**1ST IBERIAN GRID INFRASTRUCTURE CONFERENCE**
14-16 May 2007, Santiago de Compostela, Spain
www.ibergrid.eu


# D-Grid in International Context

## Lessons Learned and Recommendations

Wolfgang Gentzsch
D-Grid, RENCI, OGF, e-IRG, Duke

with support from
Tony Hey, Stephen Newhouse, et al, Satoshi Matsuoka, Kazushige Saga,
Hai Jin, Bob Jones, Charlie Catlett, Dane Skow,
D-Grid Team,
and the Renaissance Computing Institute at
UNC Chapel Hill, North Carolina



# Today's Topics


- Let me start with D-Grid
- Examples of e-Science grid projects and their Key Objectives
- Components of an e-Science infrastructure and Grid middleware
- Challenges for research and industry
- Sustainability of e-Infrastructures
- e-Science applications
- Attracting and integrating new Grid Communities
- Lessons learned and recommendations

# D-Grid at a Glance


## Building a National e-Infrastructure for Research and Industry

- 01/2003: Pre-D-Grid Working Groups ➔ Recommendation to Government
- 09/2005: D-Grid-1: early adopters, 'Services for Science'
- 01/2007: D-Grid-2: new communities, 'Service Grids'
- 01/2008: D-Grid-3: Service Grids for research and industry

- D-Grid-1: 25 MEuro > 100 Orgs > 200 researchers
- D-Grid-2: 25 MEuro > 50 addl Orgs > 200 addl researchers
- D-Grid-3: Call in May 2007

➢ **Important:**

- ➢ Sustainable production grid infrastructure after the end of the funding
- ➢ Integration of new communities
- ➢ Evaluating business models for grid services

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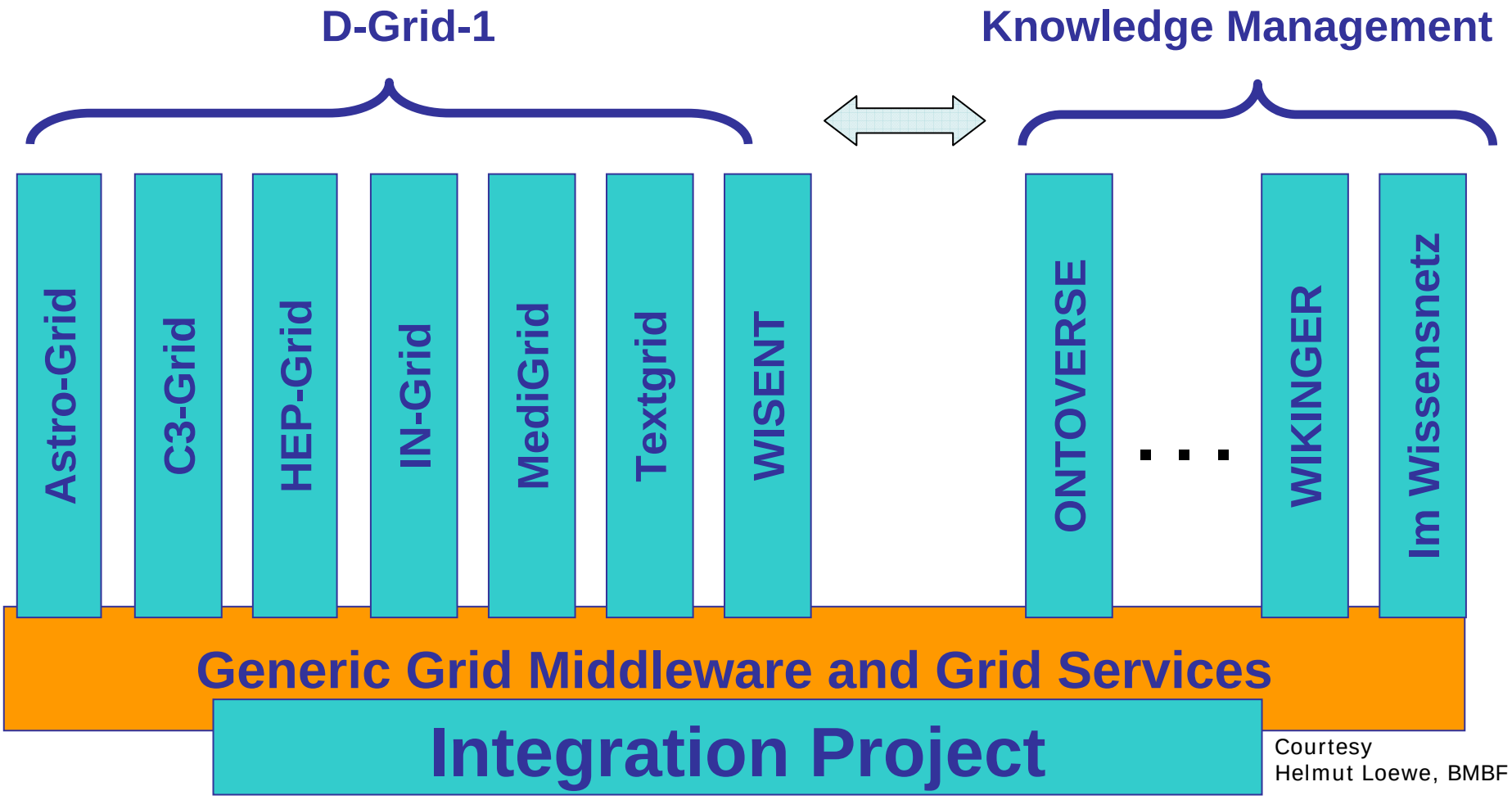
# D-Grid




Courtesy
Helmut Loewe, BMBF

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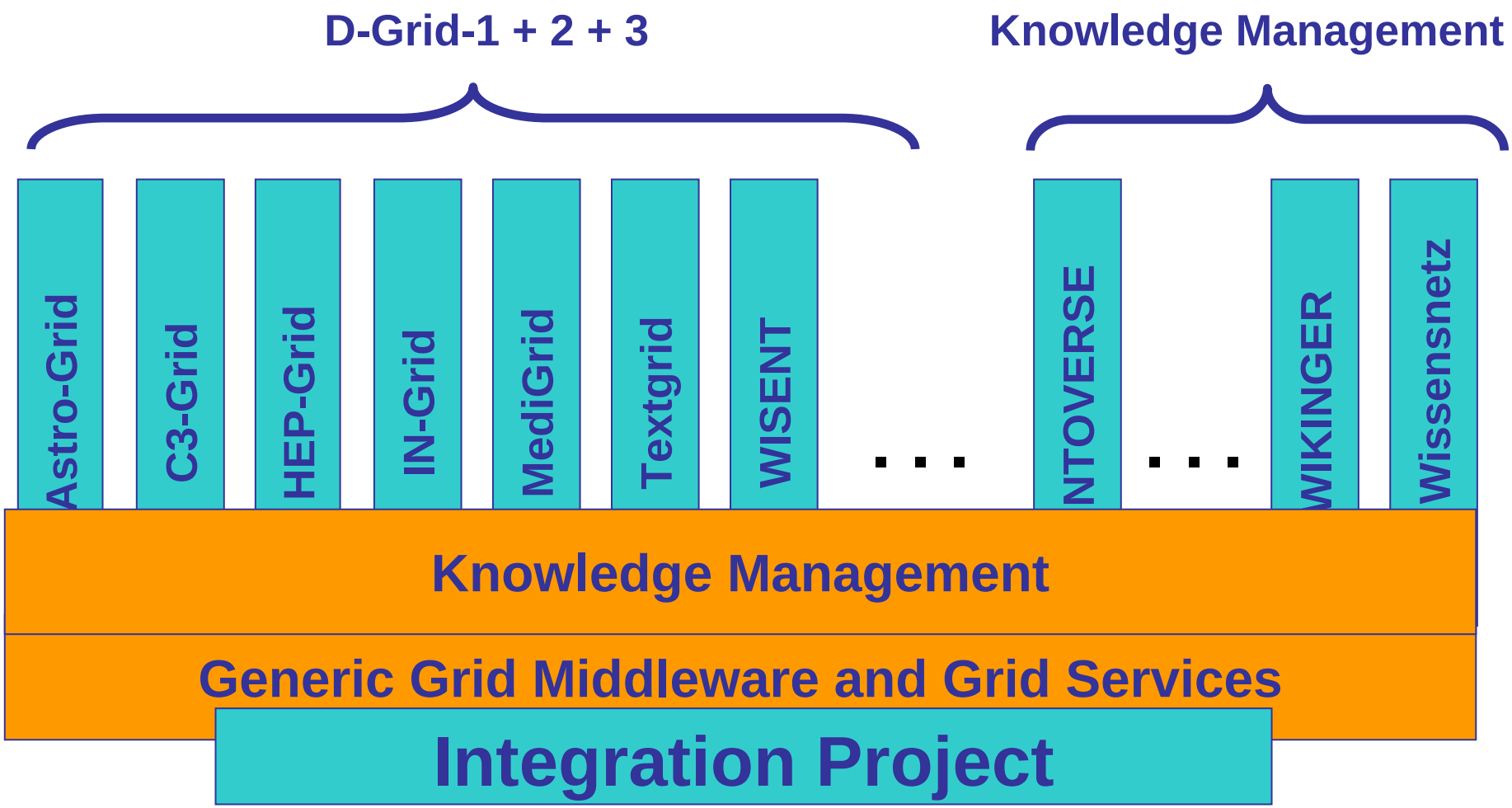
# D-Grid



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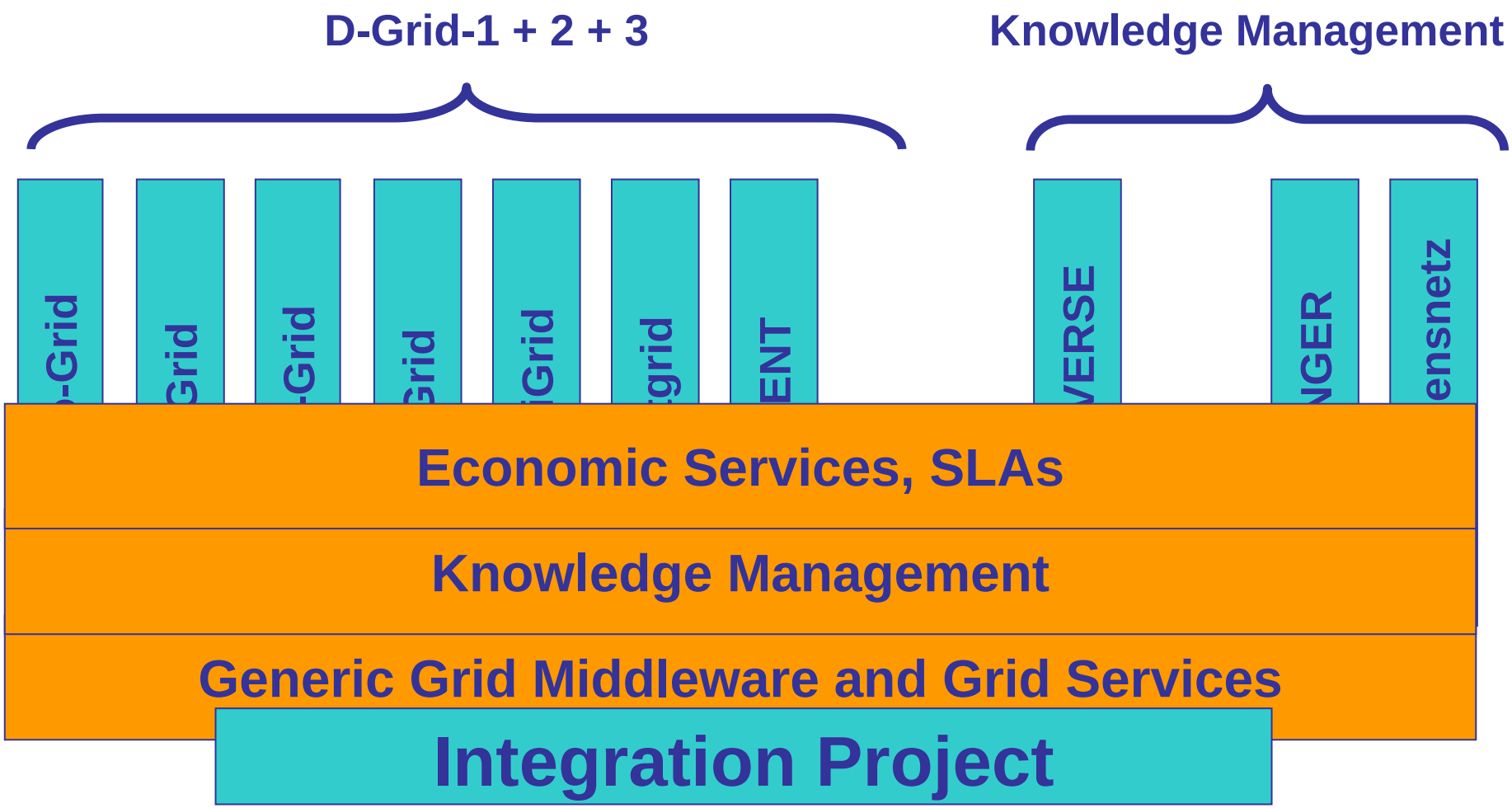

