LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

MNM TEAM
MUNICH NETWORK MANAGEMENT TEAM

LRZ

User Support for Extreme Scale Computing at the LRZ

Dieter Kranzlmüller

Munich Network Management Team
Ludwig-Maximilians-Universität München (LMU) &
Leibniz Supercomputing Centre (LRZ)
of the Bavarian Academy of Sciences and Humanities

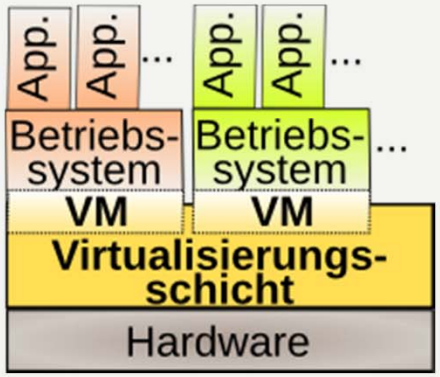

TUM
TECHNISCHE UNIVERSITÄT MÜNCHEN
Garching
lrz
Isar
München
LMU
LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN
der Bundeswehr
Universität München
Neubiberg

Networks

Grid computing

Cloud Computing

High Performance Computing



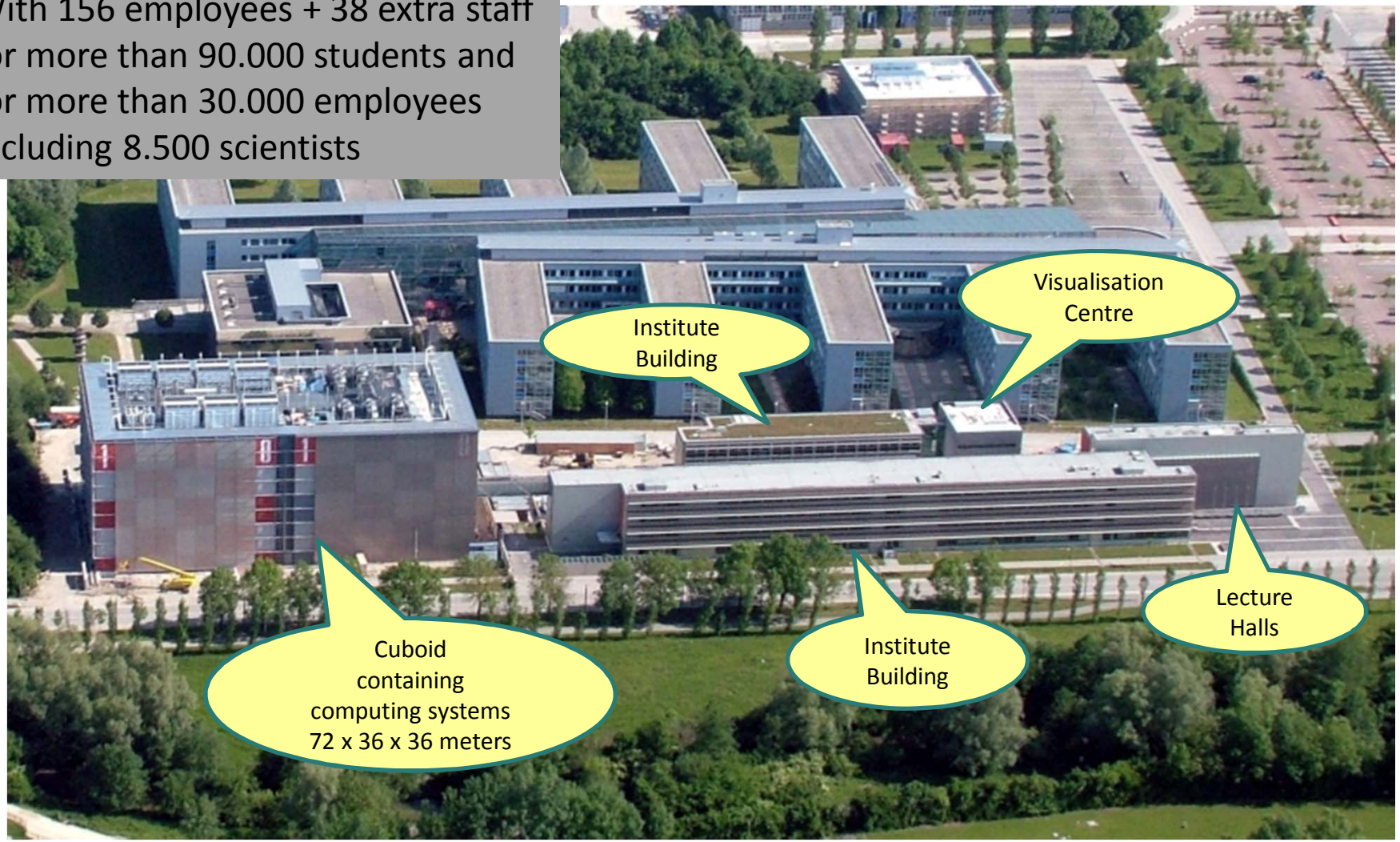
Service Management

Virtualization

IT Security

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

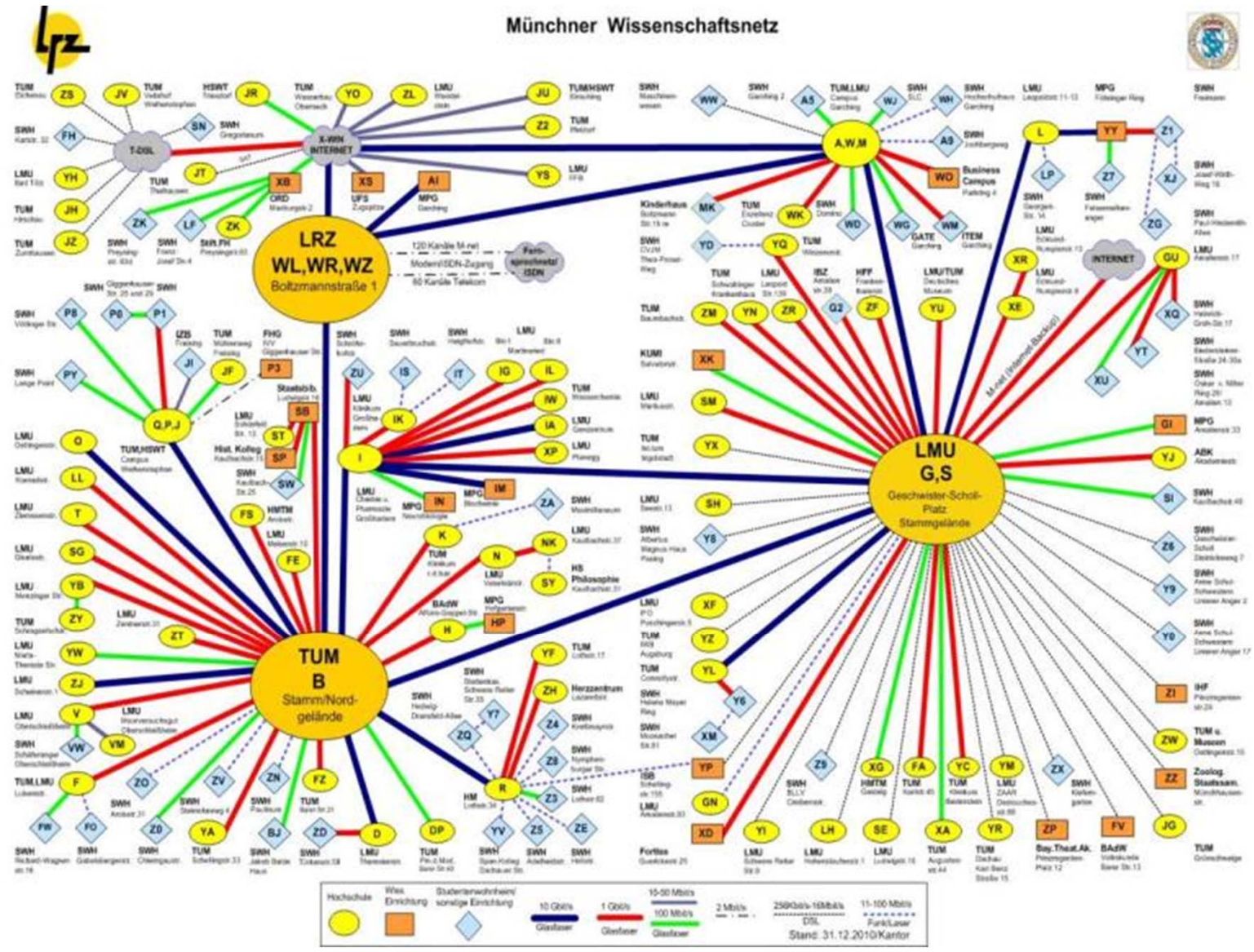


- Computer Centre for all Munich Universities

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, …)

