LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

MNM TEAM
MUNICH NETWORK MANAGEMENT TEAM

LRZ

Hydrometeorological and Hydroclimatological Science on European e-Infrastructures

Dieter Kranzlmüller

Munich Network Management Team

Ludwig-Maximilians-Universität München (LMU)
&
Leibniz Supercomputing Centre
of the Bavarian Academy of Sciences and Humanities

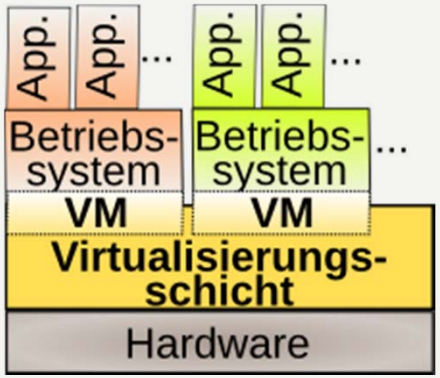

TUM
TECHNISCHE UNIVERSITÄT MÜNCHEN
Garching
lrz
Isar
München
LMU
LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN
der Bundeswehr
Universität München
Neubiberg

Networks

Grid computing

Cloud Computing

High Performance Computing



Virtualization

Service Management

IT Security

iPhone 4s:

- Apple A5 Processor
  - Apple/Samsung System-on-a-Chip (SoC)
  - Presented on 2 March 2011
- Basis: ARM-Architecture
  - Clock frequency: 1 GHz
  - 2 ARM-A9 Cores
- Additional: Graphicsprocessor PowerVR SGX 543MP2
  - 2 Cores - Imagination Technologies

www.apple.com

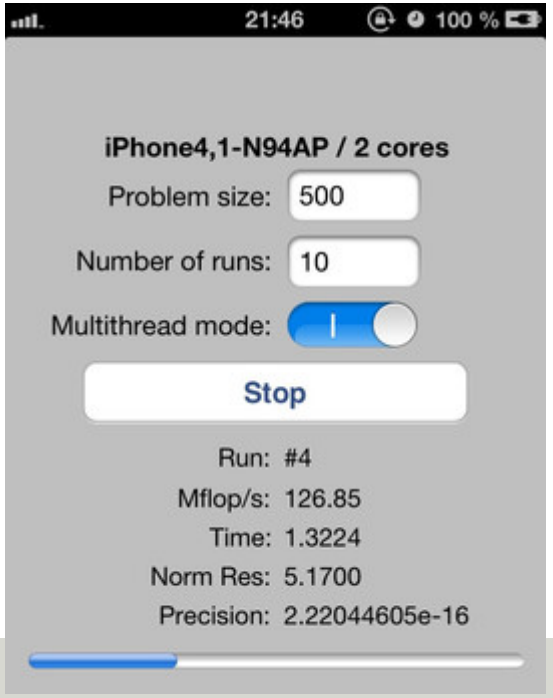
Linpack Benchmark

- Author: Jack Dongarra, University of Tennessee, Knoxville

Jack Dongarra
@ Johannes Kepler University Linz

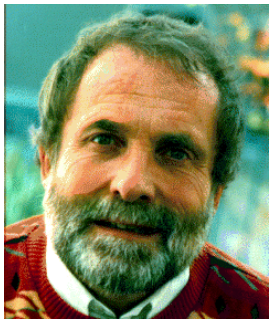
Linpack Benchmark

- Author: Jack Dongarra, University of Tennessee, Knoxville
- Widely used benchmark to measure computers
- Performance data available for all relevant systems
- First results published in 1979
- Solver for systems of linear equations
  ➔ regular problem
- Parameter: Scaling the problem size
- Optimization of software is allowed



Top 500 Supercomputer

- http://www.top500.org
- Statistics about Computers (for vendors, users, …)
- Ranked according to Linpack Benchmark
- Twice a year since 1993
- Authors:
  - Jack Dongarra, Univ. Tennessee
  - Hans-Werner Meuer, Univ. Mannheim
  - Erich Strohmaier & Horst Simon (NERSC/LBNL)



Top 500 Supercomputer (Juni 2012)

Rank	Site	System	Cores	(TFlop/s)	(TFlop/s)	(kW)
1	National University of Defense Technology China	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3120000	33862.7	54902.4	17808
2	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560640	17590.0	27112.5	8209
3	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1572864	17173.2	20132.7	7890
4	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705024	10510.0	11280.4	12660
5	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786432	8586.6	10066.3	3945
6	Texas Advanced Computing Center/Univ. of Texas United States	**Stampede** - PowerEdge C8220, Xeon E5-2680 8C 2.700GHz, Infiniband FDR, Intel Xeon Phi SE10P Dell	462462	5168.1	8520.1	4510
7	Forschungszentrum Juelich (FZJ) Germany	**JUQUEEN** - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect IBM	458752	5008.9	5872.0	2301
8	DOE/NNSA/LLNL United States	**Vulcan** - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect IBM	393216	4293.3	5033.2	1972
9	Leibniz Rechenzentrum Germany	**SuperMUC** - iDataPlex DX360M4, Xeon E5-2680 8C 2.70GHz, Infiniband FDR IBM	147456	2897.0	3185.1	3423
10	National Supercomputing Center in Tianjin China	**Tianhe-1A** - NUDT YH MPP, Xeon X5670 6C 2.93 GHz, NVIDIA 2050 NUDT	186368	2566.0	4701.0	4040
11	Total Exploration Production France	**Pangea** - SGI ICE X, Xeon E5-2670 8C 2.600GHz, Infiniband FDR SGI	110400	2098.1	2296.3	2118
12	CINECA Italy	**Fermi** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	163840	1788.9	2097.2	822

www.top500.org

Top 500 Supercomputer (Juni 2012)

Rank	Site	System	Cores	(TFlop/s)	(TFlop/s)	(kW)
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		16C 1.60GHz,	786432	8586.6	10066.3	3945

Exa	1.000.000.000.000.000.000	Quintillion
Peta	1.000.000.000.000.000	Quadrillion
Tera	1.000.000.000.000	Trillion
Giga	1.000.000.000	Billion
Mega	1.000.000	Million
Kilo	1.000	Thousand

www.top500.org

Tianhe-2 Supercomputer

Tianhe-2 (Milky Way 2)

National University
of Defense Technology
China

33,86 Pflop/s Linpack
54,90 Pflop/s Peak

3.120.000 Cores
17,8 MW Power

Top 500 Supercomputer (Juni 2012)

Rank	Site	System	Cores	(TFlop/s)	(TFlop/s)	(kW)
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www.top500.org

Titan am Oakridge National Laboratory

NSA Utah Data Center

aka **Intelligence Community Comprehensive National Cybersecurity Initiative Data Center**

Camp Williams, Bluffdale, Utah

1,5 million square feet
2 billion US$ building
2 billion US$ hardware
65 MW power
1 Yottabyte Storage

To process “all forms of communication, including the complete contents of private emails, cell phone calls, and Internet searches, as well as all sorts of personal data trails - parking receipts, travel itineraries, bookstore purchases, and other digital 'pocket litter'.”

Top 500 Supercomputer (Juni 2012)

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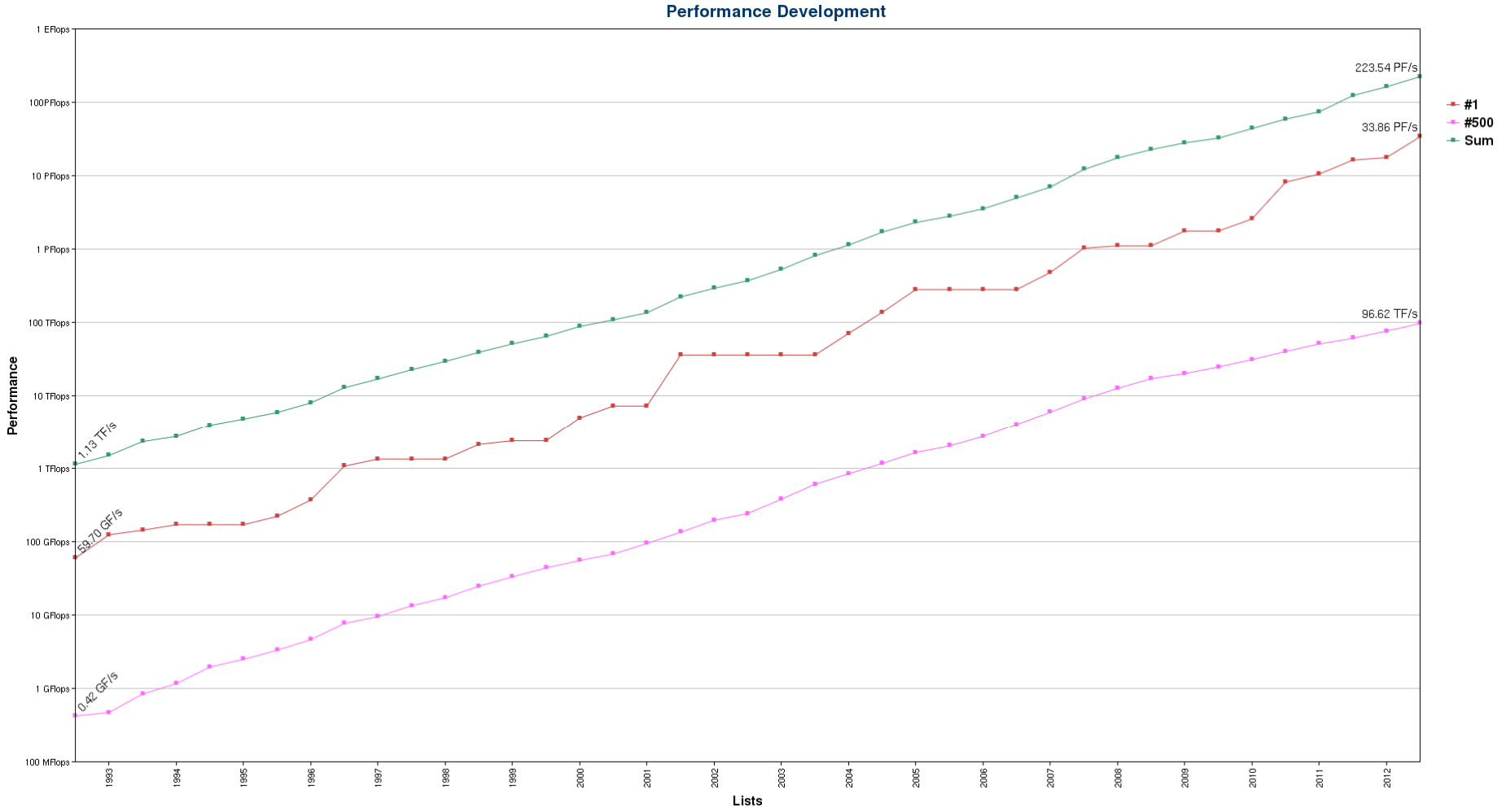
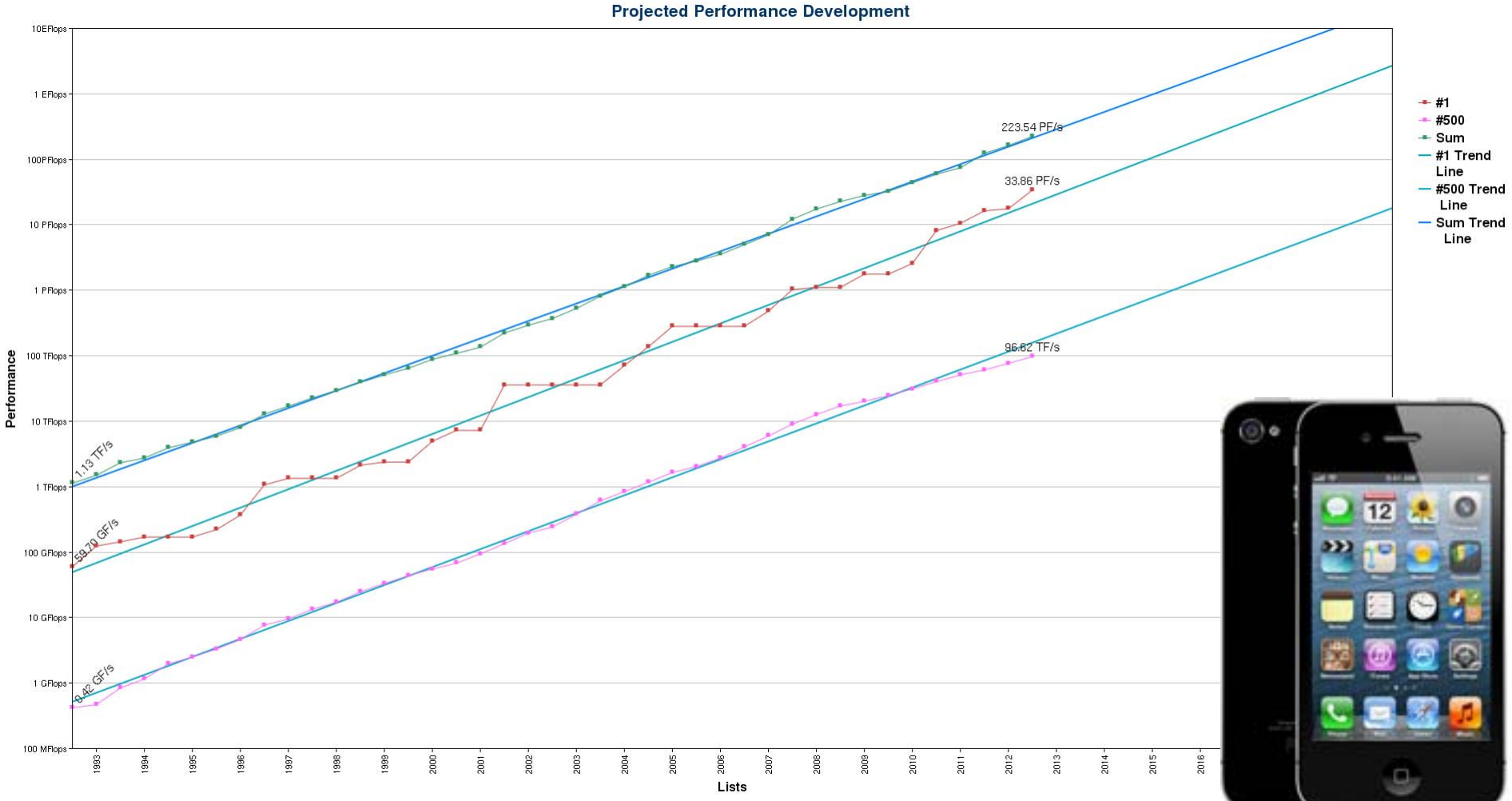
www.top500.org

Top 500 Performance Development



Top 500 Projected Performance Development



www.apple.com

MNM-Team AppleTV Cluster

- 4+2 Nodes, connected via 100 MBit Ethernet

ATV2 Benchmarks:

- 4 Nodes perform at **160.4** MFlops/Watt
- Power consumption approx. 10 Watts (total for all 4 nodes)

➔ Power efficiency = 16 MFlops/Watt

First Google Production Cluster

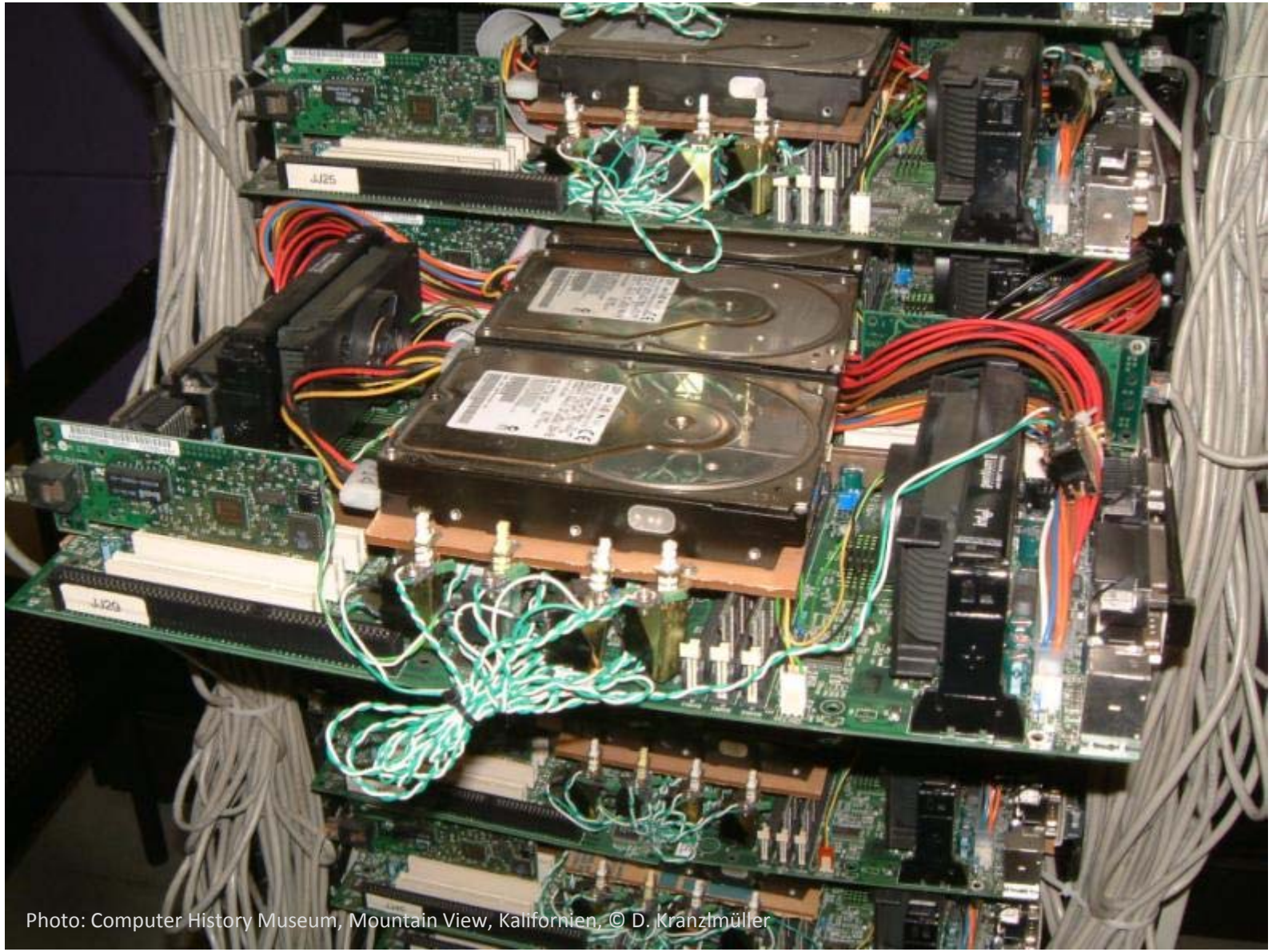
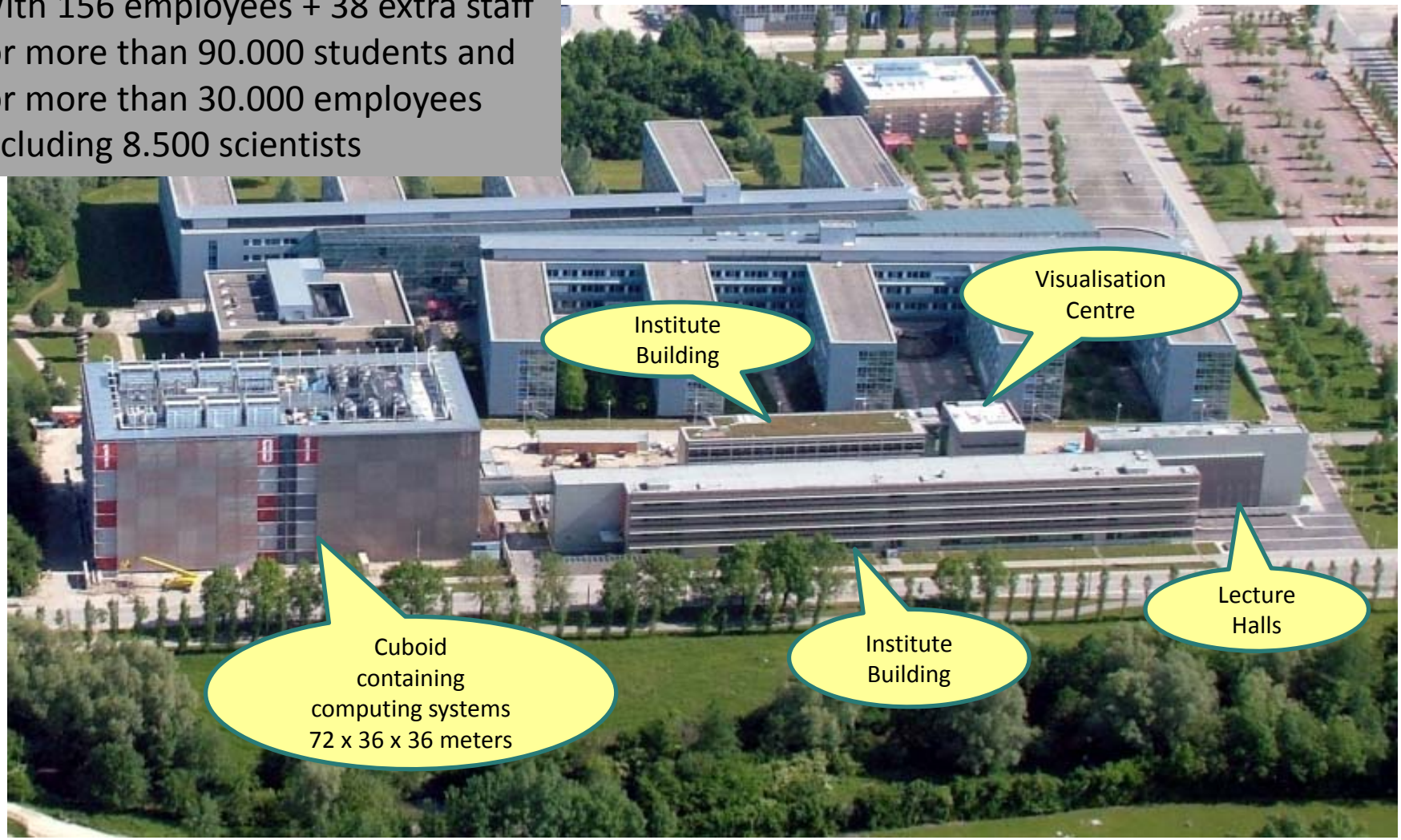


Photo: Computer History Museum, Mountain View, Kalifornien, © D. Kranzlmüller

Leibniz Supercomputing Centre (LRZ)
Garching near Munich, Germany

Leibniz Supercomputing Centre
of the Bavarian Academy of Sciences and Humanities

With 156 employees + 38 extra staff
for more than 90.000 students and
for more than 30.000 employees
including 8.500 scientists