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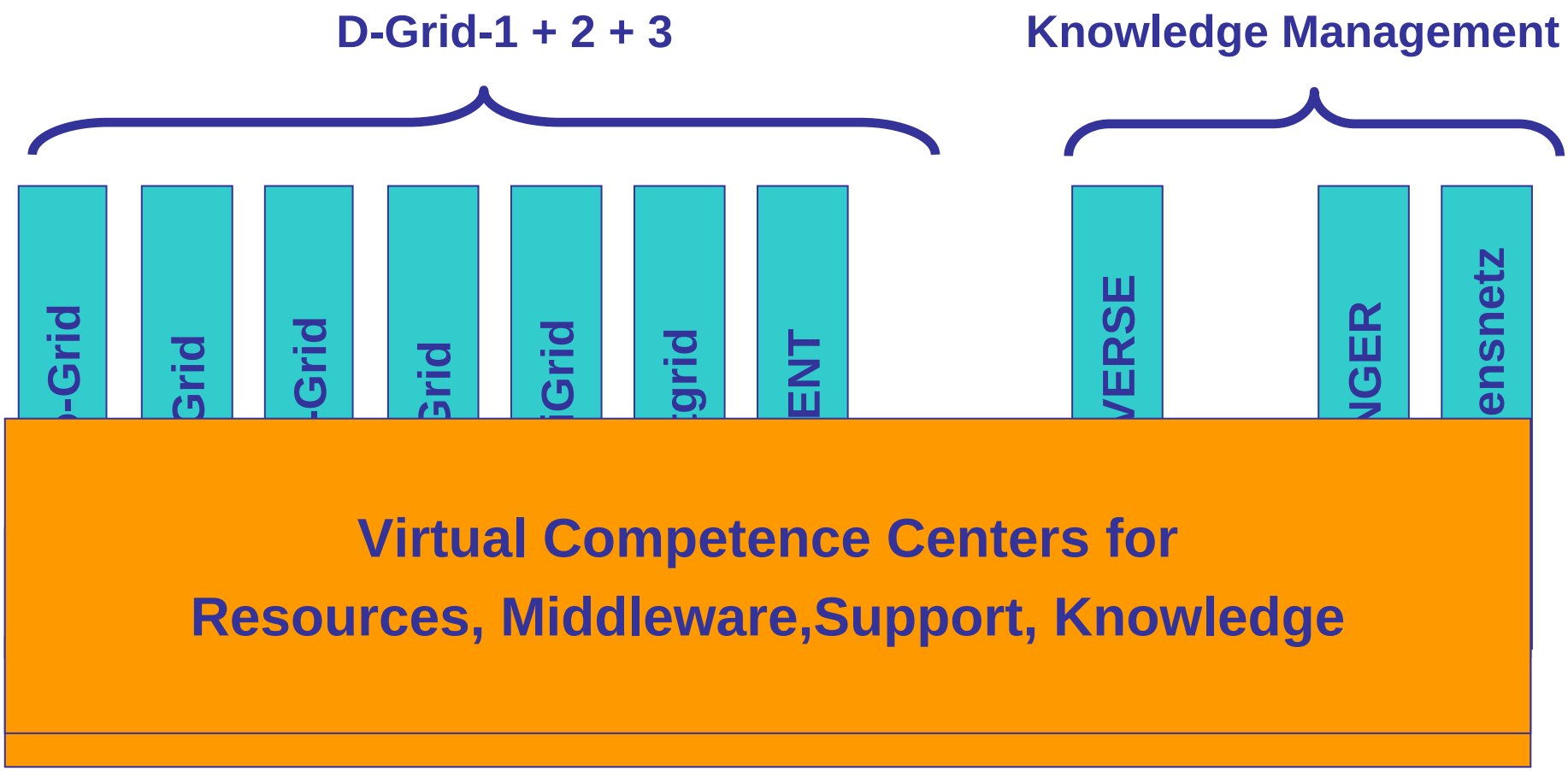
# D-Grid



# Core D-Grid

**Objective:**

- establishment and operation of the Core D-Grid infrastructure by the D-Grid integration project (DGI)
- evaluation of interoperability and performance of resources

**The Core D-Grid comprises:**

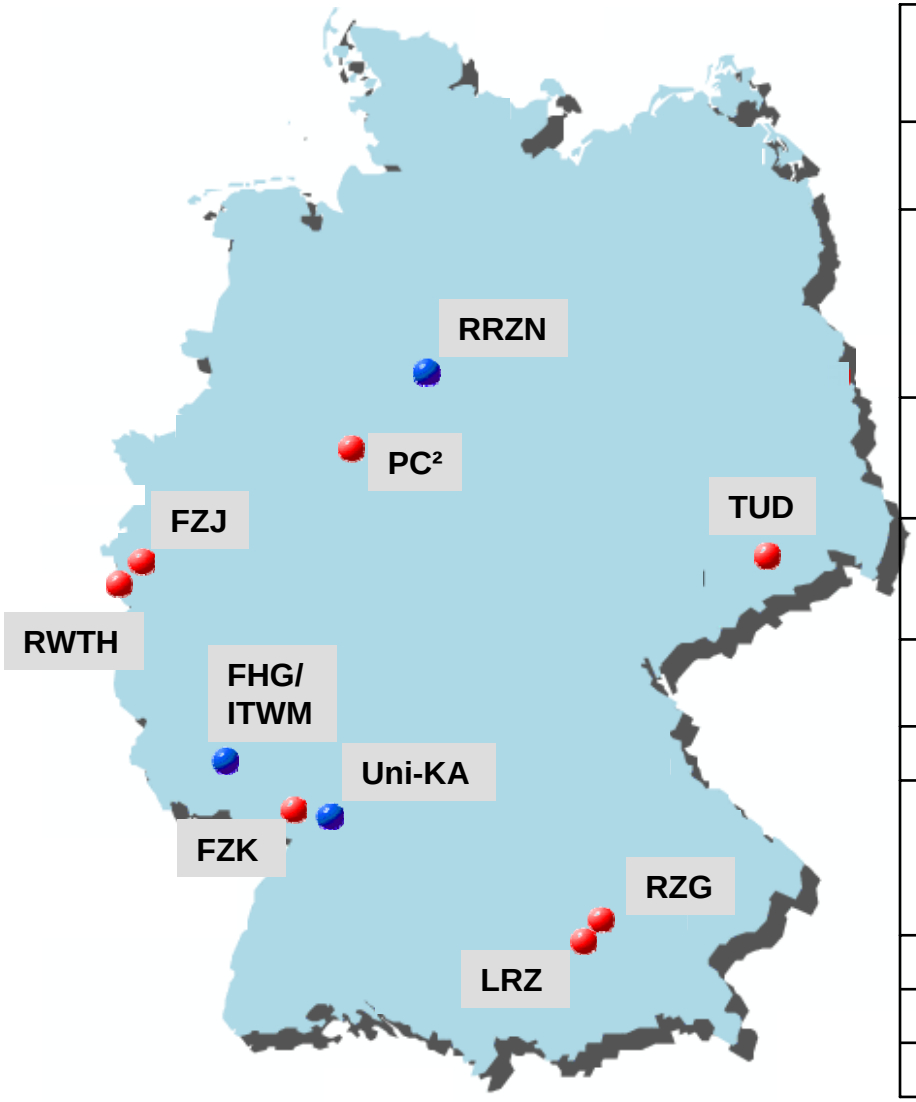
- Acquisition and integration of compute and storage resources
- Implementation and provision of middleware (Globus, gLite, UNICORE)
- Attachment of storage robots to the storage element of the D-Grid software (dCache, SRM/SRB)
- Admission of users to resources and applications (AA)
- Operation of a virtual Grid Operating Center (GOC)

# Requirements for Core Grid Resources

## Additional 5.3 Mio Euro Investment in D-Grid Hardware in December 2006

- Each resource with full middleware stack (GT4, gLite, UNICORE)
- Storage systems accessible through DGI tools (dCache, SRB, OGSA-DAI,...)
- Resources should be available for ALL communities (DGrid1 and DGrid2)
- Sustainability at least until the end of resource life cycle
- Different resources from different grid communities in one location have to be consolidated

# GOC, German Core Grid sites, Phase 1




| Site | Resource | Amount |
|---|---|---|
| FZJ/ZAM | IBM Supercomputer with 8,5 TFlops<br>STK data robot system with 2,8 PByte | 32 CPUs<br>**300 TByte** |
| FZK/IWR | 8 nodes Opteron 2x2.2 GHz<br>8 processors of a system NEC SX-5<br>1 p630 with 4 processors<br>1 SX-6i to do tests<br>2 nodes Opteron 2x2.2 GHz to do tests | 100%<br>50%<br>50%<br>50%<br>50% |
| LRZ | SGI high performance system with 20 TFlop/s<br>Intel IA32 and IA 64 Cluster,<br>IBM p690, SunFire 80 | 5%<br>5%<br>5% |
| MPI / RZG | IBM supercomputer with 4,5 TFlops,<br>PC cluster with 2 TFlops<br>Data robot system with 8 PByte | 32 CPUs<br>**400 TByte** |
| PC² | Cluster of 400 Xeon 64 Bit processors, high performance visualization and FPGAs | 10% |
| RWTH/RZ | 2 SunFire 6900 with 24 UltraSPARC IV each | 100% |
| TU-Dresden/ZIH | SGI O2K(56 proc)/O3K(192 proc.) :<br>T3E (64 proc):<br>PC cluster with 30 processors,<br>end off 2005: new system with 1000 proc. | 10%<br>20%<br>20%<br>2% |
| Uni-H/RRZN | PC-Cluster mit 64 CPUs | assoc. |
| Uni-KA | PC-Pool | assoc. |
| FHG/ITWM | | assoc. |

# GOC, German Core Grid sites, Phase 2


| Institution | Gesamt | | Backbone | | AstroGrid-D | C3-Grid | HEP | InGrid | MediGRID | TextGrid | WISNET |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | | | |
| FZK | 480 | | 480 | | | | | | | | |
| FZJ | 380 | | 380 | | | | | | | | |
| DESY | 380 | | 380 | | | | | | | | |
| RRZN | 380 | | 380 | | | | | | | | |
| ZIB | 450 | | 380 | | | 70 | | | | | |
| LRZ | 380 | | 380 | | | | | | | | |
| HLRS | 480 | | 380 | | | | | 100 | | | |
| ZIH/TUD | 380 | | 280 | | | | | | 100 | | |
| FhG SCAI | 200 | | 100 | | | | | 100 | | | |
| | | | | | | | | | | | |
| AIP/AEI | 150 | | | | 150 | | | | | | |
| MPA/MPE | 150 | | | | 150 | | | | | | |
| ZAH | 150 | | | | 150 | | | | | | |
| WDC Clim. | 100 | | | | | 100 | | | | | |
| Uni Köln | 70 | | | | | 70 | | | | | |
| Uni Do. | 150 | | | | | 70 | 80 | | | | |
| LMU | 100 | | | | | | 100 | | | | |
| Uni Freiburg | 100 | | | | | | 100 | | | | |
| Uni Wup. | 100 | | | | | | 100 | | | | |
| GSI | 50 | | | | | | 50 | | | | |
| Uni Marburg | 100 | | | | | | | 100 | | | |
| Uni Siegen | 100 | | | | | | | 100 | | | |
| FhG IAO | 30 | | | | | | | | 30 | | |
| GWDG | 270 | | | | | | | | 170 | 100 | |
| OFFIS | 190 | | | | | | | | | | 190 |
| DLR-DFD | 50 | | | | | | | | | | 50 |
| | | | | | | | | | | | |
| | | | | | | | | | | | |
| | | | | | | | | | | | |
| Gesamt: | 5370 | | 3140 | | 450 | 310 | 430 | 400 | 300 | 100 | 240 |

# Core D-Grid Infrastructure


- 8 DGI Centers to build the resource and service backbone for all communities, plus 17 local resources
- All centers are responsible for a reliable and sustainable grid operation
- Backbone resources are available for all communities exclusively for grid-related activities
- Each Grid Community is building a community resource infrastructure with similar quality and services
- FZK in Karlsruhe provides supervision, coordination, monitoring as part of this 2-tier architecture

# DGI Services, Available March 2007

- Sustainable grid operation environment with a set of core D-Grid middleware services for all grid communities
- Central registration and information management for all resources
- Packaged middleware components for gLite, Globus and Unicore and for data management systems SRB, dCache and OGSA-DAI
- D-Grid support infrastructure for new communities with installation and integration of new grid resources into D-Grid Help-Desk, Monitoring System and central Information Portal