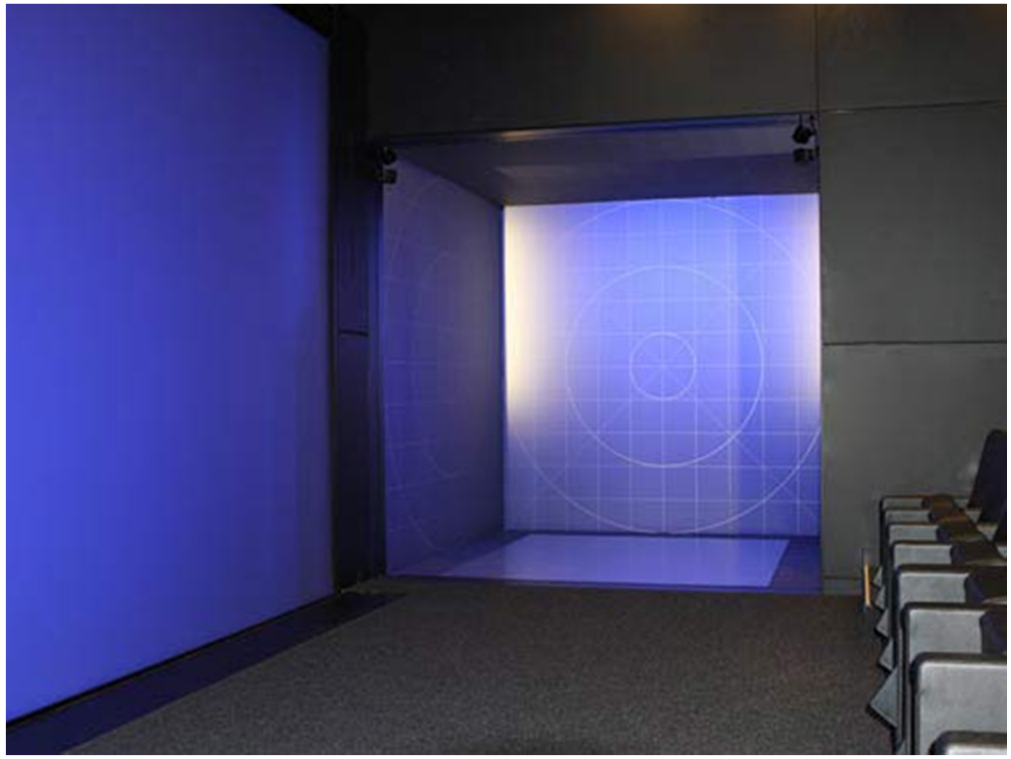
The Munich Scientific Network (MWN)



- Regional Computer Centre for all Bavarian Universities

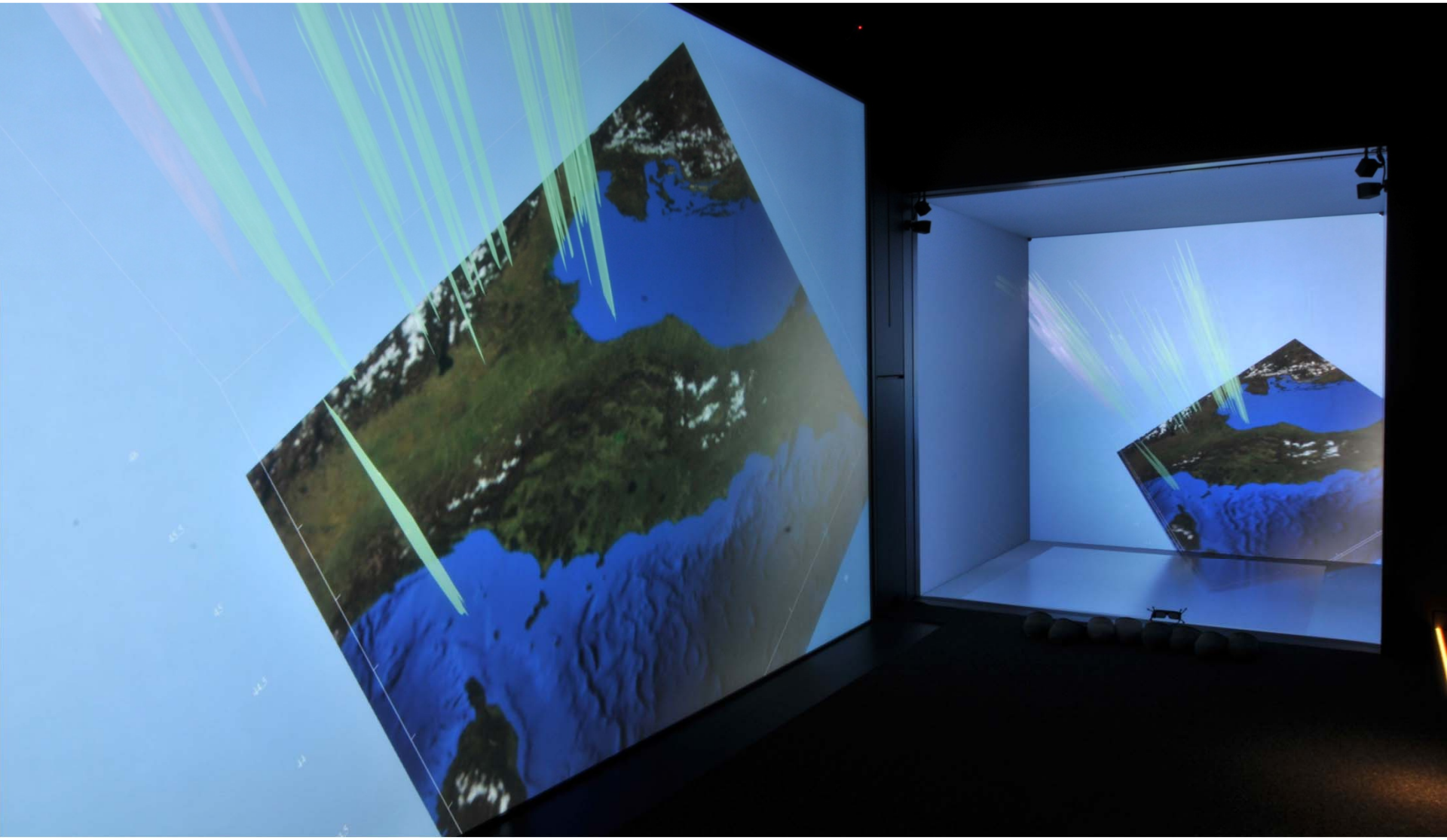
- Computer Centre for all Munich Universities

Virtual Reality and Visualisation Centre (V2C)



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

DRIHM – Distributed Research Infrastructure for Hydrometeorology

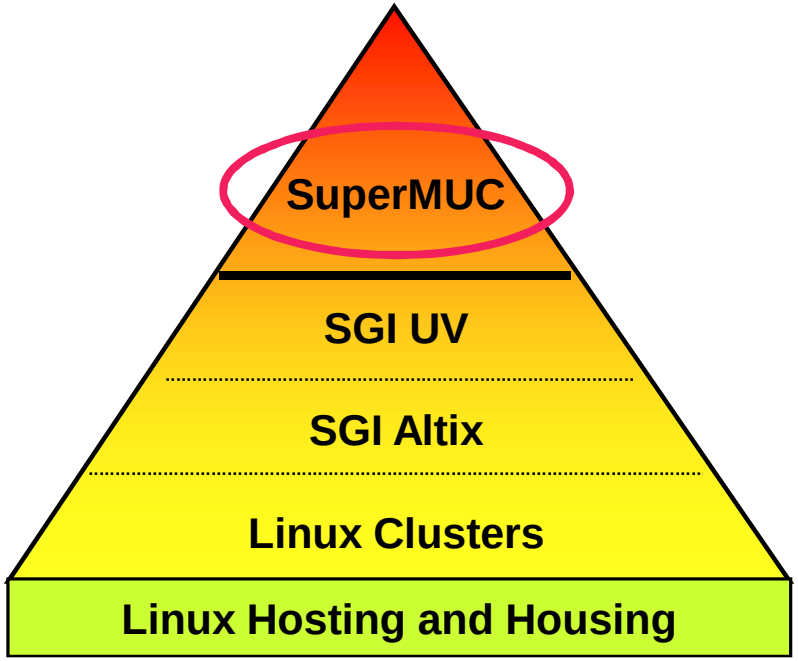


- National Supercomputing Centre
- Regional Computer Centre for all Bavarian Universities
- Computer Centre for all Munich Universities

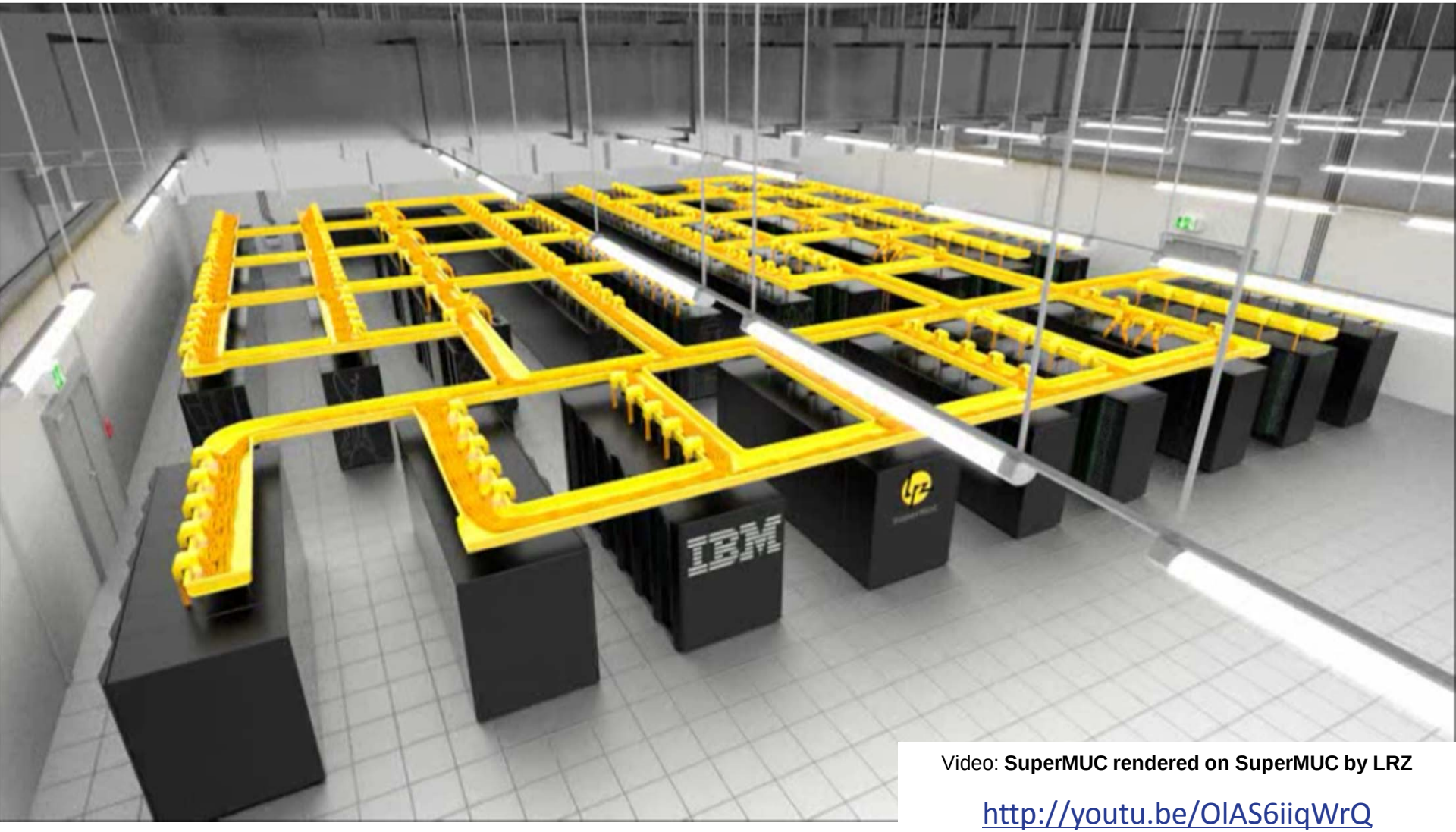
Gauss Centre for Supercomputing (GCS)