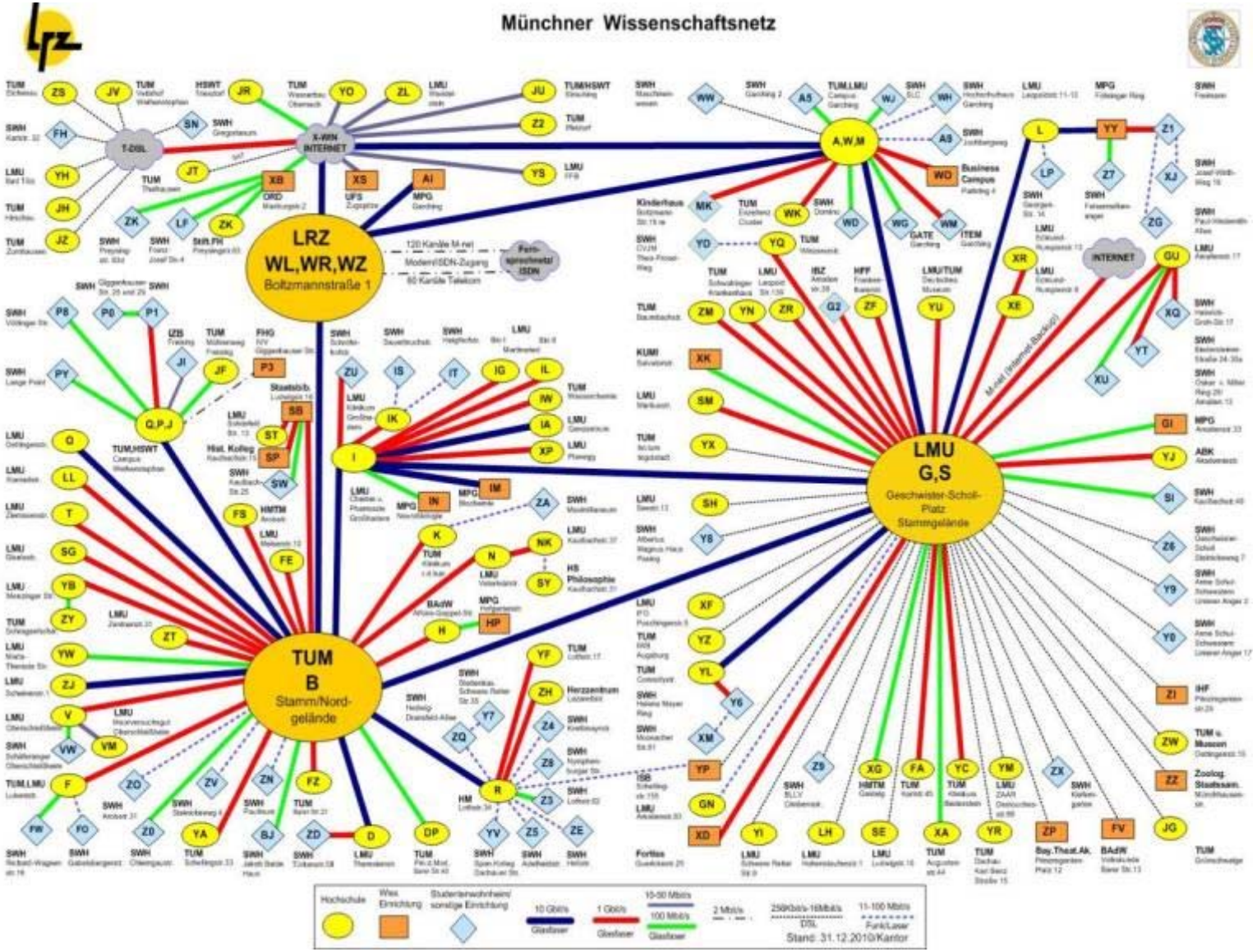


- Computer Centre for all Munich Universities

IT Service Provider:
- Munich Scientific Network (MWN)
- Web servers
- e-Learning
- E-Mail
- Groupware
- Special equipment:
  - Virtual Reality Laboratory
  - Video Conference
  - Scanners for slides and large documents
  - Large scale plotters

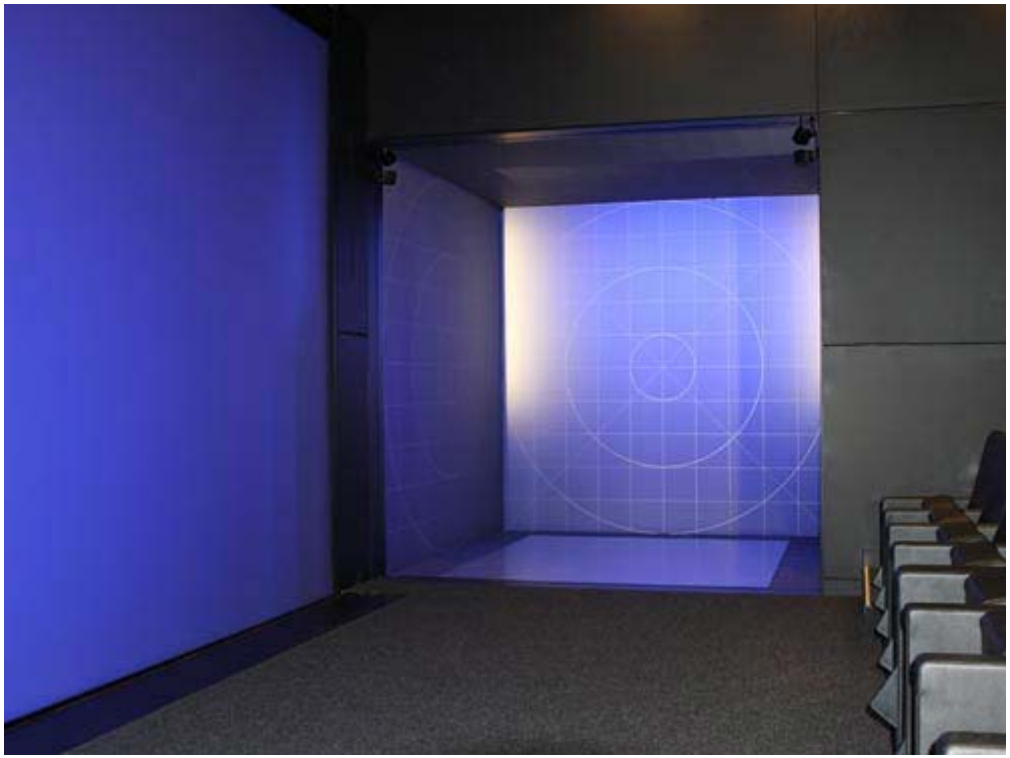
IT Competence Centre:
- Hotline and support
- Consulting (security, networking, scientifc computing, …)
- Courses (text editing, image processing, UNIX, Linux, HPC, …)

The Munich Scientific Network (MWN)



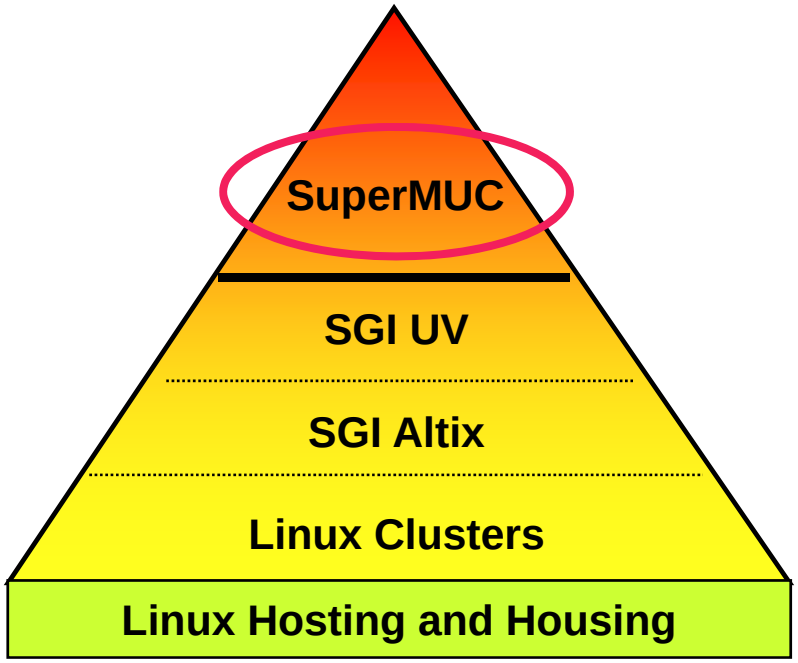
- Regional Computer Centre for all Bavarian Universities
- Computer Centre for all Munich Universities

Virtual Reality and Visualisation Centre (V2C)



5-sided projection room +
large-scale high-resolution powerwall

- European Supercomputing Centre
- National Supercomputing Centre
- Regional Computer Centre for all Bavarian Universities
- Computer Centre for all Munich Universities



SuperMUC @ LRZ

SuperMUC @ LRZ

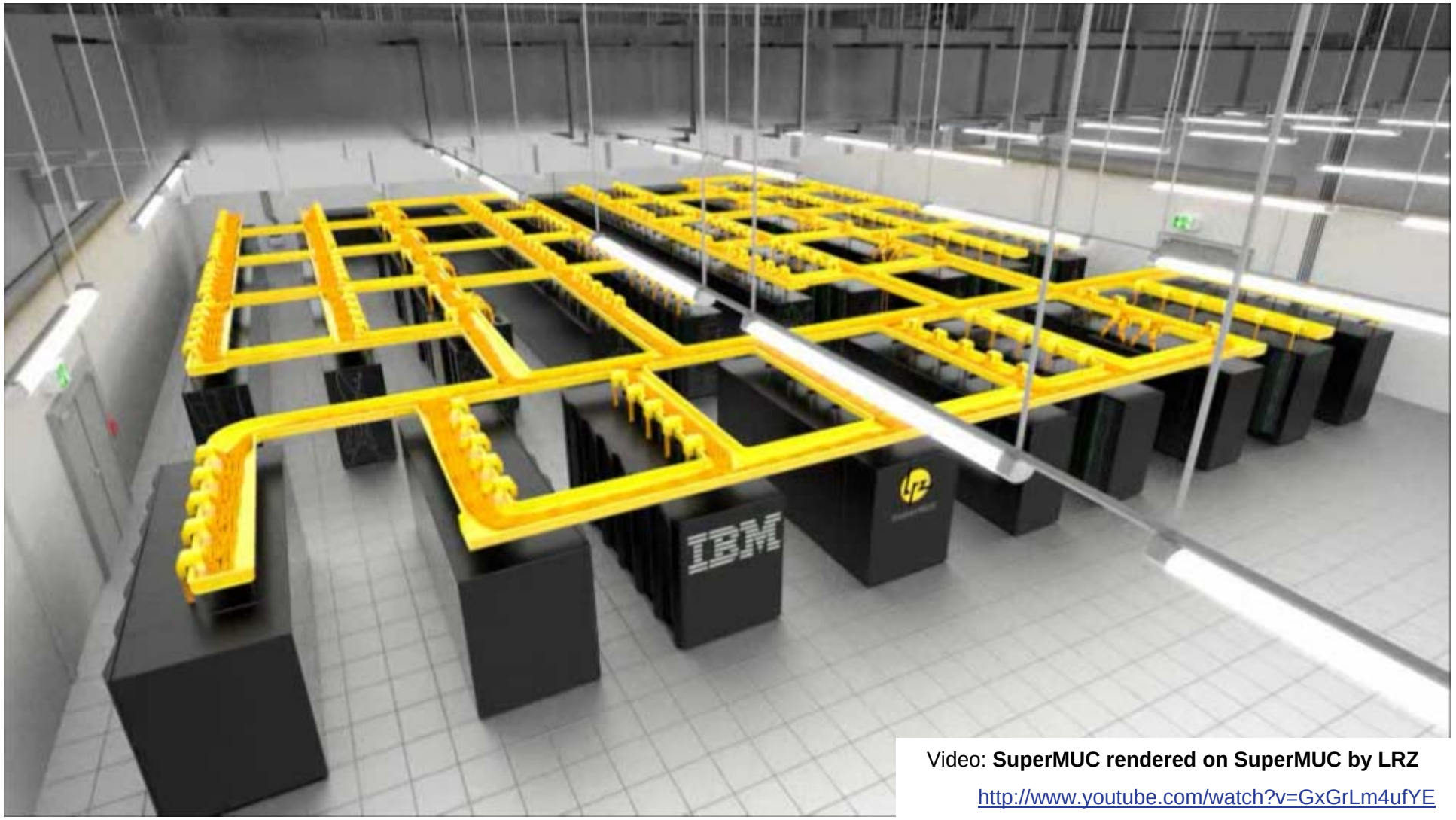
- Fastest Computer in Europe
  Worldwide Position 5 on Top 500, June 2012

Top 500 Supercomputer (Juni 2012)

Rank	Site	Computer/Year Vendor	Cores	R_{max}	R_{peak}	Power
1	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom / 2011 IBM	1572864	16324.75	20132.66	7890.0
2	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect / 2011 Fujitsu	705024	10510.00	11280.38	12659.9
3	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom / 2012 IBM	786432	8162.38	10066.33	3945.0
4	Leibniz Rechenzentrum Germany	**SuperMUC** - iDataPlex DX360M4, Xeon E5-2680 8C 2.70GHz, Infiniband FDR / 2012 IBM	147456	2897.00	3185.05	3422.7
5	National Supercomputing Center in Tianjin China	**Tianhe-1A** - NUDT YH MPP, Xeon X5670 6C 2.93 GHz, NVIDIA 2050 / 2010 NUDT	186368	2566.00	4701.00	4040.0
6	DOE/SC/Oak Ridge National Laboratory United States	**Jaguar** - Cray XK6, Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA 2090 / 2009 Cray Inc.	298592	1941.00	2627.61	5142.0
7	CINECA Italy	**Fermi** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom / 2012 IBM	163840	1725.49	2097.15	821.9
8	Forschungszentrum Juelich (FZJ) Germany	**JuQUEEN** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom / 2012 IBM	131072	1380.39	1677.72	657.5
9	CEA/TGCC-GENCI France	**Curie thin nodes** - Bullx B510, Xeon E5-2680 8C 2.700GHz, Infiniband QDR / 2012 Bull	77184	1359.00	1667.17	2251.0
10	National Supercomputing Centre in Shenzhen (NSCS) China	**Nebulae** - Dawning TC3600 Blade System, Xeon X5650 6C 2.66GHz, Infiniband QDR, NVIDIA 2050 / 2010 Dawning	120640	1271.00	2984.30	2580.0

www.top500.org

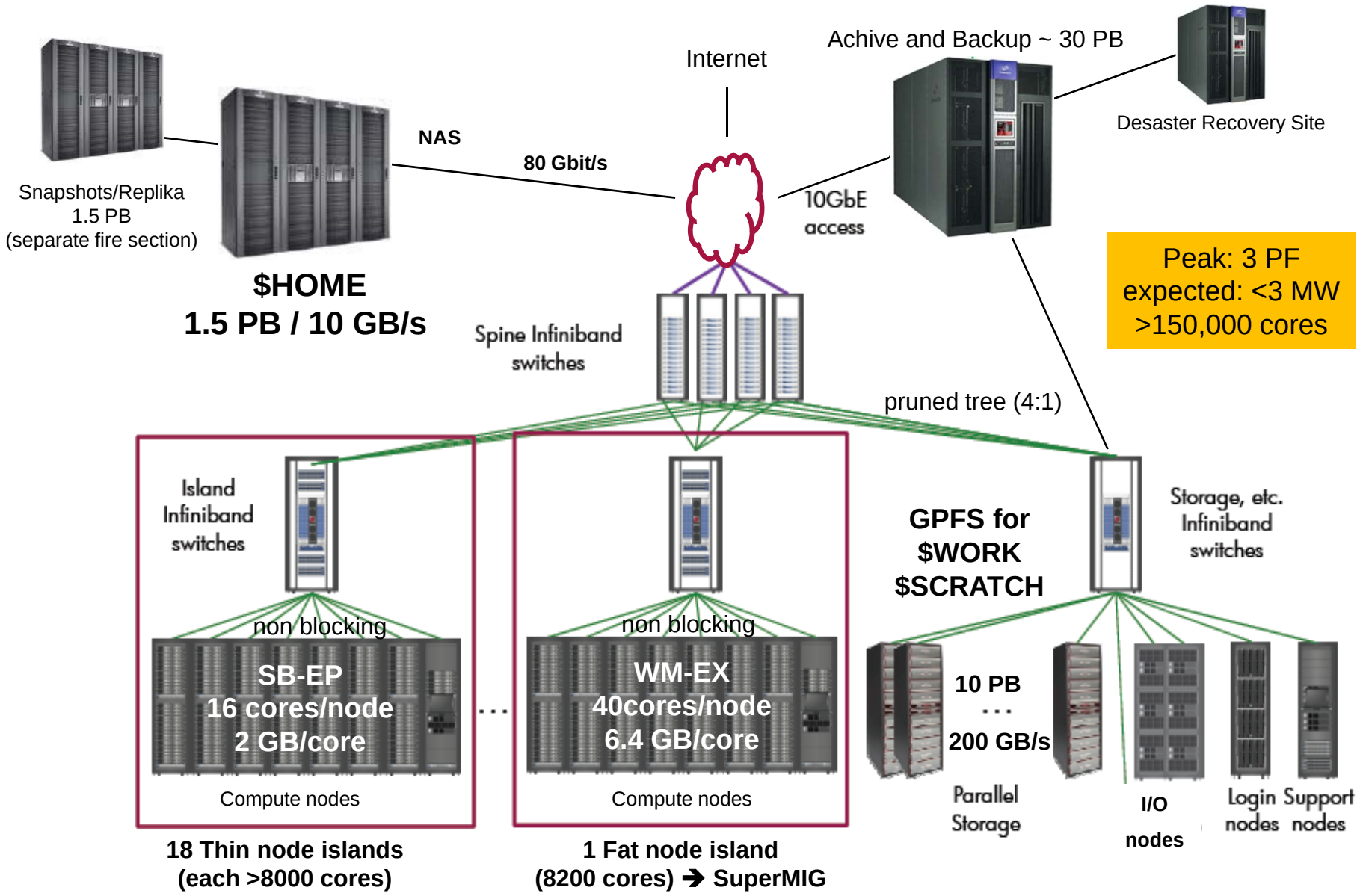
PRACE Tier-0 at LRZ: SuperMUC



Video: **SuperMUC rendered on SuperMUC by LRZ**

http://www.youtube.com/watch?v=GxGrLm4ufYE

PRACE Tier-0 @ LRZ: SuperMUC



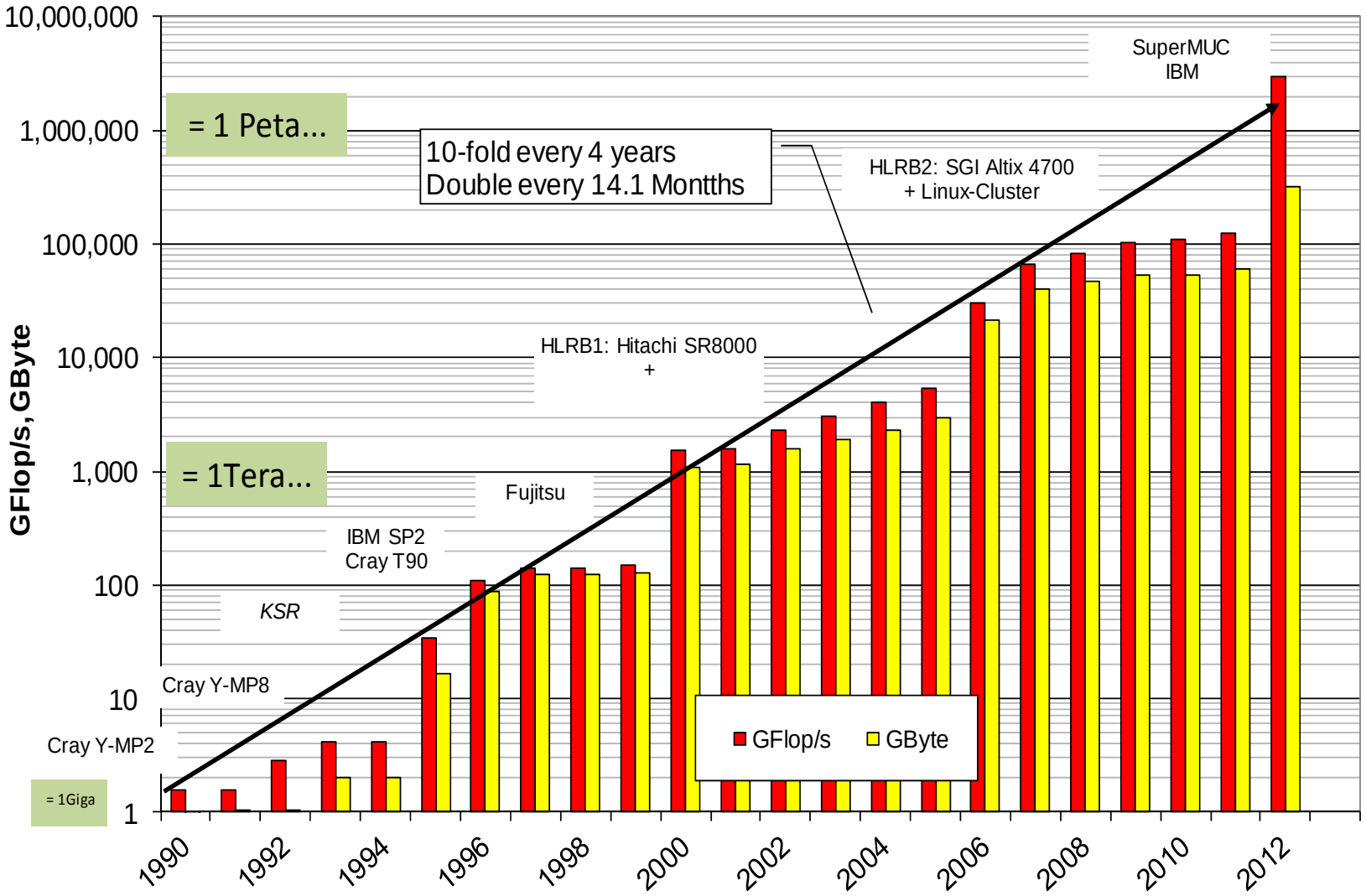
LRZ Building Extension

Picture: Horst-Dieter Steinhöfer

Figure: Herzog+Partner für StBAM2 (staatl. Hochbauamt München 2)