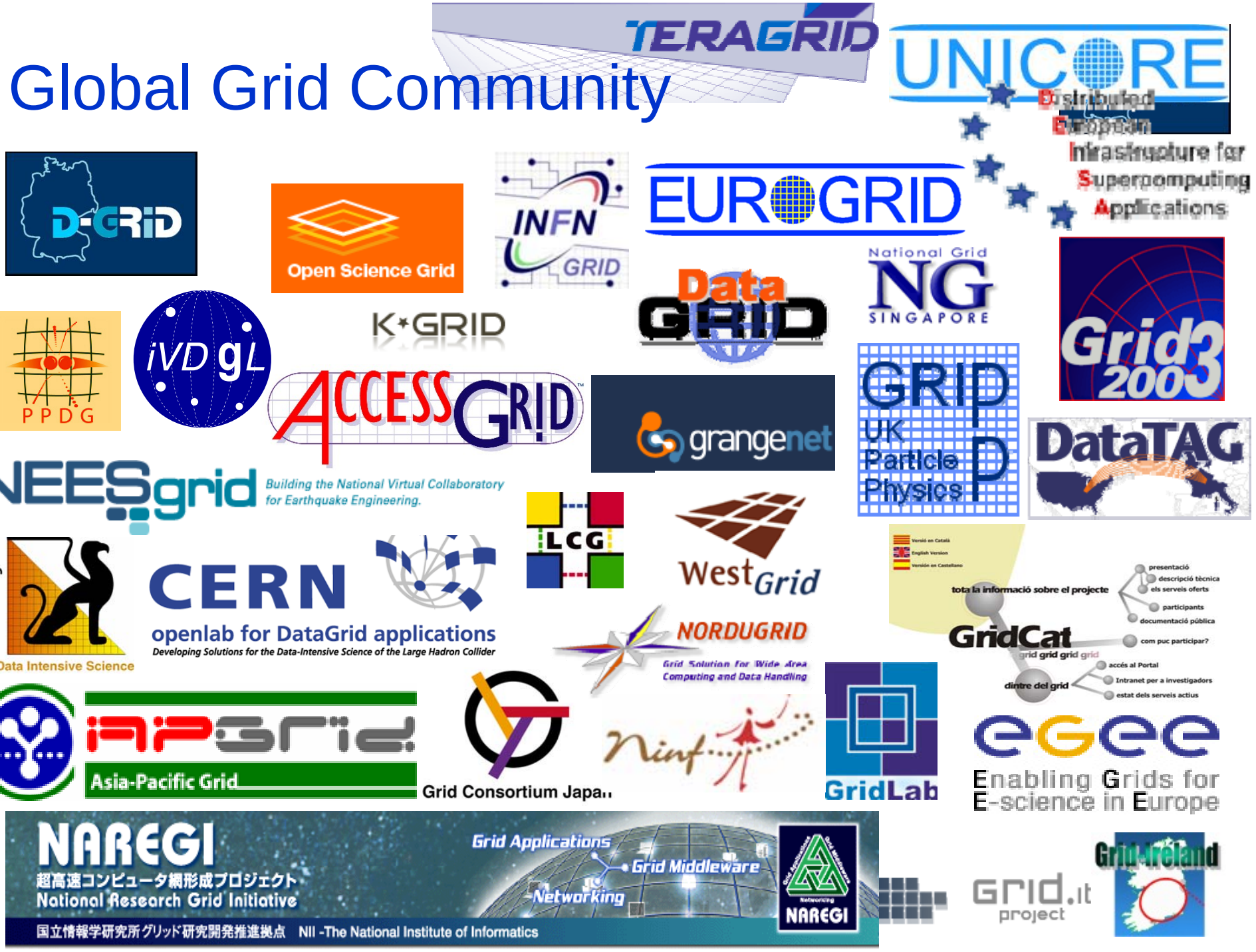
# DGI Services, March 2007, cont.


- Tools for managing VOs based on VOMS and Shibboleth
- Test implementation for Monitoring & Accounting for Grid resources, and first concept for a billing system
- Network and security support for Communities (firewalls in grids, alternative network protocols,...)
- DGI operates „Registration Authorities“, with internationally accepted Grid certificates of DFN & GridKa Karlsruhe
- Partners support new D-Grid members with building their own „Registration Authorities“

# DGI Services, March 2007, cont.


- DGI will offer resources to other Communities, with access via gLite, Globus Toolkit 4, and UNICORE
- Portal-Framework Gridsphere can be used by future users as a graphical user interface
- For administration and management of large scientific datasets, DGI will offer dCache for testing
- New users can use the D-Grid resources of the core grid infrastructure upon request

# Global Grid Community



# Components of e-Science Infrastructures

1. Resources: Networks with computing and data nodes, etc.
2. Development/support of standard middleware & grid services
3. Internationally agreed AAA infrastructure
4. Discovery services and collaborative tools
5. Data provenance, curation and preservation
6. Open access to data and publications via interoperable repositories
7. Remote access to large-scale facilities:  Telescopes, LHC, ITER, ..
8. Industrial collaboration

# e-Science Grid Initiatives Investigated


| Initiative | Time | Funding | People *) | Users |
|---|---|---|---|---|
| UK e-Science-I: | 2001 - 2004 | $180M | 900 | Res. |
| UK e-Science-II: | 2004 - 2006 | $220M | 1100 | Res. Ind. |
| TeraGrid-I: | 2001 - 2004 | $90M | 500 | Res. |
| TeraGrid-II: | 2005 - 2010 | $150M | 850 | Res. |
| ChinaGrid-I: | 2003 - 2006 | 20M RMB | 400 | Res. |
| ChinaGrid-II: | 2007 – 2010 | 50M RMB *) | 1000 | Res. |
| NAREGI-I: | 2003 - 2005 | $25M | 150 | Res. |
| NAREGI-II | 2006 - 2010 | $40M *) | 250 | Res. Ind. |
| EGEE-I: | 2004 - 2006 | $40M | 800 | Res. |
| EGEE-II: | 2006 - 2008 | $45M | 1000 | Res. Ind. |
| D-Grid-I: | 2005 - 2008 | $25M | 220 | Res. |
| D-Grid-II: | 2007 - 2009 | $25M | 220 (= 440) | Res. Ind. |

*) estimate

# Main Objectives of e-Science Projects


**UK e-Science:**

To enable the next generation of multi-disciplinary collaborative science and engineering, to enable faster, better or different research.

**EGEE:**

To provide a seamless Grid infrastructure for e-Science that is available for scientists 24 hours-a-day.

**ChinaGrid:**

To provide a research and education platform by using grid technology for the faculties and students among the major universities in China.

**NAREGI:**

To do research, development and deployment of science grid middleware.

**TeraGrid:**

Create a unified Cyberinfrastructure supporting a broad array of US science activities using the suite of NSF HPC facilities

**D-Grid:**

Build and operate a sustainable grid service infrastructure for German research (D-Grid1) and research and industry (D-Grid2)

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# Grid Middleware Stacks, major modules


**UK e-Science:**
Phase 1: Globus 2.4.3, Condor, SRB.
Phase 2: Globus 3.9.5 und 4.0.1, OGSA-DAI, Web services.

**EGEE:**
gLite distribution: elements of Condor, Globus 2.4.3 (via Virtual Data Toolkit).

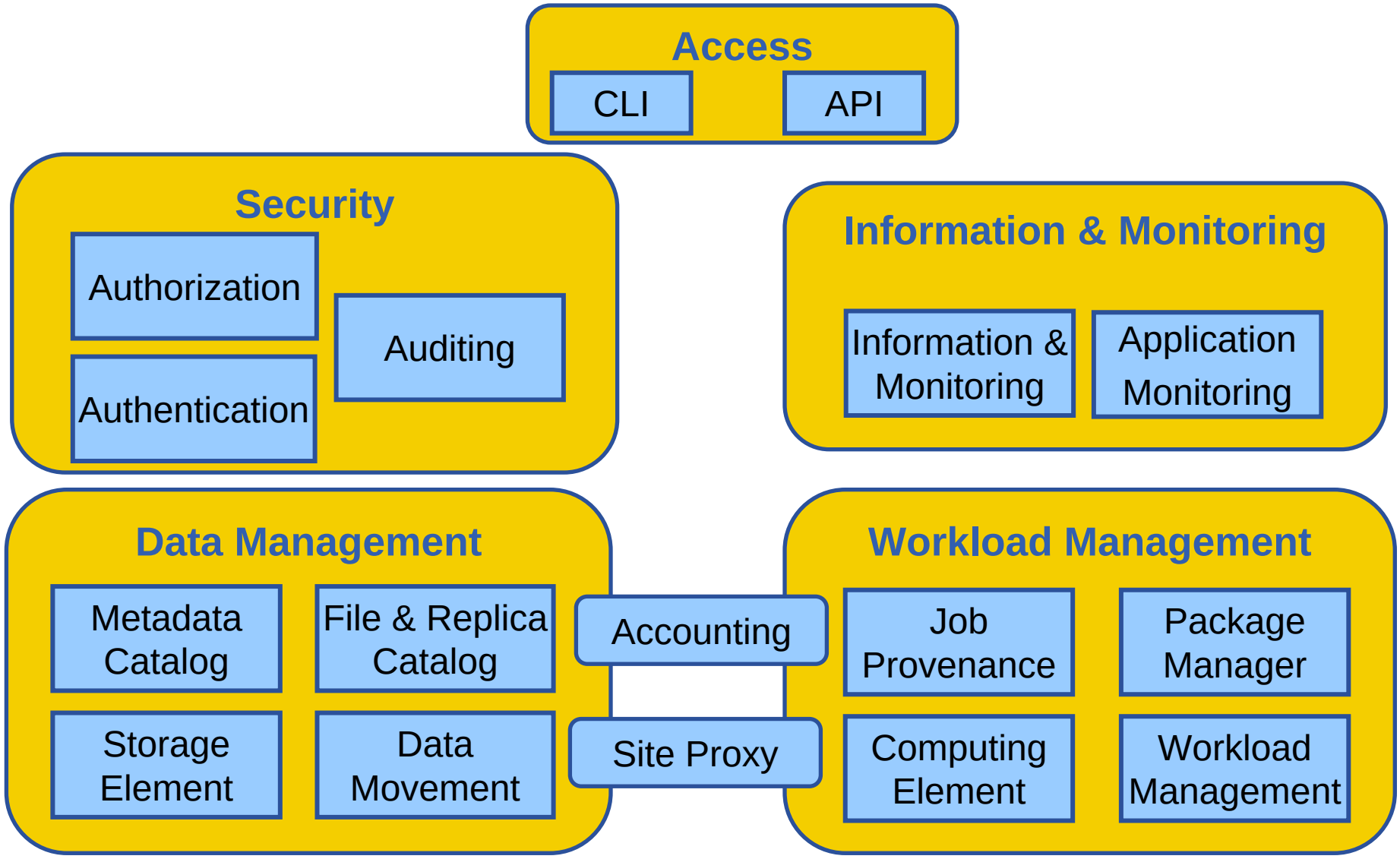
**ChinaGrid:**
ChinaGrid Supporting Platform (CGSP) 1.0 is based on Globus 3.9.1, and CGSP 2.0 is implemented based on Globus 4.0.

**NAREGI:** NAREGI middleware and Globus 4.0.1 GSI and WS-GRAM

**TeraGrid:**
GT 2.4. and 4.0.1: Globus GRAM, MDS for information, GridFTP & TGCP file transfer, RLS for data replication support, MyProxy for credential mgmnt

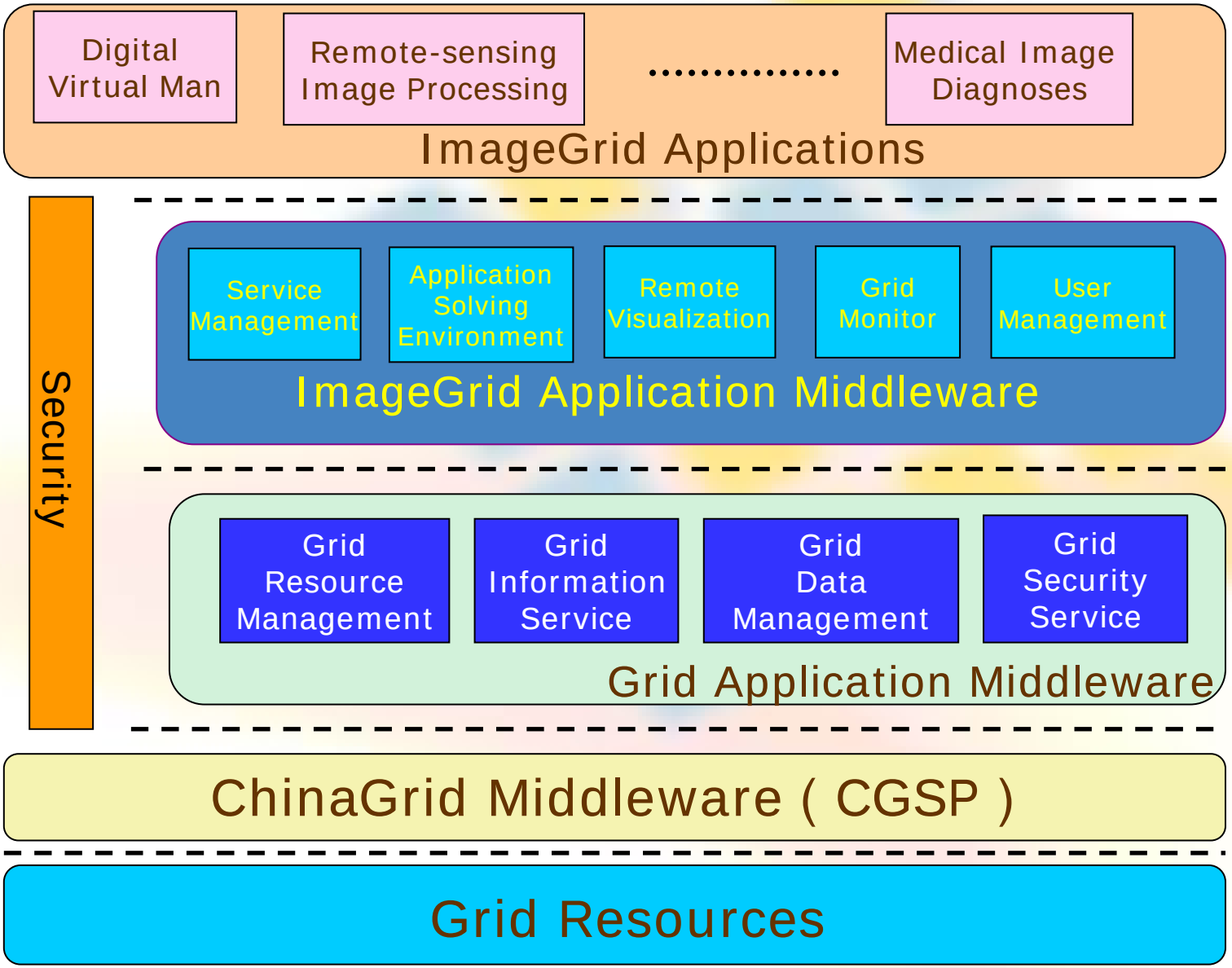
**D-Grid:**
Globus 4.0.3, Unicore 5, gLite (GT 2.4.3), dCache, SRB, OGSA-DAI, GridSphere, GAT, VOMS and Shibboleth