- Combination of the 3 German national supercomputing centers:
  - John von Neumann Institute for Computing (NIC), Jülich
  - High Performance Computing Center Stuttgart (HLRS)
  - Leibniz Supercomputing Centre (LRZ), Garching n. Munich
- Founded on 13. April 2007
- Hosting member of PRACE
  (Partnership for Advanced Computing in Europe)

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



SuperMUC @ LRZ



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

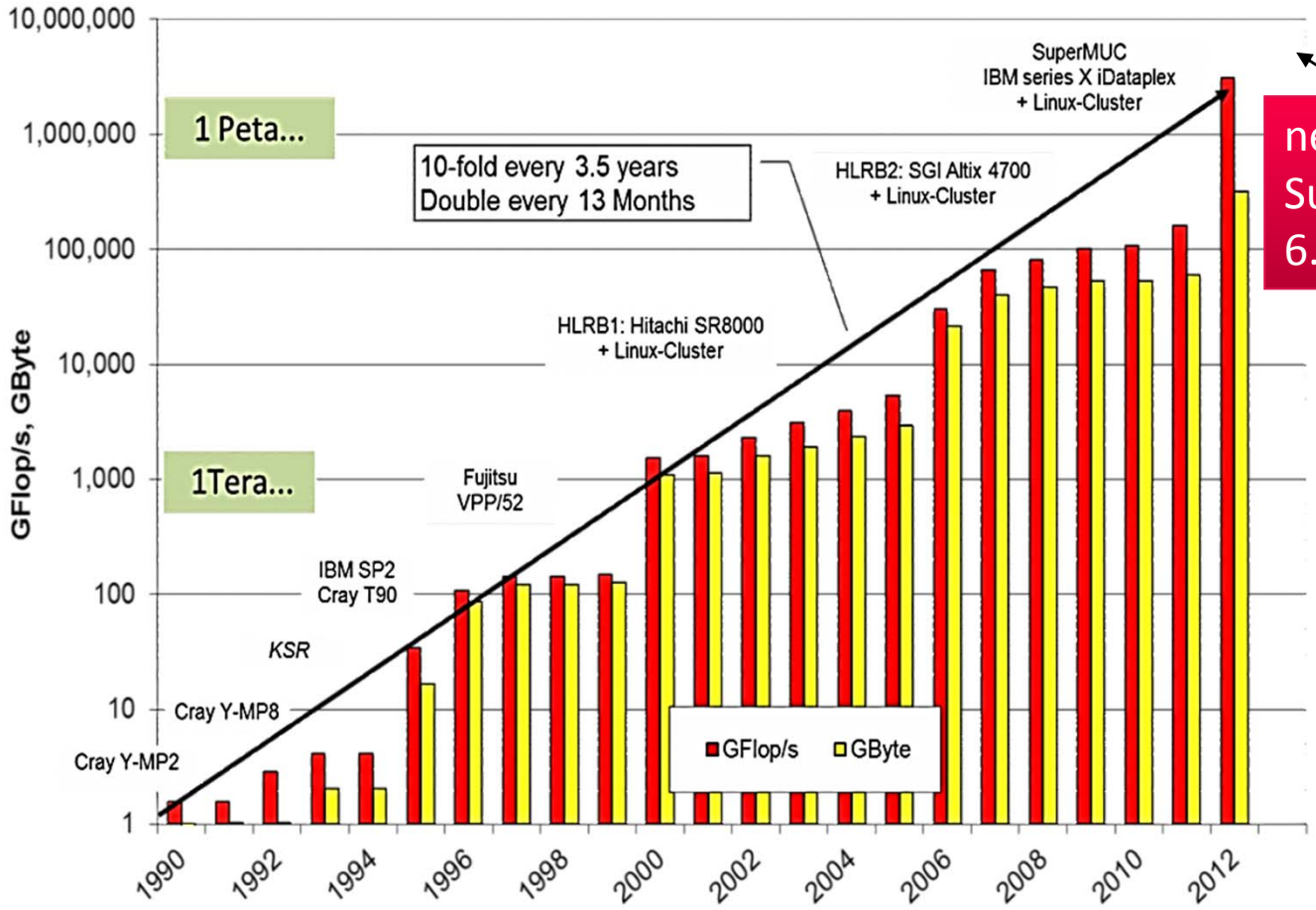
http://youtu.be/OlAS6iiqWrQ

Top 500 Supercomputer List (June 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

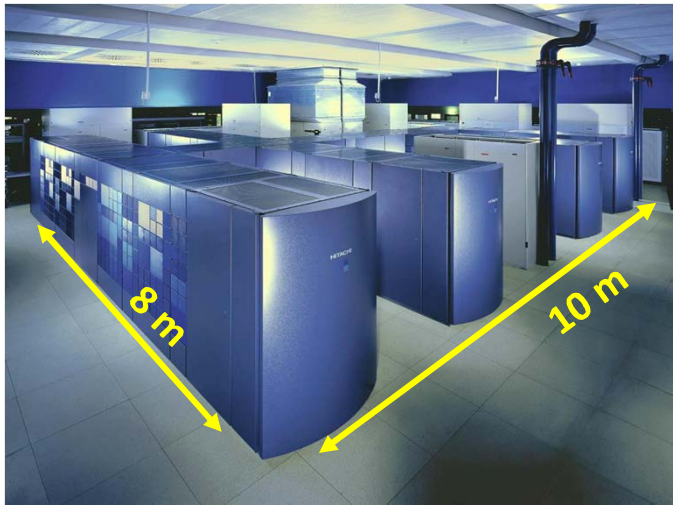
www.top500.org

LRZ Supercomputers



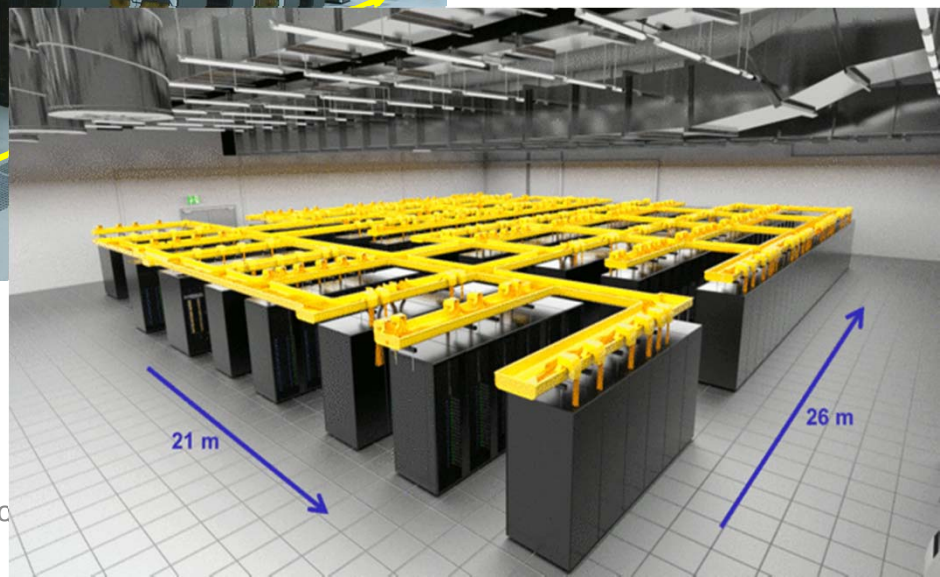
next to come (2014):
SuperMUC Phase II
6.4 PFlop/s

