

Many Different Types of GRIDS ?

Cycle Scavenging GRIDS - desktop to

Supercomputers

Application Specific GRIDS (e.g. distributed computing, simulations, interactive response, etc.)

Data GRID (large amounts of distributed data, data tends to be computed)

DataGRID or DatabaseGRID, (Genomics, Ensembl, Proteins etc.)

Service GRID (Astronomical combined data, PLANT, etc. on genome, protein databases)

Collaborative GRID (virtual reality, etc. on...steering ...)

Integration (heterogeneous dbs)

...other GRID classifications...



An Evolving and Wider Vision

Thinking about The GRID is evolving to encompass not just computational and data resources but to...

The decision maker, researcher, Doctor, surgeon...

In his own Virtual Organisation of collaborators

is provided with his own virtual col-laboratory, virtual environment, workbench environment...

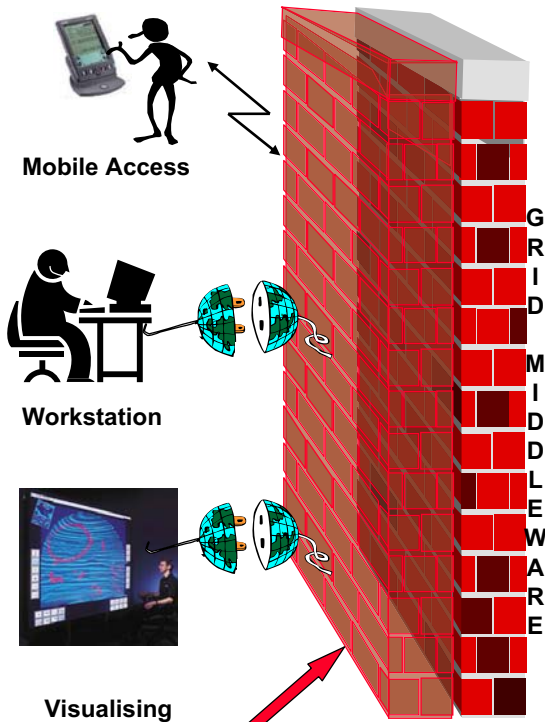
In which computers and technology make available to him in a transparent and easy fashion, independent of location and time...

All services that he/she needs for the best decision making...

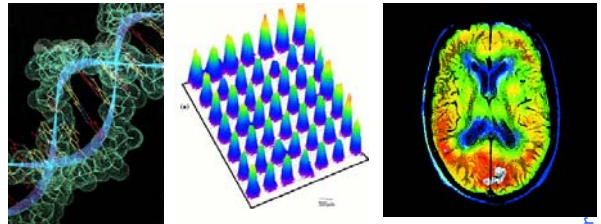
which may be information of all types from databases (including e.g. medical records...), compute power for applications (e.g. modelling), access to colleagues for consultation,

And the GRID is just an enabling technology in this vision

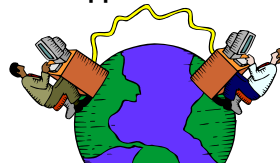
The User connects to his "Virtual Laboratory" or "Workbench Environment"



Supercomputer, PC-Cluster



Data-storage, Sensors, Experiments, Grid enabled Applications



Internet, networks

Integrating framework middleware

Examples of Different GRIDS

Simple Cycle-stealing GRIDS

SETI@home

Oxford University/United Devices: screening Anthrax toxin, Smallpox, certain cancers...

Pharmaceutical companies:

Novartis 2700 computers used to discover one most promising drug candidate

Plans to extend to much wider network

Ask a question you thought you could never ask
Reduce a "batch" problem to an interactive question!

A major change in productive working!

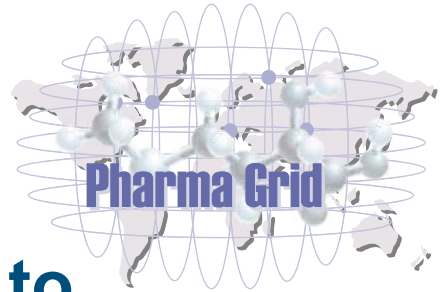
"Crunch GRIDS"

Aim: to be able to ask questions that did not make sense before because they took too much time

Reduce a "batch" problem to an interactive question!

Computer Farms
and "Cycle Harvesting"

The example of  NOVARTIS



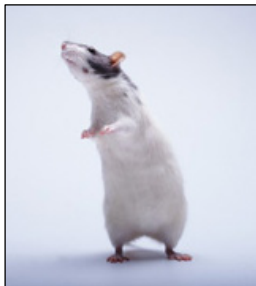
Pharma Grids – Key to Pharmaceutical Innovation?

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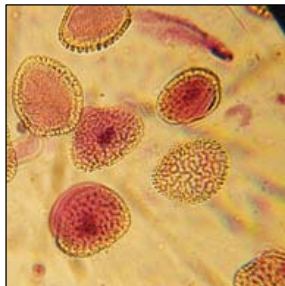
The Evolving *in silico* Science Platform

Evolution of the Pharmaceutical Industry:

In Vivo



In Vitro

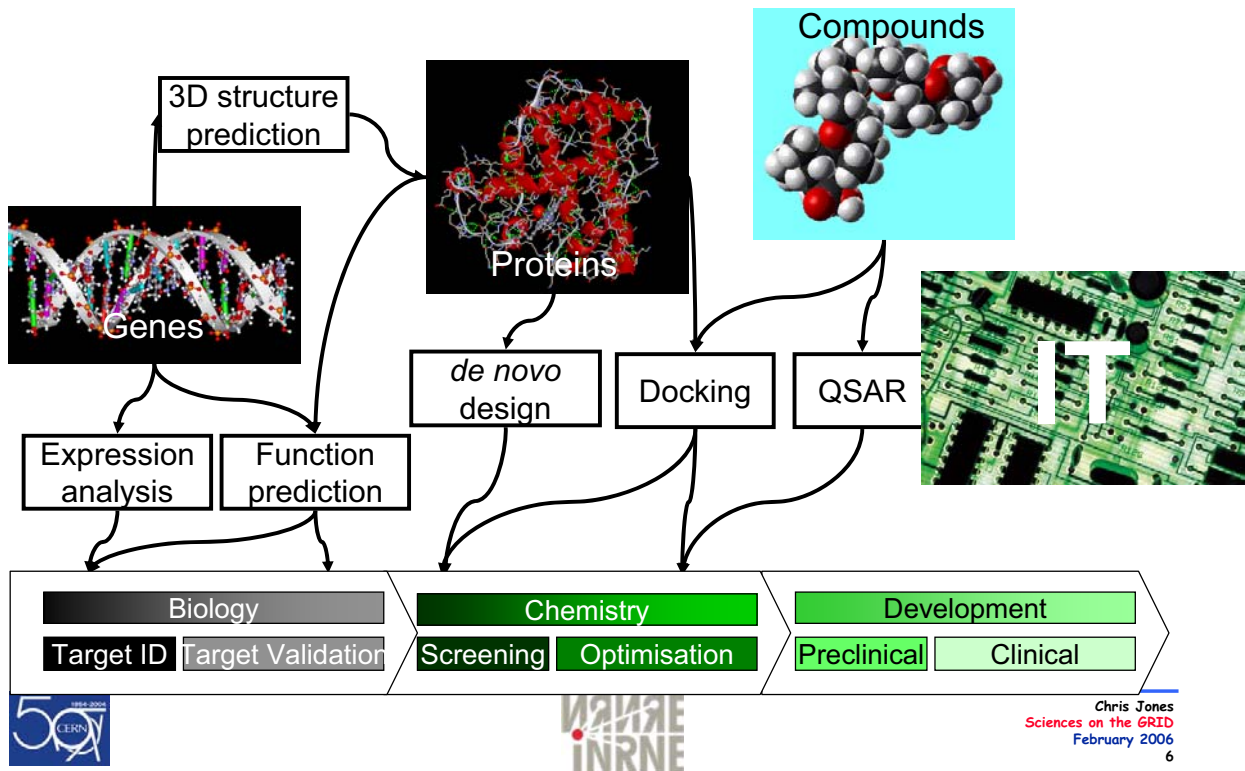


In Silico



[Time]

The Contribution of IT to Drug Discovery is Increasing



Novartis Has Implemented a Globally Coherent Pharma Grid Strategy

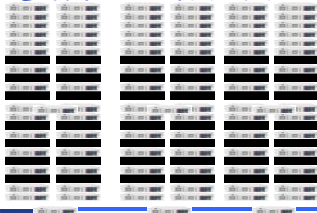
Users and applications :



Cluster existing HPC infrastructure :



Large shared Linux Clusters



Shared PC grid



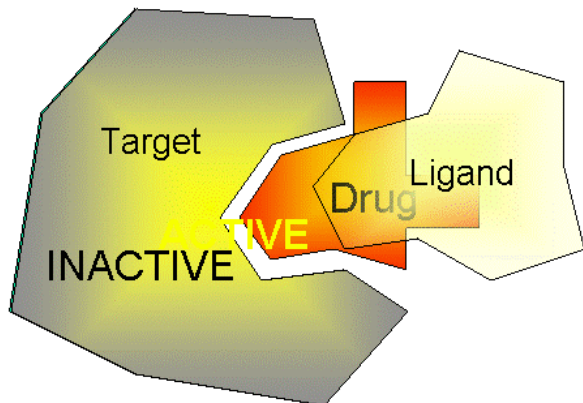
Shared Multi-processor servers



External Collaborations

Chris Jones
Sciences on the GRID
February 2006

Influencing Bio-molecular Processes



Target = enzyme, receptor, nucleic acid, ...