# gLite Grid Middleware Services

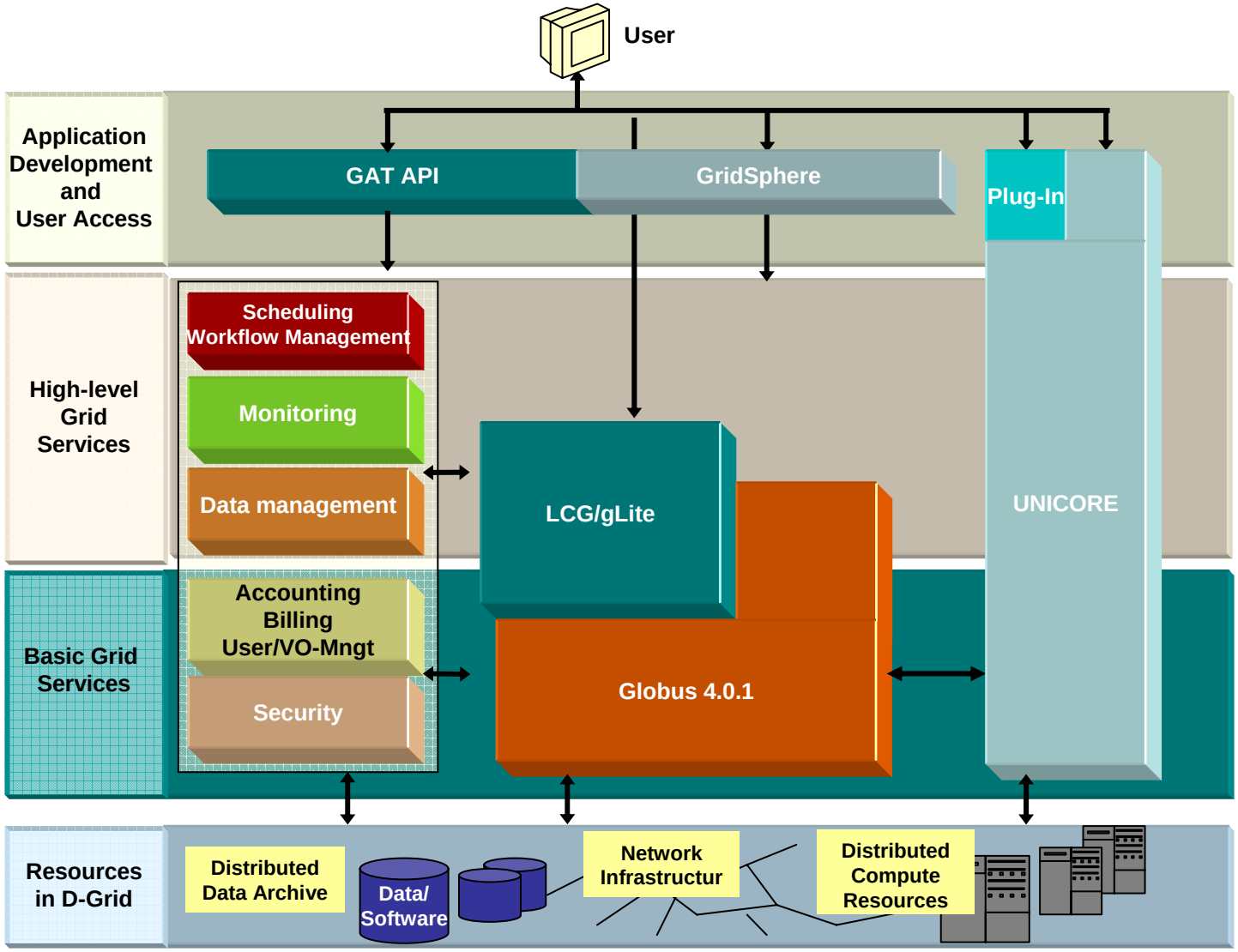



**Overview paper http://doc.cern.ch//archive/electronic/egee/tr/egee-tr-2006-001.pdf**

# ChinaGrid Middleware



# D-Grid Middleware



# Sustainability


**UK e-Science:**
National Grid Service (NGS), Grid Operations Support Center (GOSC),
National e-Science Center (NeSC), Regional e-Science Centers,
Open Middleware Infrastructure Institute (OMII), Digital Curation Center (DCC)

**EGEE:**
Plans to support a European Grid Initiative (EGI), together with NGIs, to provide persistent grid service federating national grid programmes starting in late 2007

**ChinaGrid:**
Increasing numbers of grid applications using CGSP grid middleware packages

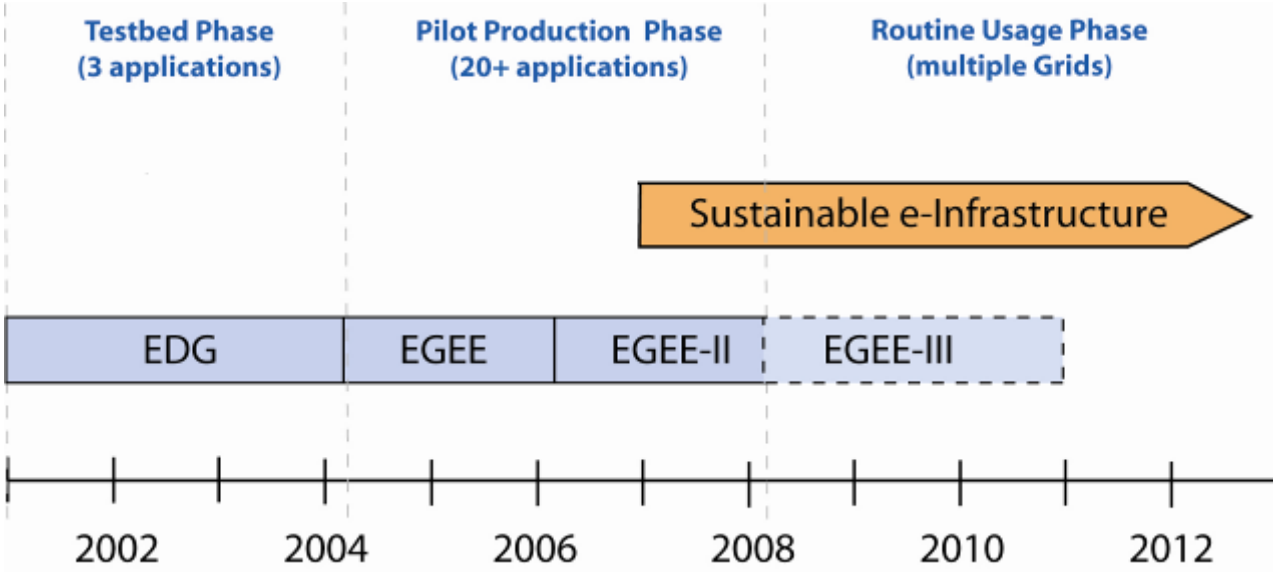
**NAREGI:**
Software will be managed and maintained by Cyber Science Infrastructure Center of the National Institute of Informatics

**TeraGrid:**
5-year Agreement with NSF Cyberinfrastructure Office. Partnerships with peer grid efforts and commercial web services activities in order to integrate broadly. Science Gateways.

**D-Grid:**
DGI WP 4: Long-term funding, WP Sustainability, economic models, service centers

# Sustainability: Beyond EGEE-II

- **Need to prepare for permanent Grid infrastructure**
  - Maintain Europe's leading position in global science Grids
  - Ensure a reliable and adaptive support for all sciences
  - Independent of short project funding cycles
  - Modelled on success of GÉANT
    - Infrastructure managed in collaboration with national grid initiatives



# D-Grid: Towards a Sustainable Infrastructure for Science and Industry


- Govt is changing policies for resource acquisition (HBFG ! ) to enable a service model
- 2nd Call: Focus on Service Provisioning for Sciences & Industry
- Strong collaboration with: Globus Project, EGEE, Deisa, CrossGrid, CoreGrid, GridCoord, GRIP, UniGrids, NextGrid, …
- Application and user-driven, not infrastructure-driven
- Focus on implementation and production, not grid research, in a multi-technology environment (Globus, Unicore, gLite, etc)
- D-Grid is the Core of the German e-Science Initiative

# e-Science Applications


**UK e-Science:**
Particle physics, astronomy, chemistry, bioinformatics, healthcare, engineering, environment, pharmaceutical, petro-chemical, media and financial sectors

**EGEE:**
2 pilot applications (physics, life science) and applications from other 7 disciplines.

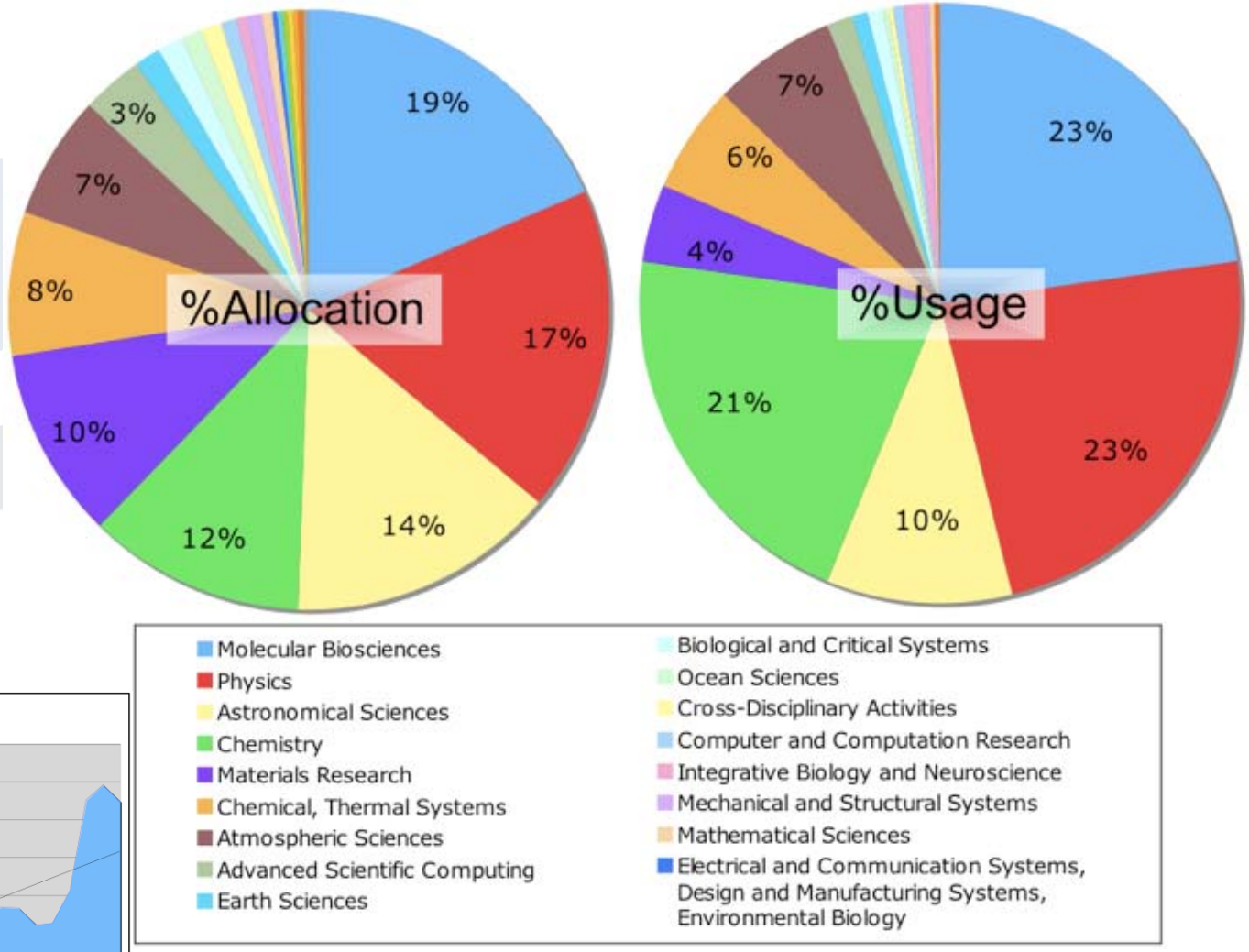
**ChinaGrid:**
Bioinformatics, image processing, computational fluid dynamics, remote education, and massive data processing