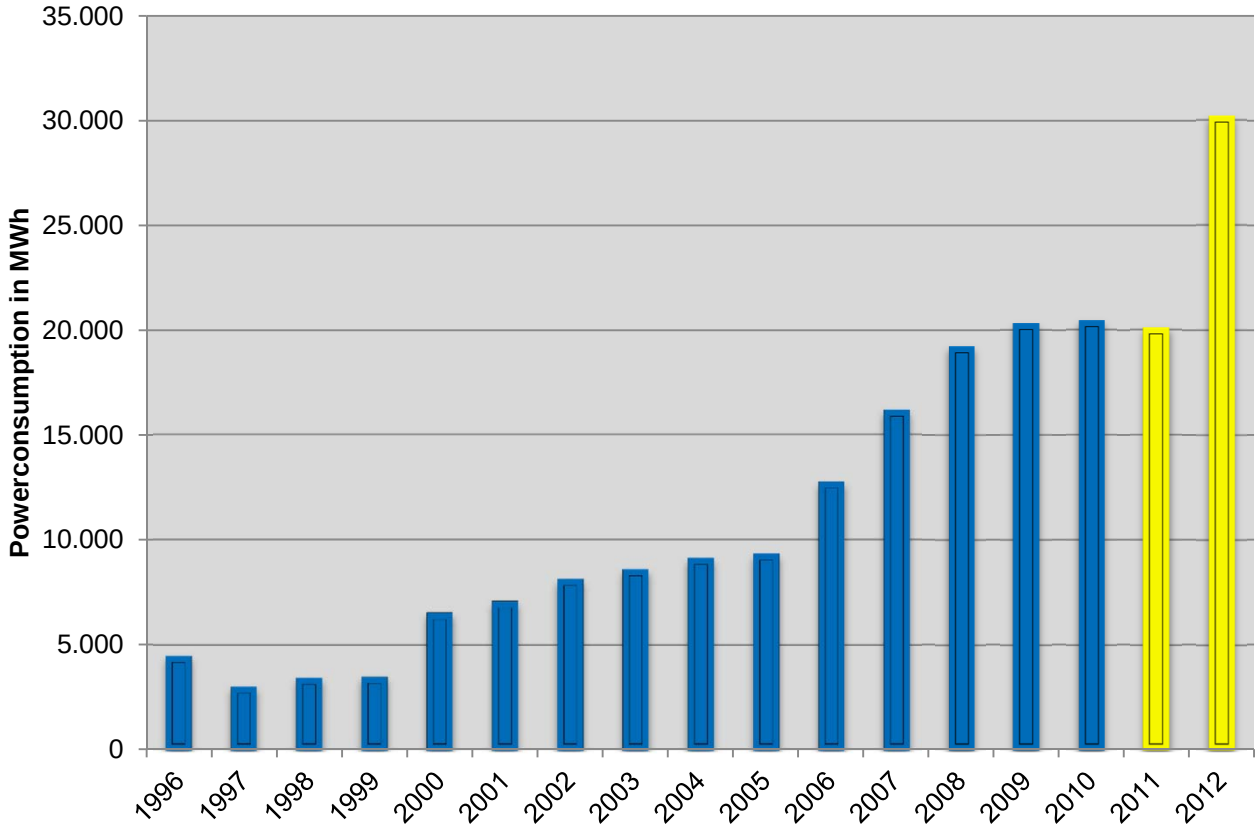
Picture: Ernst A. Graf

Energy Efficient Supercomputing at LRZ



Power Consumption and Cooling

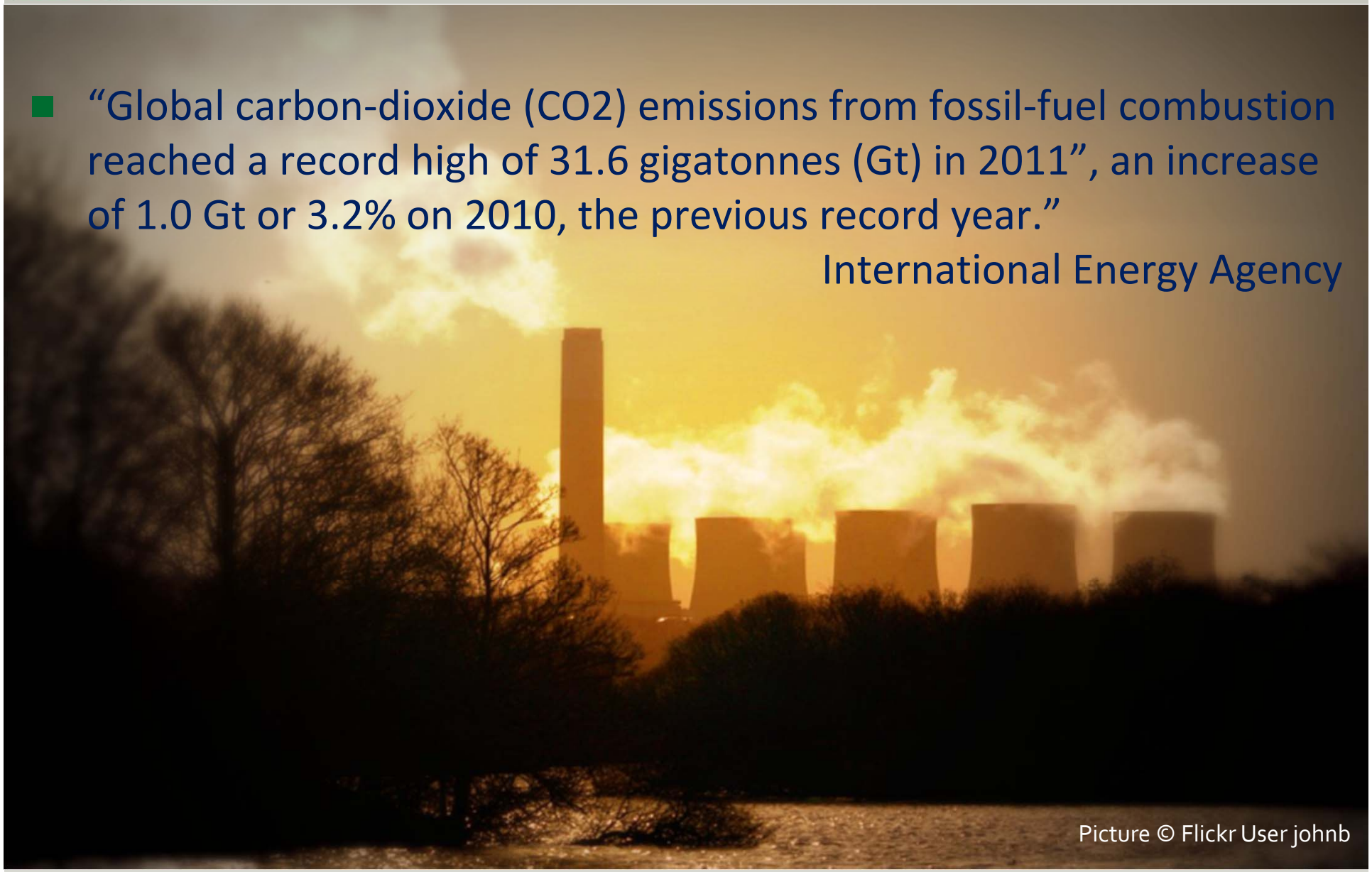
Energy Consumption at LRZ



ICT and Global Warming

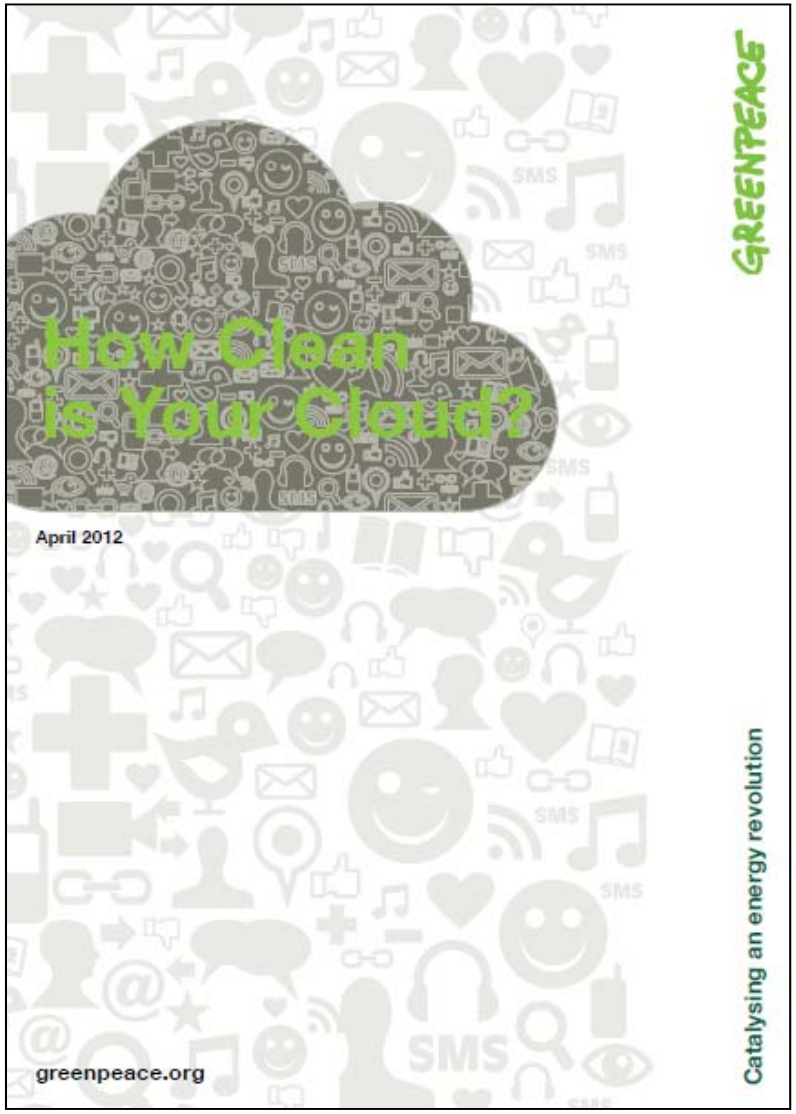
- "Global carbon-dioxide (CO2) emissions from fossil-fuel combustion reached a record high of 31.6 gigatonnes (Gt) in 2011", an increase of 1.0 Gt or 3.2% on 2010, the previous record year."

  International Energy Agency



Picture © Flickr User johnb

Energy Consumption in Computing Centres?



http://www.greenpeace.org/international/Global/international/publications/climate/2012/iCoal/HowCleanisYourCloud.pdf

ICT and Global Warming

- ICT industry is responsible for around 2-3% of the global carbon footprint

  The Organisation for Economic Co-operation and Development (OECD)

- Energy Consumption 2008 in Germany: 616,6 TWh
- Energy Consumption in HPC & Datenzentren: 10,1 TWh

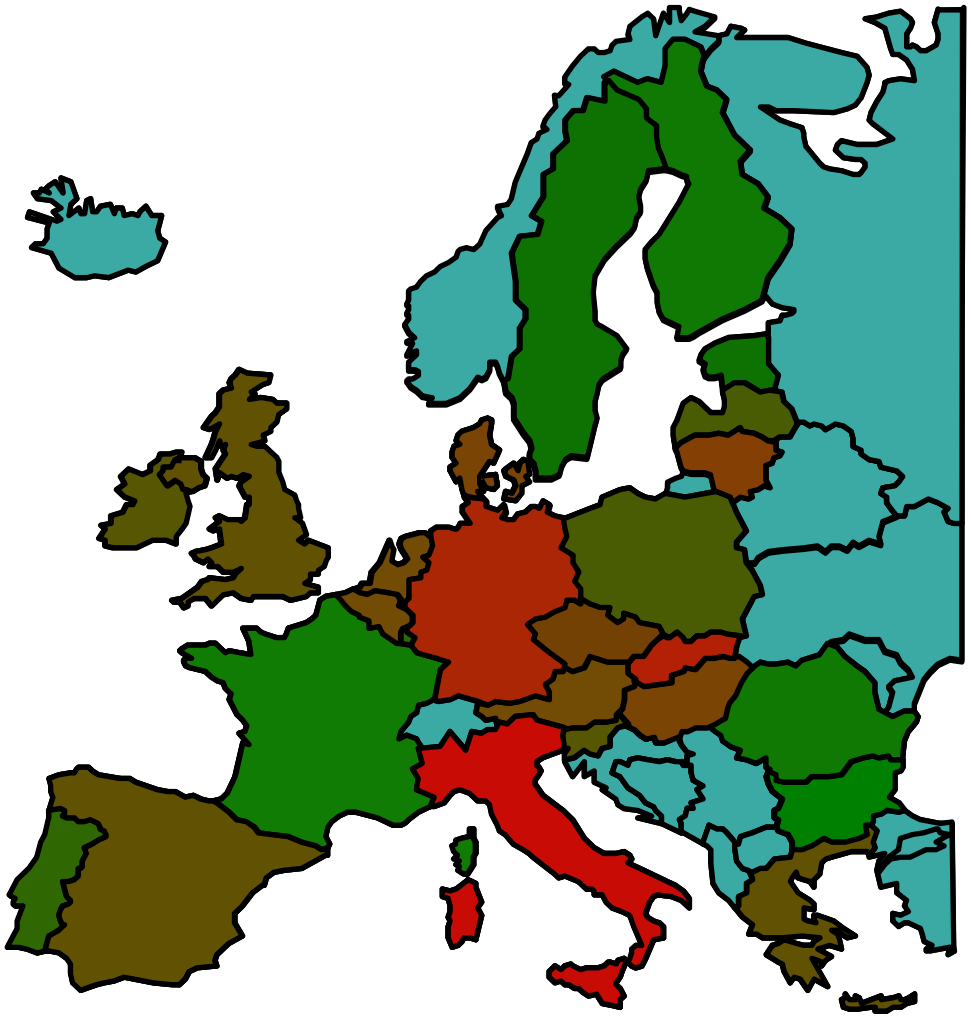
  ➔ ca. 1.6% - 6.4 Millionen Tonnen CO2

  Federal Ministry of Economics and Technology, Germany

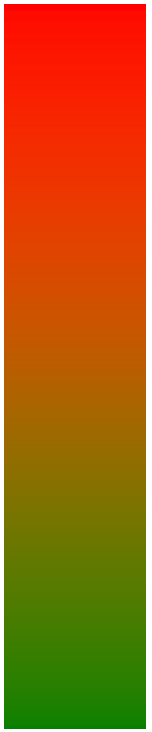
- "ICT is fundamental to measuring — and directly improving — energy efficiency across all industries, including its own, which makes it different from all other industry sectors."

Stephan Scholz, CTO Nokia Siemens Networks
at the UN Climate Change Conference,
Copenhagen, Denmark, in December 2009

Financial Consequences (Power Bill)

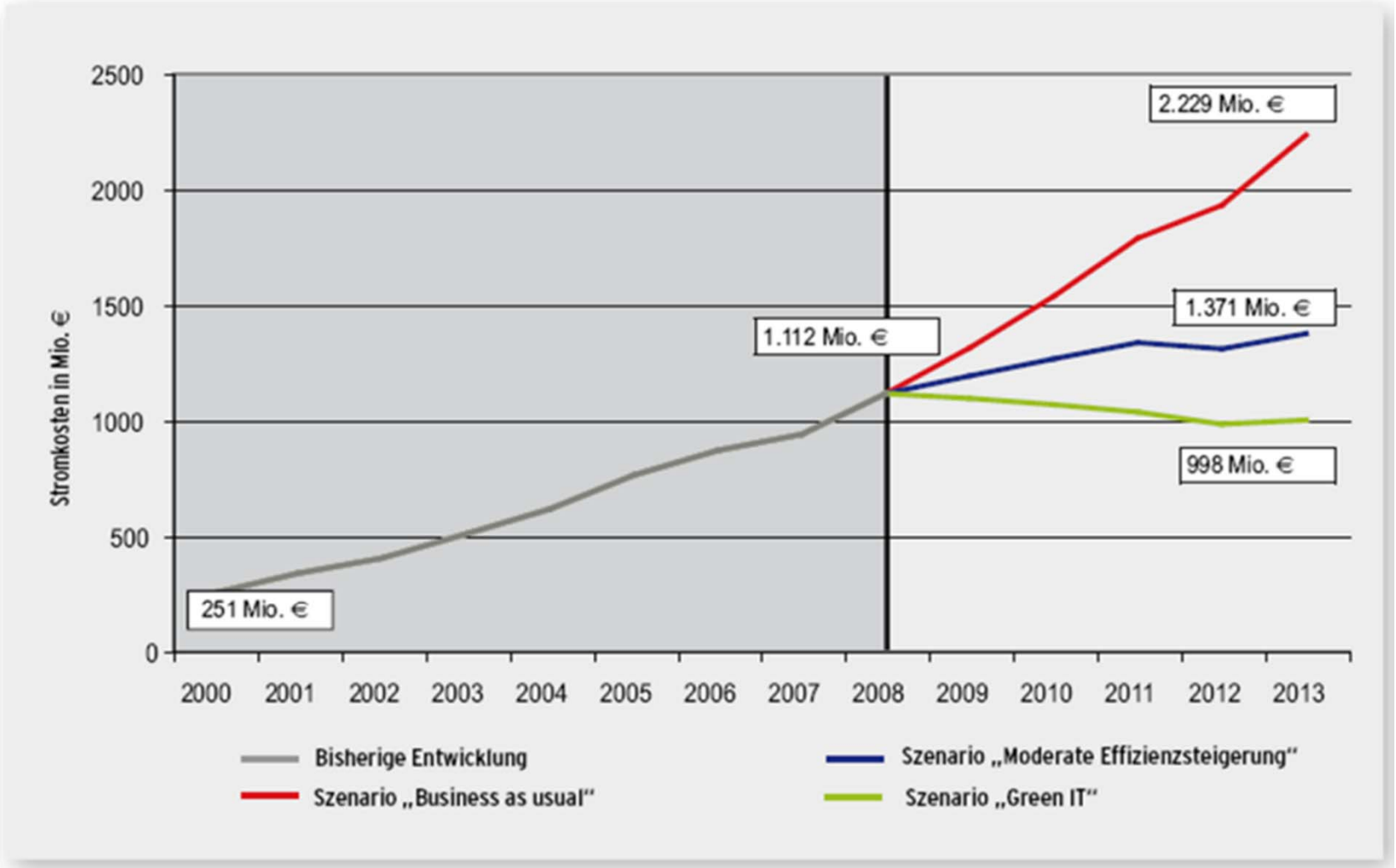


€ / KWh
for industrial customers



Source: energy.eu (effective April 2011)

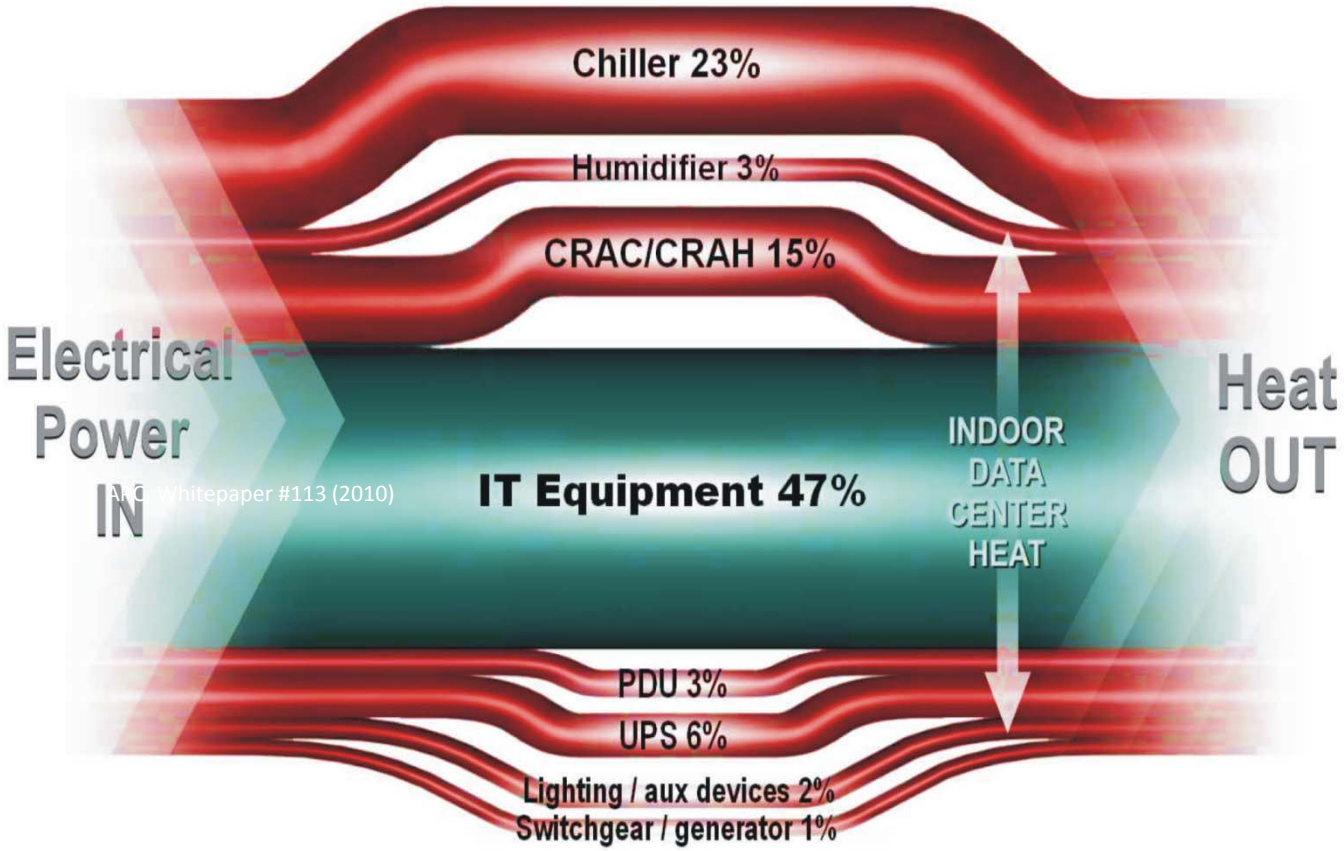
Energy costs of Germany Data Centres



Quelle: Borderstep 2008

Energy Consumption in Data Centres

- Data Centres are "Heaters with integrated logic"

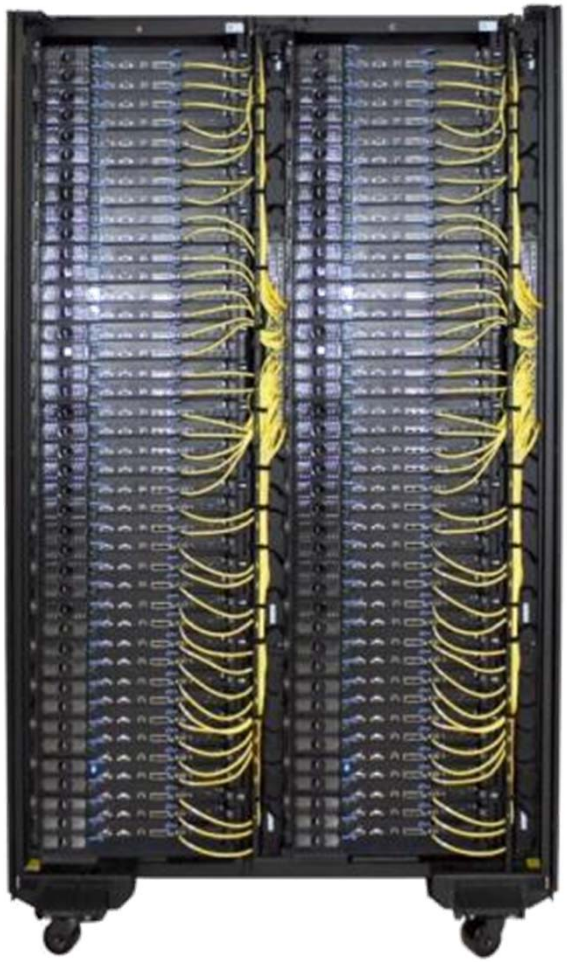


APC Whitepaper #113 (2010)

Torsten Bloth, IBM Lab Services - © IBM Corporation

SuperMUC Cooling

IBM System x iDataPlex
Direct Water Cooled Rack



iDataplex DWC Rack
w/ water cooled nodes
(front view)

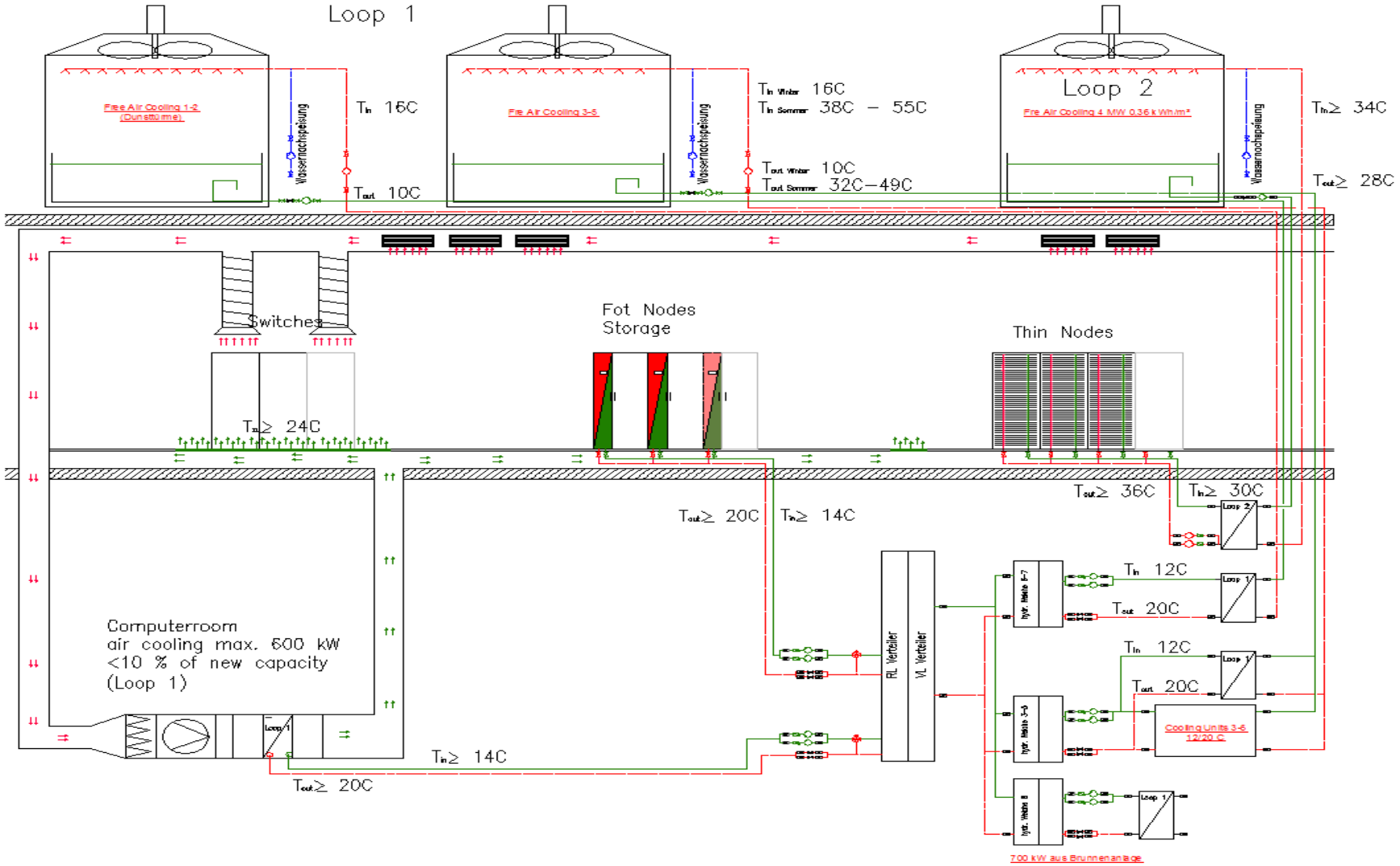
iDataplex DWC Rack
w/ water cooled nodes
(rear view of water manifolds)