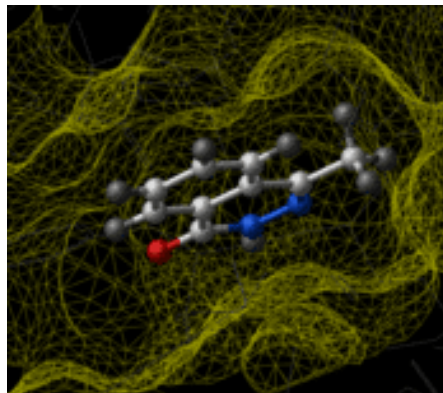
Ligand = substrate, hormone, other messenger, ...

Virtual Screening by *in silico* Docking

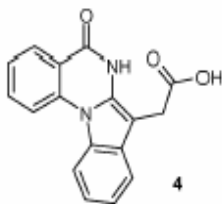


Docking
Process
and
Selection
of
possible
hits

< 100
Compounds



Results



Conclusion

We have identified a 7-substituted indoloquinazoline compound as a novel inhibitor of protein kinase CK2 by **virtual screening of 400 000 compounds**, of which a dozen were selected for actual testing in a biochemical assay. The compound inhibits the enzymatic activity of CK2 with an IC₅₀ value of 80 nM, making it **the most potent inhibitor of this enzyme ever reported**. Its high potency, associated with **high selectivity**, provides a valuable tool for the study of the biological function of CK2.

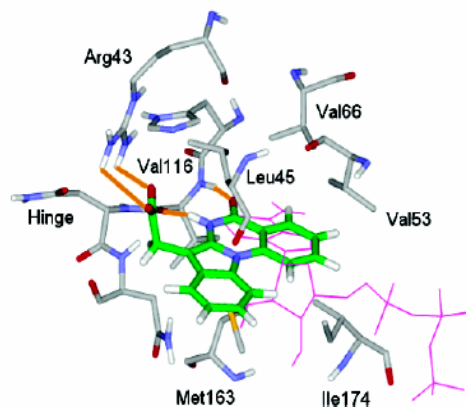


Figure 3. Relative binding modes of compound **4** (green) and the ATP analogue extracted from the crystallographic template structure 1DAW (magenta) in the human CK2 α active site. The hydrogen bonds formed with Arg 43 and Val 116 are indicated as orange lines.

Table 2. Selectivity Profile of Compound **4** in Terms of % of Inhibition of the Catalytic Activity of the Kinases at a Compound Concentration of 10 μ M

CK2	c-Abl	HER-1	HER-2	KDR	Flt-3	IGF-1R	c-Raf-1	PDGFR- β	c-Kit	Flt-4	Flt-1	Tek	PKA	c-src	CDK1	PKB	PKD1	Ins-R	FGFR-1	c-Met
97	25	12	29	54	41	44	30	11	31	30	21	36	51	0	51	30	9	23	32	40

Virtual Docking Accelerates the Docking Process at Negligible Additional Cost

Task: DOCK, ~320,000 molecules

Virtual docking of compounds from the Novartis Library into the 3D structure of a protein (target)

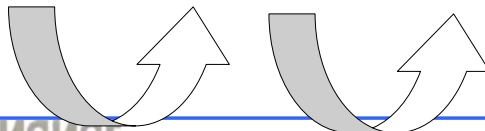
Elapsed time Hrs.

Elapsed time days

Elapsed time years

Devices in Grid:

55,794	547	6
2,325	23	
6.4		
	561	1200



WIRRE
INRNE

An aerial photograph of Basel, Switzerland, showing the Rhine river flowing through the city. The river is a deep blue, and a long bridge spans across it in the middle ground. The city is densely packed with buildings of various heights and colors, mostly in shades of grey and brown. In the background, the city extends to the horizon under a clear blue sky with some light clouds. The text is overlaid in the bottom right corner in a bold, yellow font.

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"Crunch GRIDS"

"Cycle Scavenging" with screen saver technology
(as used by SETI@Home)

Example of Oxford University, United Devices, IBM, Accelrys
www.GRID.org

In silico screening to select best molecules for *in vitro* bio-assay.

- Cancer
- Anthrax Toxin
- Smallpox



Grid.org

LigandFit

computational chemistry

NT_0.1.5 (2814)

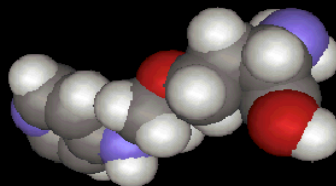
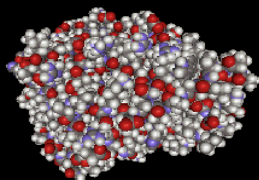
LIFE SCIENCES

Currently working on:
generating energy grid

Current Prospective Ligand 3D Structure:

168 hits

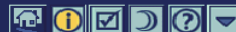
Current Protein Target:



Legend:

● Carbon	● Hydrogen	● Iron
● Oxygen	● Potassium	● Iodine
● Nitrogen	● Sodium	● Other

22 of 30 ligands processed





The Cancer Project

➤ Goal

- Exhaustive screen of 12 targets identified in multiple cancers using the world's largest molecular library

➤ Challenge

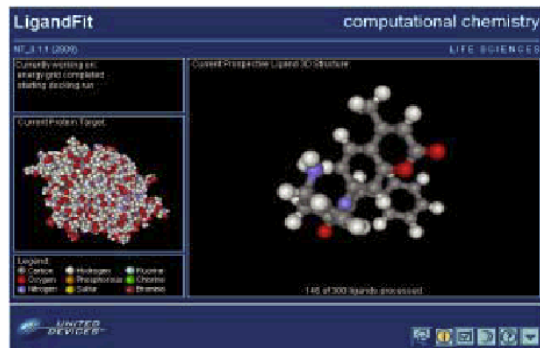
- Massive computational power was required to realize Oxford's vision

➤ Solution Highlights

- Built a working Public Grid dedicated to Life Science research
- Accomplished the initial stage of the project in less than 12 months

➤ Results

- Over 2.5M nodes from around the world are part of Grid.org
- Total CPU time for project was over 190,000 years
- Results published in Nature Drug Discovery



But these are simple GRIDS

The Vision in Life Sciences, and in many other sciences, is to use the GRID NOT just for cycle harvesting or scavenging, but to extend human capabilities with e.g.

Service GRIDS

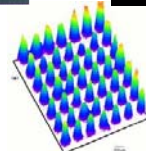
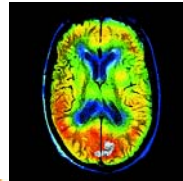
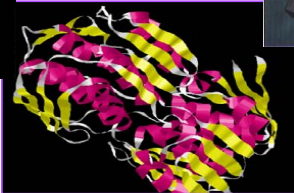
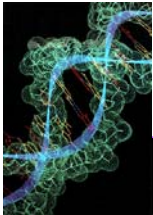
Information/Knowledge GRIDS

More informed decisions

Whilst many services and much information are potentially available to the decision maker today,

in practice there are so many barriers that such access and integration are not even considered

The vision is hence of the research worker or doctor able to make much more informed decisions because so many new services and information are available to support the decision.





Virtual Observatories

An example of a **SERVICE GRID**

Astrophysicists have images of objects in many **different wavelengths**, in **different distributed heterogeneous databases**:

Optical

Infrared

X-ray

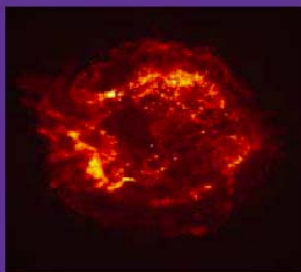
Radio

Etc.