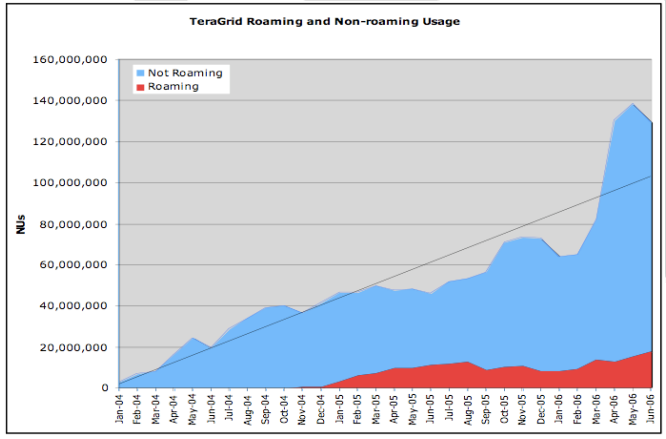
**NAREGI:**
Nano-science applications

**TeraGrid:**
Physics (Lattice QCD calculations, Turbulence simulations, Stellar models), Molecular Bioscience (molecular dynamics), Chemistry, Atmospheric Sciences

**D-Grid-1:**
Astrophysics, high-energy physics, earth science, medicine, engineering, humanities

# TeraGrid Usage



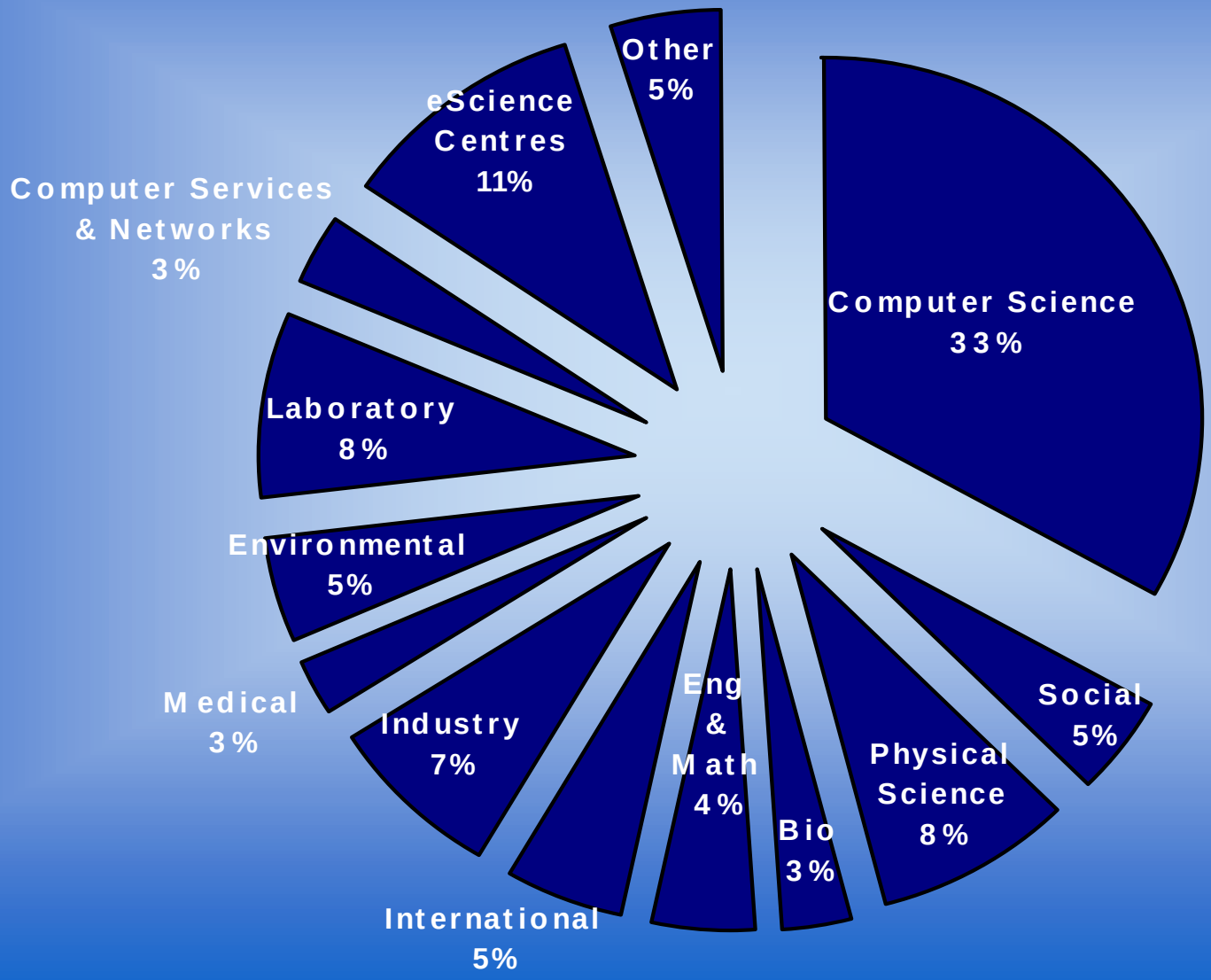

*Charlie Catlett (cec@uchicago.edu)*



TeraGrid

AHM 2004 Attendees

# The UK e-Science Community

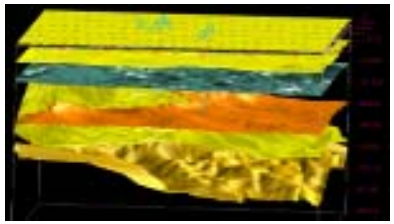
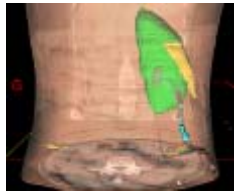


# Applications on EGEE

- **More than 25 applications from 9 domains**
  - Astrophysics
  - Computational Chemistry
  - Earth Sciences
  - Financial Simulation
  - Fusion
  - Geophysics
  - High Energy Physics
  - Life Sciences
  - Multimedia
  - Material Sciences
  - …..





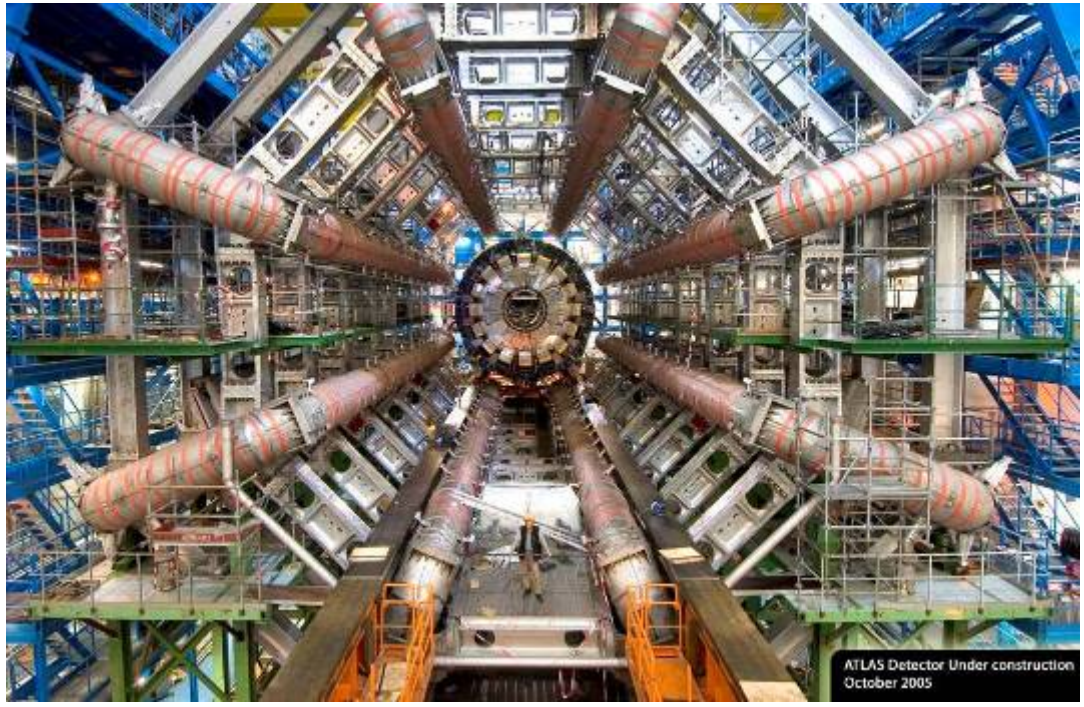



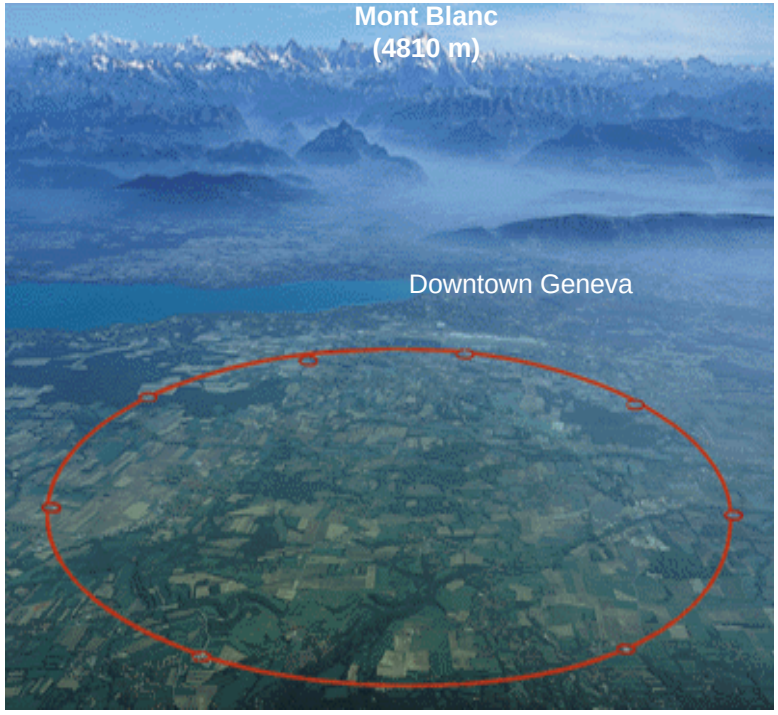

Book of abstracts: http://doc.cern.ch//archive/electronic/egee/tr/egee-tr-2006-005.pdf

# High Energy Physics

## Large Hadron Collider (LHC):

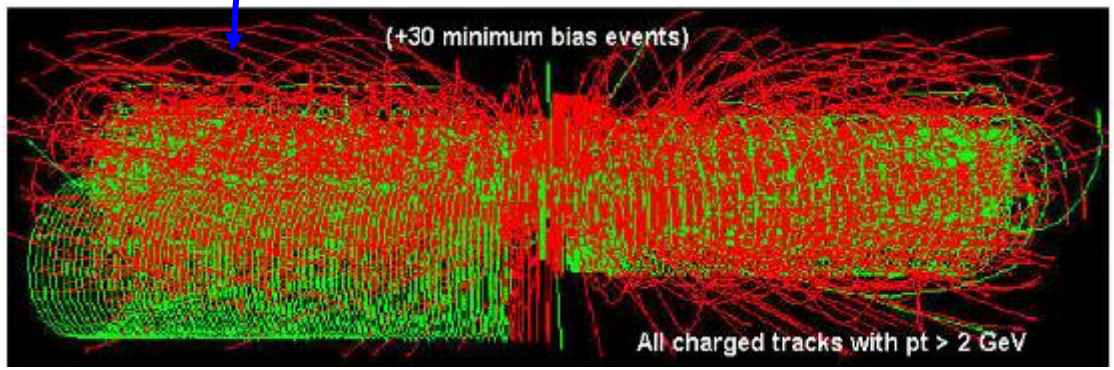
- One of the most powerful instruments ever built to investigate matter
- 4 Experiments: ALICE, ATLAS, CMS, LHCb
- 27 km circumference tunnel
- Due to start up in 2007

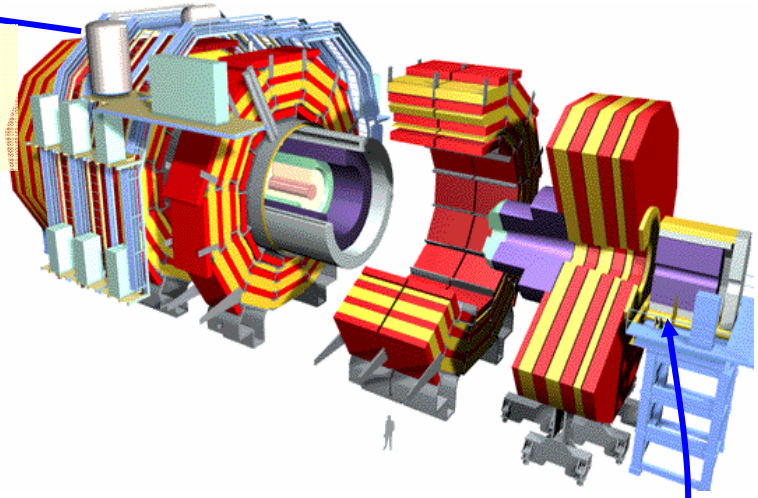


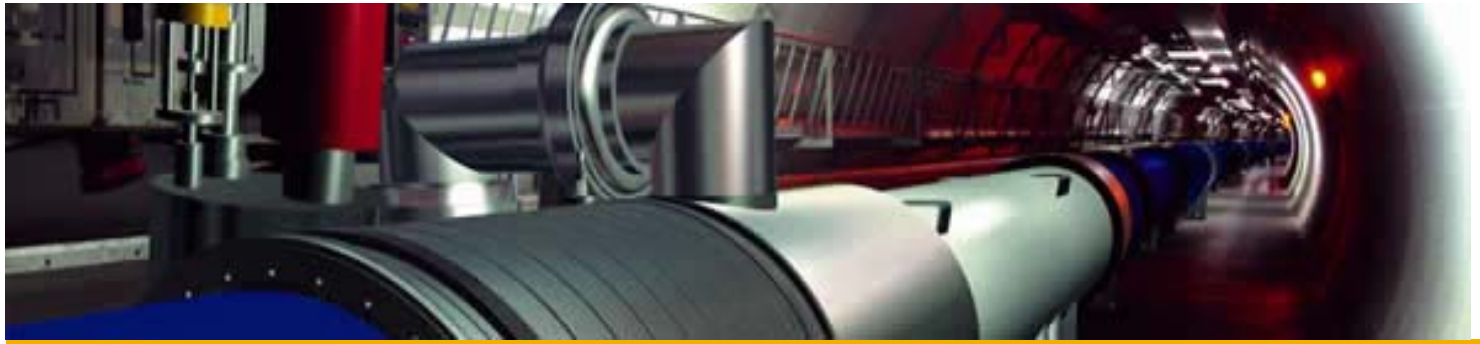
# Large Hadron Collider data

This is reduced by online computers that filter out a few hundred “good” events/sec.