Torsten Bloth, IBM Lab Services - © IBM Corporation

IBM iDataplex dx360 M4

Torsten Bloth, IBM Lab Services - © IBM Corporation

Cooling Concept – Dedicated Free Cooling



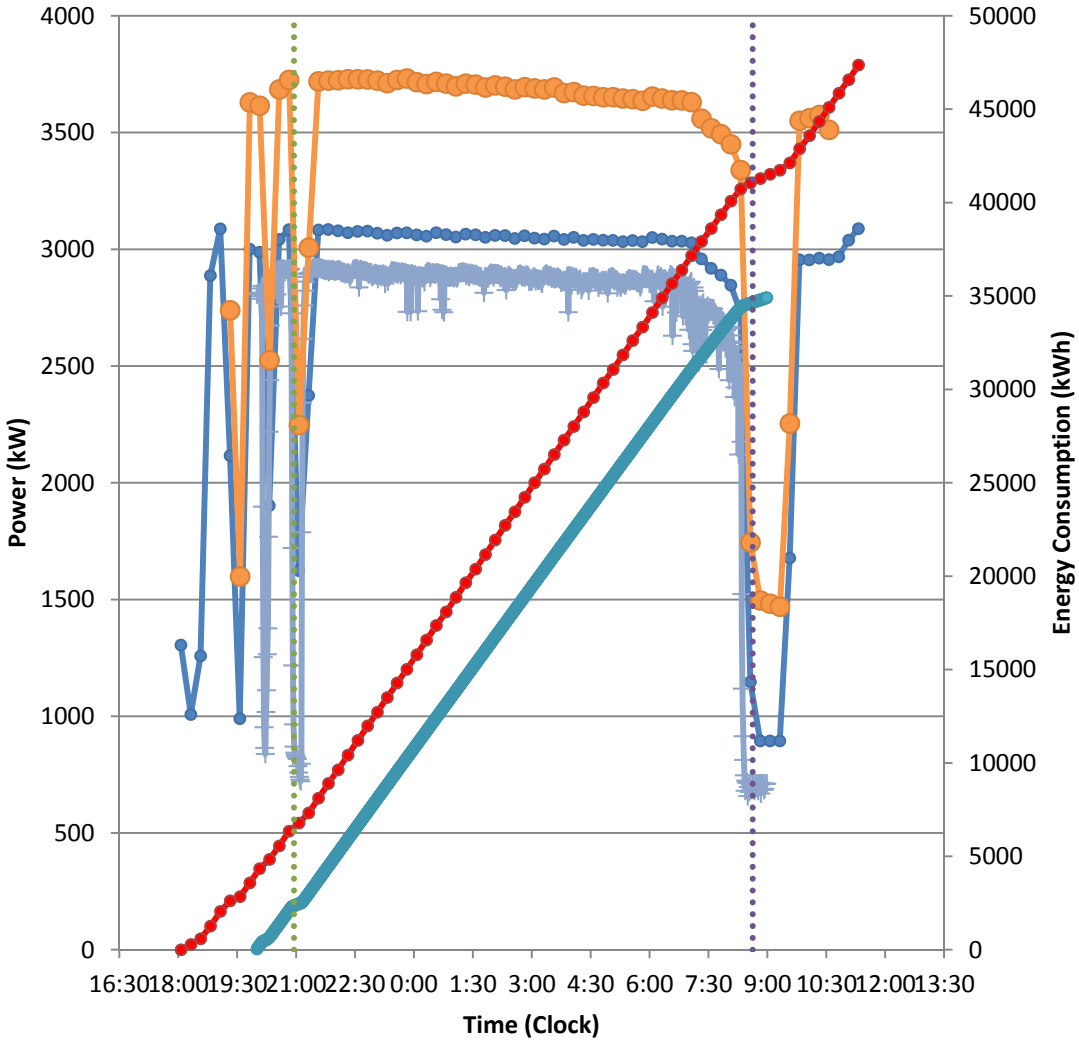
Cooling Infrastructure 3rd Floor

Pictures: StBAM2 (staatl. Hochbauamt München 2)

Cooling Infrastructure Rooftop

Picture: StBAM2 (staatl. Hochbauamt München 2)

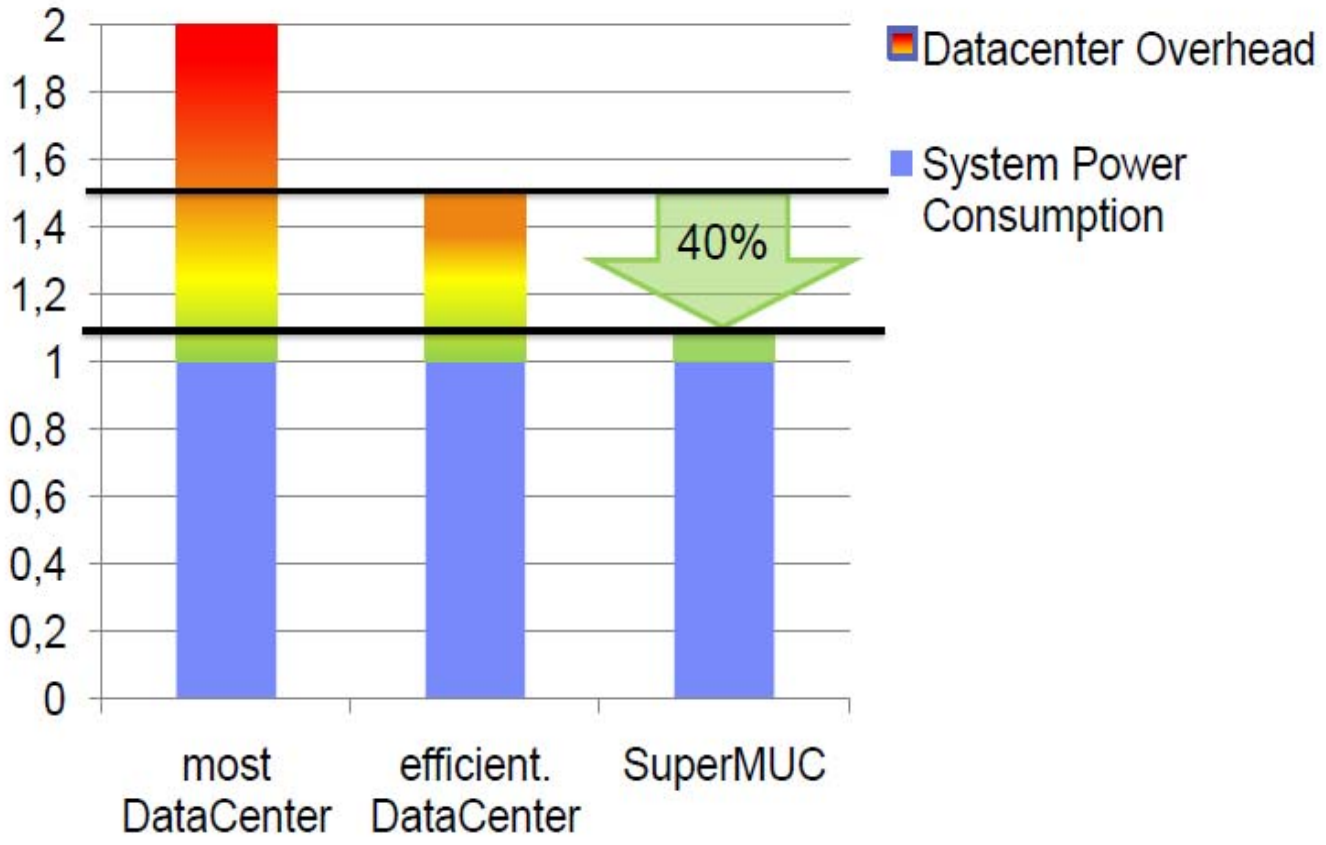
SuperMUC HPL Energy Consumption



Energy efficiency *(single number in GFlops/Watt)*
9,380E-01 (PDU, 10 minutes resolution, whole run)
9,359E-01 (PDU, 1 minutes resolution, whole run, without cooling)
9,359E-01 (PDU, 1 minutes resolution, whole run, cooling included)
8,871E-01 (machine room measurement, whole run)
7,296E-01 (infrastructure measurement, whole run)

SuperMUC & Green IT

Cost Advantage with impoverd PUE and reduced CO_2:



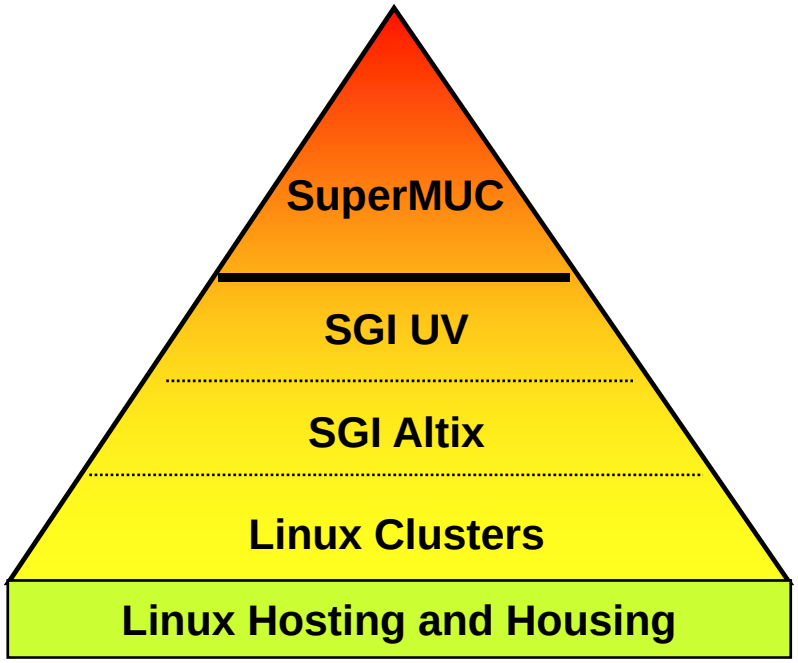
SuperMUC - Energy Efficient Supercomputing

- Probably **most powerful x86-system in Europe** (3PetaFlops peak)
- Use for science in Europe (PRACE), Germany (GCS) and Bavaria (KONWIHR)
- System with >150.000 cores, 324 TeraByte Main Memory
- **Most energy efficient General Purpose Supercomputer** in Europe in 2012
  - Hot liquid cooling
  - Reuse of waste heat
  - Hardware and software tools for clock scaling and optimization („dynamic frequency scaling“, „CPU throttling“ WIKIPEDIA)

Energy Efficiency at LRZ

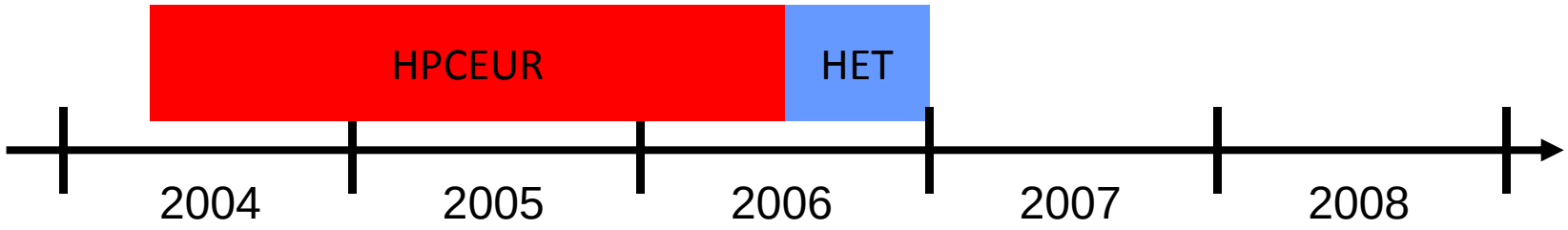
- **Measures** around SuperMUC
  - New Contract (Spot Market / Evaluation of alternative Technologies)
  - Optimization of Building and Cooling Infrastructure (additional cooling loop)
  - Hot liquid cooling PUE < 1,1
  - Cooperation LRZ / TUM / LMU / IBM on Tools and Provider / User Strategies
  - Cooperation with Building Management YIT
- PRACE
  - 1 IP – Evaluation Prototype SGI Ultraviolet
  - 2 IP – Evaluation Prototype T-Platforms
- Exascale EU Project DEEP:
  - System based on „Accelerator – Architecture“ (Intel MIC)
  - Cooling and Prototype Evaluation
- Exascale EU Project Mont-Blanc
  - System based on low-power commercially available embedded CPUs
  - Next-generation HPC machine with a range of embedded technology
  - Software applications to run on this new generation of HPC systems

- European Supercomputing Centre
- National Supercomputing Centre
- Regional Computer Centre for all Bavarian Universities
- Computer Centre for all Munich Universities

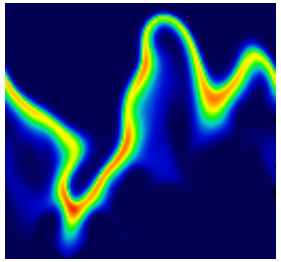


PRACE – Partnership for Advanced Computing in Europe

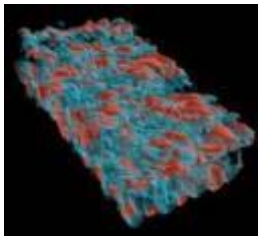
PRACE – Partnership for Advanced Computing in Europe



The European Scientific Case

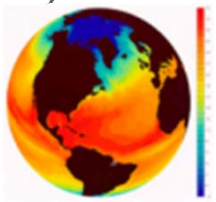
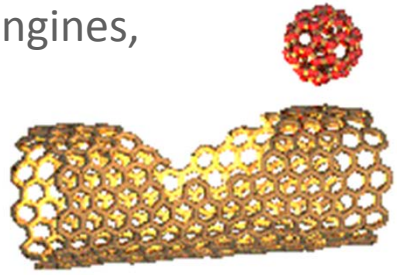
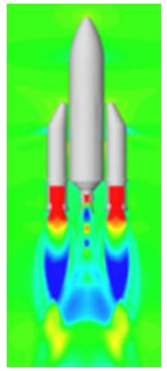
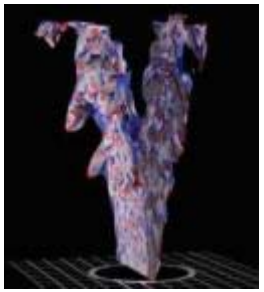



- Weather, Climatology, Earth Science
  - degree of warming, scenarios for our future climate.
  - understand and predict ocean properties and variations
  - weather and flood events
- Astrophysics, Elementary particle physics, Plasma physics
  - systems, structures which span a large range of different length and time scales
  - quantum field theories like QCD, ITER



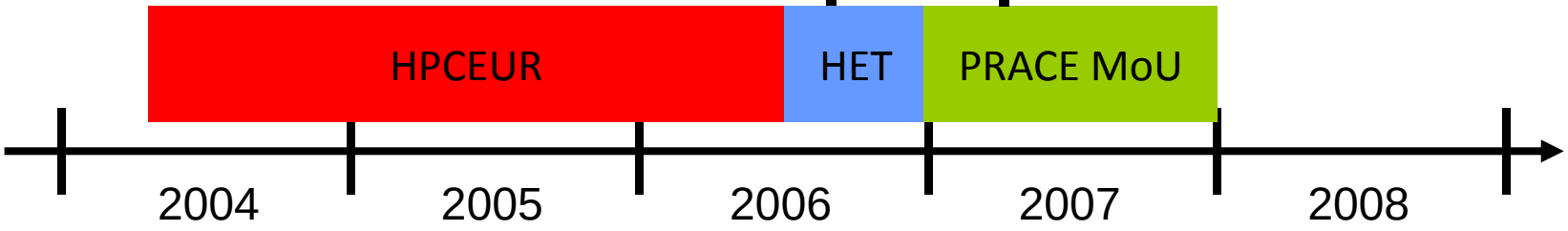
- Material Science, Chemistry, Nanoscience
  - understanding complex materials, complex chemistry, nanoscience
  - the determination of electronic and transport properties
- Life Science
  - system biology, chromatin dynamics, large scale protein dynamics, protein association and aggregation, supramolecular systems, medicine

- Engineering
  - complex helicopter simulation, biomedical flows, gas turbines and internal combustion engines, forest fires, green aircraft,
  - virtual power plant

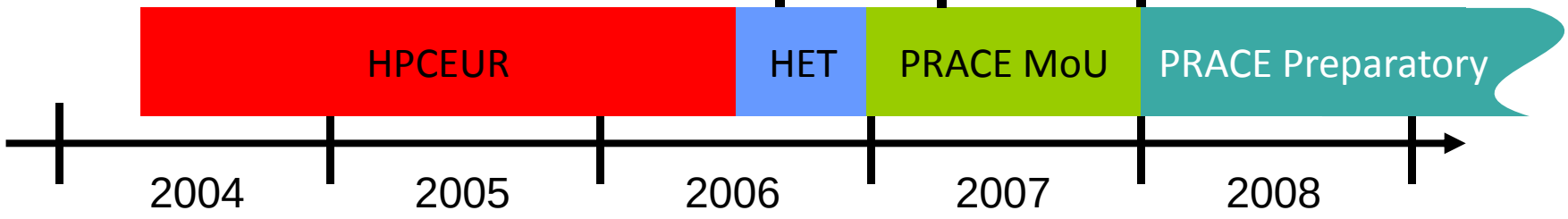
PRACE Timeline

PRACE – Partnership for Advanced Computing in Europe

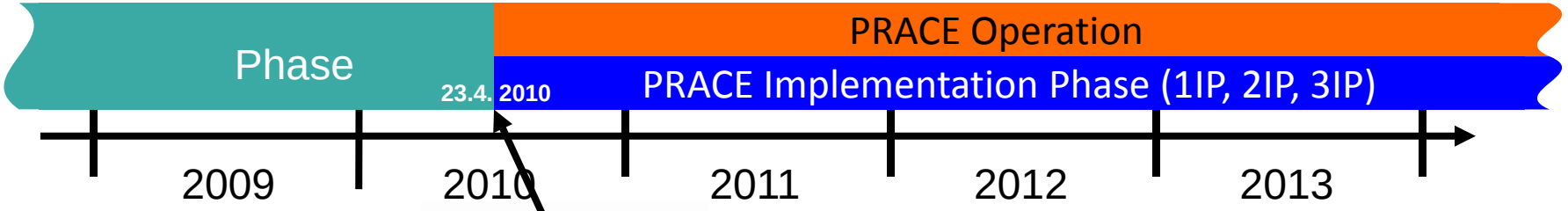


PRACE Timeline

PRACE – Partnership for Advanced Computing in Europe



EU-Grant: INFSO-RI-211528, 10 Mio. €



PRACE

PRACE (AISBL), a legal entity with (current) seat location in Brussels

PRACE Research Infrastructure Created

- Establishment of the legal framework
  - PRACE AISBL created with seat in Brussels in April (Association Internationale Sans But Lucratif)
  - 20 members representing 20 European countries
  - Inauguration in Barcelona on June 9

Gauss Centre for Supercomputing (GCS)

- Joint activity of the **3 German National HPC Centres**
  - John von Neumann Institut für Computing (NIC), Jülich
  - Leibniz Supercomputing Centre (LRZ), Garching near Munich
  - Höchstleistungsrechenzentrum Stuttgart (HLRS), Stuttgart

- **Largest and most powerful supercomputer infrastructure in Europe**

- Foundation of GCS (e.V.) April, 13th, 2007.
- Principal Partner in PRACE
  (Partnership for Advanced Computing in Europe)

PRACE Research Infrastructure Created

- Establishment of the legal framework
  - PRACE AISBL created with seat in Brussels in April (Association Internationale Sans But Lucratif)
  - 20 members representing 20 European countries
  - Inauguration in Barcelona on June 9

- Funding secured for 2010 - 2015
  - 400 Million € from France, Germany, Italy, Spain
    Provided as Tier-0 services on TCO basis
  - Funding decision for 100 Million € in The Netherlands expected soon
  - 70+ Million € from EC FP7 for preparatory and implementation
    Grants INFSO-RI-211528 and 261557
    Complemented by ~ 60 Million € from PRACE members

PRACE Tier-0 Systems

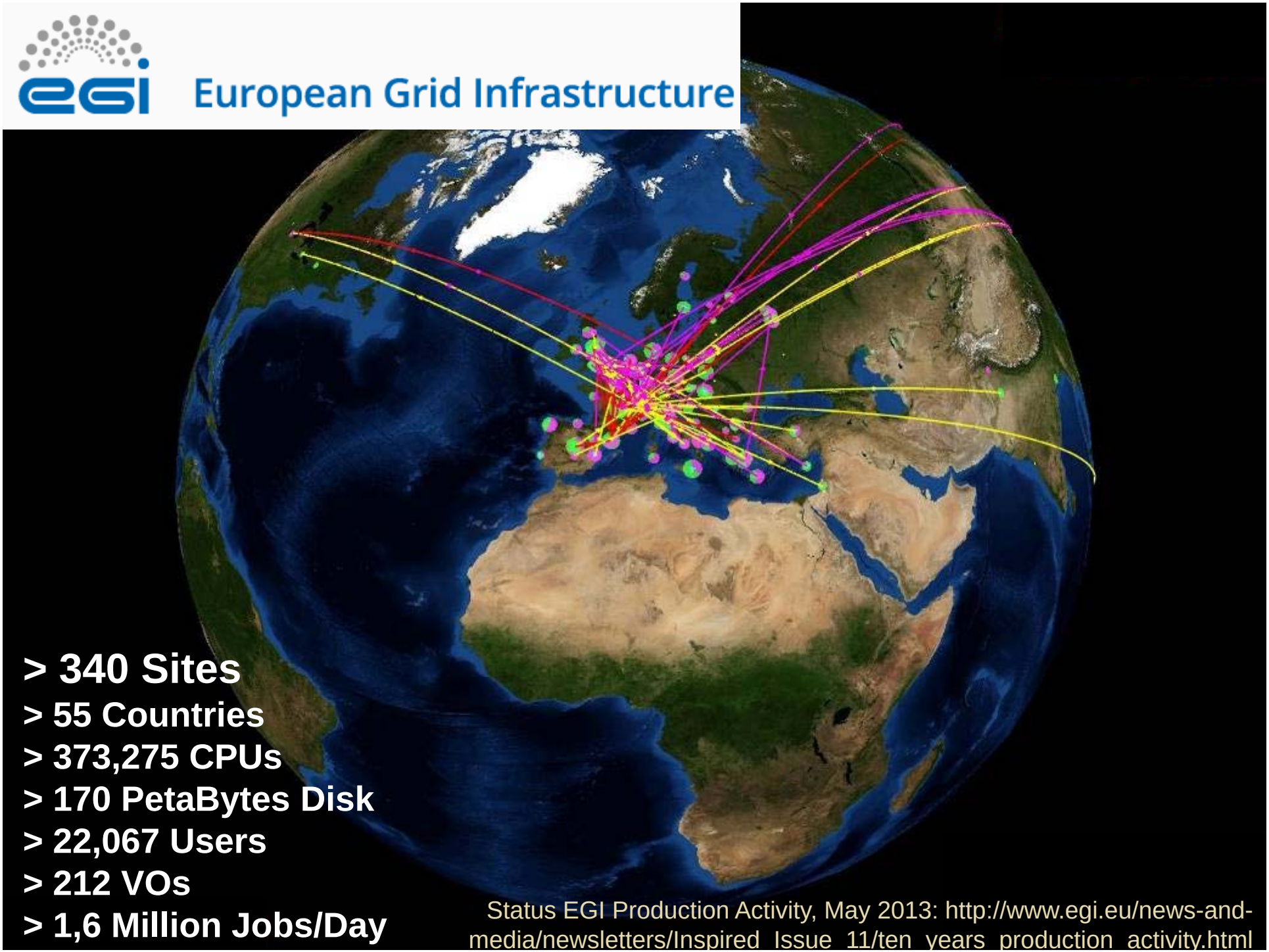
- 1st Tier-0 System
  - **Jugene**: BlueGene/P in GCS@Juelich
  - 72 Racks, 1 PFlop/s peak
  - 35% of capacity provided to PRACE
- 2nd Tier-0 System
  - **Curie**: Bull Cluster with Intel CPUs operated by CEA
  - 1.6 PFlop/s peak in Oct. 2011 (1st step in 10/2010)
  - Largest fraction of capacity provided to PRACE
- Next Procurements (in alphabetical order)
  - BSC, CINECA, GCS@HLRS, GCS@LRZ
  - Procurement plan based on analysis of user requirements and market

PRACE Tier-0 Access

- Single pan-European Peer Review
- Early Access Call in May 2010
  - 68 proposals asked for 1870 Million Core hours
  - 10 projects granted with 328 Million Core hours
  - Principal Investigators from D (5), UK (2) NL (1), I (1), PT (1)
  - Involves researchers from 31 institutions in 12 countries
- 1st Regular Call closed on August 2010
  - 58 proposals received asked for 2900 million core hours
  - 33 proposals have fulfilled the technical assessment
  - 360 million core hours available
    for a 12 months allocation period starting November 2010
- Further calls being scheduled (every 6 months)
  - 2nd regular call will include both Jugene and Curie