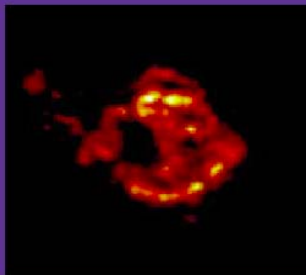
Share all these images in Virtual Observatories

In order to **COMPARE** images you need **MORE** than the Web

multi- λ
views of a
Supernova
Remnant



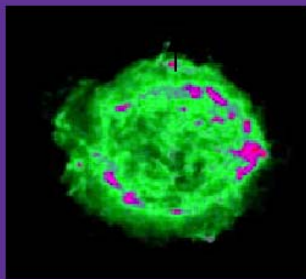
Shocks seen in the X-ray



Dust seen in the IR



Heavy elements
seen in the optical



Relativistic electrons
seen in the radio

Information / Knowledge GRIDS in Life Sciences

Many Active Projects

Discovery Net Snapshot

In Real Time

Scientific Information

Scientific Discovery

Discovery Workflow

Real Time Data Integration

Discovery Services

Dynamic Application Integration

Interactive Visual Analysis

Using Distributed Resources

Literature

Databases

Operational Data

Images

Instrument Data



Chris Jones
Sciences on the GRID
February 2006

MyGrid

Personalised
extensible environments for
data-intensive
in silico experiments

in biology

Professor Carole Goble,
University of Manchester

Dr Alan Robinson,
EBI

EMBL
European Bioinformatics Institute



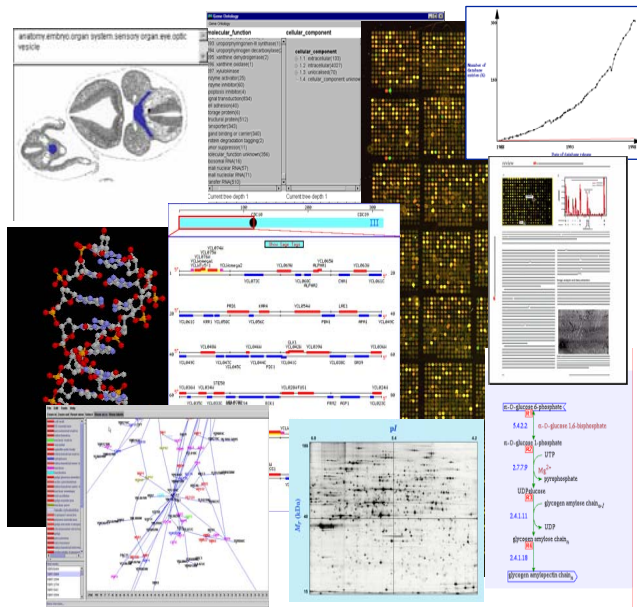
myGrid Project

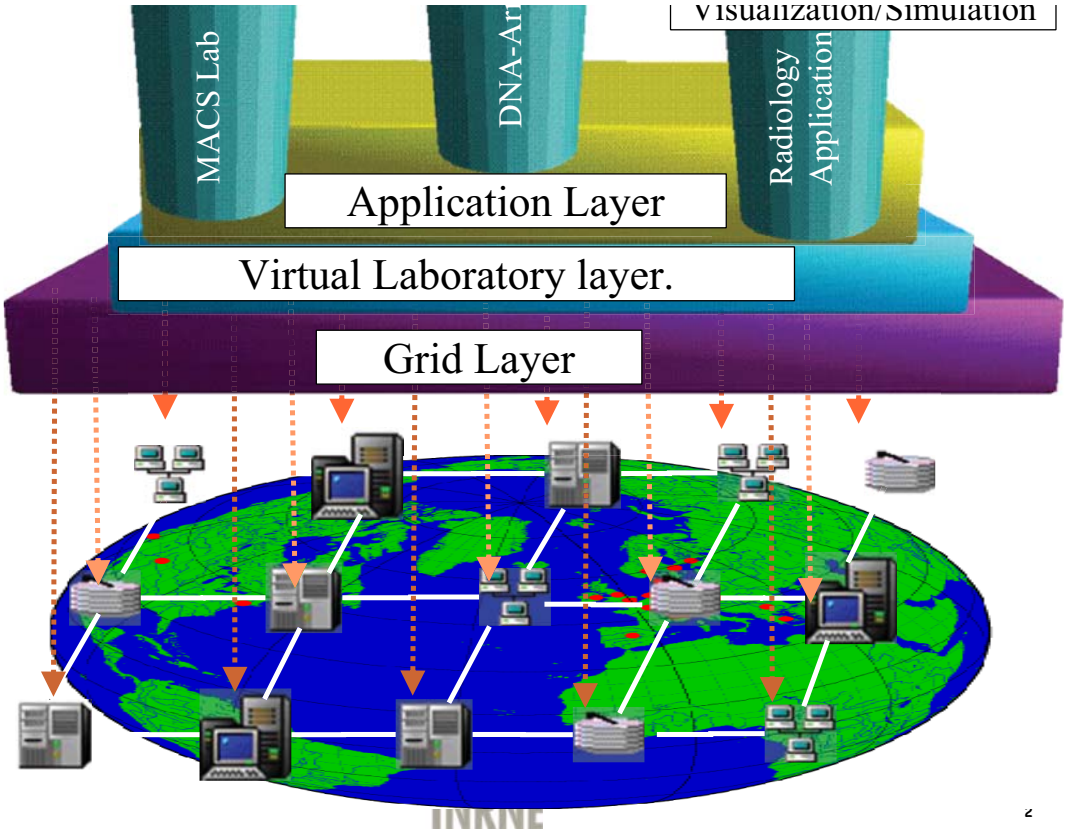
Imminent 'deluge' of data

Highly heterogeneous

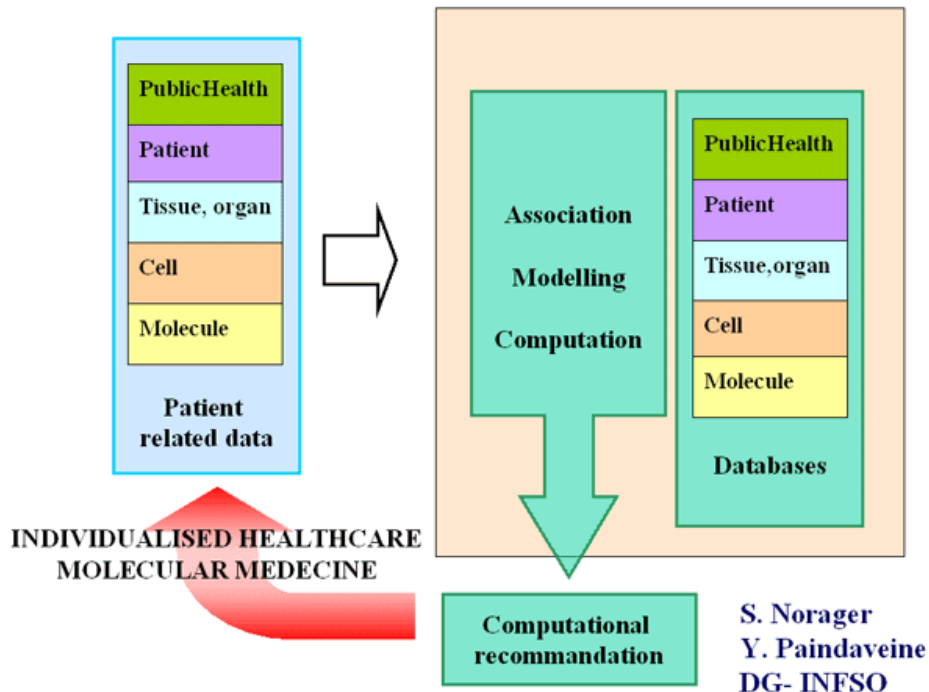
Highly complex and inter-related

Convergence of data and literature archives





HealthGRID - DG-INFSO



Health GRIDS

HEALTHGRID



Second European HealthGRID Conference

Third conference in Oxford, March 2005

Definition of "Health" is broad (see next)

There is a useful Web Site with much information linked

<http://www.healthgrid.org>

Presentation from Ignacio Blanquer.pdf



White Paper for EU in final draft

There are many issues in the use of informatics in the domain of health, but there are many people working





The Biomedical Informatics Research Network

**The Merger of Advanced Imaging
with Advanced Cyber Infrastructure**

Mark H. Ellisman

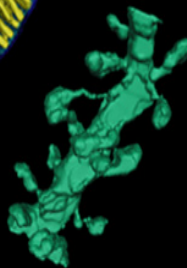
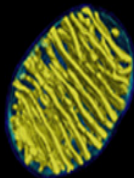
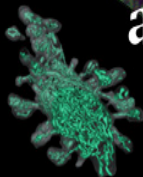
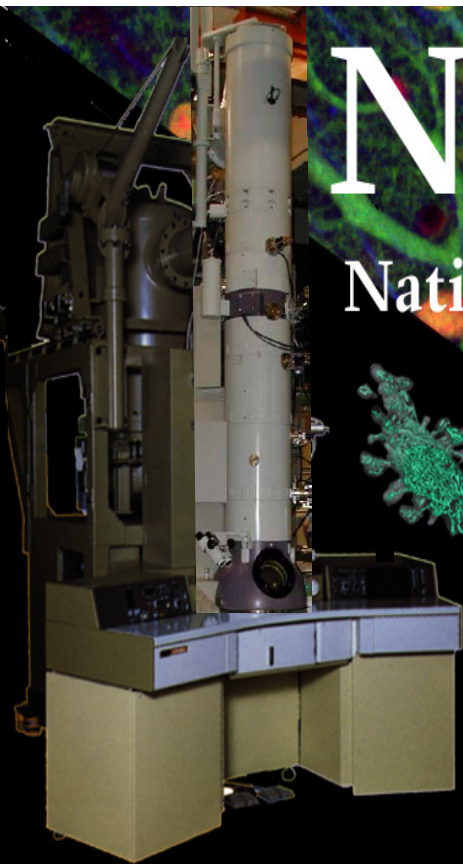
University of California San Diego

National Center for Microscopy and Imaging Research

N C M I R

National Center for Microscopy
and Imaging Research

An NIH sponsored Research Resource





Modern 3D Transmission Electron Microscope

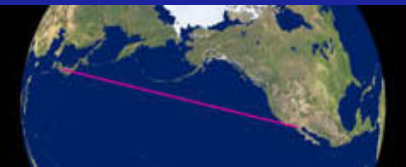
extreme penetration!