SuperMUC and its predecessors



SuperMUC and its predecessors

SuperMUC and its predecessors



LRZ Building Extension

Picture: Horst-Dieter Steinhöfer

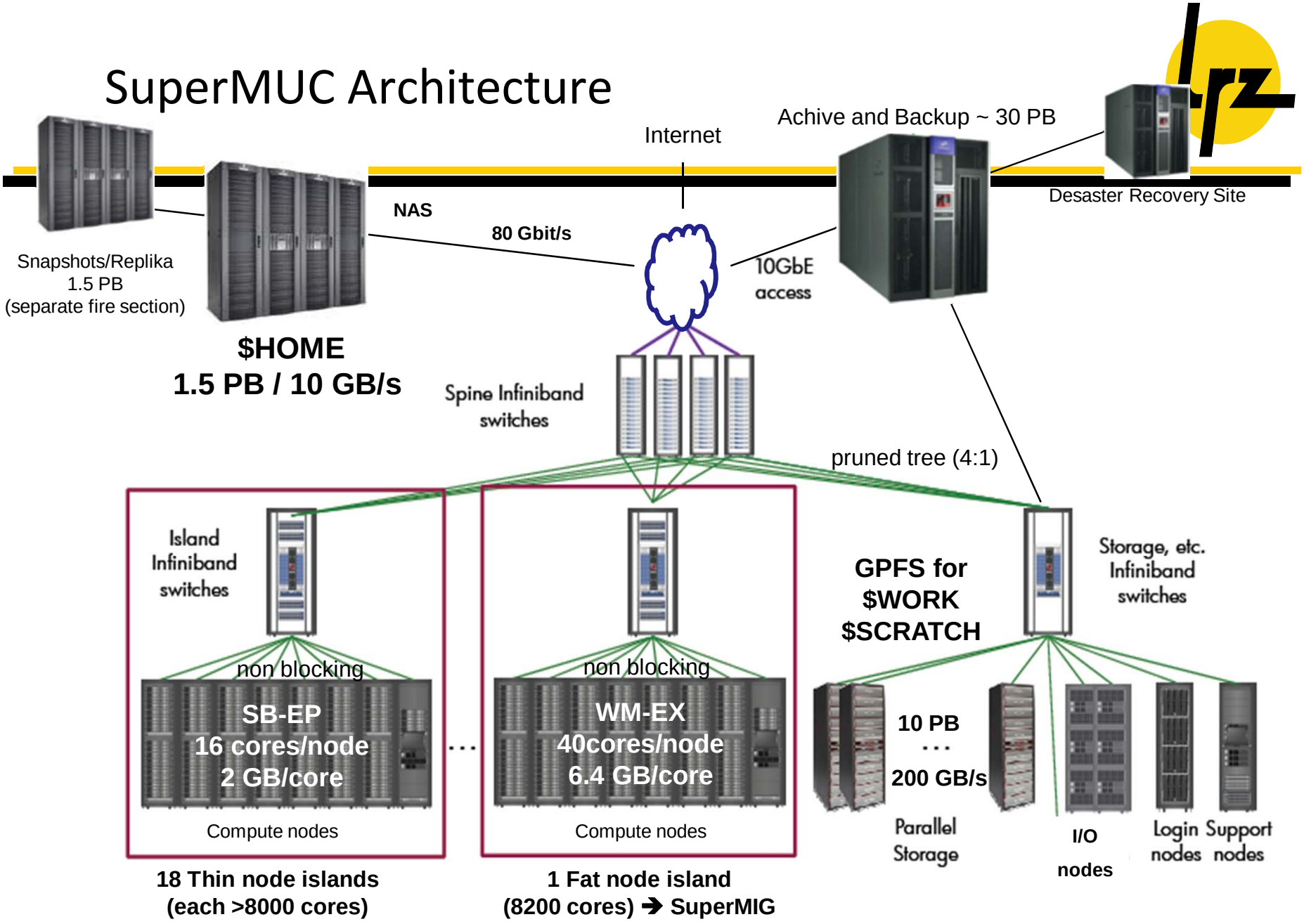
Figure: Herzog+Partner für StBAM2 (staatl. Hochbauamt München 2)

Picture: Ernst A. Graf

Increasing numbers

Date	System	Flop/s	Cores
2000	HLRB-I	2 Tflop/s	1512
2006	HLRB-II	62 Tflop/s	9728
2012	SuperMUC	3200 Tflop/s	155656
2014	SuperMUC Phase II	3.2 + 3.2 Pflop/s	229960

SuperMUC Architecture



LRZ Application Mix

- **Computational Fluid Dynamics: Optimisation of turbines and wings, noise reduction, air conditioning in trains**
- **Fusion: Plasma in a future fusion reactor (ITER)**
- **Astrophysics: Origin and evolution of stars and galaxies**
- **Solid State Physics: Superconductivity, surface properties**
- **Geophysics: Earth quake scenarios**
- **Material Science: Semiconductors**
- **Chemistry: Catalytic reactions**
- **Medicine and Medical Engineering: Blood flow, aneurysms, air conditioning of operating theatres**
- **Biophysics: Properties of viruses, genome analysis**
- **Climate research: Currents in oceans**

LRZ Extreme Scale Workshop

- **July 2013:**

  First SuperMUC Extreme Scale Workshop

- **Participants:**
  - 15 international projects
- **Prerequisites:**
  - Successful run on 4 islands (32768 cores)
- **Participating Groups (Software packages):**
  - LAMMPS, VERTEX, GADGET, WaLBerla, BQCD, Gromacs, APES, SeisSol, CIAO
- **Successful results (> 64000 Cores):**
  - Invited to participate in PARCO Conference (Sept. 2013) including a publication of their approach

LRZ Extreme Scale Workshop

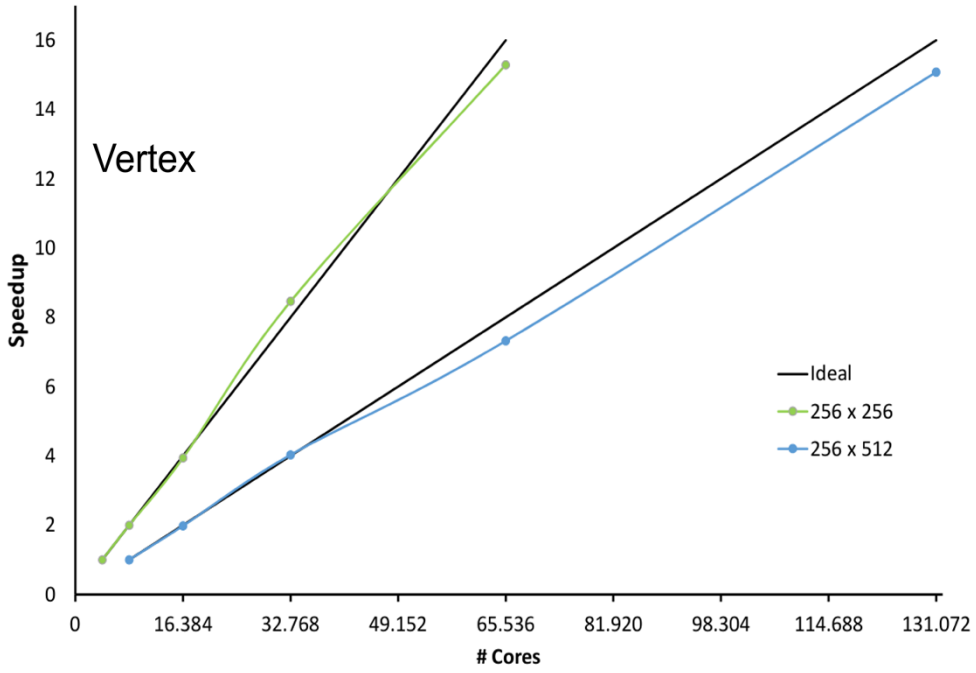
- **Regular SuperMUC operation**
  - 4 Islands maximum
  - Batch scheduling system
- **Entire SuperMUC reserved 2,5 days for challenge:**
  - 0,5 Days for testing
  - 2 Days for executing
  - 16 (of 19) Islands available
- **Consumed computing time for all groups:**
  - 1 hour of runtime = 130.000 CPU hours
  - 1 year in total

Results (Sustained TFlop/s on 128000 cores)

Name	MPI	# cores	Description	TFlop/s/island	TFlop/s max
Linpack	IBM	128000	TOP500	161	2560
Vertex	IBM	128000	Plasma Physics	15	245
GROMACS	IBM, Intel	64000	Molecular Modelling	40	110
Seissol	IBM	64000	Geophysics	31	95
waLBerla	IBM	128000	Lattice Boltzmann	5.6	90
LAMMPS	IBM	128000	Molecular Modelling	5.6	90
APES	IBM	64000	CFD	6	47
BQCD	Intel	128000	Quantum Physics	10	27

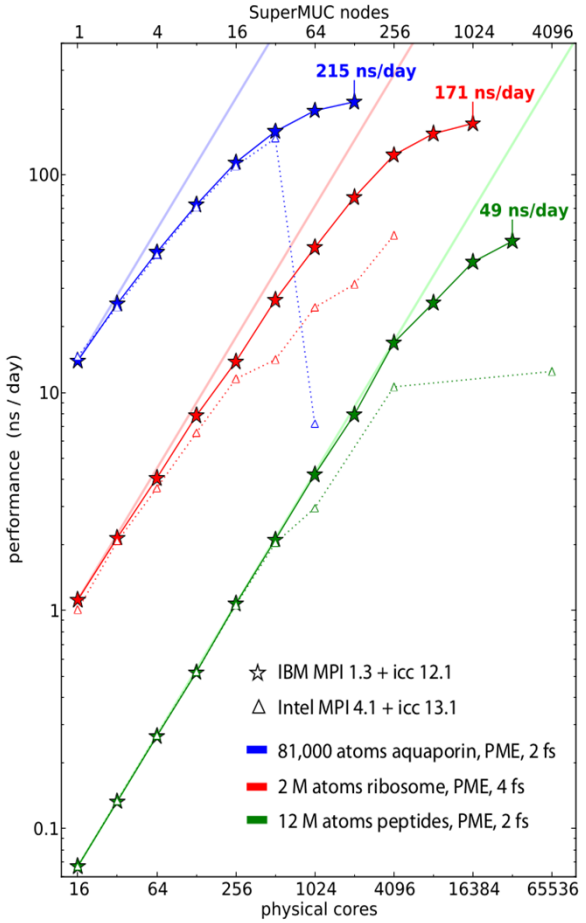
Results

- **5 Software packages were running on max 16 islands:**
  - LAMMPS
  - VERTEX
  - GADGET
  - WaLBerla
  - BQCD
- **VERTEX reached 245 TFlop/s on 16 islands (A. Marek)**



Results

- **4 Software packages were running on max 8 islands:**
  - Gromacs
  - APES
  - SeisSol
  - CIAO
- **GROMACS reached 201 TFlop/s on 8 islands (C. Kutzner)**



Lessons learned

- **Hybrid (MPI+OpenMP) on SuperMUC still slower than pure MPI (e.g. GROMACS), but applications scale to larger core counts (e.g. VERTEX)**
- **Core pinning needs a lot of experience by the programmer**
- **Parallel IO still remains a challenge for many applications, both with regard to stability and speed.**
- **Several stability issues with GPFS were observed for very large jobs due to writing thousands of files in a single directory. This will be improved in the upcoming versions of the application codes.**

