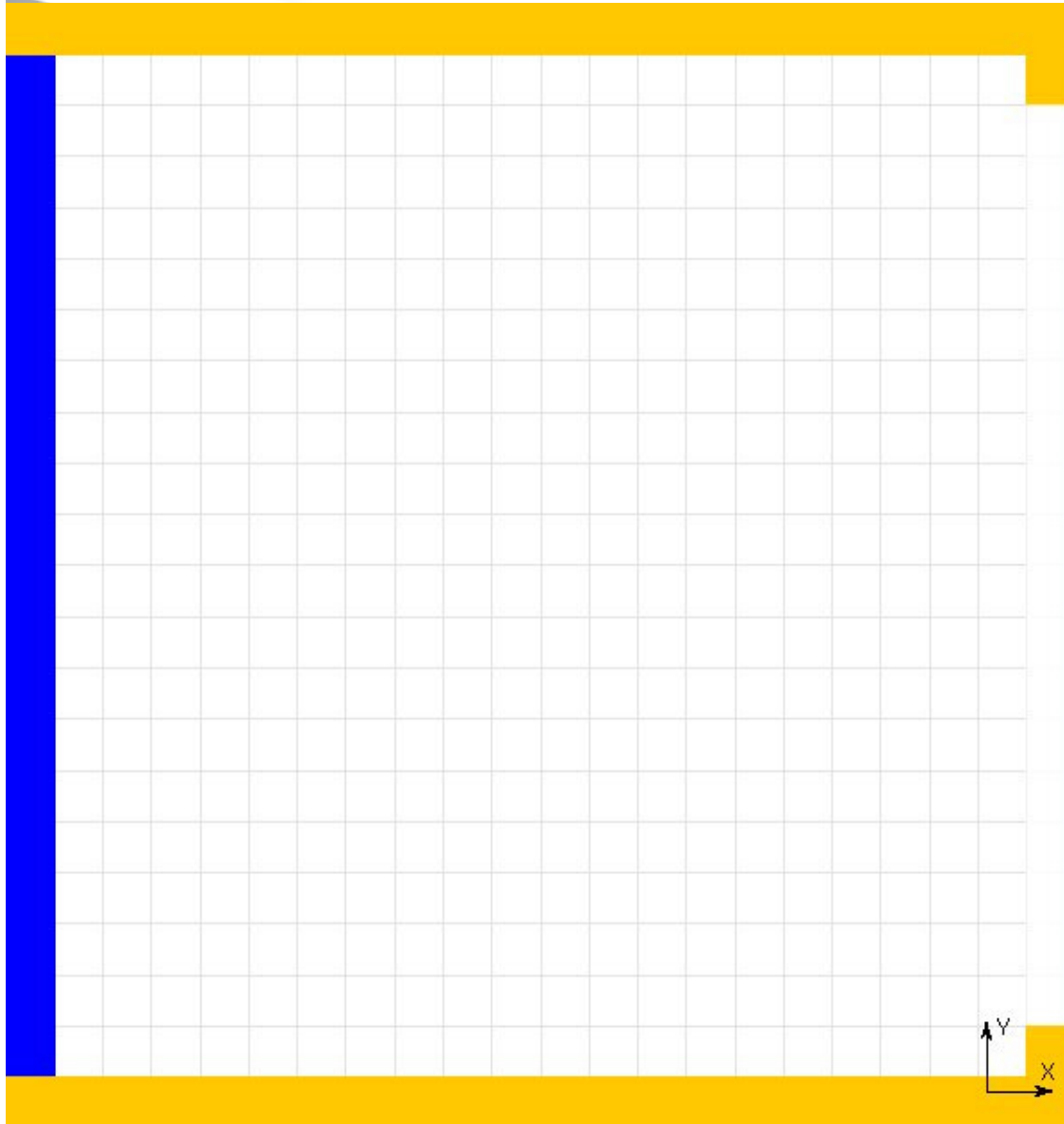
Link name:

Link address:

is public?