Ultra High Voltage EM @
Osaka Univ.

- 3 Million Electron Volts
- 15 Meters Tall
- 140 Tons
- \$\$\$ > 50M US Dollars
- only one of these



Trans-Pacific Telemicroscopy



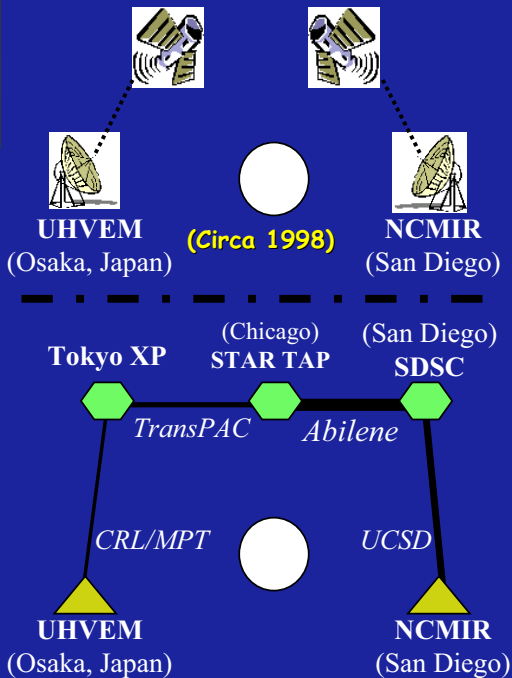
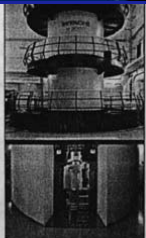
NET NEWS

Microscopy Across an Ocean

A big push by biologists to use computer networks to operate rare instruments from afar passed a major milestone on 25 June: Scientists took a spin on the world's most powerful electron microscope in Japan—while sitting 6000 kilometers away in California.

Six years ago, University of California, San Diego, neuroscientist Mark Ellisman thrilled audiences at a conference in Chicago by using the Internet to control an electron microscope in San Diego. Several U.S. agencies jumped in to fund projects for operating microscopes by remote control, and by now at least a dozen groups are doing so in the United States. Ellisman's team has since moved on to the Mount Everest of microscopes: Osaka University's Ultra High Voltage Electron Microscope, a 3,000,000-volt behemoth that can create three-dimensional images from much thicker samples (such as biological cells) than ordinary microscopes can. Ellisman and his U.S. and Japanese colleagues wondered if they could operate this instrument's roomful of controls from across the Pacific Ocean.

They showed they could. Over 5 hours, San Diego scientists imaged nerve cells from a rat and a frog without setting foot in Japan, controlling things like focus and specimen position across a private data line while the images came in across a satellite video link. Ellisman says this lays the groundwork for researchers all over the United States and Japan to borrow each others' specialized microscopes, probably via a high-speed Internet link, "within a year or two."



Now part of a production environment using IPv6

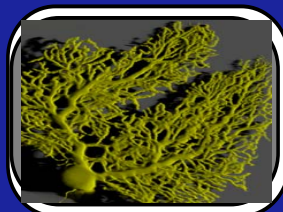
TELEMICROSCOPY & GRID - BASED COMPUTING

REMOTE ACCESS FOR DATA ACQUISITION AND ANALYSIS

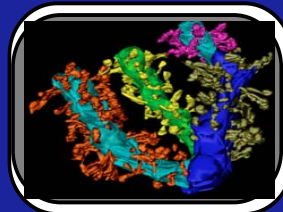
DATA ACQUISITION



DATA ANALYSIS



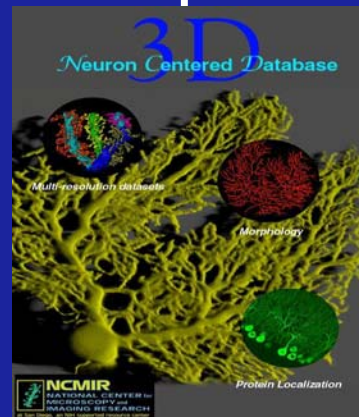
ADVANCED
COMPUTER
GRAPHICS



NETWORK



QuickTime™ and a YUV420 codec decompressor are needed to see this picture.



MULTI-
SCALE
DATA-
BASES

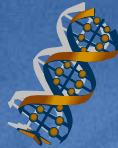
IMAGING
INSTRUMENTS

COMPUTATIONAL
RESOURCES

International Infrastructures for Science and Industry



Earth
Sciences



Life Sciences



Computer and
Information
Sciences

General Overview



Multidisciplinary
Research

$$E=MC^2$$

Math and
Physical Science



New Materials,
Technologies
and Processes



Social Sciences

Fabrizio Gagliardi
Director, Technical Computing, Microsoft EMEA

The e-Science Vision

- ◆ e-Science is about multidisciplinary science and the technologies to support such distributed, collaborative scientific research
 - Many areas of science are in danger of being overwhelmed by a 'data deluge' from new high-throughput devices, sensor networks, satellite surveys ...
 - Areas such as bioinformatics, genomics, drug design, engineering, healthcare ... require collaboration between different domain experts
- 'e-Science' is a shorthand for a set of technologies to support collaborative networked science

e-Science and the Grid

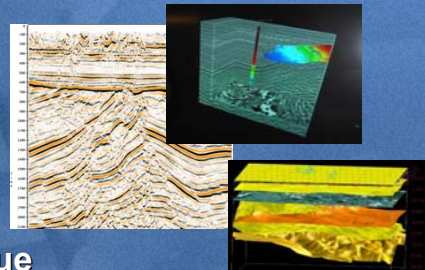
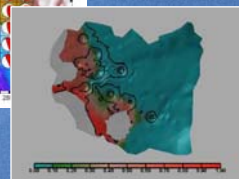
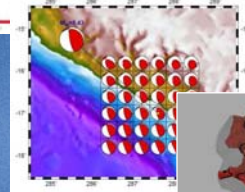
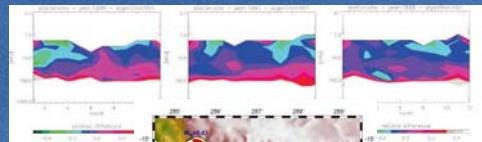
- ◆ **Cyberinfrastructure and e-Infrastructure**
 - In both the US and Europe there is a vision for the 'cyberinfrastructure' required to support the e-Science revolution
 - Set of Middleware Services supported on top of high bandwidth academic research networks
- ◆ **Similar to vision of the Grid as a set of services that allows scientists – and industry – to routinely set up 'Virtual Organizations' for their research – or business**
 - Many companies emphasize computing cycle aspect of Grids
 - The 'Microsoft Grid' vision should be more about data management than about compute clusters

Need for e-Infrastructures

- ◆ Science, industry and commerce are more and more digital, process vast amounts of data and need massive computing power
- ◆ We live in a “flat” world:
 - Science is more and more an international collaboration and often requires a multidisciplinary approach
- ◆ Need to use technology for the good cause
 - Fight Digital/Divide
- ◆ Industrial uptake has become essential

Some examples (from EU-EGEE): Earth sciences applications

- ◆ **Satellite Observations:**
 - ozone profiles
- ◆ **Solid Earth Physics**
 - Fast Determination of mechanisms of important earthquakes
- ◆ **Hydrology**
 - Management of water resources in Mediterranean area (SWIMED)
- ◆ **Geology**
 - Geocluster: R&D initiative of the Compagnie Générale de Géophysique



More examples: MAGIC, cosmic physics

- ◆ Ground based Air Cerenkov Telescope 17 m diameter

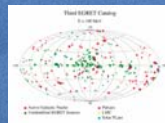
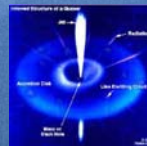
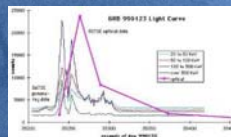
- ◆ Physics Goals:

- Origin of VHE Gamma rays
- Active Galactic Nuclei
- Supernova Remnants
- Unidentified EGRET sources
- Gamma Ray Burst

- ◆ MAGIC II will come 2007

- ◆ Grid added value

- Enable “(e-)scientific” collaboration between partners
- Enable the cooperation between different experiments
- Enable the participation on Virtual Observatories



and more: Computational Chemistry

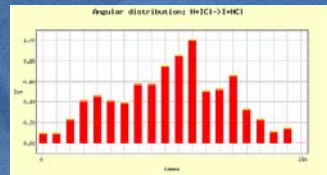
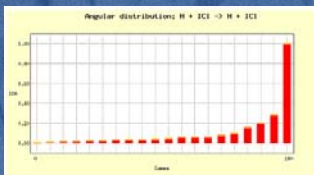
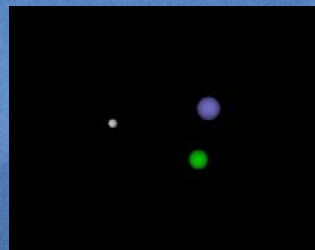
◆ The Grid Enabled Molecular Simulator (GEMS)

➤ Motivation:

- Modern computer simulations of biomolecular systems produce an abundance of data, which could be reused several times by different researchers.
 - ➔ data must be catalogued and searchable

➤ GEMS database and toolkit:

- autonomous storage resources
- metadata specification
- automatic storage allocation and replication policies
- interface for distributed computation



Planck: Cosmological studies

On the Grid:

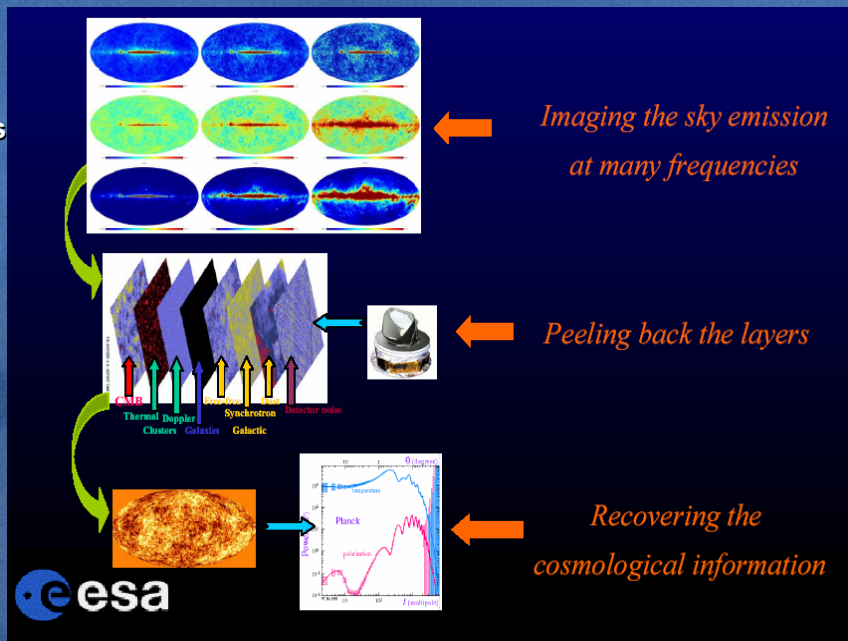
- > 12 time faster
- (but ~5% failures)

Complex data structure

- → data handling important

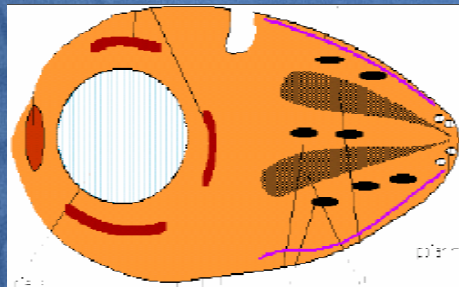
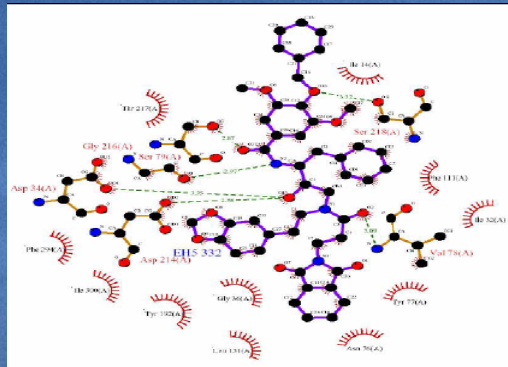
The Grid as

- collaboration tool
- common user-interface
- Flexible environment
- new approach to data and S/W sharing



Drug Discovery: a new hope for developing countries

- ◆ **Grid-enabled drug discovery process**
 - Reduce time required to develop drugs
 - Develop the next steps of the process (molecular dynamics)
- ◆ **Data challenge proposal for docking on malaria**
 - Never done on a large scale production infrastructure
 - Never done for a neglected disease
- ◆ **Data challenge during the summer**
 - 5 different structures of the most promising target
 - Output Data: 16,5 million results, ~10 TB
- ◆ **Added value**
 - Facilitates inclusion of developing countries
 - Tool to enhance collaboration building
 - Facilitate distributed software development for complex integrated workflows



Earth Science Activity

David Weissenbach (IPSL)
weissenb@ccr.jussieu.fr



EGEE is funded by the European Union under contract IST-2003-508833

EARTH SCIENCE

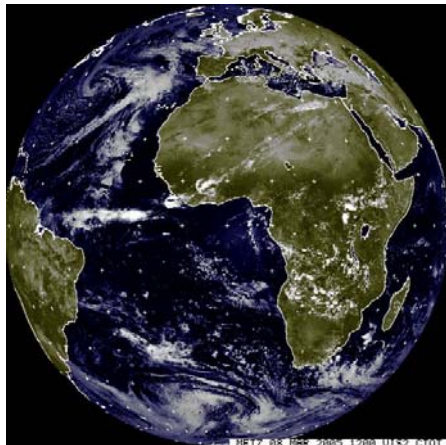
The Earth is a complex system, centre of a large variety of phenomena.

Its description is separated in various independent domains with interfaces between them

Solid Earth Ocean Atmosphere

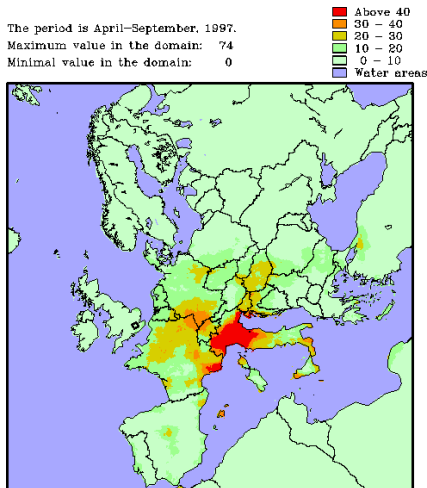
The approach could be based on physics, chemistry and/or biology

➔ The community is constituted by many small groups, that aggregate for projects (and separate afterwards).



Pollution (T.ostromsky ceco@parallel.bas.bg)

- BAS(Bulgaria): implementation of a large scale air pollution model on EGEE, for evaluation of the concentrations of a large variety of chemical species, responsible for the air pollution
- Model based on a parallel architecture
 - Distribution of computation
 - Development of new advanced splitting scheme (planned)



Difficulties:

- Large sets of data input and output: need a specific management
- Optimisation to take full advantage of the Grid

Recent past history

- ◆ Meta-computing and distributed computing
early examples in the 80' and 90' (CASA, I-Way, Unicore, Condor etc.)
- ◆ EU-US workshop in Annapolis in 1999 on
large scientific data bases:
<http://www.cacr.caltech.edu/euus/>
- ◆ EU FP5 and US Trillium and national Grids
- ◆ EU FP6, US OSG, NAREGI/Japan...