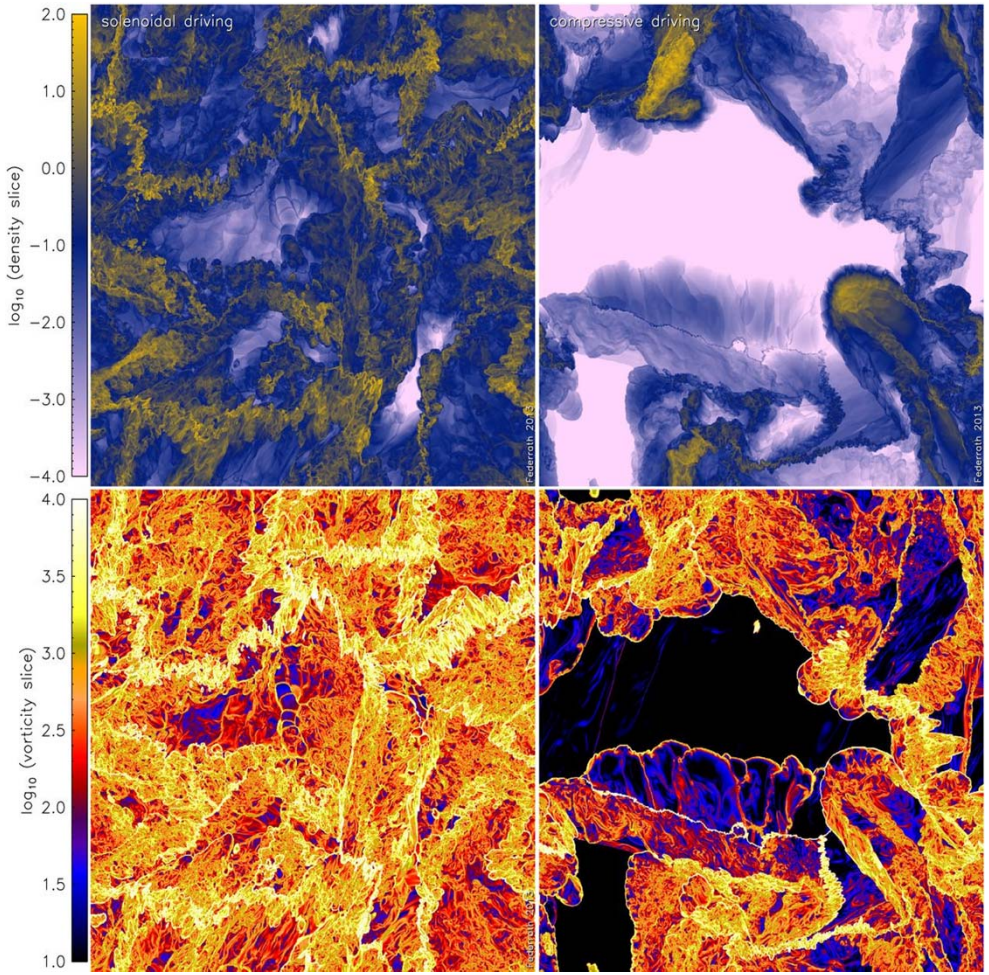
LRZ Extreme Scale Suite (LESS)

- **Platform and architecture agnostic framework for automatic compilation and submission of validation and test jobs**
- **Framework source originates from DEISA benchmark suite**
- **Extended in EU Project Scalalife to Gromacs, Dalton and Discrete**
- **Implemented in XML and perl**
- **System architecture is described as XML file**
- **Many system architectures available**
  - Hardware: SGI Altix, UV, ice, IBM dataplex, cell, CRAY, generic x86
  - Compilers: icc, gcc, xlc
  - Batch systems: PBS, SLURM, Loadleveller, ...
- **Software Packages: BQCD, GROAMCS, Lammps, Gadget, APES,CIAO, SeisSol, GPI, pbdMPI, doRedis, Blender**

Next Steps

- **LRZ Extreme Scale Benchmark Suite (LESS) will be available in two versions: public and internal**
- **All teams will have the opportunity to run performance benchmarks after upcoming SuperMUC maintenances**
- **Next workshop will be June/July 2014**
- **Initiation of the LRZ Partnership Initiative piCS**

Astrophysics: world's largest simulations of supersonic, compressible turbulence with a numerical grid resolution of 4096^3 points.



Slices through the three-dimensional gas density (top panels) and vorticity (bottom panels) for fully developed, highly compressible, supersonic turbulence, generated by solenoidal driving (left-hand column) and compressive driving (right-hand column), and a grid resolution of 4096^3 cells.

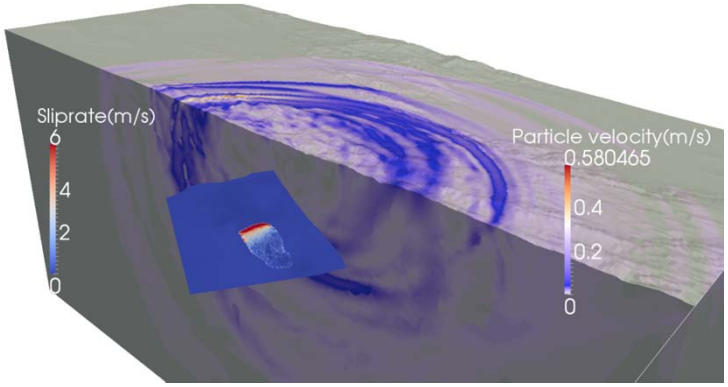
Federrath C MNRAS 2013;mnras.stt1644

MONTHLY NOTICES *of the* Royal Astronomical Society

SeisSol – Earthquake Simulation at Petascale

Key Features

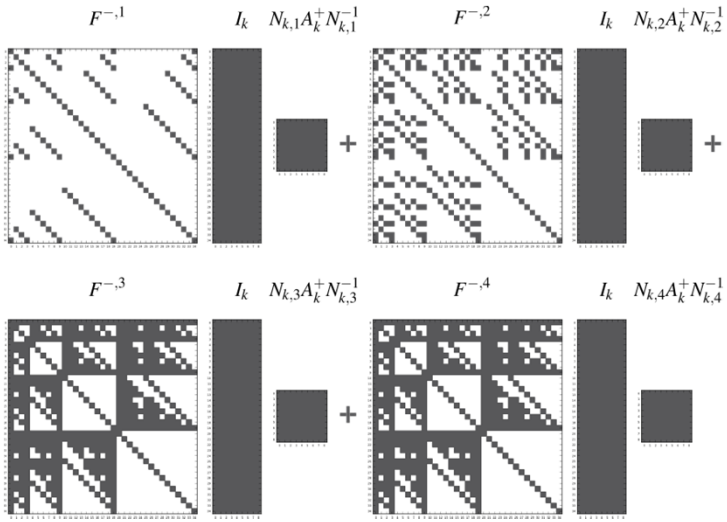
- ADER-DG: high approximation order in space and time
- Adaptive tetrahedral meshes for highly complex geometries
- Dynamic rupture simulation coupled to seismic wave propagation



1994 Northridge Earthquake (A. Gabriel)

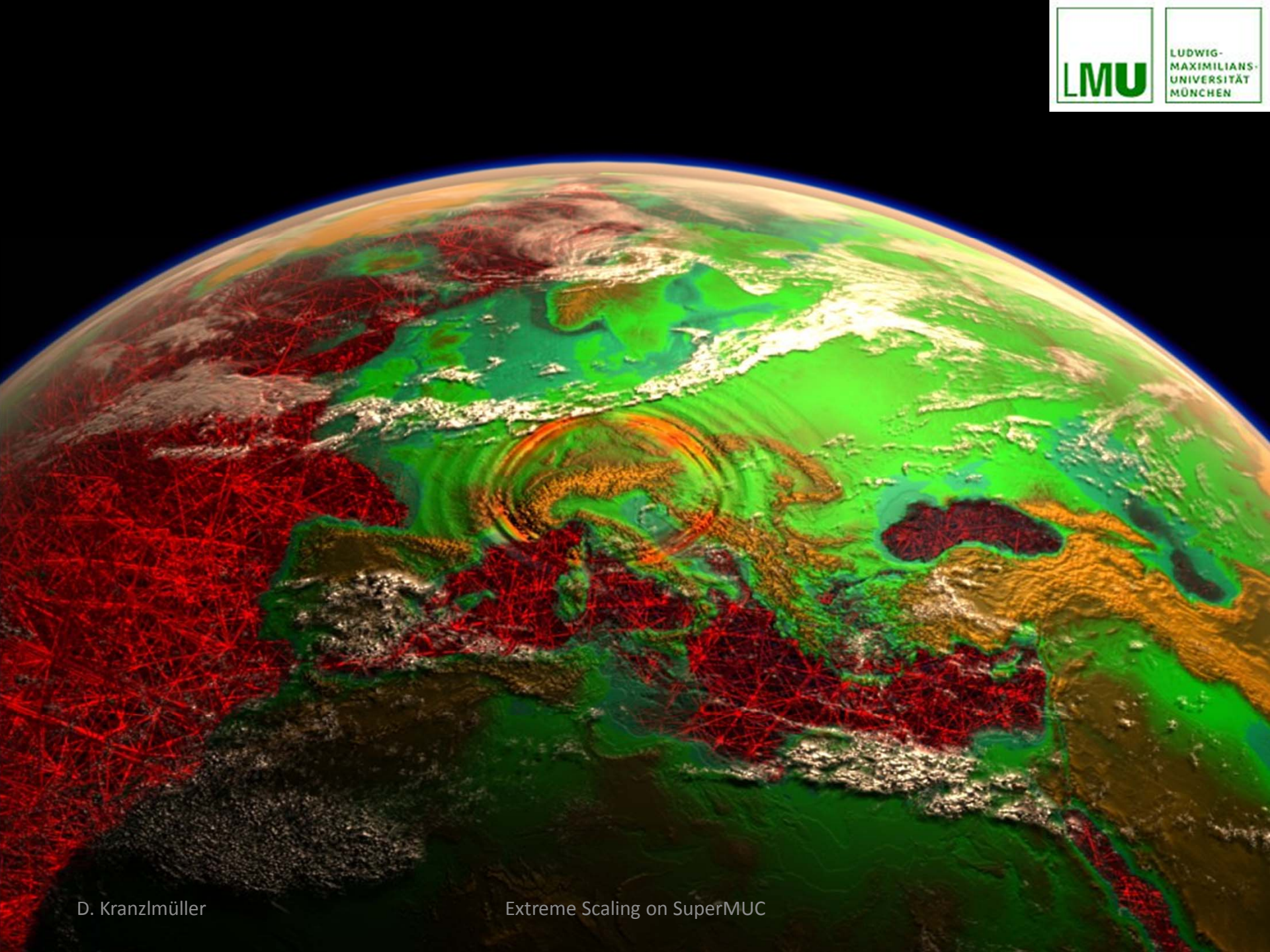
Code Generation for Matrix Kernels:

- Optimal code generation in an offline pre-compile phase
- Generation of vector instruction when the auto-vectorizer fails
- Selection of the optimal kernel (sparse or dense) for every matrix and numerical order



Several sparsity patterns of a 5th-order discretization

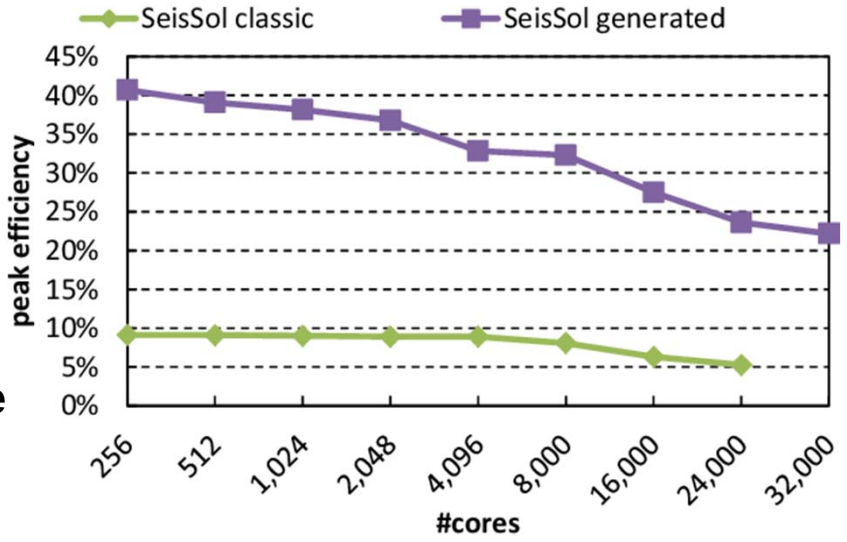
Check-out detailed poster @SC'13!



~1 PF Sustained Performance on SuperMUC

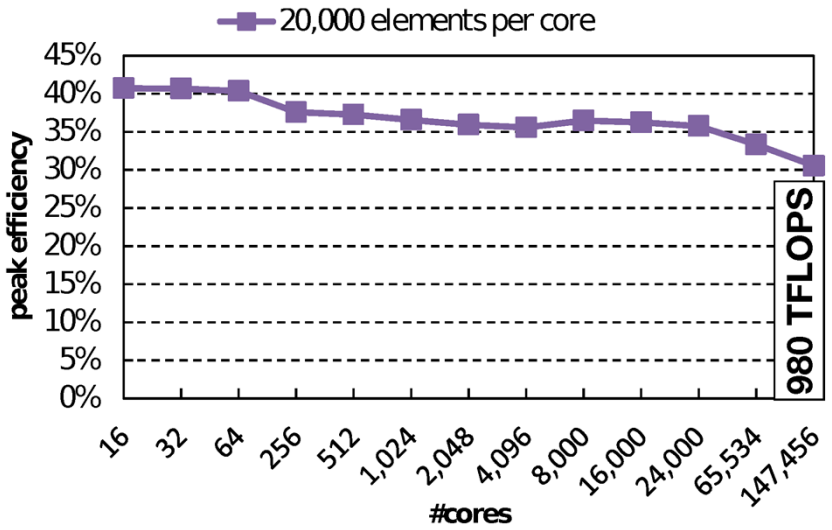
Strong Scaling Benchmark Run:

- ❑ 20,000 elements per core (recursively generated mesh on cube domain)
- ❑ 6th order (1.5 trillion unknowns) using 30% of SuperMUC's memory
- ❑ 0.98 PF, more than 30% of peak performance



Weak Scaling Study:

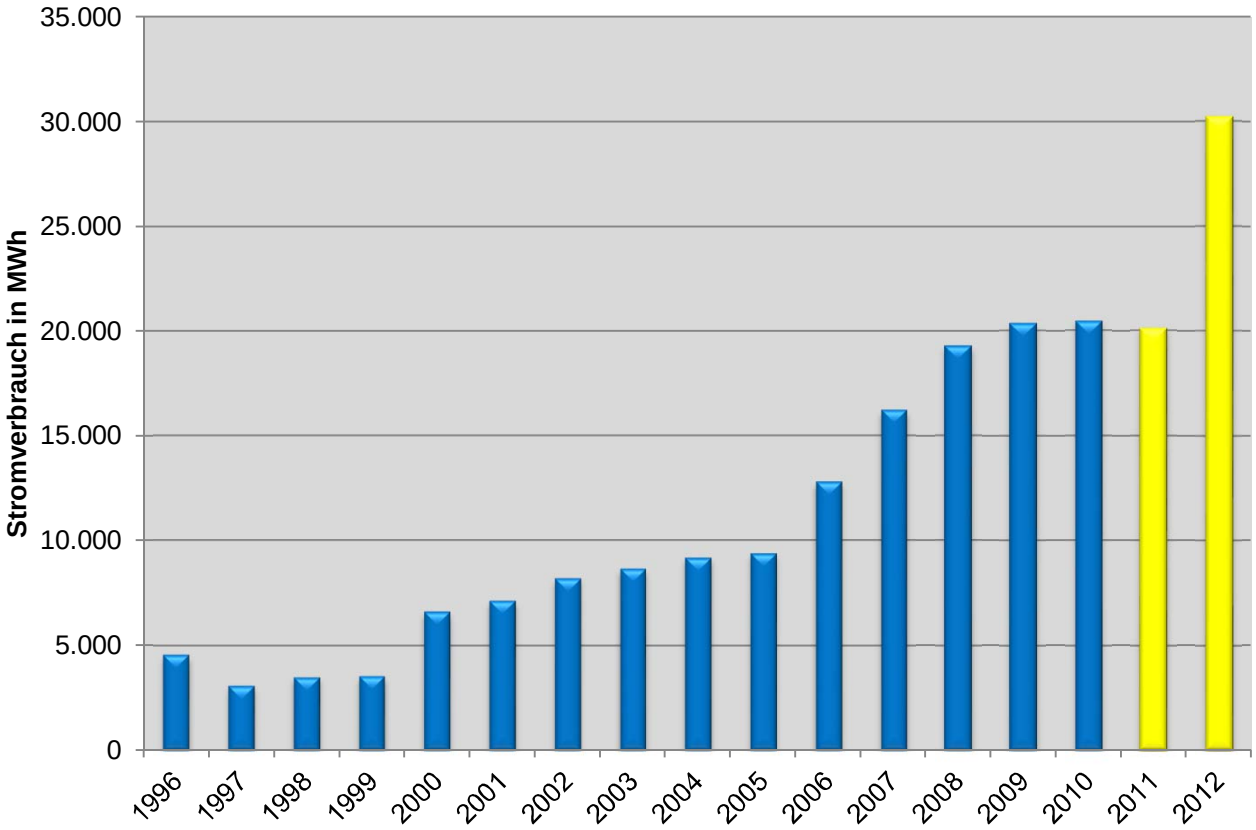
- SCEC LOH.1 , 7,252,482 cells
- 6th order (3.6 billion unknowns)
- 2.25 TF on 256 cores (40.6% peak)
  153 TF on 32K cores (21.6% peak)
- 4.5x speedup in time to solution due to kernel generation



Check-out detailed poster @SC'13!