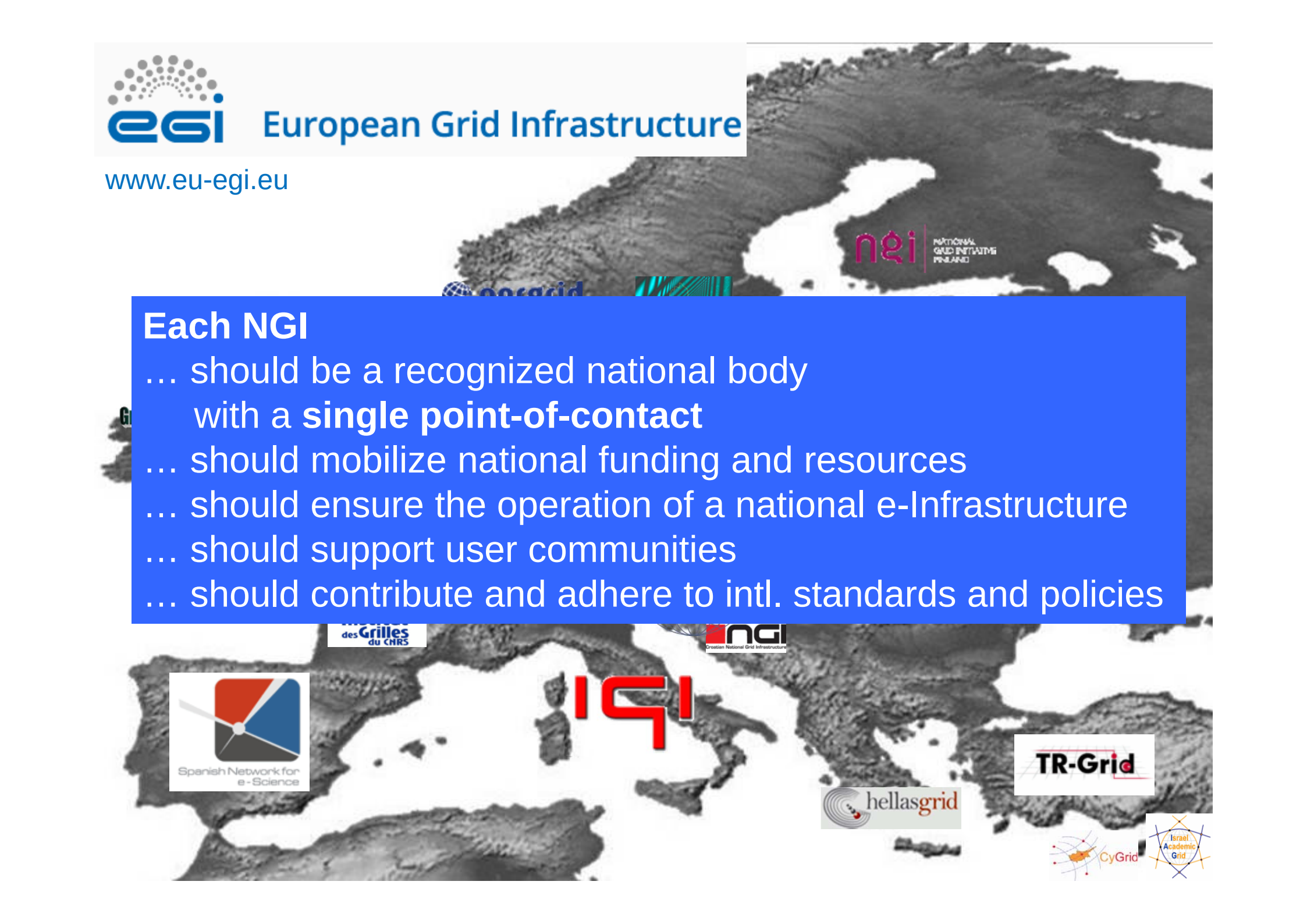
Interconnecting distributed computers

European Grid Infrastructure



> 340 Sites
> 55 Countries
> 373,275 CPUs
> 170 PetaBytes Disk
> 22,067 Users
> 212 VOs
> 1,6 Million Jobs/Day

Status EGI Production Activity, May 2013: http://www.egi.eu/news-and-media/newsletters/Inspired_Issue_11/ten_years_production_activity.html


European Grid Infrastructure
www.eu-egi.eu
Each NGI
… should be a recognized national body
with a single point-of-contact
… should mobilize national funding and resources
… should ensure the operation of a national e-Infrastructure
… should support user communities
… should contribute and adhere to intl. standards and policies
ngi
NATIONAL GRID INITIATIVE FINLAND
des Grilles du CNRS
NGI
Croatian National Grid Infrastructure
IGI
Spanish Network for e-Science
TR-Grid
hellasgrid
CyGrid
Israel Academic Grid

European Grid Infrastructure

Objectives:

- Ensure the long-term sustainability of the European e-infrastructure
- Coordinate the integration and interaction between National Grid Infrastructures
- Operate the European level of the production Grid infrastructure for a wide range of scientific disciplines to link National Grid Infrastructures

EGI Grid Infrastructure should be

- a large-scale, production Grid infrastructure
- built on national grids that interoperate seamlessly at many levels,
- offering reliable and predictable services to a wide range of applications

EGI Operations Tasks

- Operation of tools and services
- Grid configuration repositories
- Grid accounting repositories
- Grid repositories for SLA compliance and performance monitoring
- Grid operations portal
- NGI Grid oversight

- Security
- Security policy development and maintenance
- Coordination of security and incident response
- Expert team for security vulnerabilities

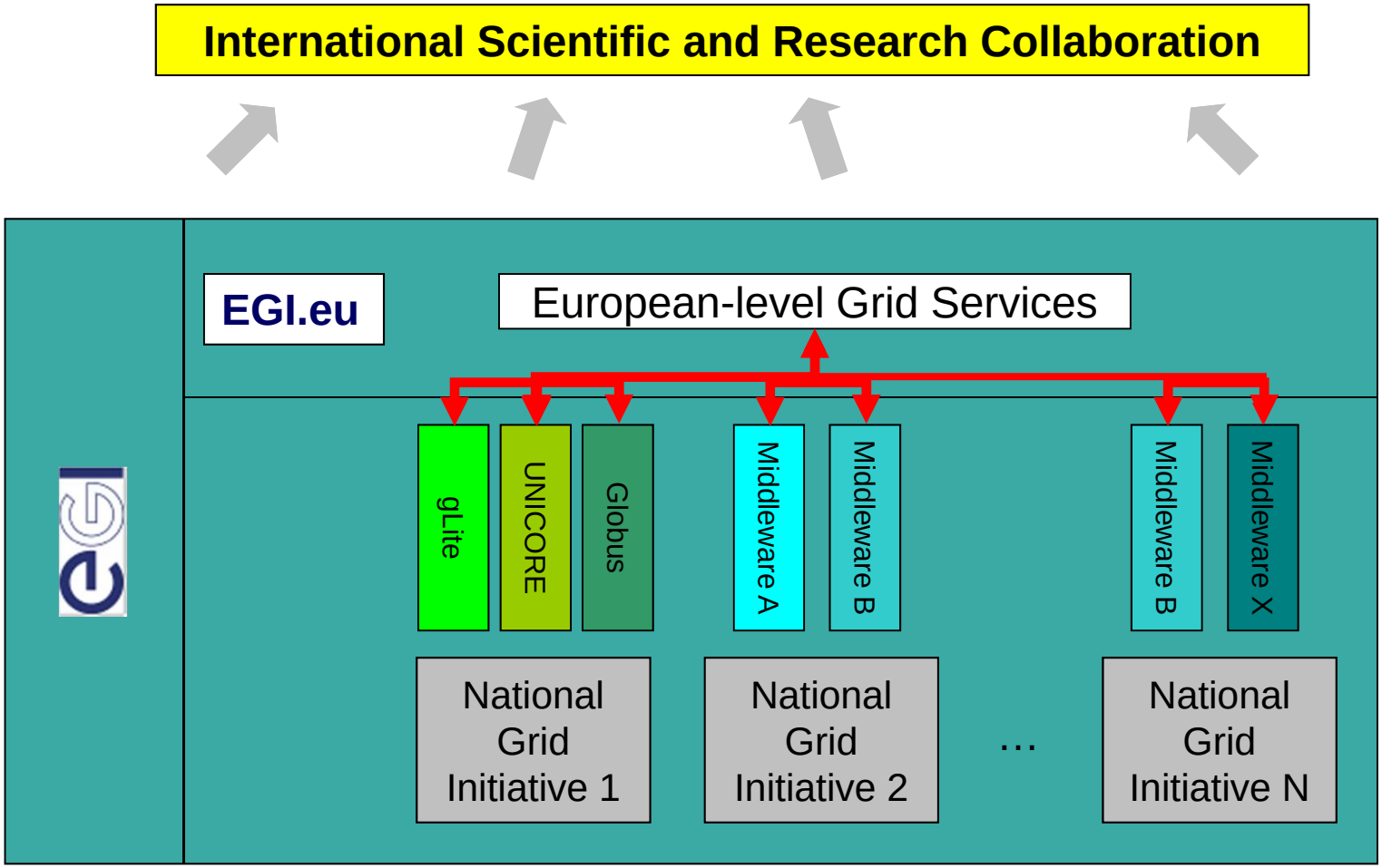
- User support
- Central ticket handling system
- Gathering requirements for user support tools

- Other international tasks
- MW deployment/roll-out and support
- Resource allocation & brokering support
- Interoperations between NGI's and with other grids
- Network support

EGI Blueprint Proposal (V3.0)
http://www.eu-egi.eu/blueprint.pdf

- Functions of EGI
- Financing of EGI
- Transition to EGI

EGI Infrastructure



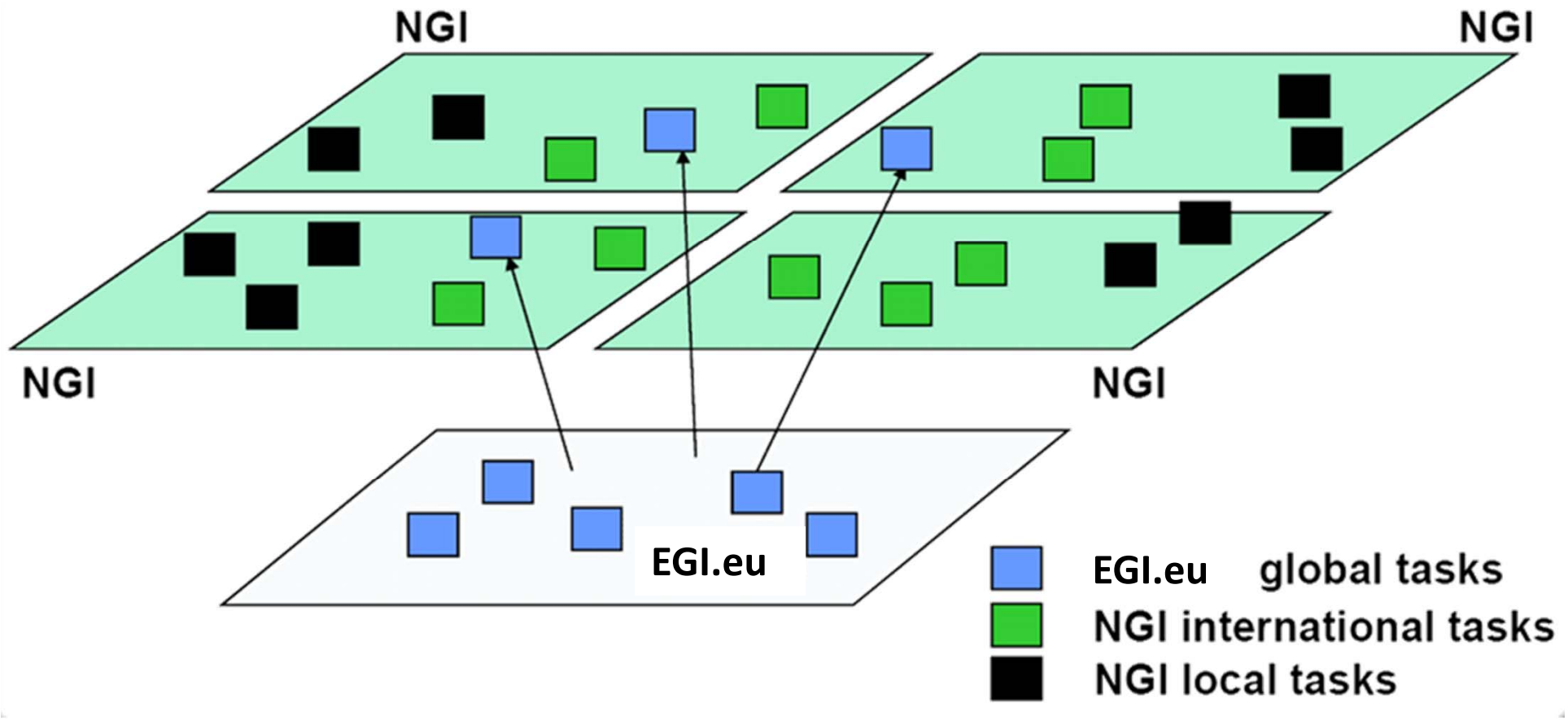
ComputingService (DB)

name	type	domainID	informa...	sourceAddr	insertTime
UNICORE 6 Target System Factory Service			CIS	134.94.105.15	2008-09-16 14:18:37.0
alnitak.ari.uni-heidelberg.de	org.teragrid.ws-gram	AstroGrid-D	MDS4	129.187.254.39	2008-08-07 11:25:16.0
anticyclone.dkrz.de	org.teragrid.ws-gram	dkrz.de	MDS4	129.187.254.39	2008-08-07 11:25:17.0
aprilia.izbi.uni-leipzig.de	org.teragrid.ws-gram		MDS4	129.187.254.39	2008-08-07 11:25:16.0
arminius-grid.uni-paderborn.de	org.teragrid.ws-gram	PC2	MDS4	129.187.254.39	2008-08-07 11:25:16.0
astar.aip.de	org.teragrid.ws-gram	AstroGrid-D	MDS4	129.187.254.39	2008-08-07 11:25:16.0
astrodata01.gac-grid.org	org.teragrid.ws-gram	AstroGrid-D	MDS4	129.187.254.39	2008-08-07 11:25:16.0
bladekemper21.informatik.tu-muenchen.de	org.teragrid.ws-gram	AstroGrid-D	MDS4	129.187.254.39	2008-08-07 11:25:16.0
buran.aei.mpg.de	org.teragrid.ws-gram	AstroGrid-D	MDS4	129.187.254.39	2008-08-07 11:25:16.0
c3grid-gt.E-Technik.Uni-Dortmund.DE	org.teragrid.ws-gram	c3grid-gt.e-t...	MDS4	129.187.254.39	2008-08-07 11:25:17.0
c3grid.rrz.uni-koeln.de	org.teragrid.ws-gram	de.uni-koeln	MDS4	129.187.254.39	2008-08-07 11:25:17.0
cashmere.aip.de	org.teragrid.ws-gram	AstroGrid-D	MDS4	129.187.254.39	2008-08-07 11:25:16.0
ce-1-fzk.gridka.de	pbspro-gLite3	FZK-LCG2	BDII	iwrdmon-bdii.fzk.de	2008-09-19 17:13:20.0
ce-2-fzk.gridka.de	pbspro-gLite3	FZK-LCG2	BDII	iwrdmon-bdii.fzk.de	2008-09-19 17:13:20.0
ce-3-fzk.gridka.de	pbspro-gLite3	FZK-LCG2	BDII	iwrdmon-bdii.fzk.de	2008-09-19 17:13:20.0

VO-specific View (OGSA-DAI)

```
SQLQuery: SELECT name, type, totalJobs, runningJobs, waitingJobs, informationProvider FROM ComputingService_VO
VO: vi
uk.org.ogsadai.resource.request.status.COMPLETED
| name                                    | type                | totalJobs | runningJobs | waitingJobs | informationProvider |
| arminius-grid.uni-paderborn.de          | org.teragrid.ws-gram | 0         | 0           | 0           | MDS4                |
| dgiref-globus.fzk.de                    | org.teragrid.ws-gram | 0         | 0           | 0           | MDS4                |
| dgrid-glitec1.rz.rwth-aachen.de         | sge-dgiseq          | null      | null        | null        | BDII                |
| dmon-unic.fz-juelich.de$9115$FZJ-JUGGLE-DMON | de.fzj.unicore.tsf | 0         | 0           | 0           | CIS                 |
| udo-gt01.grid.uni-dortmund.de           | org.teragrid.ws-gram | 151       | 151         | 0           | MDS4                |
| udo-gt03.grid.tu-dortmund.de            | org.teragrid.ws-gram | 0         | 0           | 0           | MDS4                |
```

EGI Operations = EGI.eu critical services + NGI international tasks



Status EGI

EGI-InSPIRE: Integrated Sustainable Pan-European Infrastructure for Researchers in Europe

- Duration: 4 years (starting 1 May 2010)
- Costs: 70 MEUR, incl. 25 MEUR EU
- Total costs incl. NGI ressources: ca. 330 MEUR
- Partner: EGI.eu, 37 NGIs, 2 EIROs

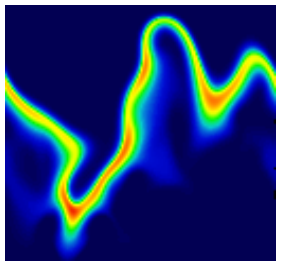
EGI.eu: EGI organization

- Location: Amsterdam, The Netherlands
- Status approved, EGI.eu Executive Board elected

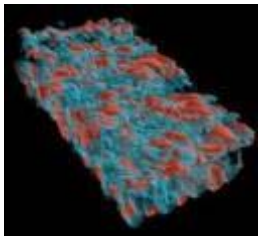
Applications on PRACE, EGI, …

The European Scientific Case

- Weather, Climatology, Earth Science
  - degree of warming, scenarios for our future climate.
  - understand and predict ocean properties and variations
  - weather and flood events

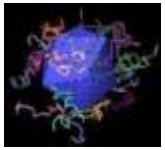
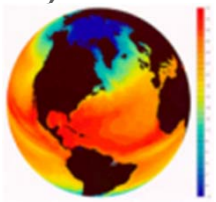
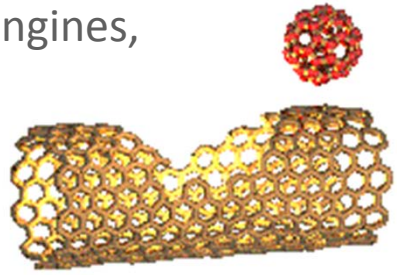
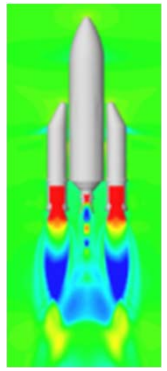
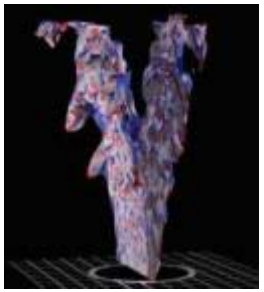



- Astrophysics, Elementary particle physics, Plasma physics
  - systems, structures which span a large range of different length and time scales
  - quantum field theories like QCD, ITER

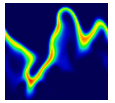


- Material Science, Chemistry, Nanoscience
  - understanding complex materials, complex chemistry, nanoscience
  - the determination of electronic and transport properties
- Life Science
  - system biology, chromatin dynamics, large scale protein dynamics, protein association and aggregation, supramolecular systems, medicine

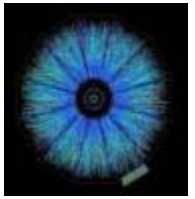
- Engineering
  - complex helicopter simulation, biomedical flows, gas turbines and internal combustion engines, forest fires, green aircraft,
  - virtual power plant

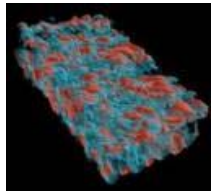






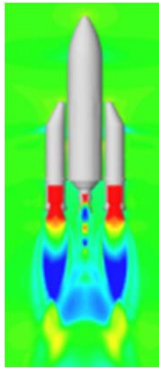
Applications @ LRZ

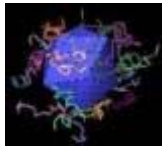


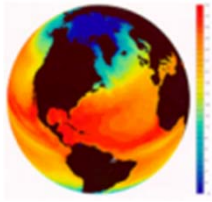
- Fluid dynamics: optimization of turbines, noise reduction, air conditioning in trains
- Fusion physics: future fusion reactor (ITER)
- Astrophysics: origins of stars and galaxies
- Solid state physics: superconductors
- Geophysics: earthquakes
- Material sciences: semiconductors
- Chemistry: catalysts
- Medicine and medical technology: blood flow, air conditioning in hospitals
- Bio sciences: virus characteristics, genome analysis
- Climate research: ocean research