GRIDs – IST in FP5 projects (~36m Euro) An integrated approach

Applications

GRIA

EGSO

CROSSGRID

Middleware
& Tools

GRIP

EUROGRID

GRIDSTART

GRIDLAB

DATAGRID

DAMIEN

DATATAG

Underlying
Infrastructures

Industry / business

Science

Current situation: accomplishments and challenges

- Many Grids around the world, very few maintained as a persistent infrastructure (a good example is the Google Grid)
- Need for public and open Grids (OSG, EGEE and related projects, NAREGI, and TERAGRID, DEISA good prototypes)
- Persistence, support, sustainability, long term funding, easy access are the major challenges

- Access to IT-resources
(connectivity, computing, data,
instrumentation...) for scientists:

- **Providing e-Infrastructure**

- Géant2
- EGEE
- DEISA
- SEE-GRID

- **Benefiting from e-Infrastructure**

- DILIGENT
- SIMDAT
- GRIDCC
- CoreGRID
- GridLab

- **Concertation: GRIDSTART, GridCoord**

- **Grid mobility: Akogrimo**

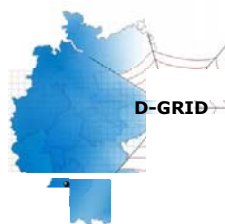


SIMDAT ##



- **Sample of National Grid projects:**

- Austrian Grid Initiative
- DutchGrid
- France:
 - e-Toile
 - ACI Grid
- Germany
 - D-Grid
 - Unicores
- Grid Ireland
- Italy
 - INFNGrid
 - GRID.IT
- NorduGrid
- UK e-Science
 - National Grid Service
 - OMII
 - GridPP project



- **EGEE**

- **Objectives**

- consistent, robust and secure service grid **infrastructure** for many applications
- improving and maintaining the **middleware**
- attracting **new resources and users** from industry as well as science

- **Structure**

- 71 leading institutions in 27 countries, federated in regional Grids
- leveraging national and regional grid activities worldwide
- funded by the EU with ~32 M Euros for first 2 years starting 1st April 2004



- **Objectives**

- Large-scale, production-quality **infrastructure** for e-Science
 - leveraging national and regional grid activities worldwide
 - consistent, robust and secure
- improving and maintaining the **middleware**
- attracting **new resources and users** from industry as well as science

- **EGEE**

- 1st April 2004 – 31 March 2006
- 71 leading institutions in 27 countries, federated in regional Grids

- **EGEE-II**

- Proposed start 1 April 2006 (for 2 years)
- Expanded consortium
 - > 90 partners in 32 countries (also non-European partners)
 - Related projects, incl.
 - *BalticGrid*
 - *SEE-GRID*
 - *EUMedGrid*
 - *EUChinaGrid*



• Infrastructure

- >170 sites
- >15 000 CPUs
- >5 PB storage
- >10 000 concurrent jobs
- >60 Virtual Organisations

• Middleware

- Now at gLite release 1.4
 - Focus on basic services, easy installation and management
 - Industry friendly open source license



Applications: >20 applications from 7 domains

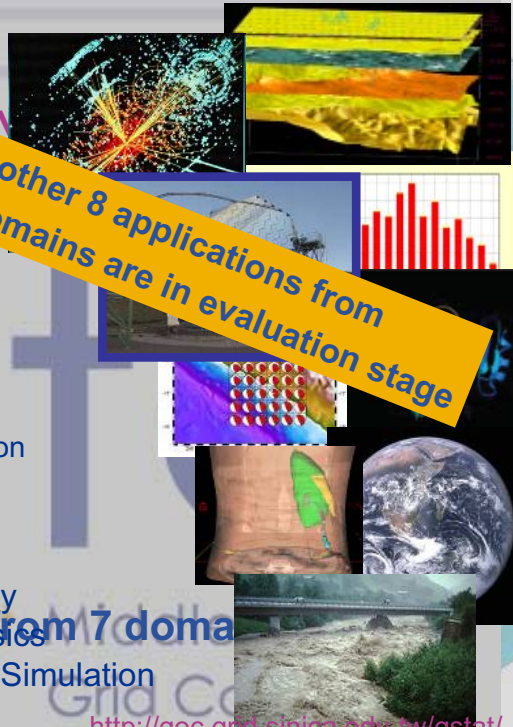
High Energy Physics

Biomedicine

Earth Sciences

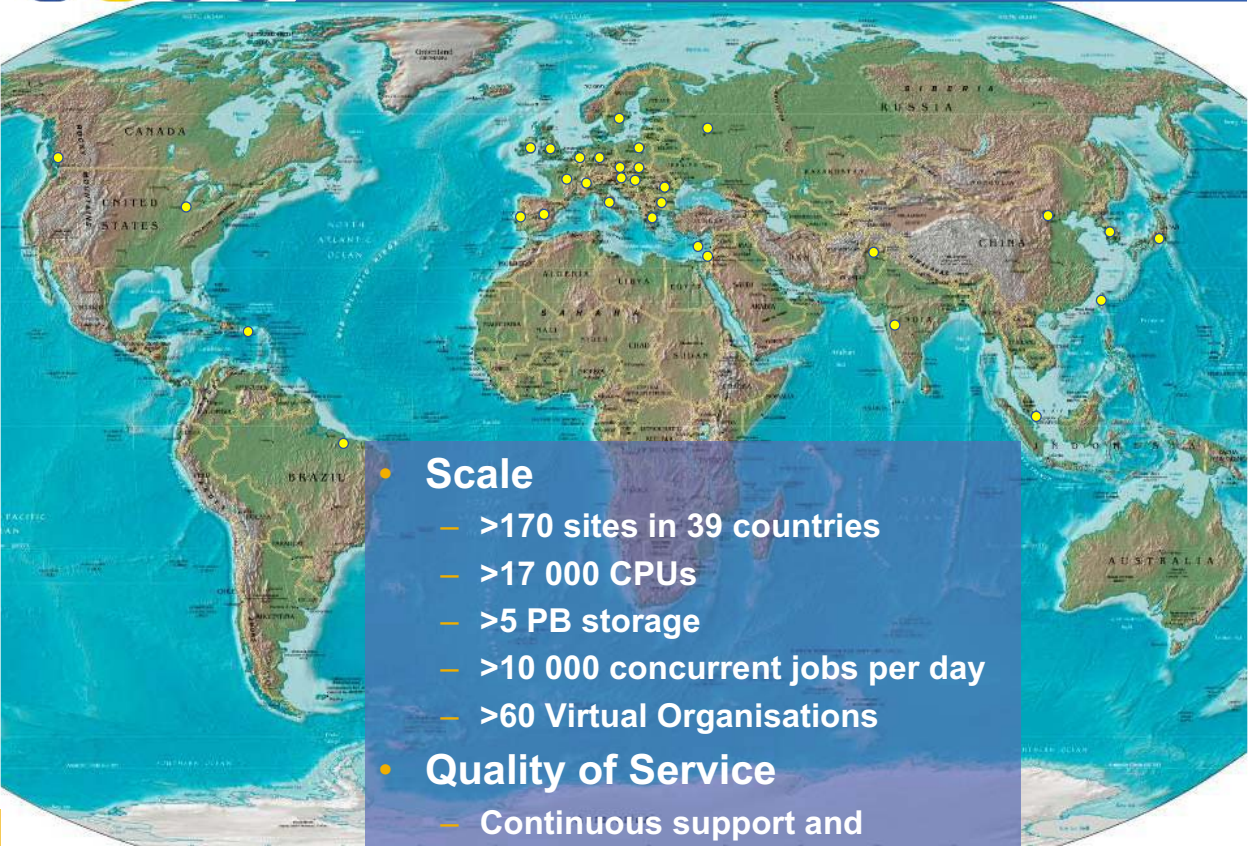
- Astronomy
- Geo-Physics
- Financial Simulation

Another 8 applications from 4 domains are in evaluation stage



<http://goc.grid.sinica.edu.tw/gstat/>

- **Infrastructure**



- **Production service**

- Based on the LCG-2 service
- With new resource centres and new applications encouraged to participate
- Stable, well-supported infrastructure, running only well-tested and reliable middleware

- **Pre-production service**

- Run in parallel with the production service (restricted nr of sites)
- First deployment of new versions of the middleware
- Applications test-bed

- **GILDA testbed**

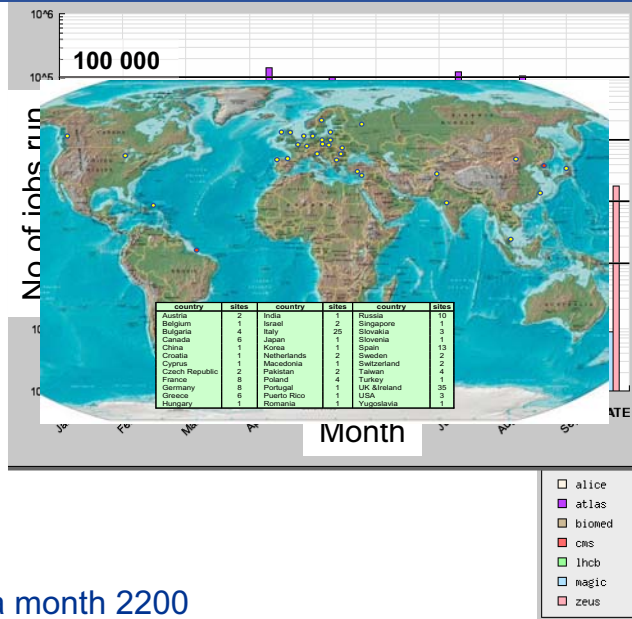
- <https://gilda.ct.infn.it/testbed.html>
- Complete suite of Grid elements and applications
 - Testbed, CA, VO, monitoring
- Everyone can register and use GILDA for training and testing



- **Scale of the production service**
 - ~16K CPUs/170 sites
 - Other national & regional grids: ~60 sites, ~6000 processors
 - greatly exceeds no of sites planned for the end of EGEE