SuperMUC @ LRZ

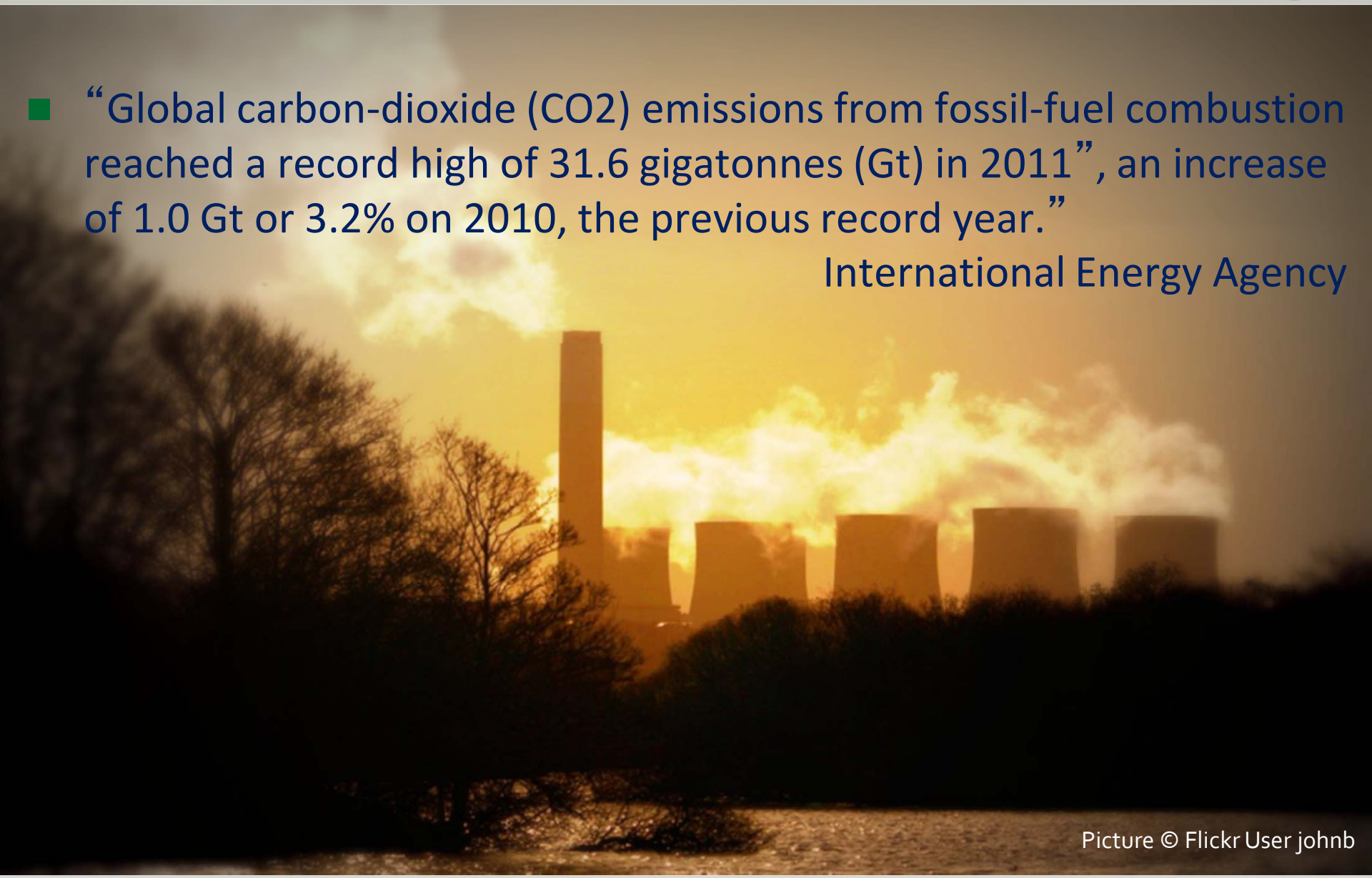
Power Consumption at LRZ



ICT and Global Warming

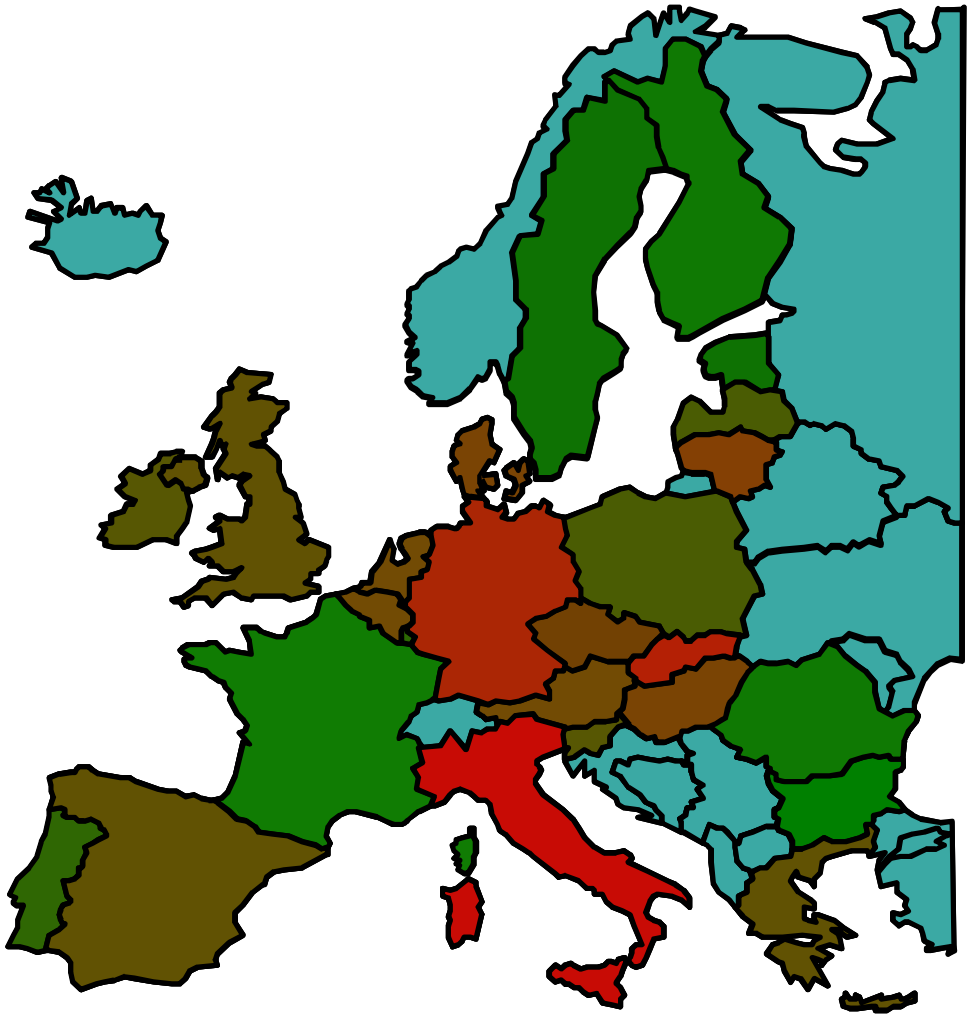
- “Global carbon-dioxide (CO2) emissions from fossil-fuel combustion reached a record high of 31.6 gigatonnes (Gt) in 2011”, an increase of 1.0 Gt or 3.2% on 2010, the previous record year.”

  International Energy Agency



Picture © Flickr User johnb

Financial Consequences (Power Bill)

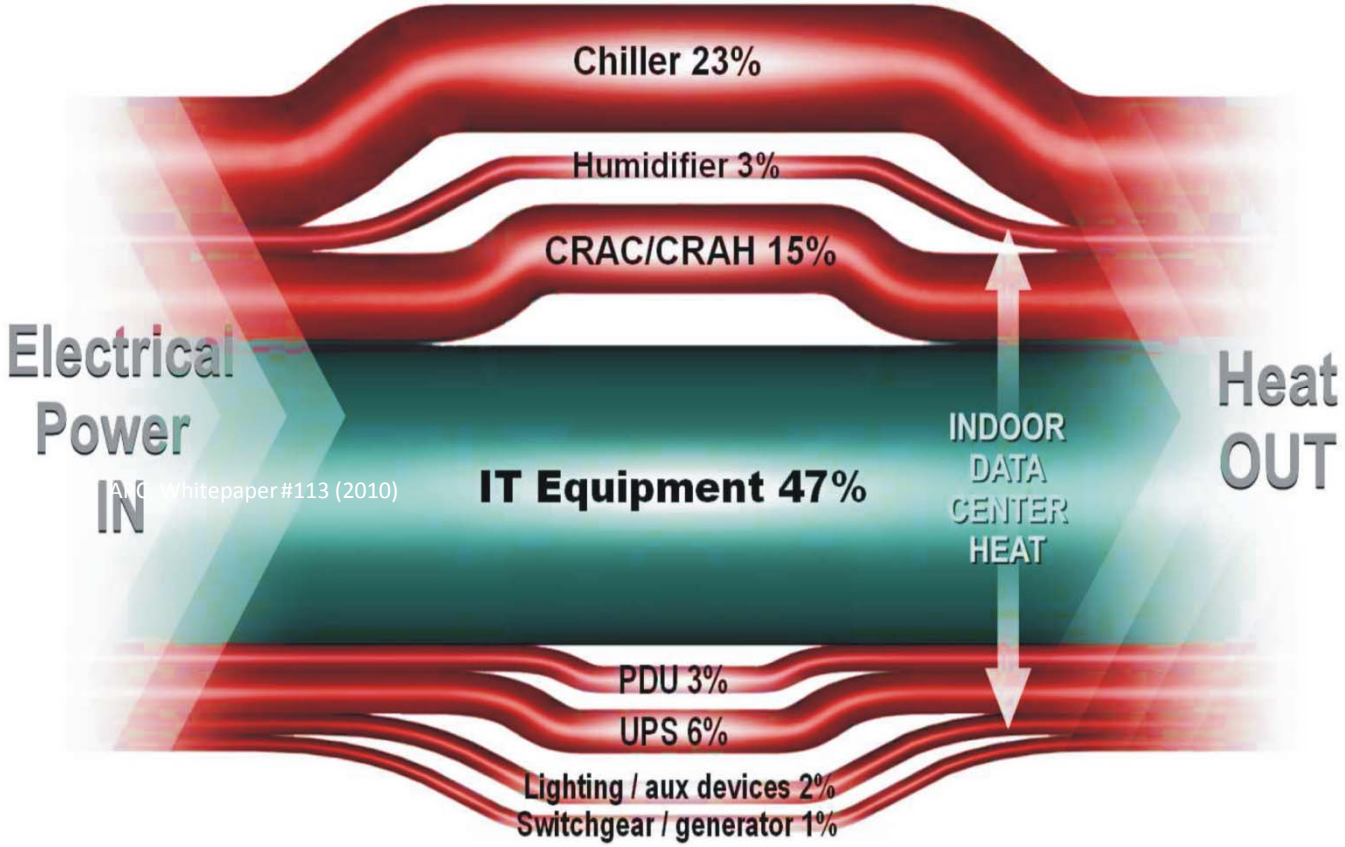


€ / KWh
for industrial customers

Source: energy.eu (effective April 2011)