Which are recorded on disk and magnetic tape at 100-1,000 MegaBytes/sec → ~15 PetaBytes per year for all four experiments



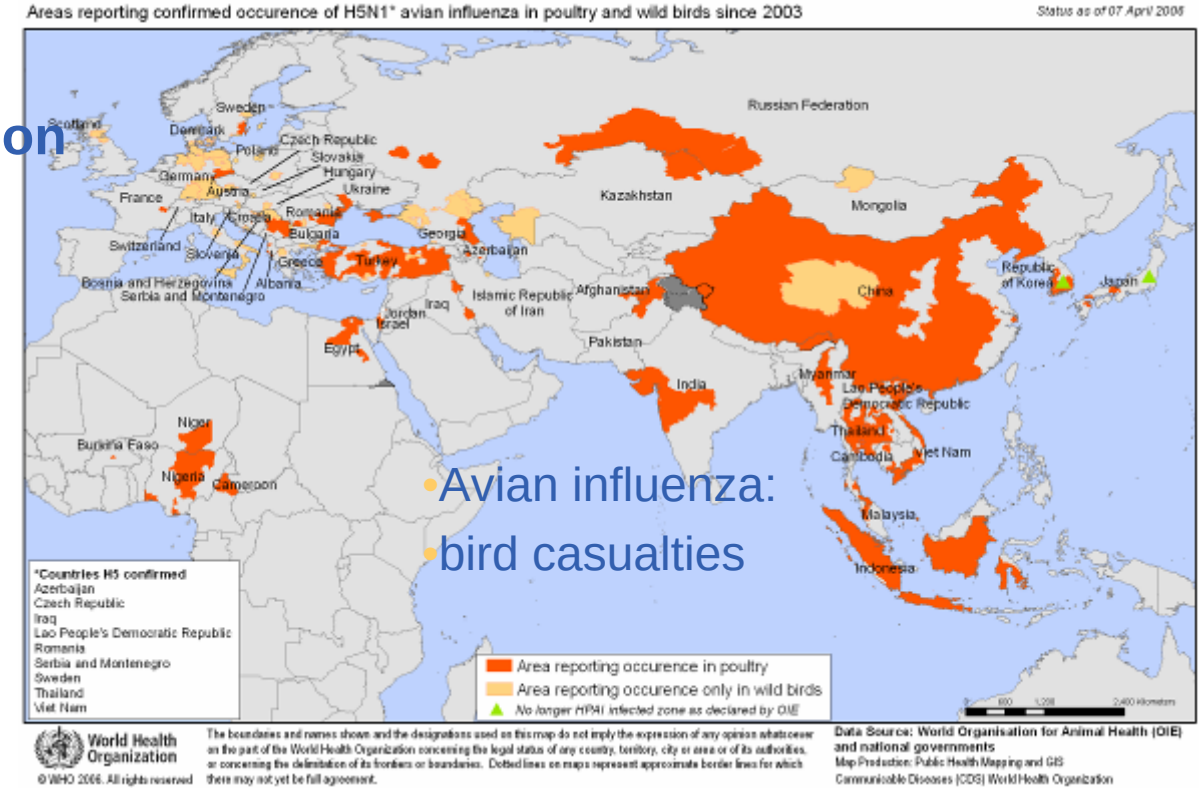
# *In silico* drug discovery

- **Diseases such as HIV/AIDS, SRAS, Bird Flu etc. are a threat to public health due to world wide exchanges and circulation of persons**

- **Grids open new perspectives to *in silico* drug discovery**
  - Reduced cost and adding an accelerating factor in the search for new drugs

**International collaboration is required for:**

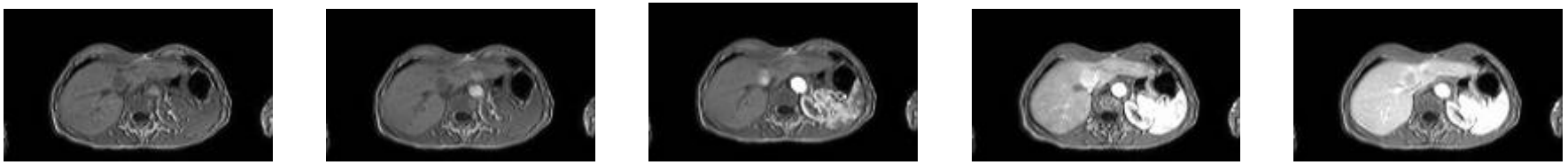
- **Early detection**
- **Epidemiological watch**
- **Prevention**
- **Search for new drugs**
- **Search for vaccines**



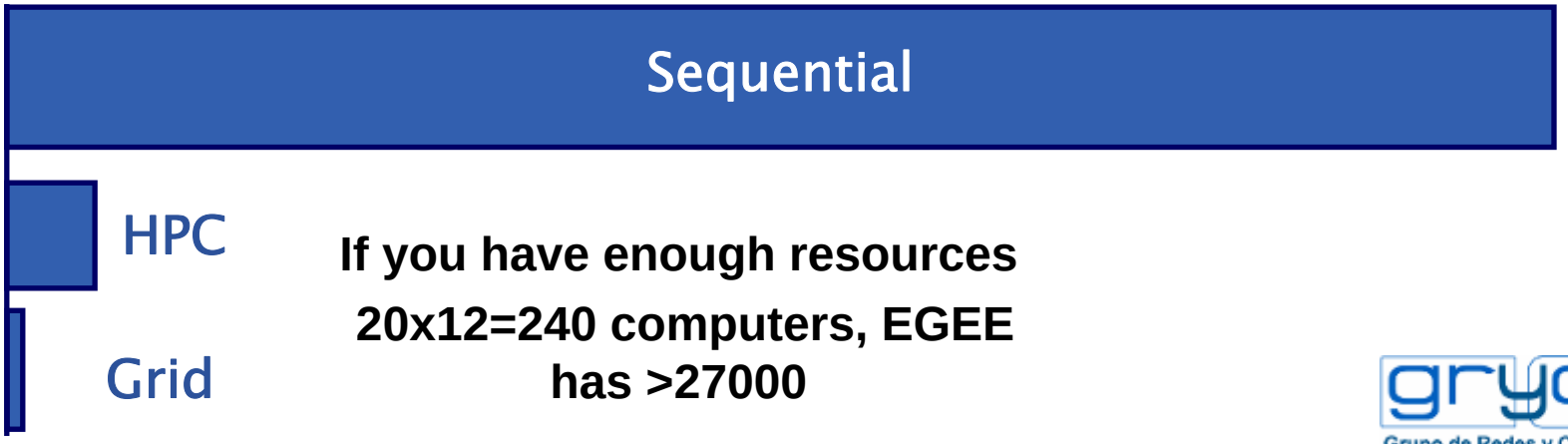

- Avian influenza:
- bird casualties

# Medical image processing: analysing tumours

- **Pharmacokinetics: contrast agent diffusion study**
  - co-registration of a time series of volumetric medical images to analyse the evolution of the diffusion of contrast agents



- **Computational Costs**
  - 20 Patients: 2623 hours (Co-registration + Parametric Image)
  - Using a 20-processor Computing Farm: 146 hours
  - Using the Grid: <20 hours



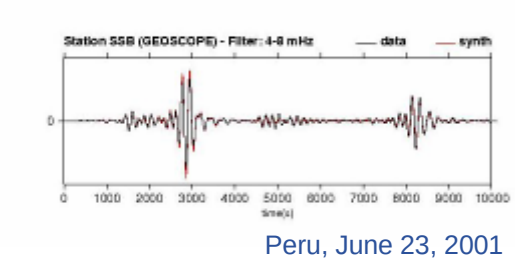

Grycap
Grupo de Redes y Computación de Altas Prestaciones

# Example: Determining earthquake mechanisms

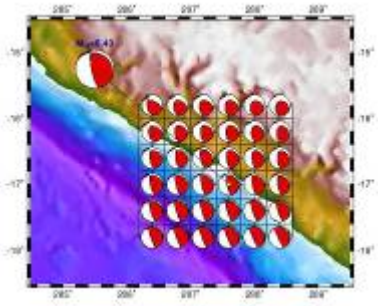
- **Seismic software application determines epicentre, magnitude, mechanism**

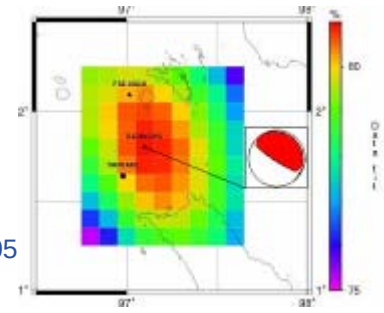
- **Analysis of Indonesian earthquake (28 March 2005)**
  - Seismic data within 12 hours after the earthquake
  - Analysis performed within 30 hours after earthquake occurred
    - 10 times faster on the Grid than on local computers
  - Results
    - Not an aftershock of December 2004 earthquake
    - Different location (different part of fault line further south)
    - Different mechanism