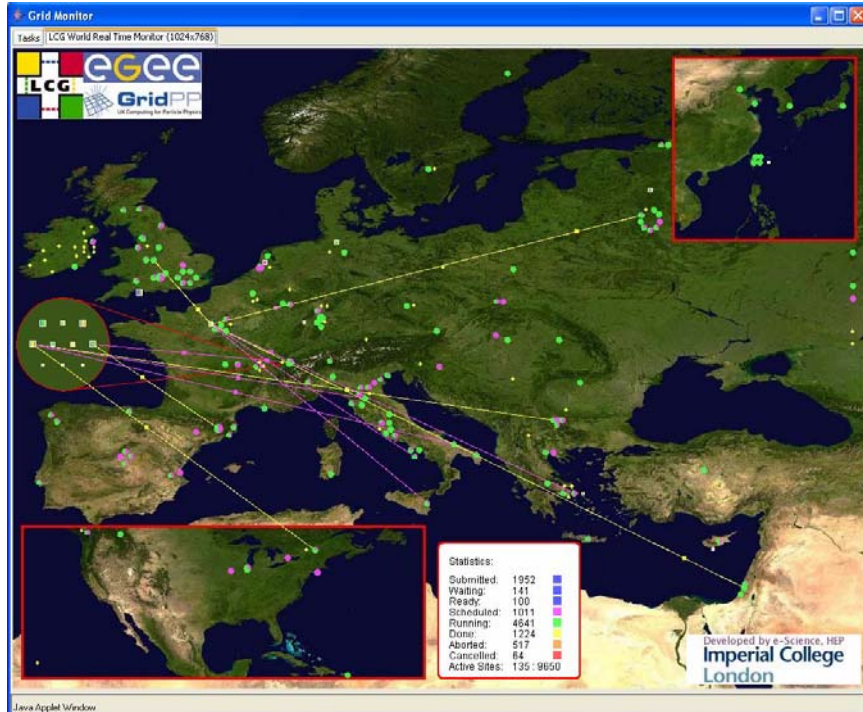
- **Interoperability demonstrated with OSG**
(ongoing work with ARC)

- **> 2.2 million jobs Jan-Oct 2005**
 - Daily averages, sustained over a month 2200 – 10 100
- ~6 M kSI2K.cpu.hours \cong ~700 cpu years



LCG2 Real Time Monitor

- Java tool
- Displays jobs running (submitted through RBs)
- Shows jobs moving around world map in real time, along with changes in status



<http://gridportal.hep.ph.ic.ac.uk/rtm/>

(snapshot 18 November 2005)

Books, Details...

The Grid - A Book

"Blueprint for a New Computing Infrastructure"

A Serious Textbook - university course level

Ian Foster and Carl Kesselman are the editors

Two chapters of **Overview**

Twenty chapters of **detailed areas**
written by appropriate experts:

challenges to be met

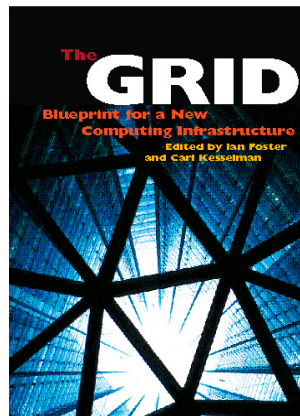
review of the state of the art

Morgan Kaufmann publishers

<http://www.mkp.com/>

*"This is a source book for the
history of the future."*

Vint Cerf, Senior Vice President,
Internet Architecture and Engineering,
MCI Communications



And another and newer book...

Grid Computing

Making the Global Infrastructure a Reality

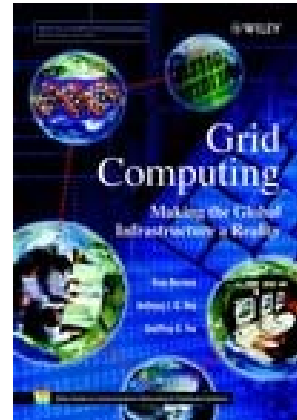
Fran Berman

Geoffrey C. Fox

Anthony J.G. Hey

Wiley

www.wiley.com



Global GRID Forum



First Meeting, joining separate Grid Forum initiatives, **Amsterdam in April 2001**, sold out with 350 people

Subsequent meetings in Washington, Rome, Toronto, Edinburgh, Chicago, excellent attendance

And growing industry attendance

As the role that industry will play in this open source - open interface unfolds



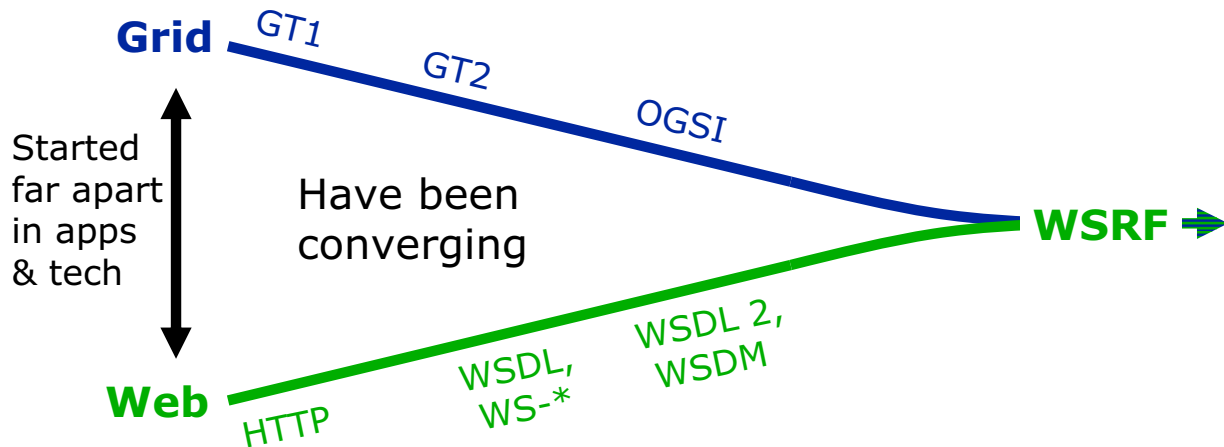
Seventh Meeting, March 2003, Japan

Eight Meeting, June 2003, Seattle...

www.ggf.org



Grid and Web Services: Convergence: Yes!



The definition of WSRF means that Grid and Web communities can move forward on a common base

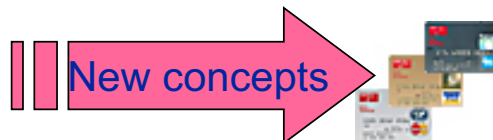
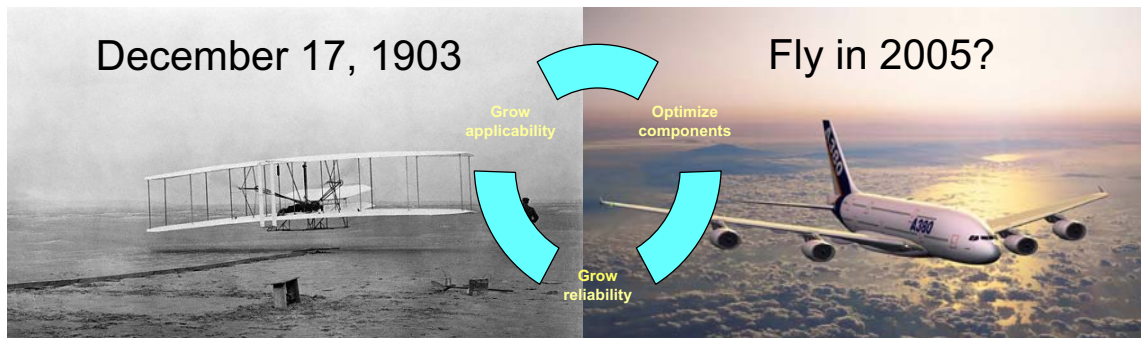
So where are we?
When is this all going to happen?

The „Kitty Hawk Project”: will it fly?

Pave the way towards achieving new functionality by
combining available components



Let's make it fly!