Add a Link

e-School: Your personal workspace



Simulation Library

Simulations Mesh oriented simulation ▾

New model Save Save As Solve model

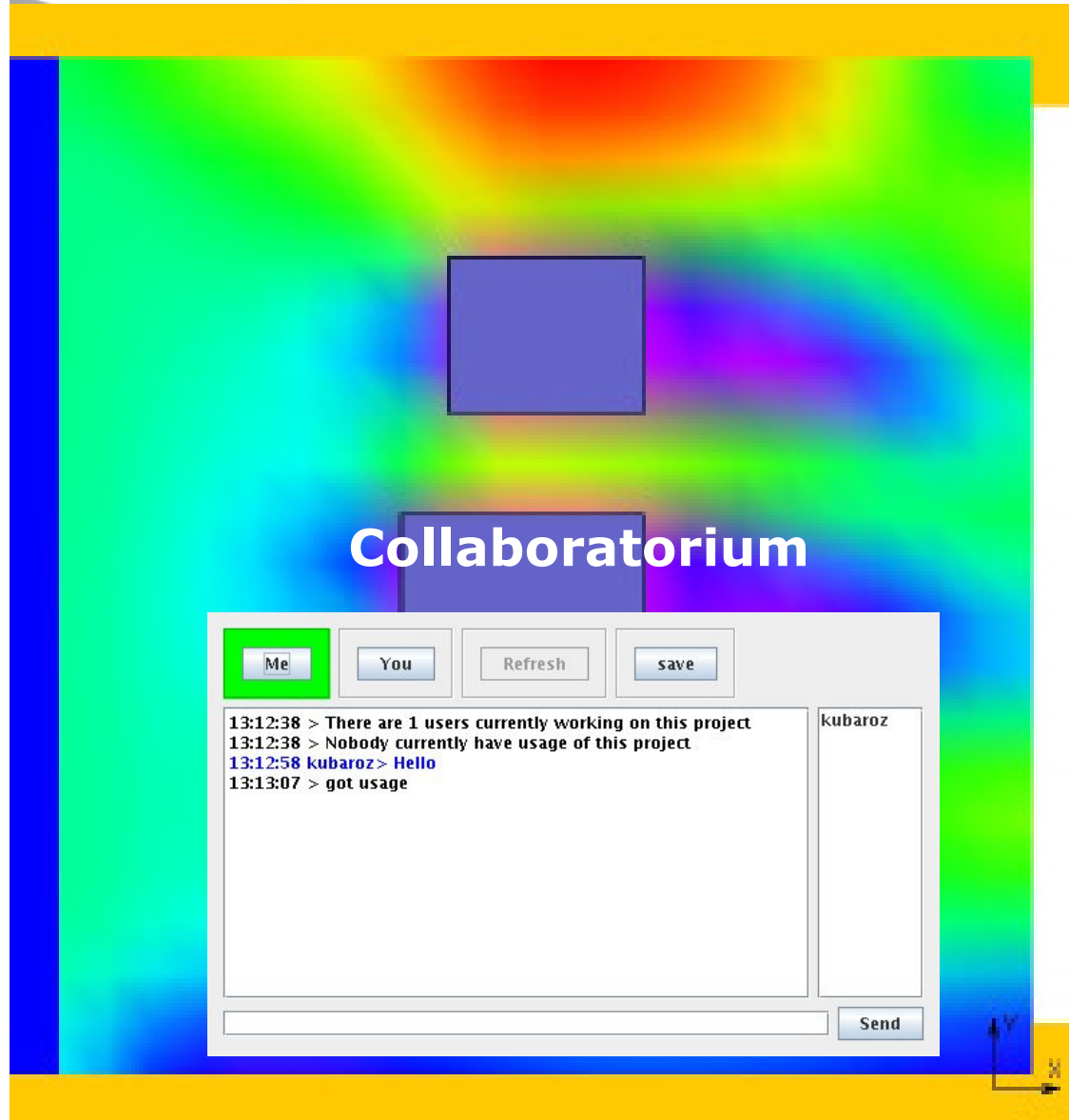
Snap to grid

Handlers

Mode Add obstacle ▾

Add obstacle

Example: interactive real-time fluid flow



Me You Refresh save

13:12:38 > There are 1 users currently working on this project
13:12:38 > Nobody currently have usage of this project
13:12:58 kubaroz > Hello
13:13:07 > got usage

kubaroz

Send

Simulation Library

Simulations: Mesh oriented simulation

New model Save Save As Back to modeling

Snap to grid


Solver parameters

Mode: Shaded Velocity Cells

Shaded Velocity Cells

Shaded Cells

Max: 19,824



Min: 1,010

Distance Learning on e-Infrastructures

Distance Learning...

- Independent of time and space
- Self-paced learning
- Teacher-independent learning
- Deductive science education
- Mostly single-learner environment.
- Linear inter-reactivity, at best
- Mostly static and repetitive

**=> Improved (but similar to)
class-room learning**

...on e-Infrastructures

- Independent of time and space
- Self-paced learning
- Teacher-independent learning
- Inquiry-based science education
- Allows for collaborating groups
- Fully nonlinear interactivity
- Highly dynamic and nonlinear
- Allows for complex simulations, data processing, and visualization
- Students and teachers become more creative, motivated and committed

=> Paradigm Shift

DEISA

Read more in:



Thank You!
GRACIAS POR SU ATENCIÓN

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