→ **Rapid analysis of earthquakes important for relief efforts**




Peru, June 23, 2001
Mw=8.4

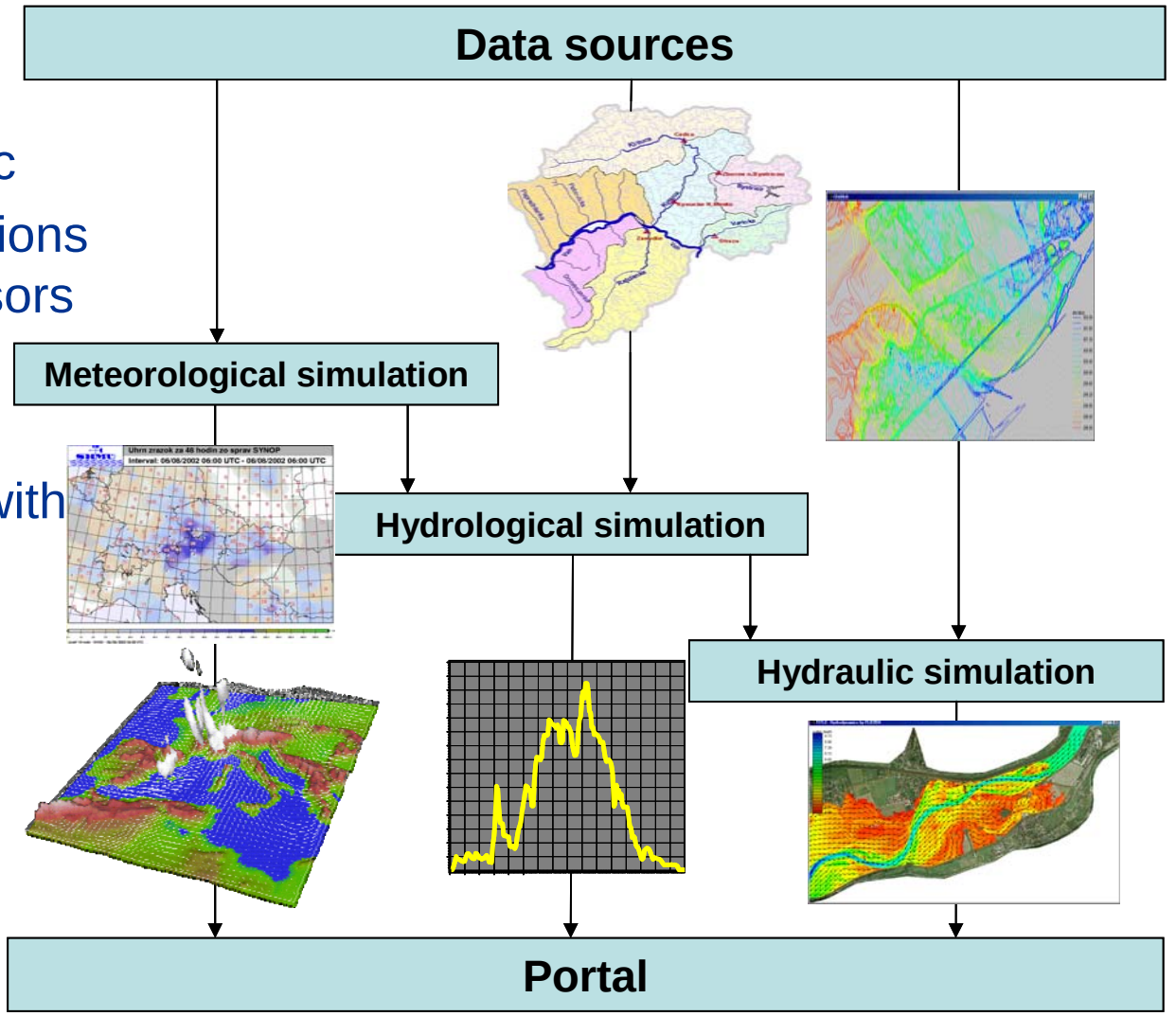




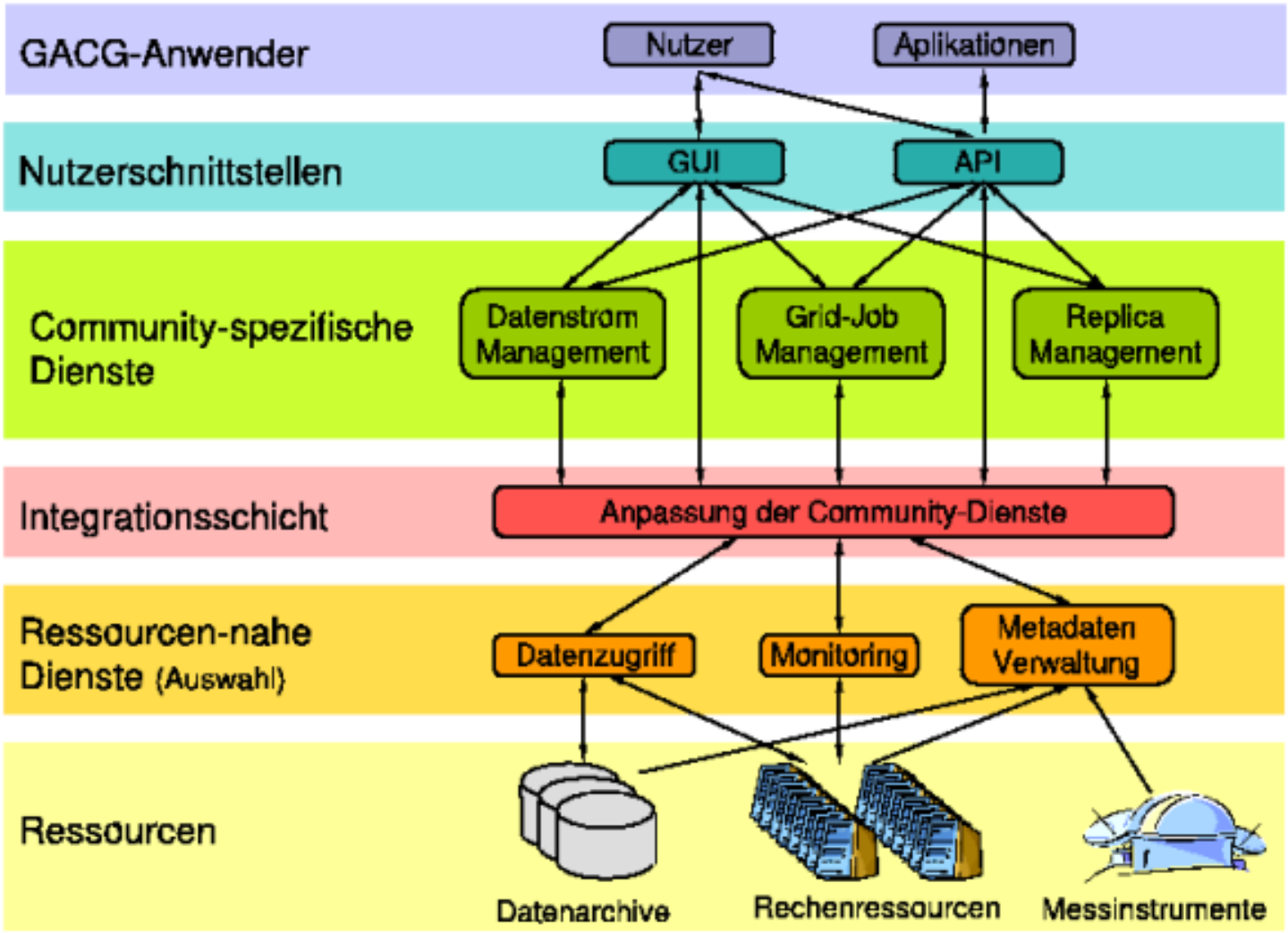
Sumatra, March 28, 2005
Mw=8.5

# Flood forecasting problem

- **Many kinds of data**
  - Meteorological, hydrological, hydraulic
  - Generated by simulations or obtained from sensors
  - Permanent or periodically updated
  - Publicly available or with restricted access



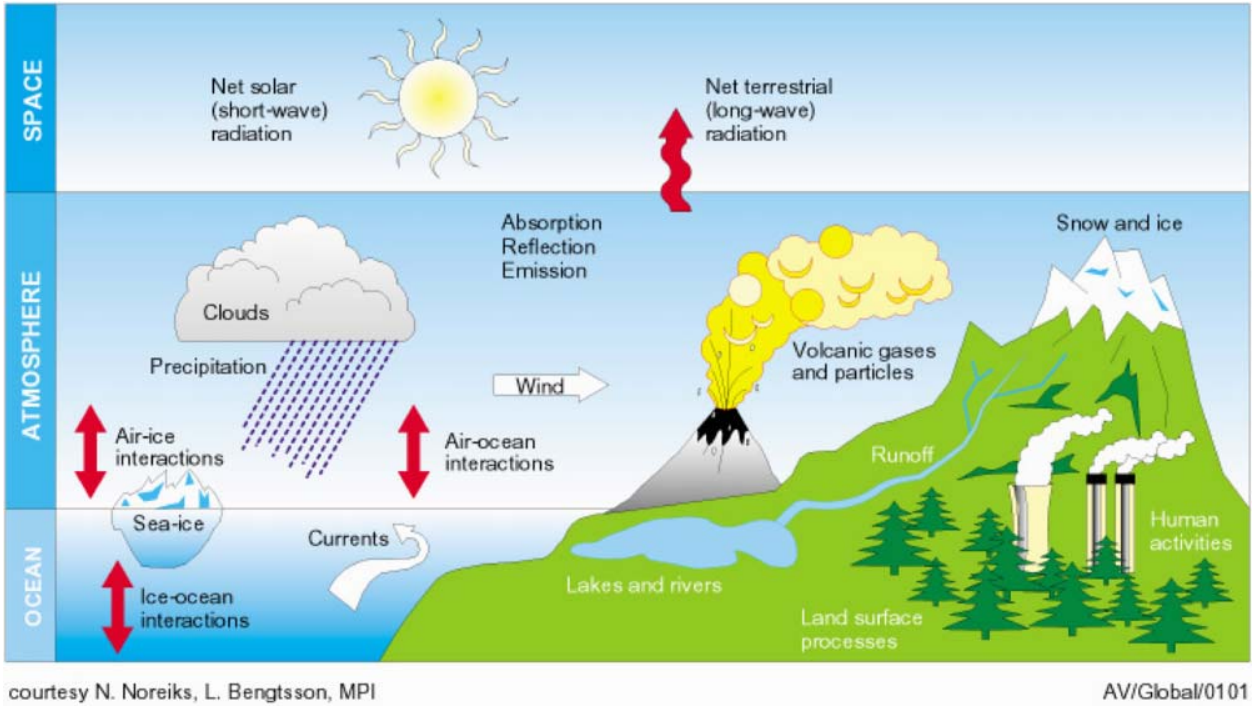
# AstroGrid


GACG-Anwender
Nutzer
Aplikationen
Nutzerschnittstellen
GUI
API
Community-spezifische Dienste
Datenstrom Management
Grid-Job Management
Replica Management
Integrationsschicht
Anpassung der Community-Dienste
Ressourcen-nahe Dienste (Auswahl)
Datenzugriff
Monitoring
Metadaten Verwaltung
Ressourcen
Datenarchive
Rechenressourcen
Messinstrumente

# C3 Grid: Collaborative Climate Community Data and Processing Grid

Climate research moves towards new levels of complexity:

Stepping from Climate (=Atmosphere+Ocean) to Earth System Modelling




**Increased Computational demand factor: O(1000 -10000)**

*Earth system model wishlist:*

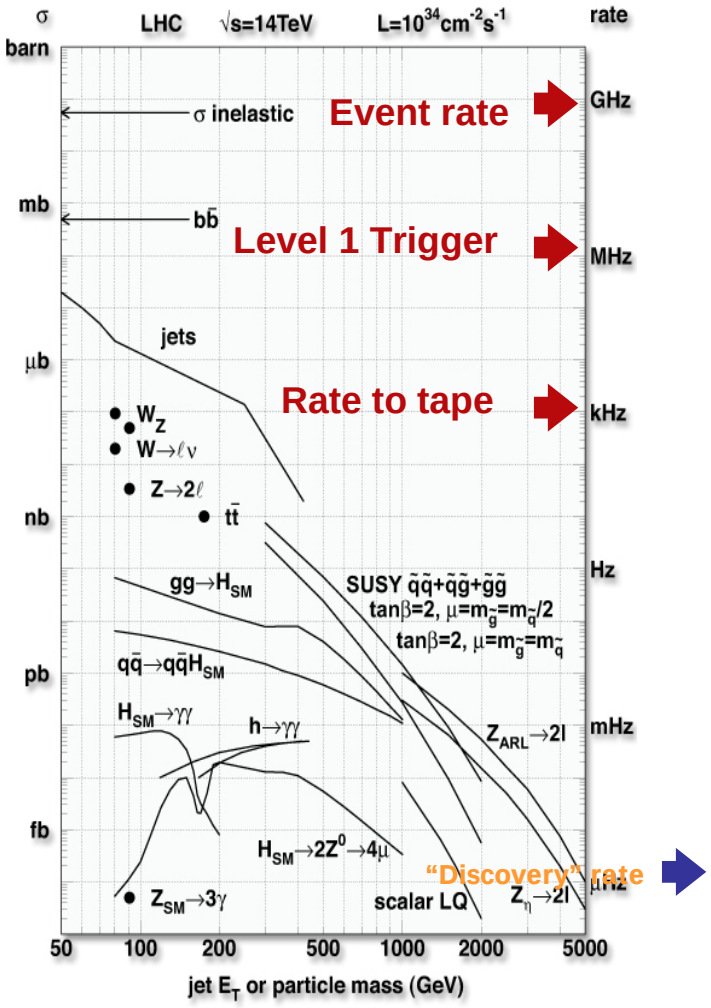
Higher spatial and temporal resolution

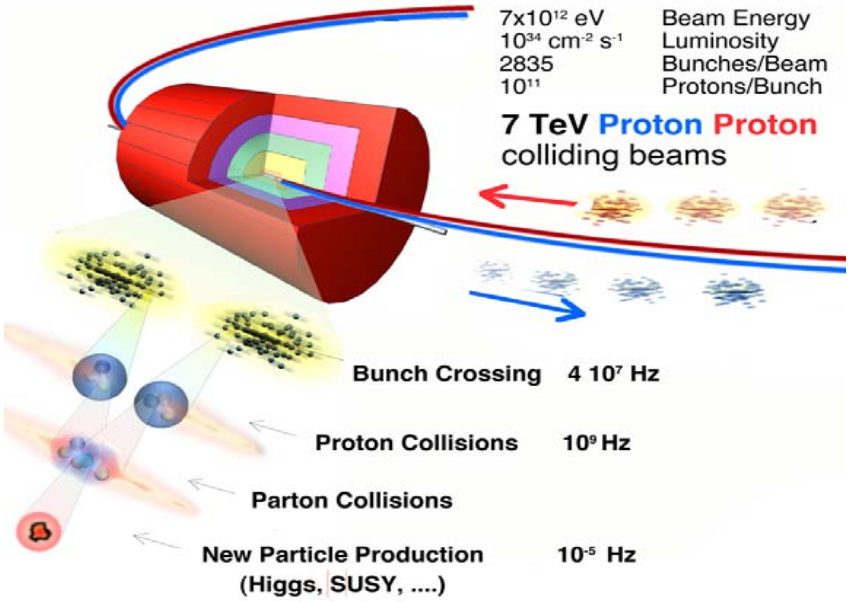
Quality: Improved subsystem models

Atmospheric chemistry (ozone, sulfates,..)

Bio-geochemistry (Carbon cycle, ecosystem dynamics,..)