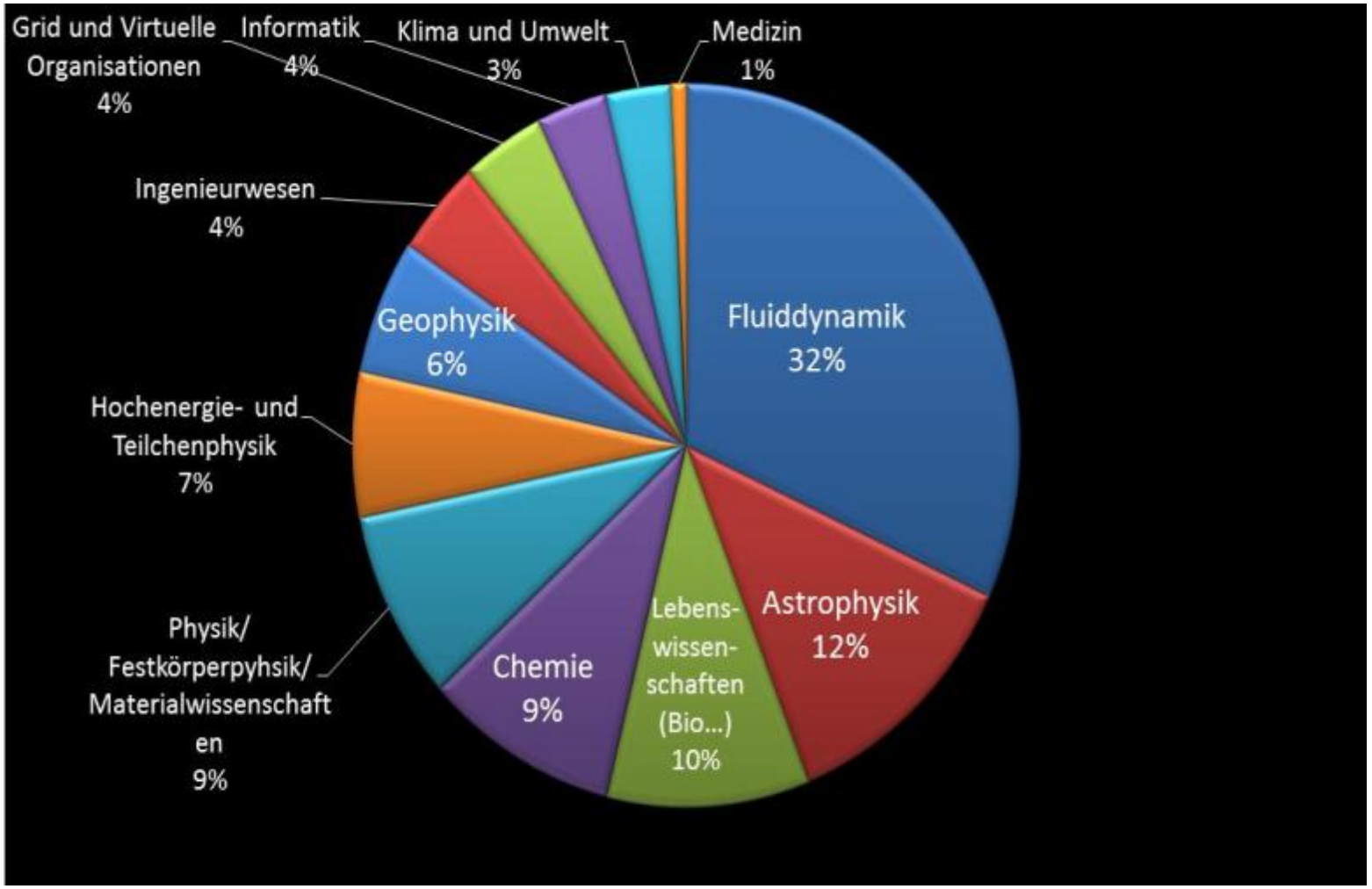




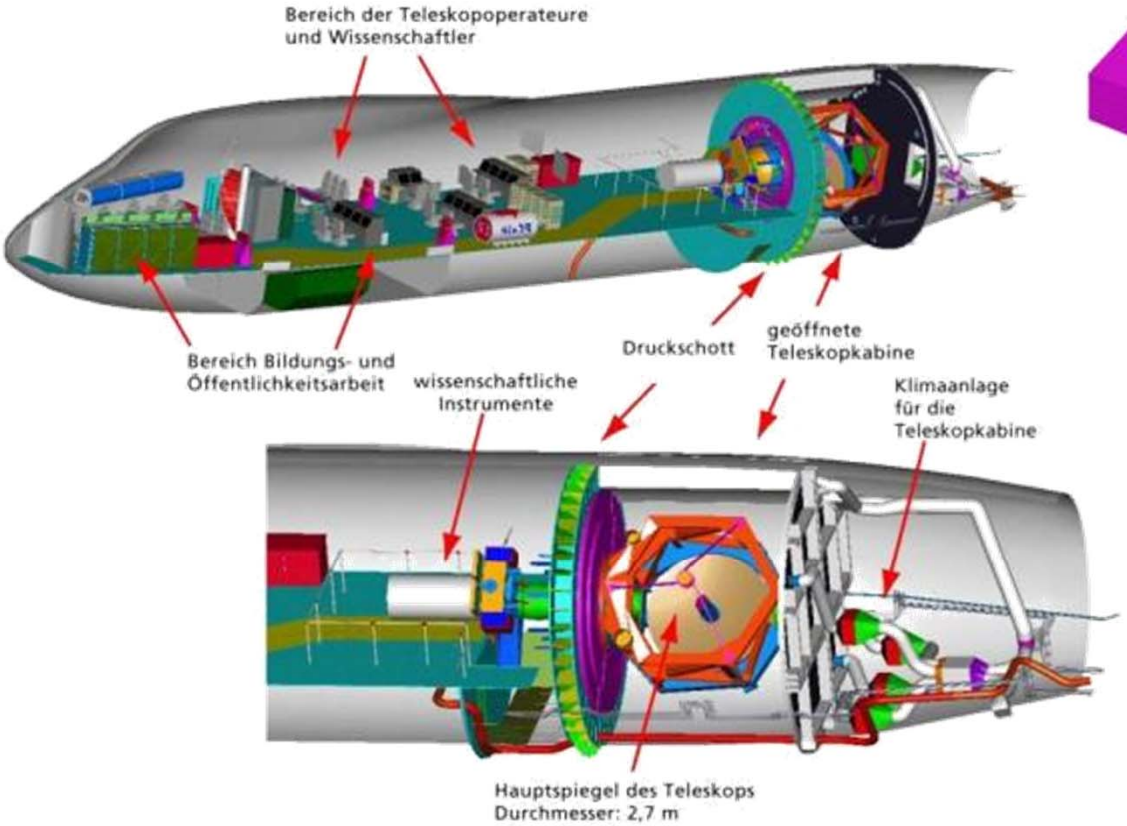




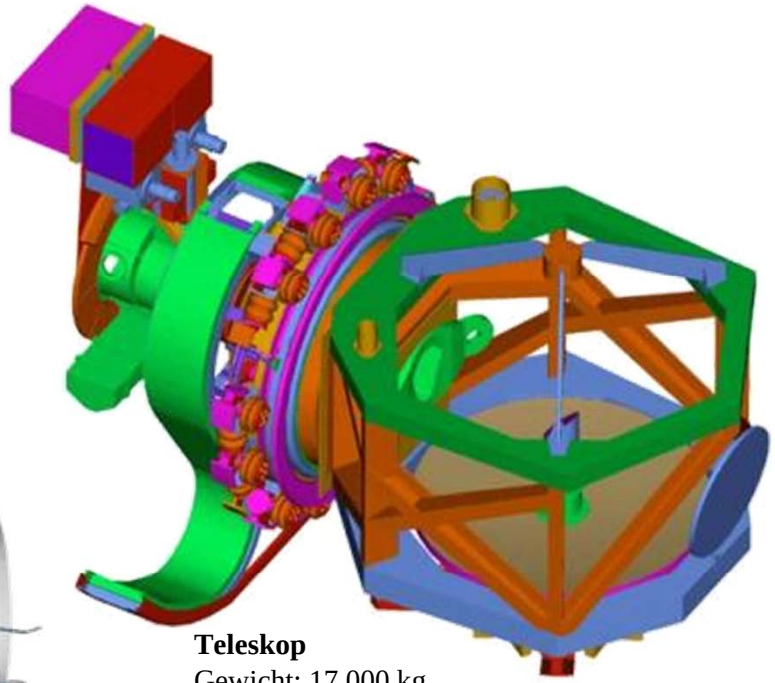
Distribution of Computing Time @ LRZ



SOFIA - Stratospheric Observatory For Infrared Astronomy



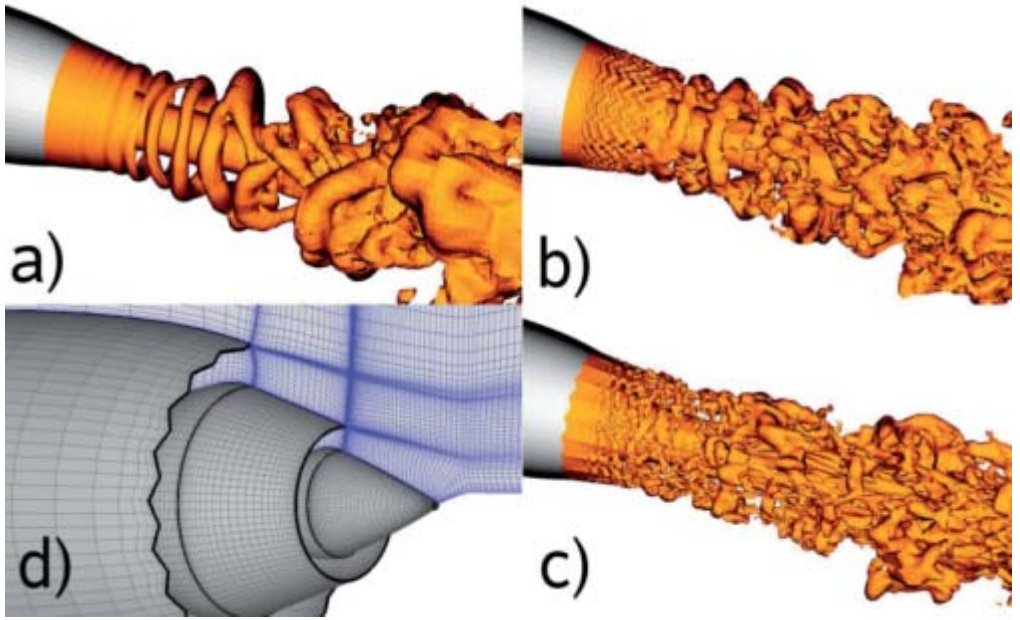
Plattform: Boeing 747 SP
Max. Bruttogewicht: 300.000 kg
Spannweite: 60m
Max. Entfernung: 15.000km



Teleskop
Gewicht: 17.000 kg
Durchmesser: 2.7m
Ansichtswinkel: 20° - 60°
Entwickelt und gebaut in Deutschland

Numerical Analysis of Turbine Noise

Rolls-Royce Trent 1000 engine on a Boing 787 Dreamliner (copyright Rolls-Royce plc 2010)



Iso-surfaces of the density showing resolved turbulent flow structures
a) standard DES;
b) modified DES, unserrated nozzle;
c) modified DES, serrated nozzle;
d) serrated short-cowl nozzle surface mesh with every second grid line shown

Institut für Strömungsmechanik und Technische Akustik, Technische Universität Berlin

Leitung

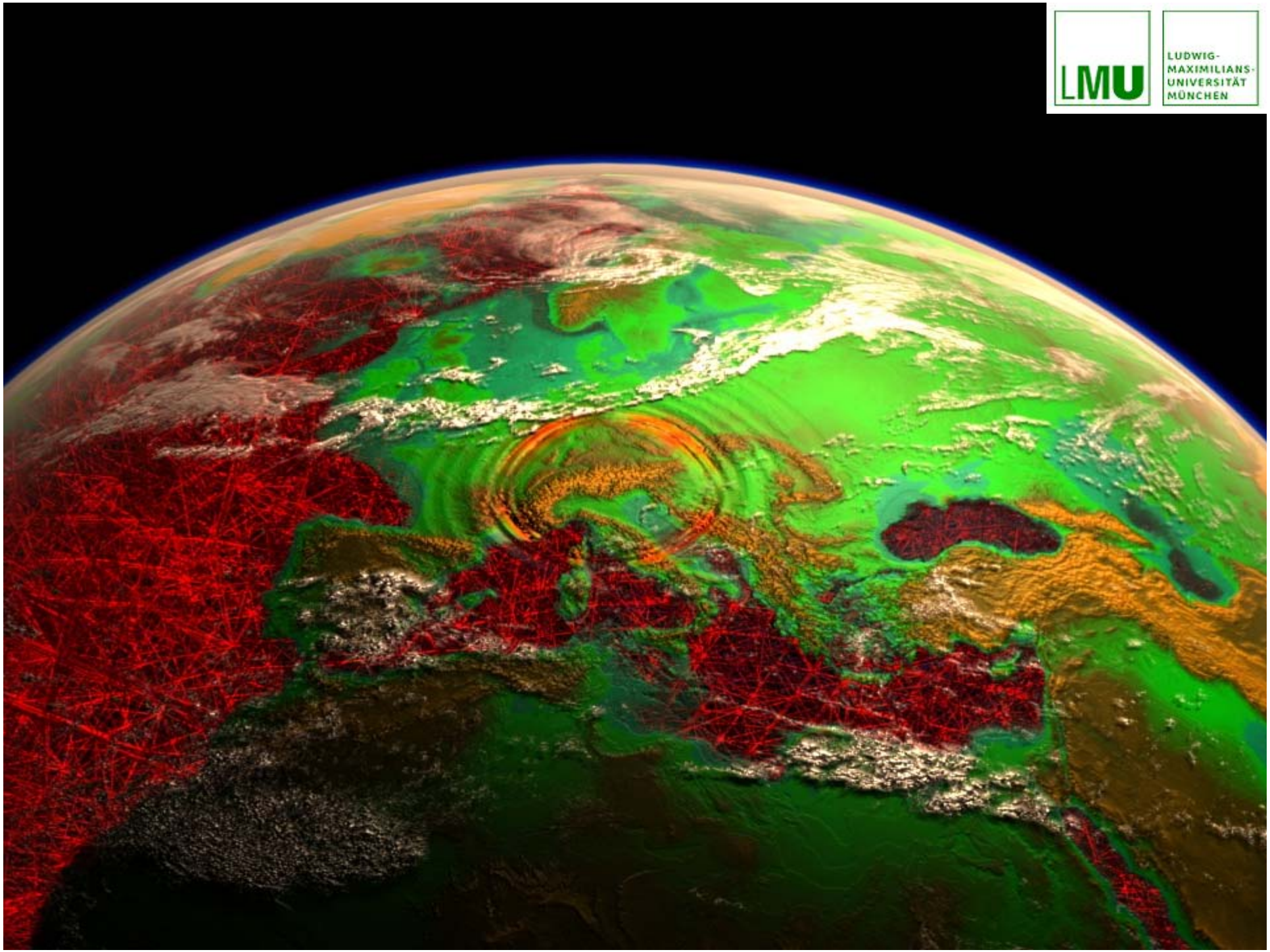
F. Thiele

Wissenschaftler

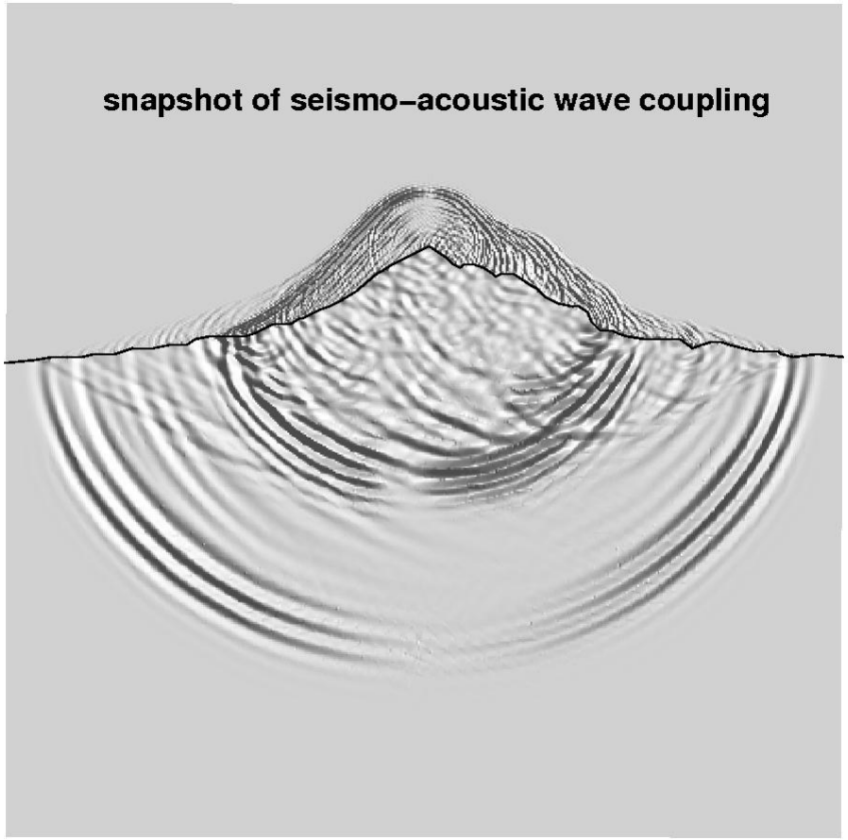
D. Eschricht, J. Yan, L. Panek and K. Tawackolian

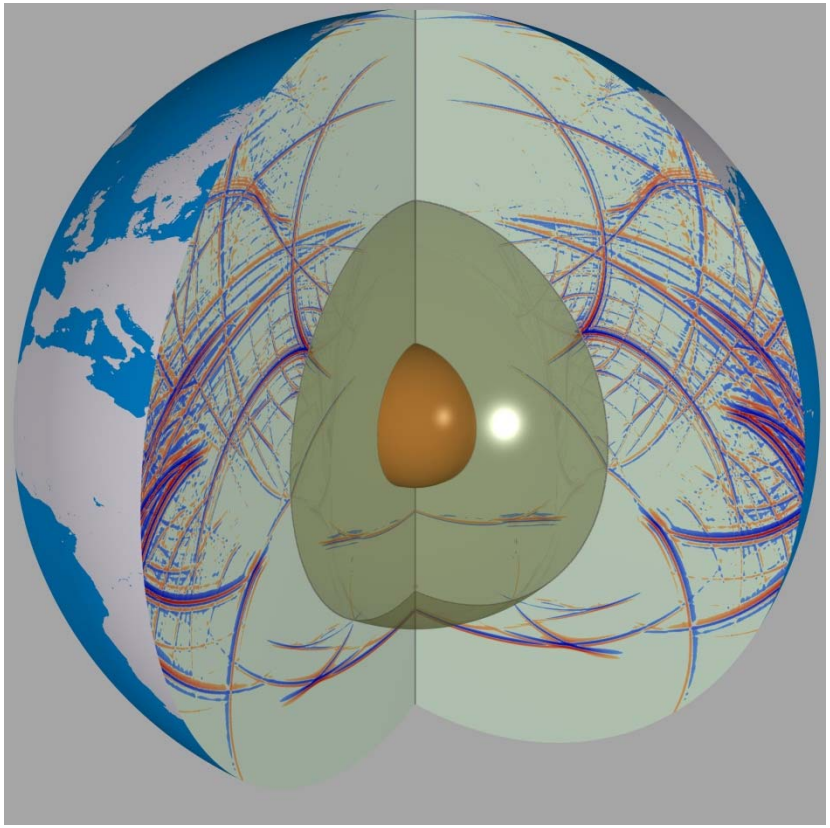
Projekt Partner

Rolls-Royce Deutschland


LMU
LUDWIG-
MAXIMILIANS-
UNIVERSITÄT
MÜNCHEN

Numerical Simulation and Visualization





Heiner Igel, Martin Käser, et al., LMU

Seismic Measurements → VERCE

Seismic Measurement Stations:

- ~ 4000 Stations
- > 180 Networks

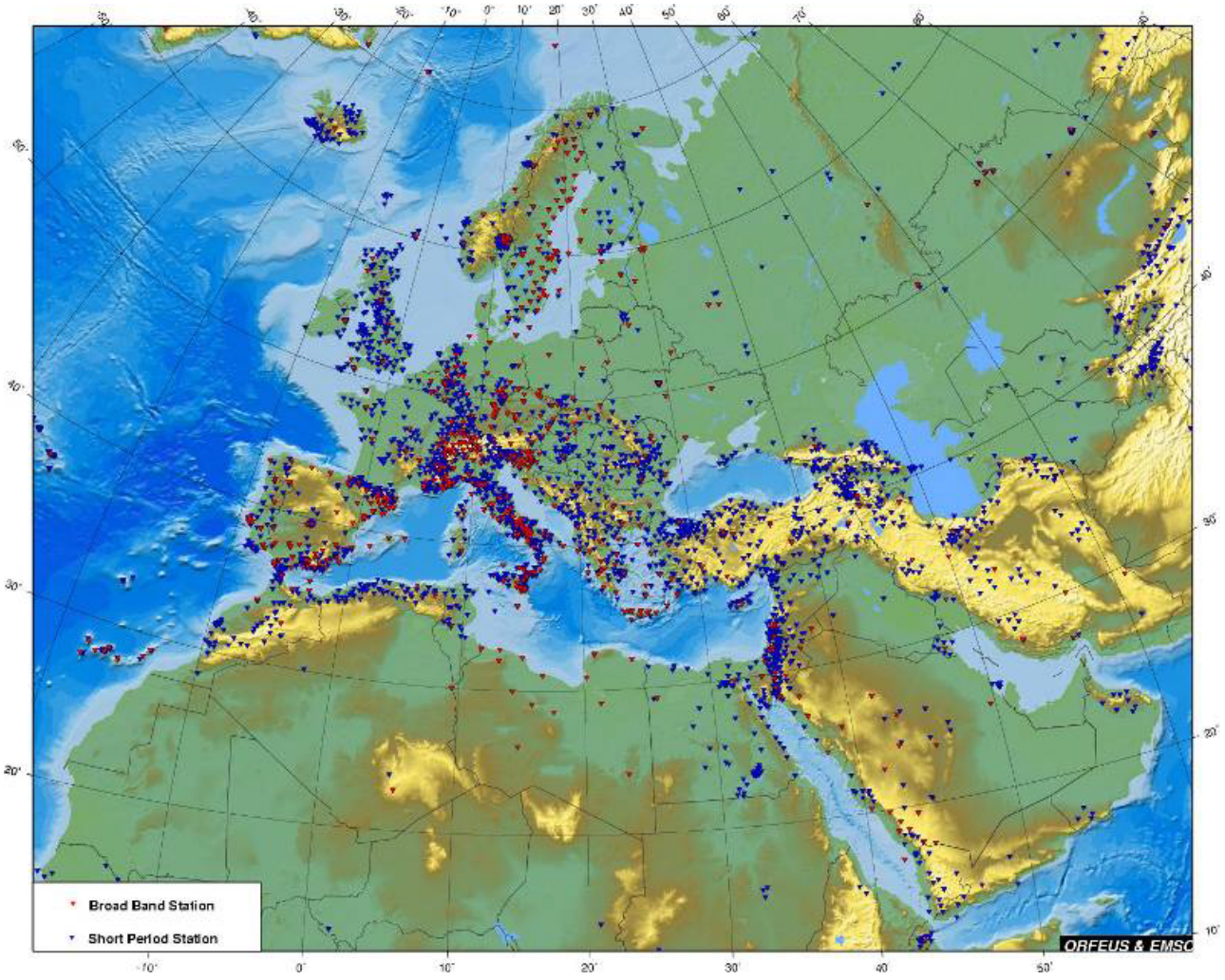
European
Data Centres:

- Parametric Data (EMSC, Paris)

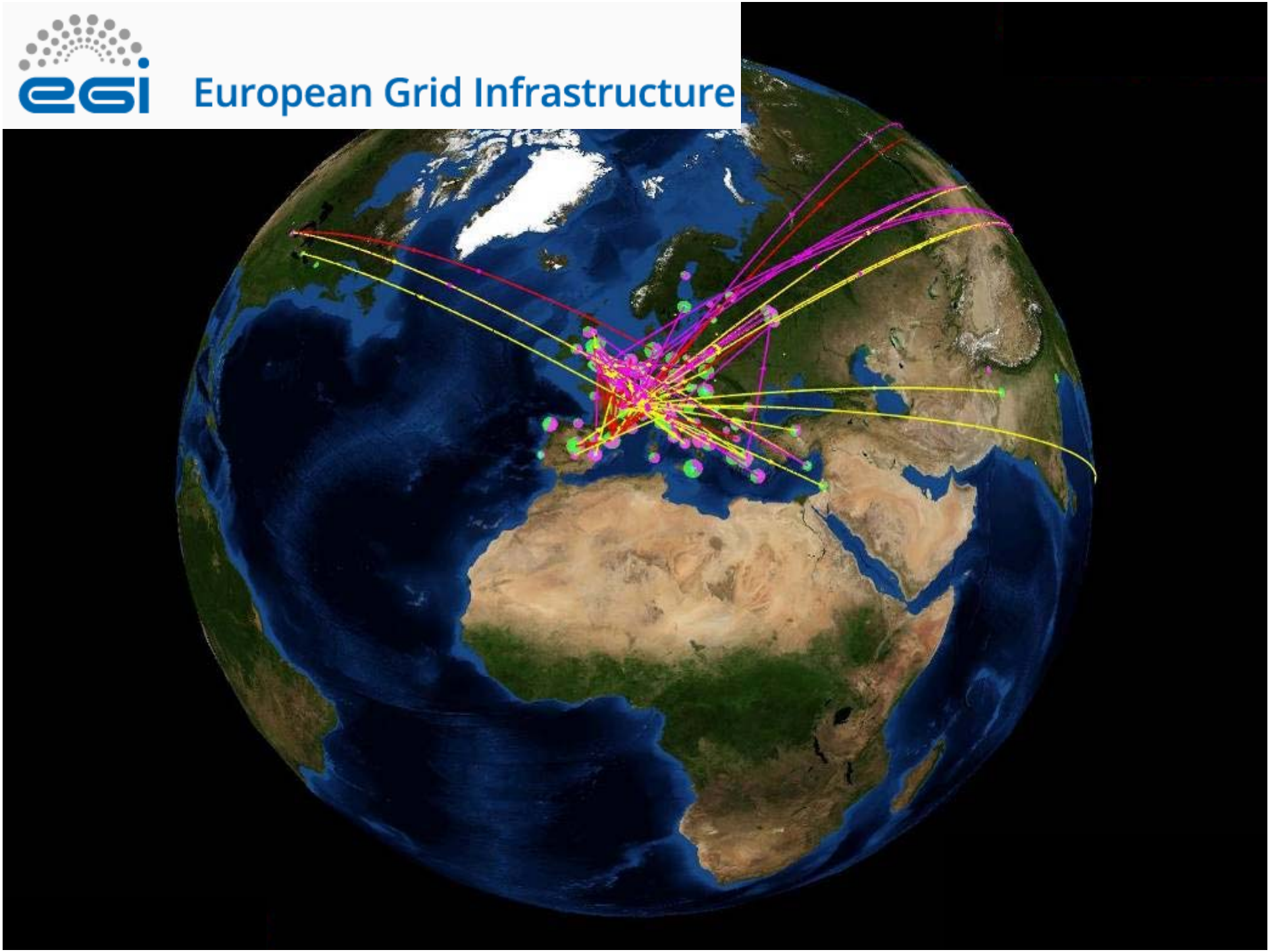
csem emsc

- Waveform Data (ORFEUS, Utrecht)