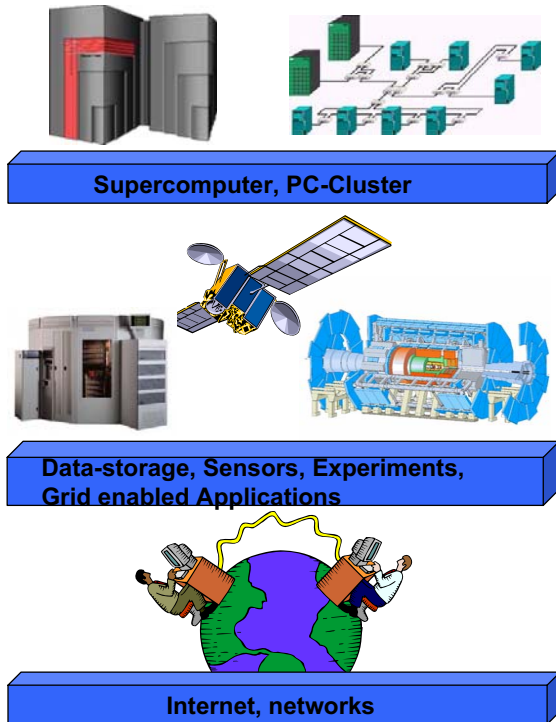
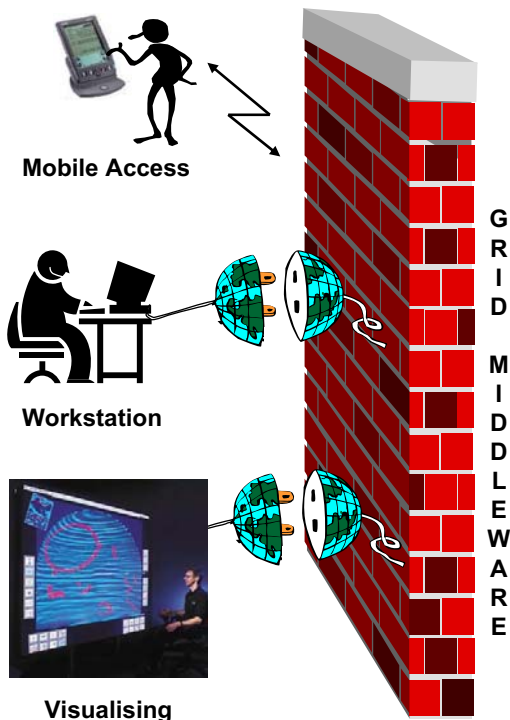


100 years of optimization and improvements

Thank You

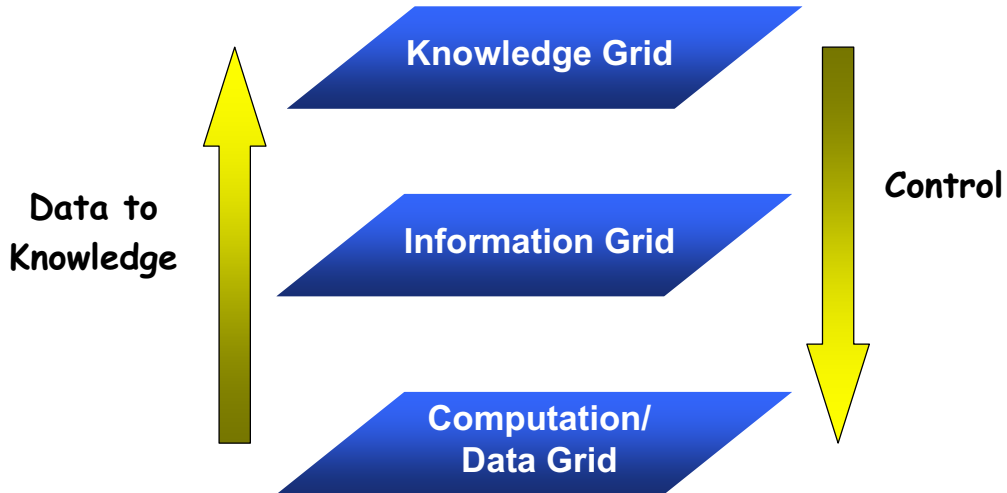


The "One-Stop Shopping" view of the GRID



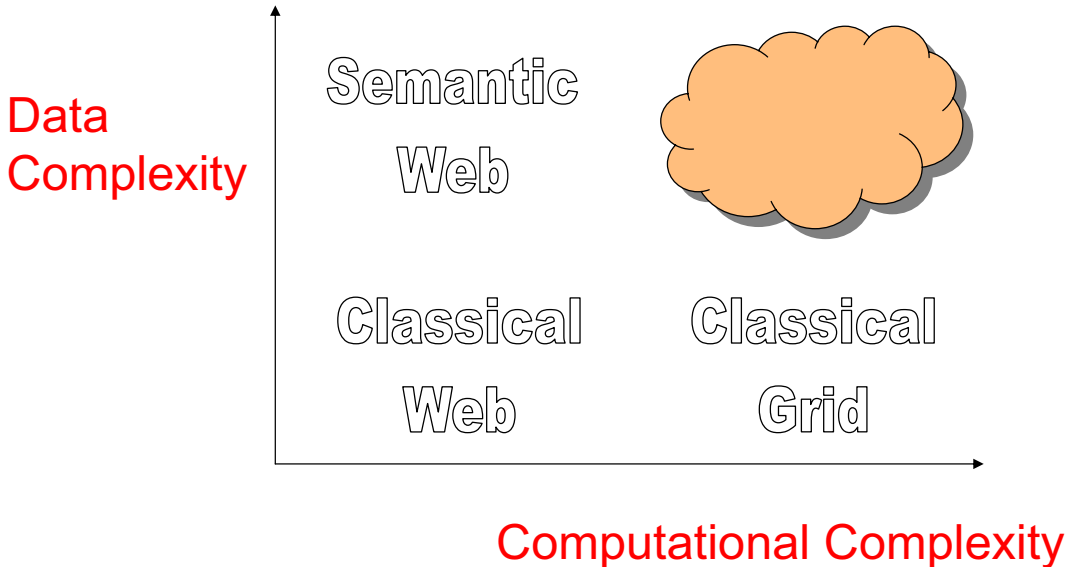
Hoffmann, Putzer, Reinefeld

Three Layer GRID Abstraction



- Data Un-interpreted bits and bytes
- Information Data equipped with meaning
- Knowledge Information applied to achieve a goal, solve a problem or enact a decision

Databases in the Grid



A final word

Of course this vision raises **many questions and obstacles that must be faced** at the same time as the technology is developed:

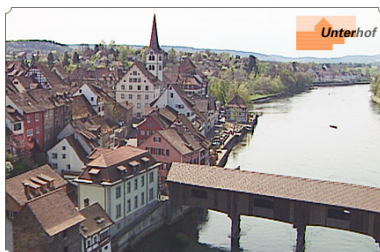
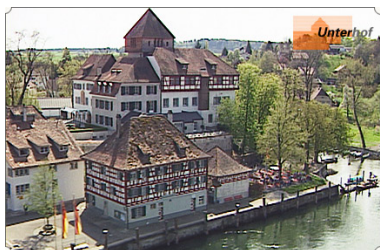
- questions of security,
- access rights,
- authentication,
- ethics,
- policies etc.

This is true of most new technologies

It is important that these issues are faced directly and not later as has been all too often the case.



PharmaGRID 2004



**2004 PharmaGRID Retreat
July 7th-9th 2004**

Seminarhotel Unterhof,

Diessenhofen, Switzerland

**Aims to bring together industry
professionals, stakeholders
and leading GRID practitioners**

For more information

www.pharmaGRID.com

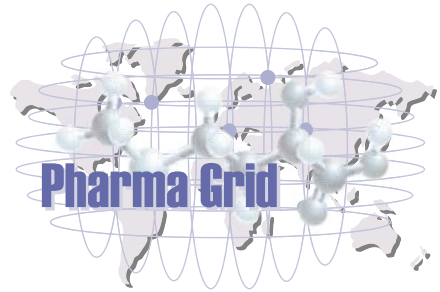
Pharma Grids: Integration Potential in Both the Private and the Public Sectors

Disease knowledge resource:

Third world diseases

Rare diseases (orphan diseases)

Lead discovery for third world
and/or rare diseases



Educational resource:

Training of health care professionals
(eLearning) (in particular in remote locations)

On-line assistance to health care professionals (in particular in remote
locations)

The University of Basel Contribution to the Dengue Knowledge Grid



www.bc2.ch/grid-forum

[BC]²

Basel Computational
Biology Conference

March 18-19
2004



Chris Jones
Sciences on the GRID
February 2006

Further Initiatives towards Knowledge Resources for Neglected Diseases

NIH:

NCCR (Natl. Center for Research Resources) and
Office of Rare Diseases; contact Dr Howard Bilofsky,
bilofsky@pcbi.upenn.edu

Virginia Bioinformatics Institute (Prof. B.Sobral)

<https://research.vbi.vt.edu>

PathPort: information resource on Anthrax, Plague, Smallpox,
many types of hemorrhagic fevers

PharmaGrid 2004 (chris.jones@cern.ch), co-sponsored and co-
organised by PRISM (www.prismforum.org)

There are issues at each layer



Data Acquisition

- In 1993 WTSI (then the Sanger Centre – named after double Nobel prize winner – Fred Sanger) started with just a few gigabytes of data

If WTSI storage had stayed in line with Moore's Law

1993	94	1995	96	1997	98	1999	2000	2001	02	2003	04	2005
20GB		40GB		80GB		160GB		320GB		640GB		1.3TB

- Within the first 6 years (1993-1999) our data store had grown to over 4.5 Terabytes (4,500 gigabytes).