# HEP-Grid: p-p collisions at LHC at CERN
## (from 2007 on)



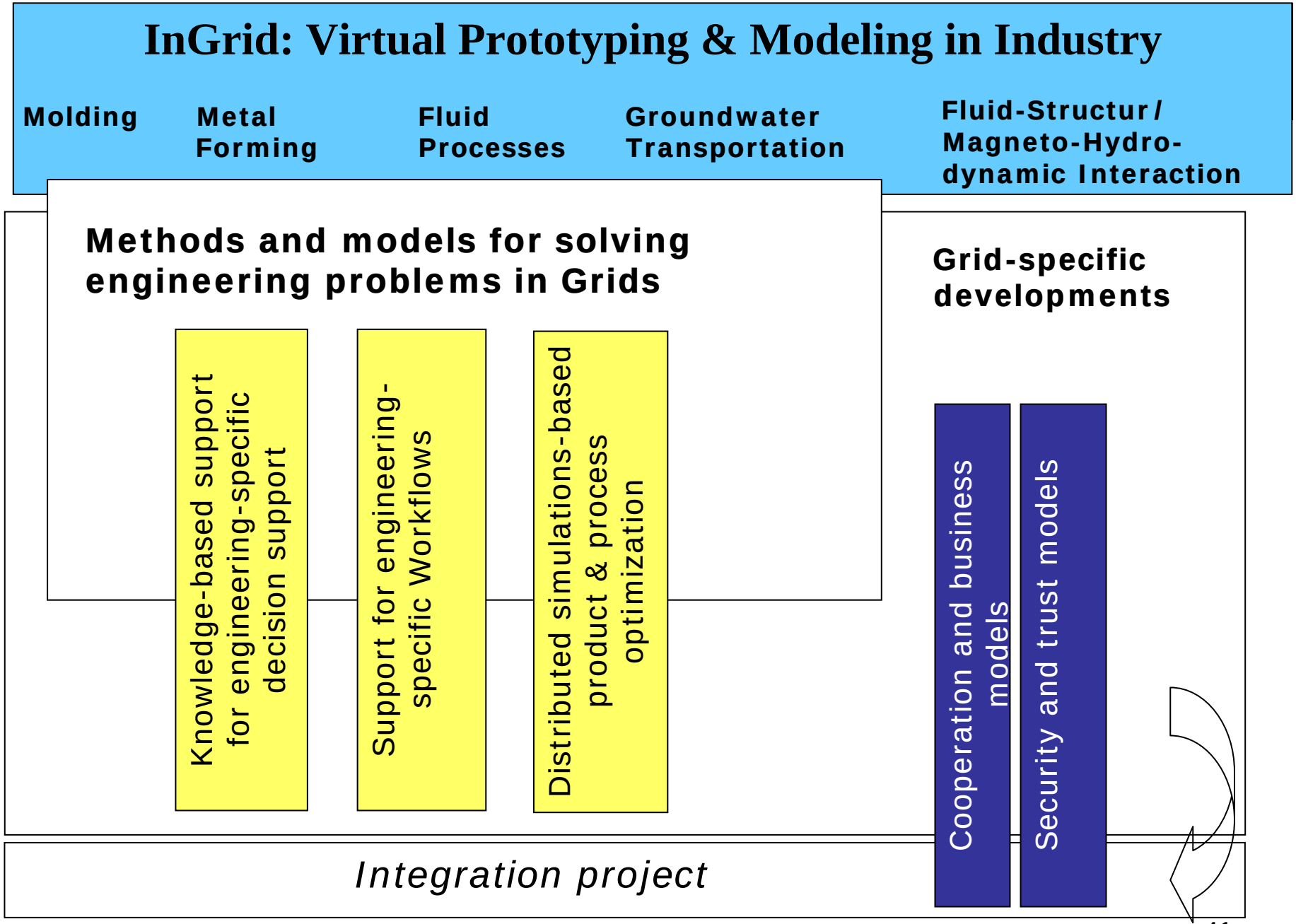




| | |
|---|---|
| **Crossing rate** | **40 MHz** |
| **Event Rates:** | **~10⁹ Hz** |
| **Max LV1 Trigger** | **100 kHz** |
| **Event size** | **~1 Mbyte** |
| **Readout network** | **1 Terabit/s** |
| **Filter Farm** | **~10⁷ Si2K** |
| **Trigger levels** | **2** |
| **Online rejection** | **99.9997% (100 Hz from 50 MHz)** |
| **System dead time** | **~ %** |
| **Event Selection:** | **~1/10¹³** |

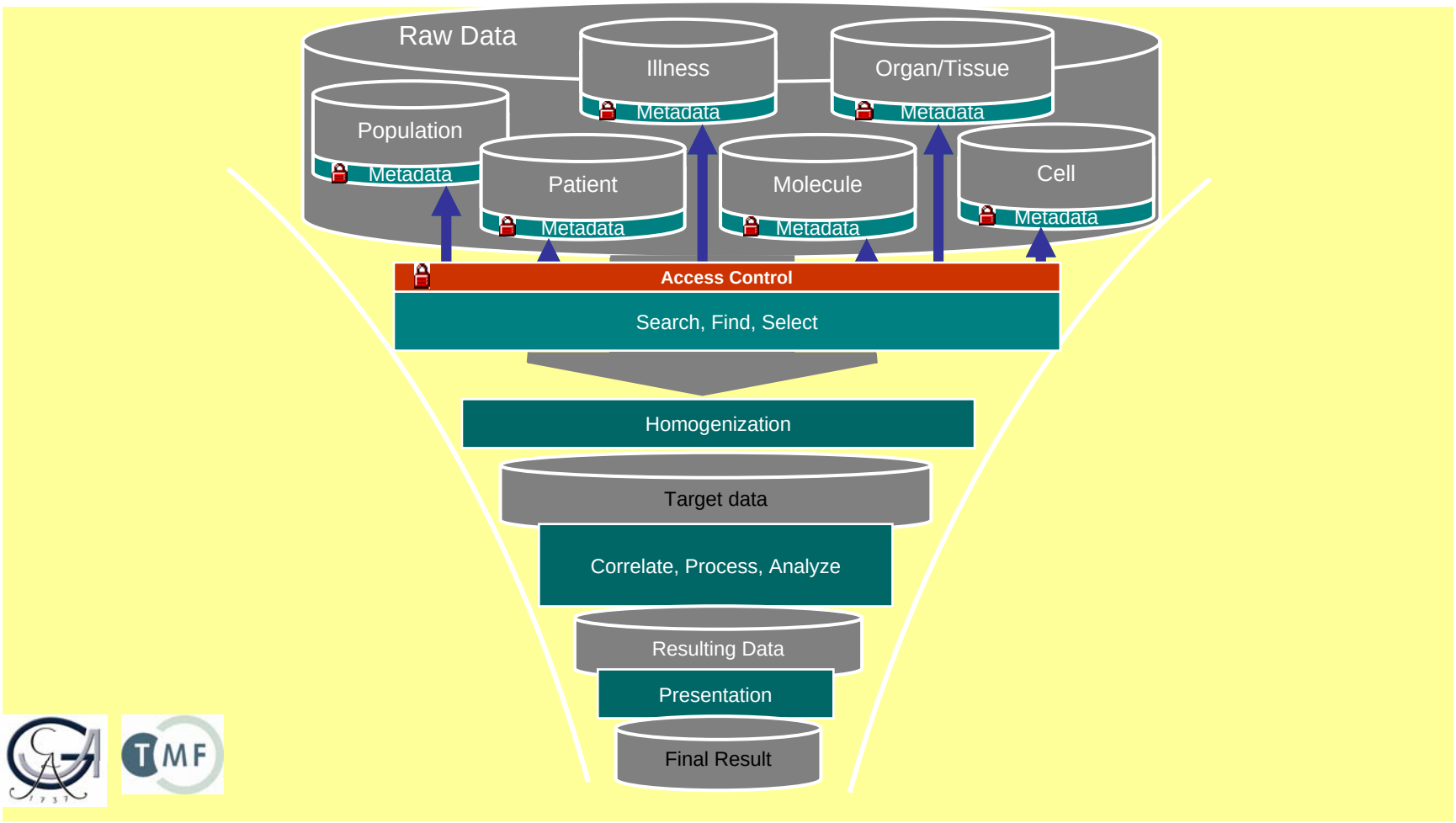
**Luminosity**
**Low 2x10³³ cm⁻² s⁻¹**
**High 10³⁴ cm⁻² s⁻¹**
**Data analysis:**
**~1PB/year**



Courtesy David Stickland


InGrid: Virtual Prototyping & Modeling in Industry
Molding
Metal Forming
Fluid Processes
Groundwater Transportation
Fluid-Structur / Magneto-Hydro-dynamic Interaction
Methods and models for solving engineering problems in Grids
Knowledge-based support for engineering-specific decision support
Support for engineering-specific Workflows
Distributed simulations-based product & process optimization
Grid-specific developments
Cooperation and business models
Security and trust models
Integration project
AP 2
AP 3
AP 4

# MediGrid: Mapping of Characteristics, Features, Raw Data, etc



# TextGrid


Modular Platform for distributed cooperative scientific text processing for the humanities

- Workbench for Publishing, Text Processing, Text Retrieval, Linking, and Workflow

- Focus of TextGrid is on:
  - Quantity: Full text instead excerpts, text and pictures
  - Speed of reprography: stability of text, volatility of medium
  - Precision: Maximum requirements on correctness
  - Availability: international open standards

# Challenges for Research and Industry


- Sensitive data, sensitive applications (medical patient records)
- Different organizations get different benefits
- Accounting, who pays for what (sharing!)
- Security policies: consistent and enforced across the grid !
- Lack of standards prevent interoperability of components
- Current IT culture is not predisposed to sharing resources
- Not all applications are grid-ready or grid-enabled
- Open source is not equal open source (read the small print)
- SLAs based on open source (liability?)
- “Static” licensing model don’t embrace grid
- Protection of intellectual property
- Legal issues (e.g. FDA, HIPAA, multi-country grids)

# Lessons Learned and Recommendations


- Continuity: Grid infrastructure should be modified and improved in large cycles only: applications depend on infrastructure !
- Sustainability: Funding should be available after end of project, to guarantee services, support and continuous improvement.
- Interoperability: Use open-source software and standards especially in the infrastructure and application middleware layer.
- Collaboration: between infrastructure developers and the applications, to best utilize grid services and to avoid application silos.
- User-Friendliness: for easy adoption for new communities. Infrastructure group should offer installation, operation and support services.
- Grid Services: Centers of Excellence should specialize on specific services, e.g. integration of new communities, grid operation, utility services, training, support, etc.
- Participation of Industry: has to be industry-driven. Push from outside, even with govmnt funding, is not promising. Success comes only from real needs e.g. through already existing collaborations between research and industry.

# D-Grid-2, Start June 2007


- 'Horizontal' Service Grids: professional Service Providers for heterogeneous user groups in research and industry

- 'Vertical' Community Service Grids using existing D-Grid infrastructure and services, supported by Service Providers

- D-Grid extensions, based on a D-Grid 1 gap analysis
  - Tools for operating a professional grid service
  - Adding business layer on top of D-Grid infrastructure
  - Pilot service phase with service providers and 'customers'

!! Reliable grid services require sustainable grid infrastructure !!

# D-Grid-2 Projects


- Grid-based platform for VOs in the **Construction** industry
- **Financial** Business Grid: A service grid architecture for the financial service industry
- Grid-based collaboration among **Aerospace** research and industry
- **Automotive**: Cooperative product design and development in simulation and production data management
- Grid-based **Enterprise Information Systems**, integration & orchestration in commercial IT systems
- **Geographical Data** infrastructure for providing and processing data and simulation for catastrophes, noise, and navigation
- Distributed analysis + exploration of **Multimedia** archives
- Grid-based **IT services** for research and education
- Horizontal integration of resource and service **Monitoring**
- Grid support for small institutions and **SMEs**

# Attract and Integrate New Communities

- First, send proposal to D-Grid-2/3/4 Call
- If approved, join D-Grid Welcome Workshops/Trainings (AHM)
- Download D-Grid software stack on your system and connect
- Your choice: Globus, gLite, Unicore
- Get support from our D-Grid Operation Centre (coming soon)
- Share (part of) your resources with D-Grid
- Port your application/s onto D-Grid infrastructure
- Develop/port/integrate app-specific middleware and tools
- Become a member of the D-Grid Steering Committee
- Develop your core community first, but then scale out
- What else ?

# Last but not least: D-Grid itself is Part of the International Grid Community


Courtesy Dieter Kranzlmueller

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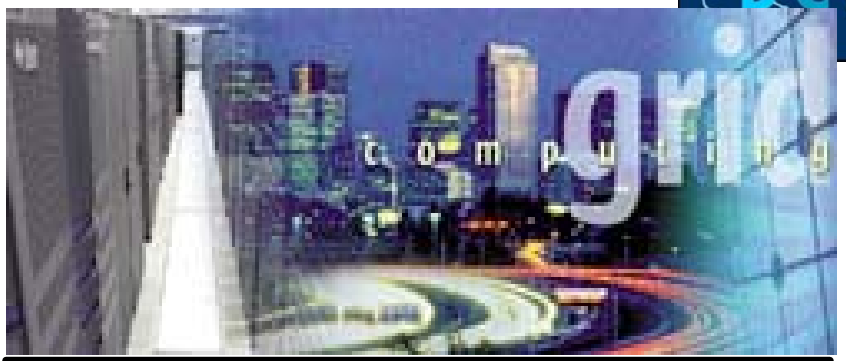
Courtesy Dieter Kranzlmueller




The Grid Engine

The Combustion Engine

The Steam Engine

# Thank You !

Slides are available

wgentzsch@d-grid.de