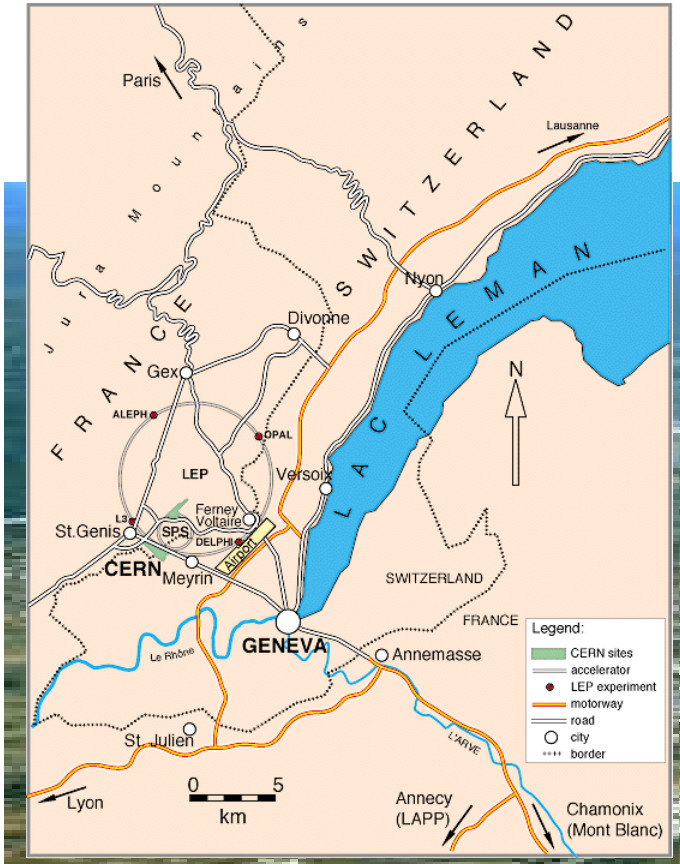
Orfeus



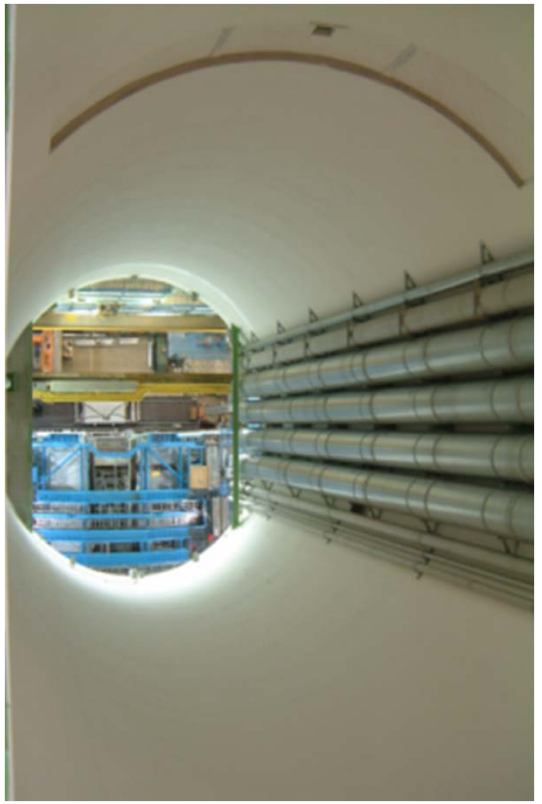
European Grid Infrastructure



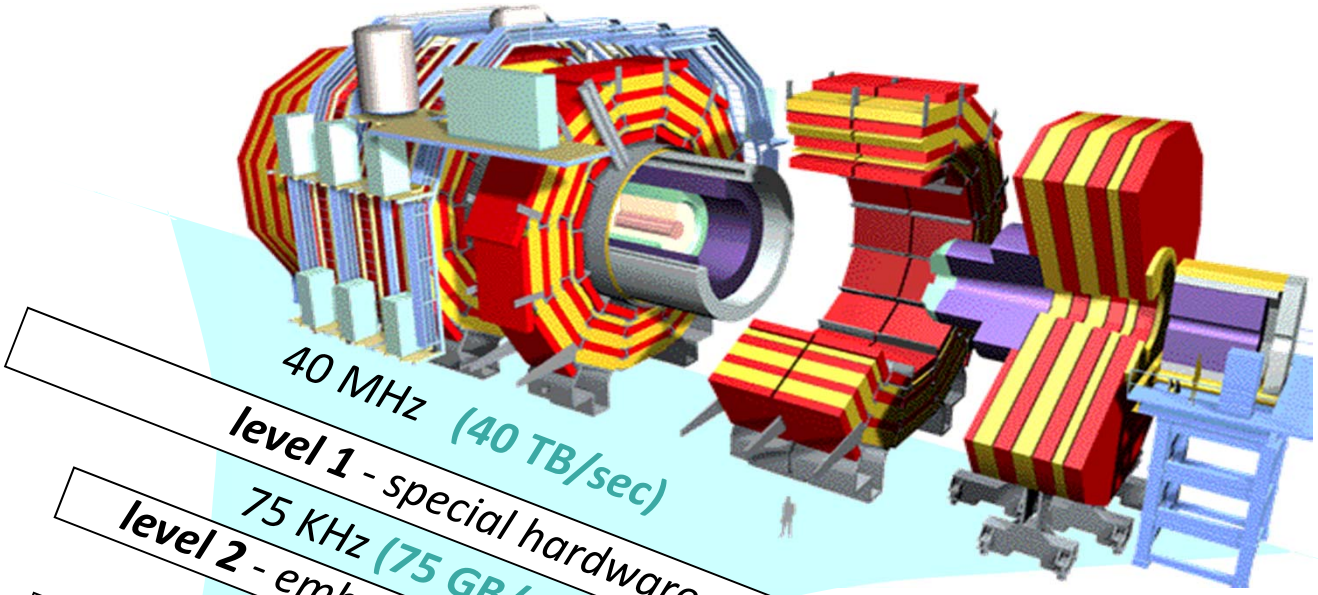
CERN – European Organisation for Nuclear Research



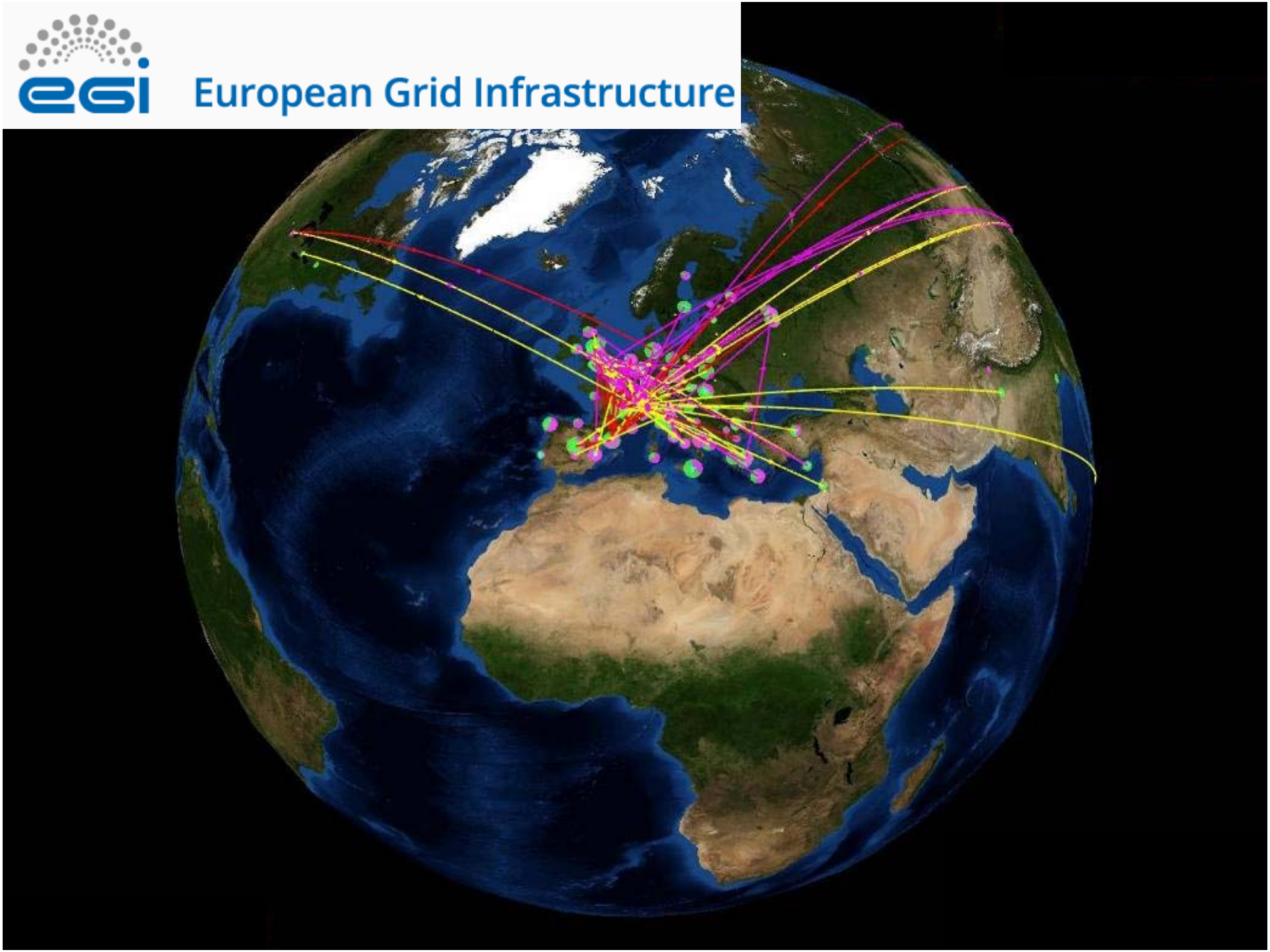
Large Hadron Collider (LHC)



LHC Detektoren

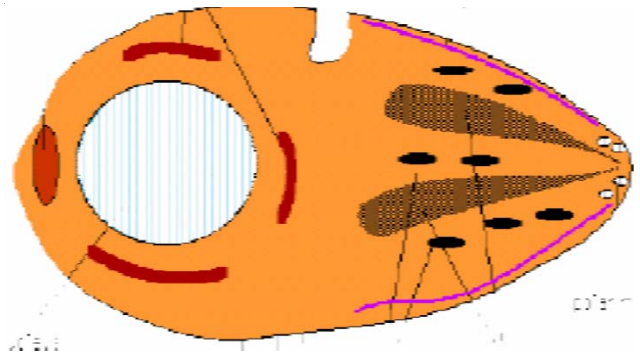


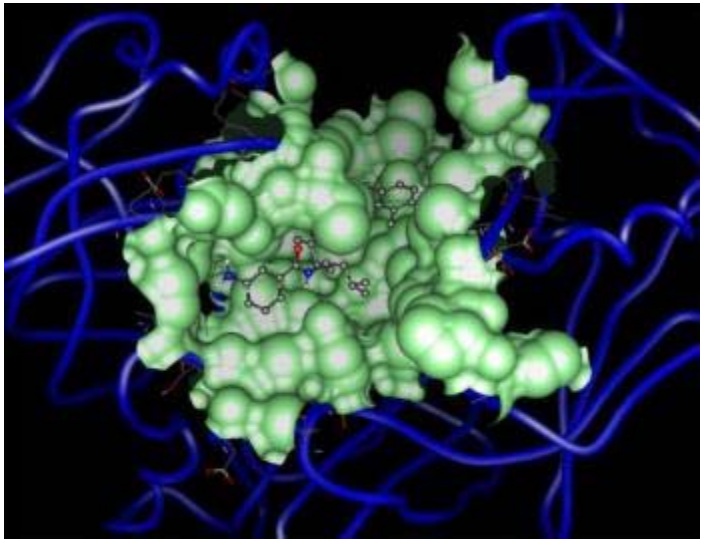
European Grid Infrastructure



WISDOM – Research on Malaria

- World-wide In Silico Docking On Malaria
- "Neglected Diseases"
- Biomedical Challenges
- Docking Experiments:
  - 46 Million Ligands
  - Runtime: 6 Weeks
  - Data: 1 TByte
  - 1000 CPUs in 15 Countries (~80 CPU Years)

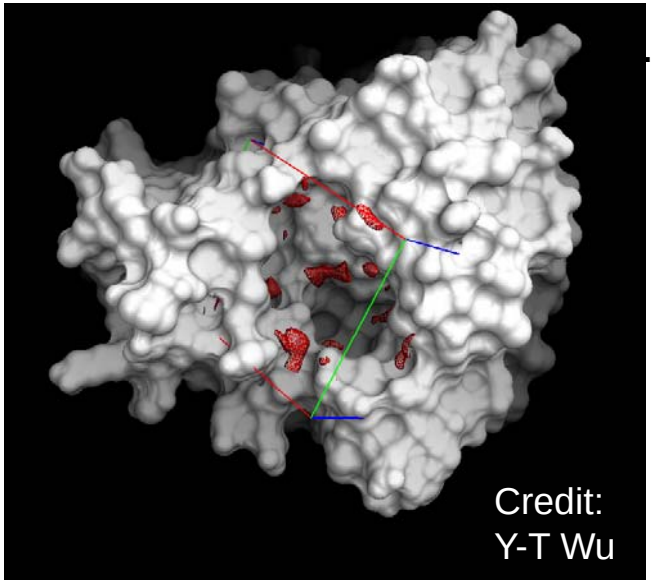




Bird Flu

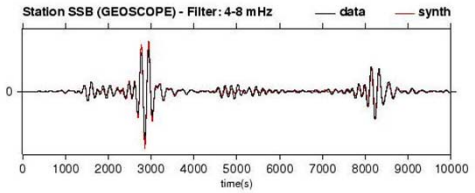
- Bird Flu H5N1
  - H5 and N1 = Proteins on the surface of the virus
- Biological Target
  - I*n silico* research of the efficiency of medicine
  - Design of potential neu medical treatments
- Data Challenge:
  - 5 Grid Projects: Auvergrid, BioinfoGrid, EGEE, Embrace, TWGrid
  - 1 Docking Software: autodock
  - 300 000 selected components
  - → >100 CPU years required to test all combinations

H5

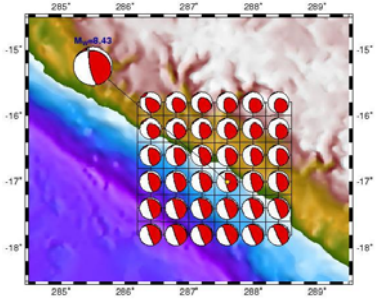


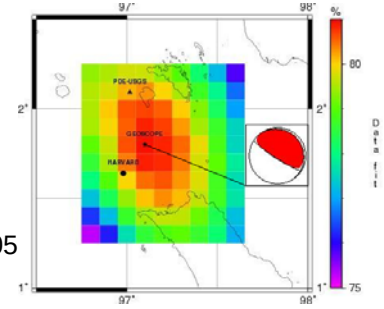
Earthquakes / Tsunamis

- Seismic software to identify epicentrum and magnitude of earthquake
- Analysis of Indonesian seaquake (28 March 2005)
  - Seismic data available within 12 hours
  - Results computed within 30 hours (10 times faster than on single computer)
- Results of simulation
  - No aftershocks to be expected
  - Epicentrum different compared to previous cases
  - Different trigger mechanism

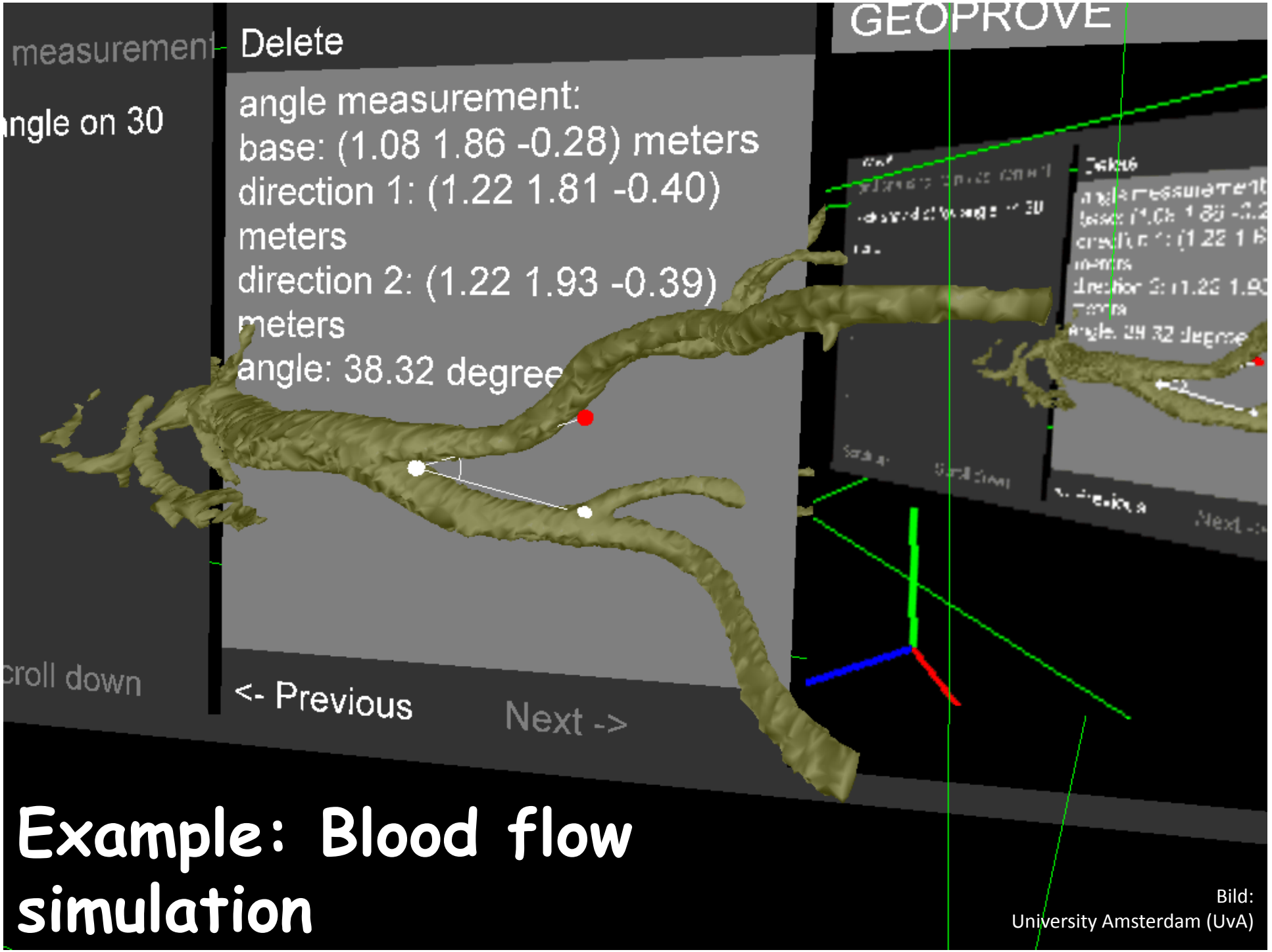


Peru, June 23, 2001
Mw=8.4



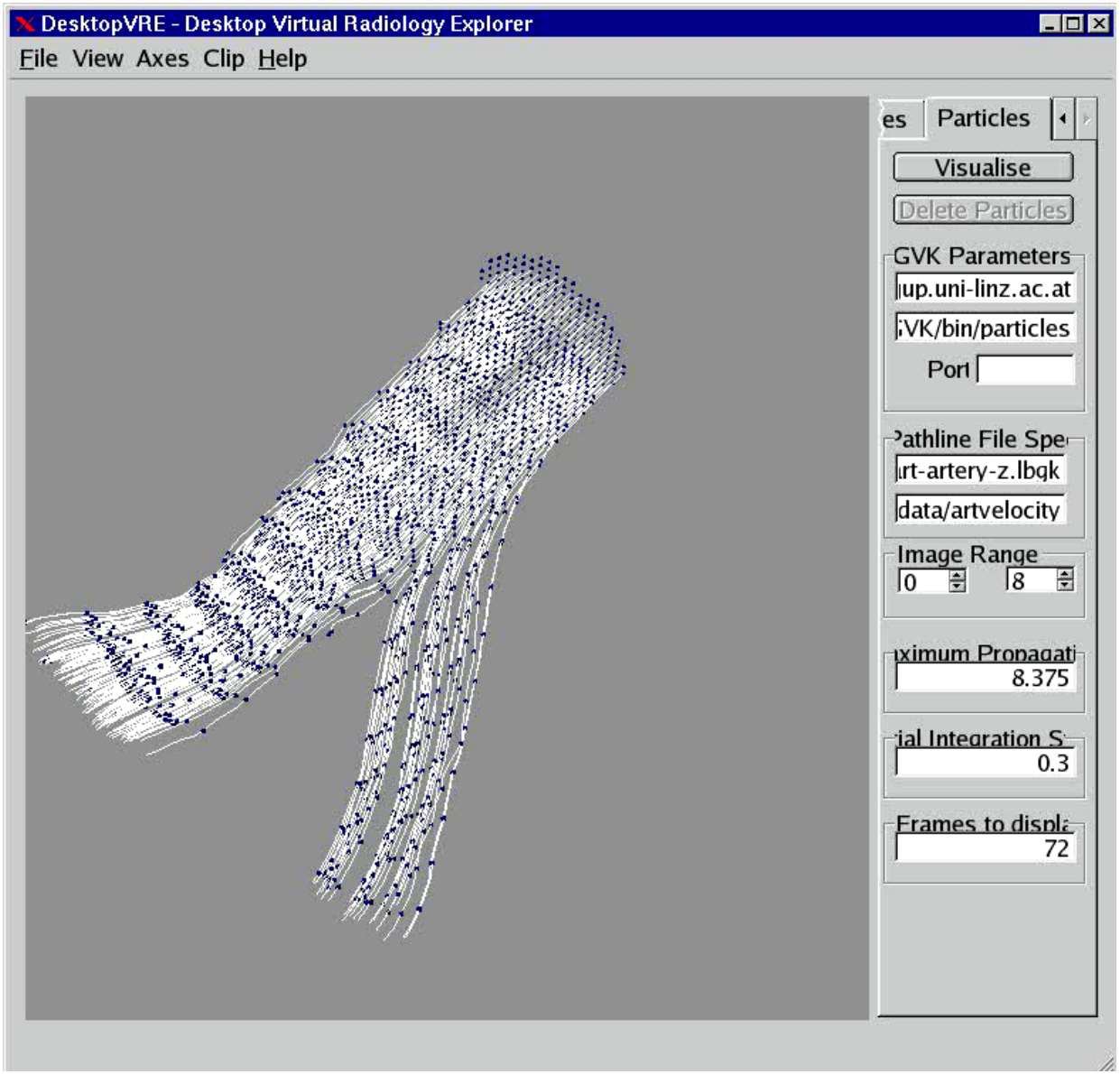


Sumatra, March 28, 2005
Mw=8.5


measurement
ngle on 30
Delete
angle measurement:
base: (1.08 1.86 -0.28) meters
direction 1: (1.22 1.81 -0.40)
meters
direction 2: (1.22 1.93 -0.39)
meters
angle: 38.32 degree
GEOPROVE
croll down
<- Previous
Next ->
Example: Blood flow simulation
Bild:
University Amsterdam (UvA)

Blood flow simulation

- Blood flow simulation in human arteries
- Real-time simulation for surgical planning
- Computation in the grid



Visualization on PSP

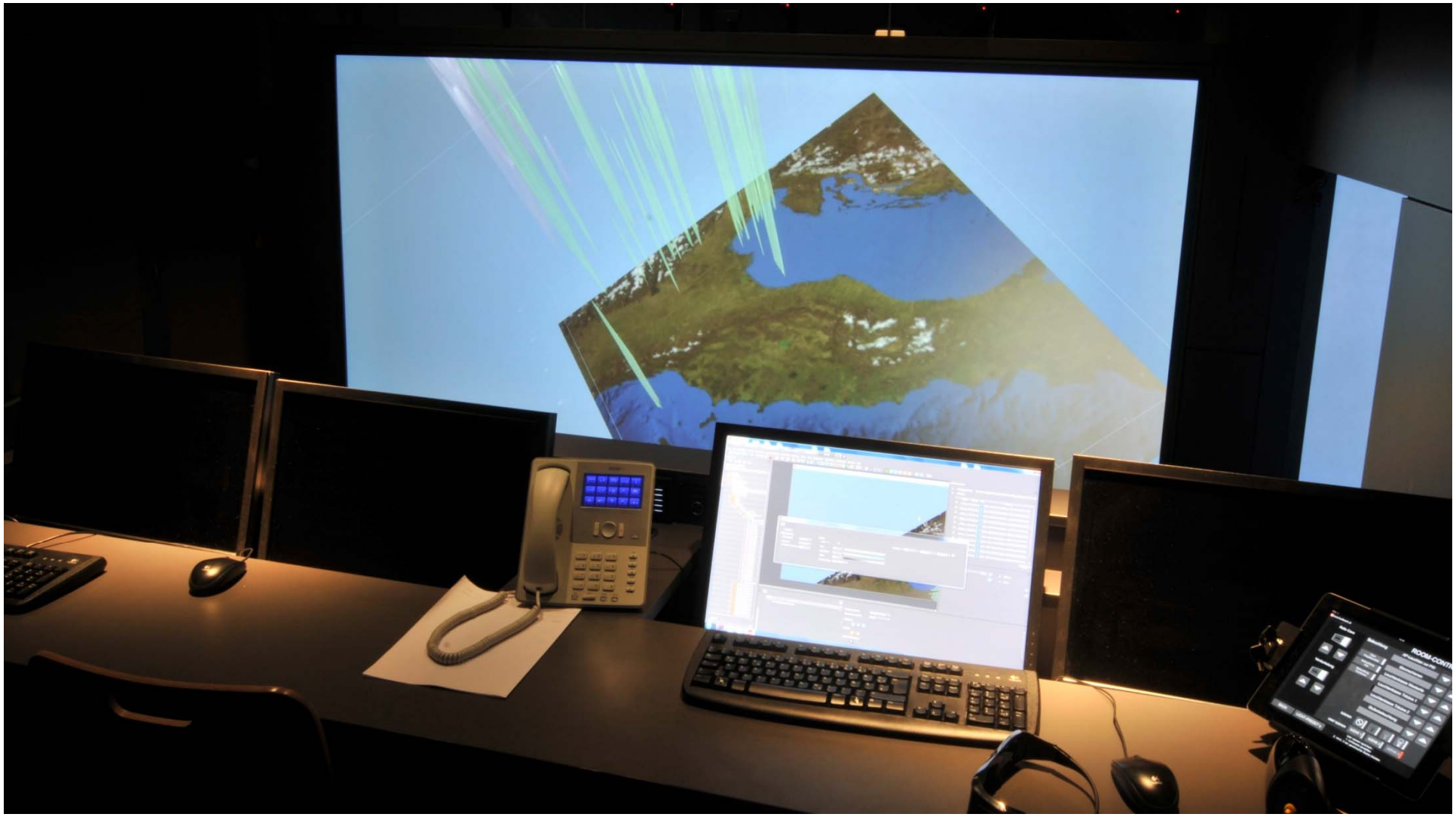
Visualization in CAVE

- Flooding simulations
- Visualization of results in the CAVE
- The "Invisible Grid"

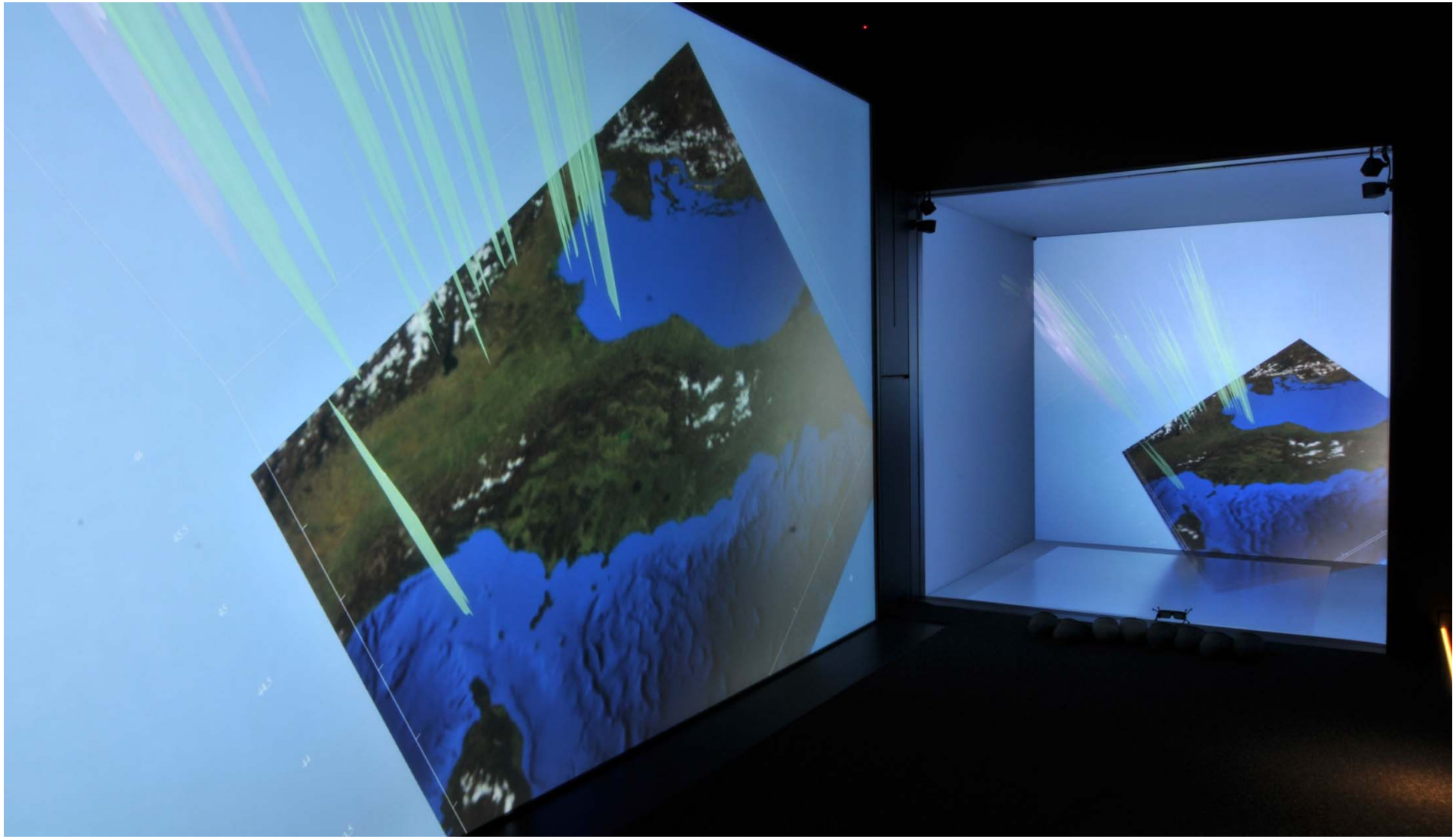
CROSSGRID

Cooperation with Slowak Academy of Sciences

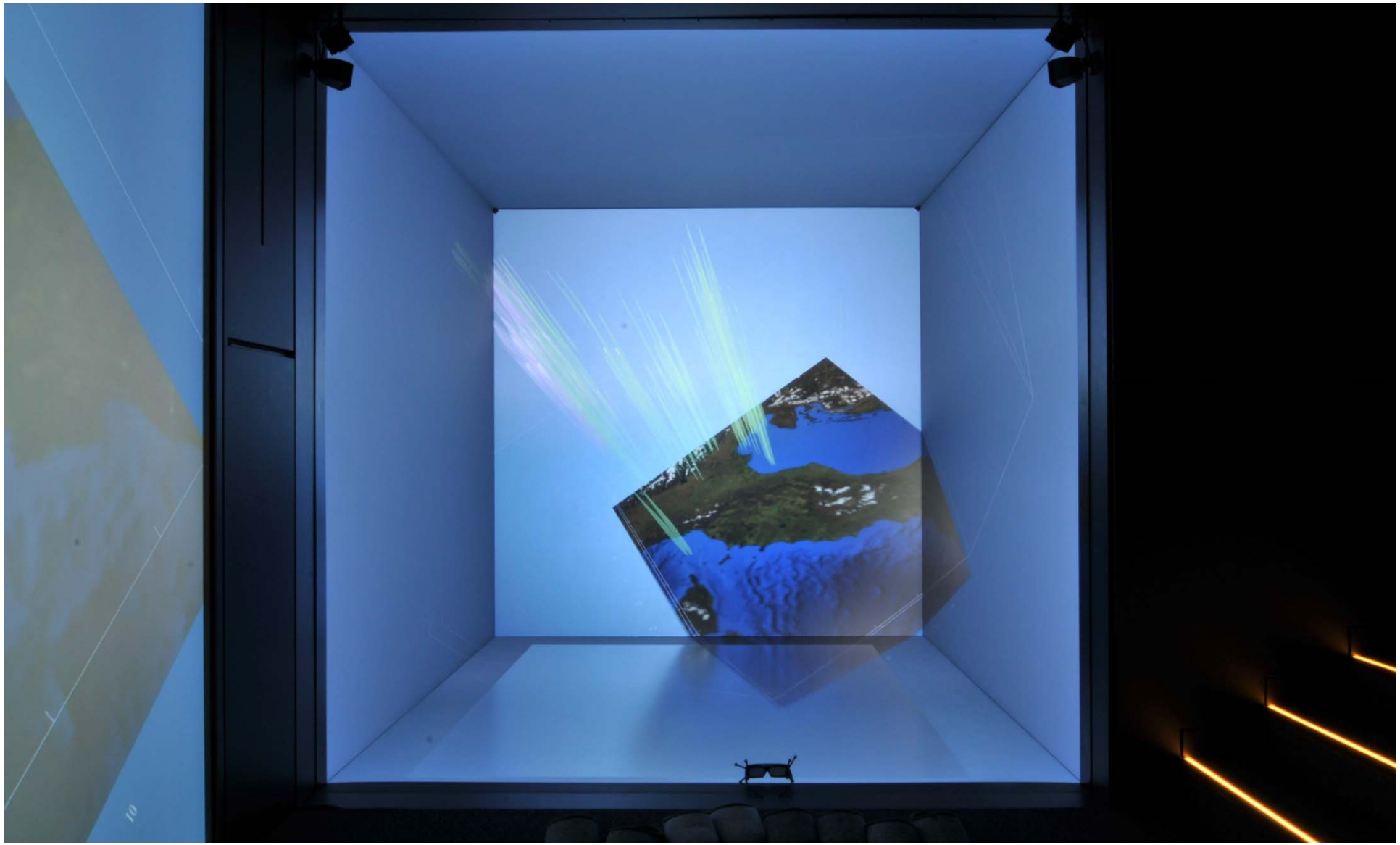
DRIHM – Distributed Research Infrastructure for Hydrometeorology



DRIHM – Distributed Research Infrastructure for Hydrometeorology



DRIHM – Distributed Research Infrastructure for Hydrometeorology



How to use these infrastructures?

Getting access

"Nice, but I just want access to some resource now"

Well, you just have to know about:

- X.509 certificates, CAs/RAs, VOMS
- AUPs, Peer reviews
- CPUh budgets, accounting
- Globus, UNICORE, gLite, ARC
- Gateways, Door nodes, Firewalls
- ….

"Why does it have to be so damn complicated??"

Scientific Quality

- Significant over-subscription of resources
  - Fair distribution of resources
    - between scientific fields: peer reviewing
    - within a scientific field: virtual organizations
  - Mutual exchange of users / jobs
    - contracts between national / regional centres
    - proof of technical suitability
- Tax-payers money
  - 1 CPUh costs roughly 0.1 – 1 €
  - Scientific projects use up 0.1 M – 5 M CPUh “for free”
    - Justification necessary

Security

- Value of assets
  - SuperMUC: 85 ➔ 133 M€
- Supercomputers and Grid interesting for
  - DDoS attacks
  - Spam mails
  - Bit coins
- Industrial users
  - Afraid of any kind of disclosure
- SLAs/Contractual penalties
  - E.g. climate/weather predictions

International Collaboration

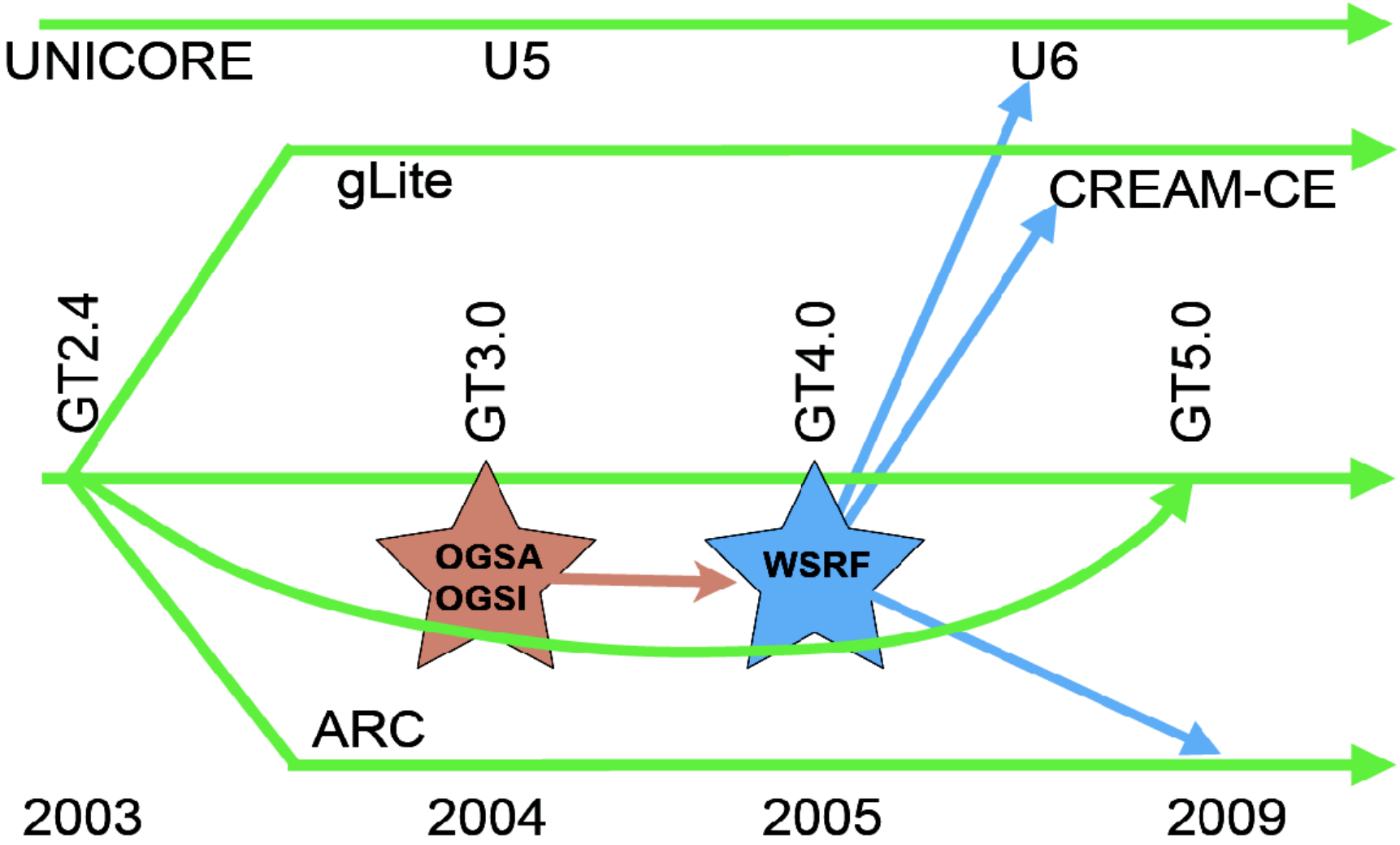
- Scientists world-wide want access to resources
  - No personal trust relationship possible
  - Trust delegation in world-wide scope
  - Trust centre infrastructure: IGTF, EUGridPMA, CAs

- Scientists want to easily change between the resources
  - Unique access to resources
  - No local account names
  - Unique identifier,
    “electronic passport”

Legal Restrictions

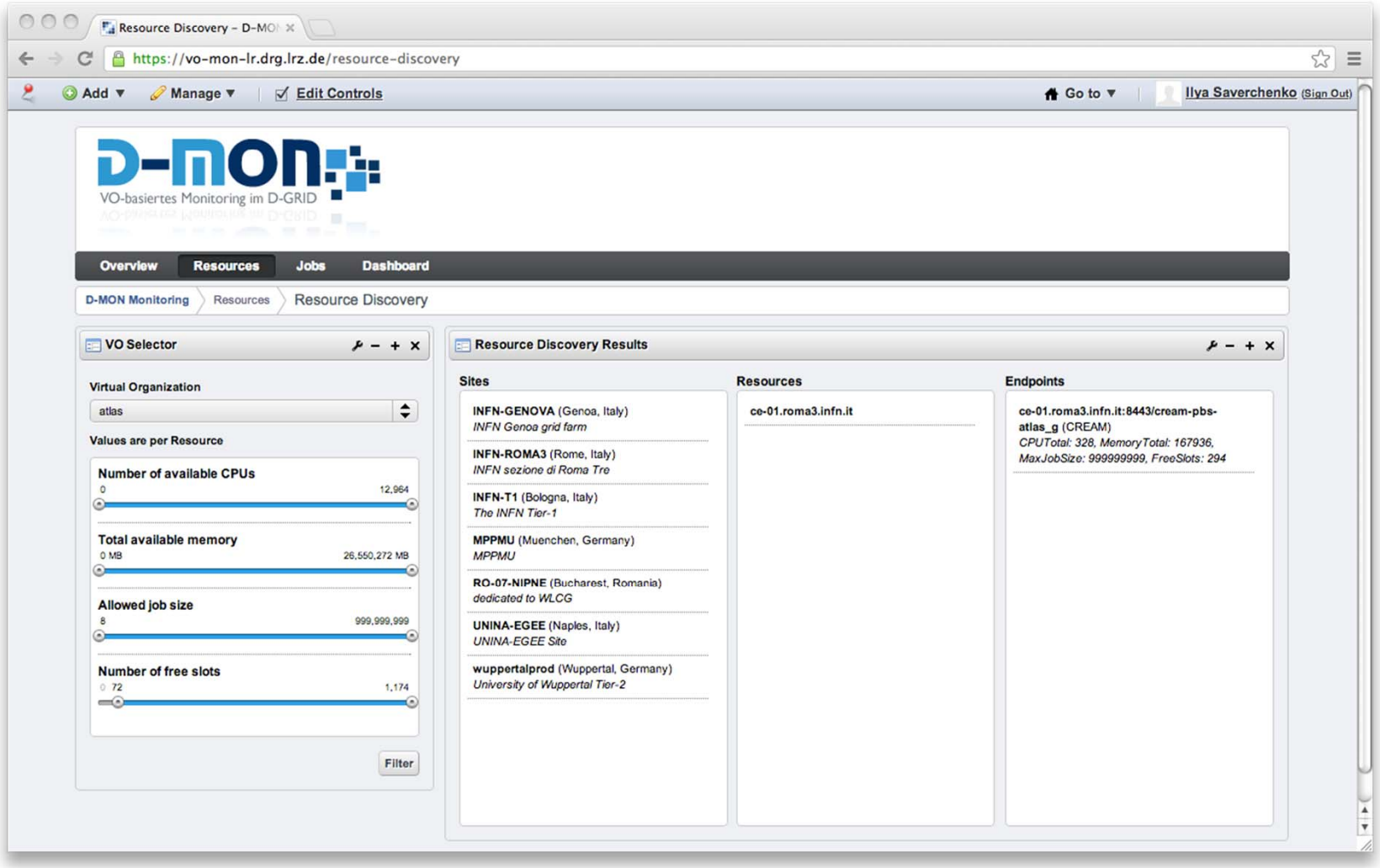
- Non-Proliferation
  - Wassenaar-Arrangement on “Dual-Use Goods and technologies”
    - relates to supercomputers AND Grids
  - Nationality of user has to be checked
  - High penalties for violation
    - e.g. in Germany: up to 500.000€ fine, 5 years jail
- National Privacy Laws
  - FR: Non-EU citizens need clearance from Security Agency
  - SE: Every business communication is public
  - NL: Private data cannot be disclosed
  - DE: Data economy (Private data must be removed after 7 days)

Software Evolution

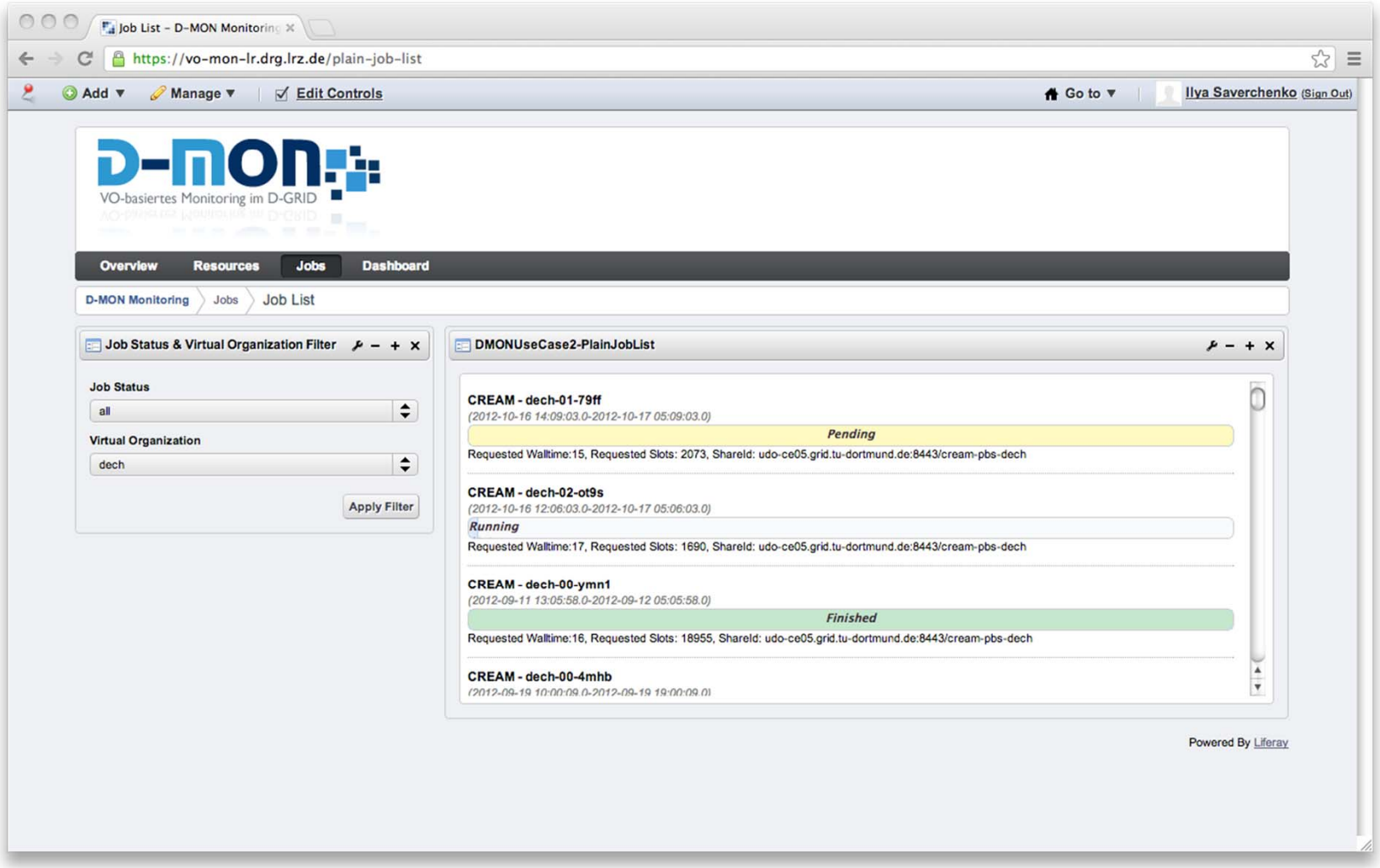


Users' Information needs

Resource & Service Discovery



Job Tracking



PRACE vs. EGI

- Fact: Funding is always limited
- Populistic view
  - PRACE: What do we need Grid/EGI for?
    Scientists want to use the one most suited HPC machine in an optimal way
  - EGI: What do we need HPC/PRACE for?
    We have sufficient resources for everything, just combine as many computers as you can get
- Optimal solution ➔ Best possible working environment for all European scientists – PRACE & EGI

Summary

- Europe provides powerful e-Infrastructures for all sciences

- Get involved:
  - Obtain your access credentials
  - Apply for compute cycles/storage
  - Communicate your requirements
  - Don‘t hesitate to ask for support
  - Attend training events
  - Provide feedback

  - Get in touch with your regional and national computing centres

  - Attend community-focused events:
    - PRACE User Forum
    - EGI Community Forum

Getting involved: PRACE & EGI

- PRACE
  - Application Guide:
    http://www.prace-ri.eu/Application-Guide
  - Help Desk and User Support:
    https://tts.prace-ri.eu/SelfService/
- EGI
  - How to:
    http://www.egi.eu/how-to/
  - Help Desk and User Support:
    https://ggus.eu/

Using European e-Infrastructures for your Research

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