Energy Consumption in Data Centres

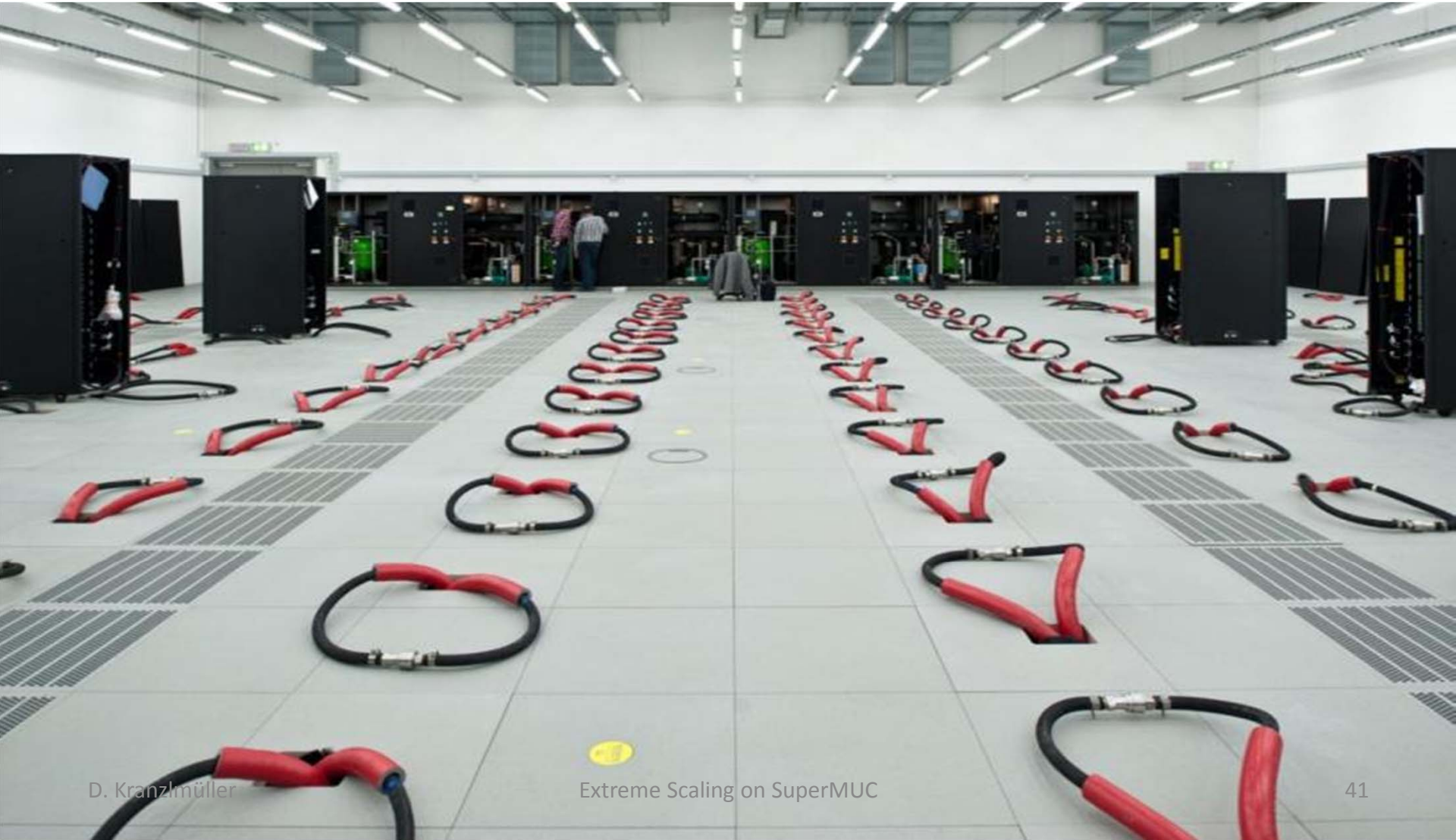
- Data Centres are "Heaters with integrated logic"



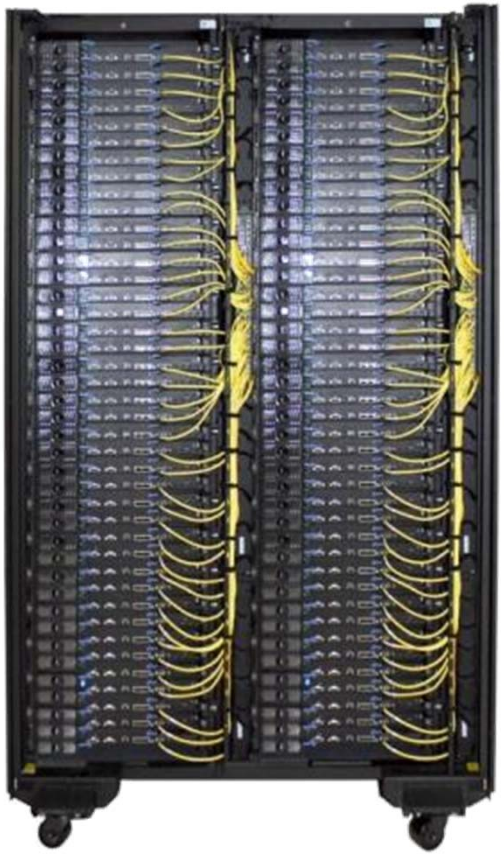
APC Whitepaper #113 (2010)

Torsten Bloth, IBM Lab Services - © IBM Corporation

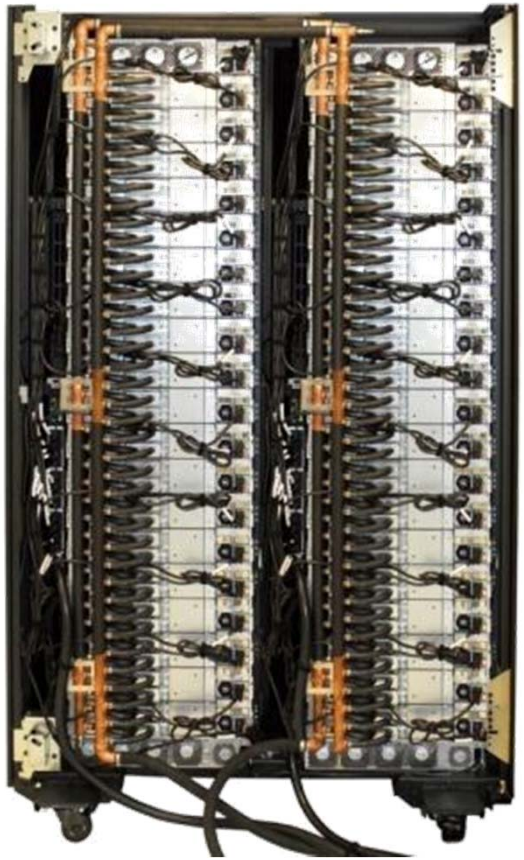
Cooling SuperMUC



IBM System x iDataPlex
Direct Water Cooled Rack



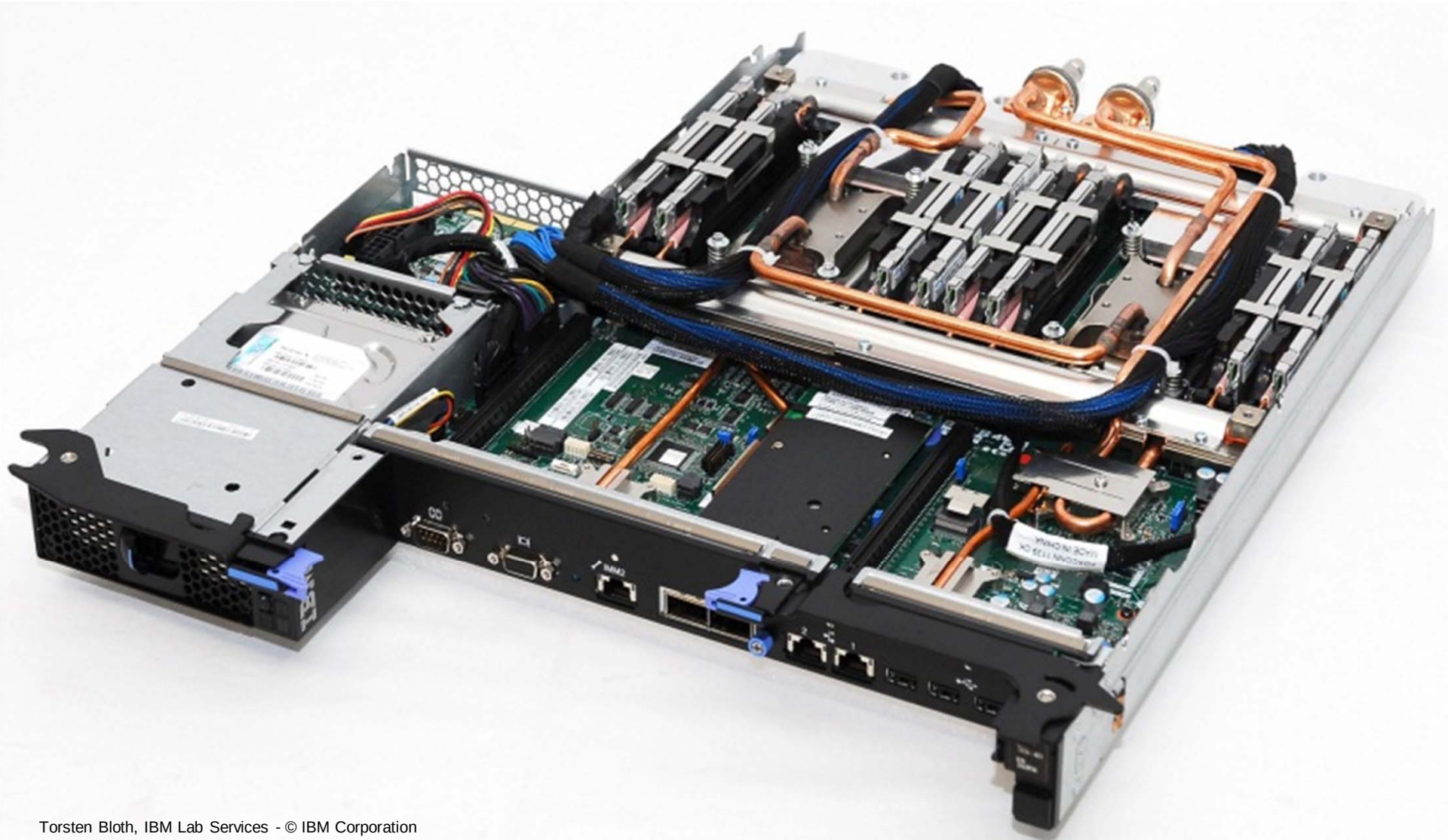
iDataplex DWC Rack
w/ water cooled nodes
(front view)



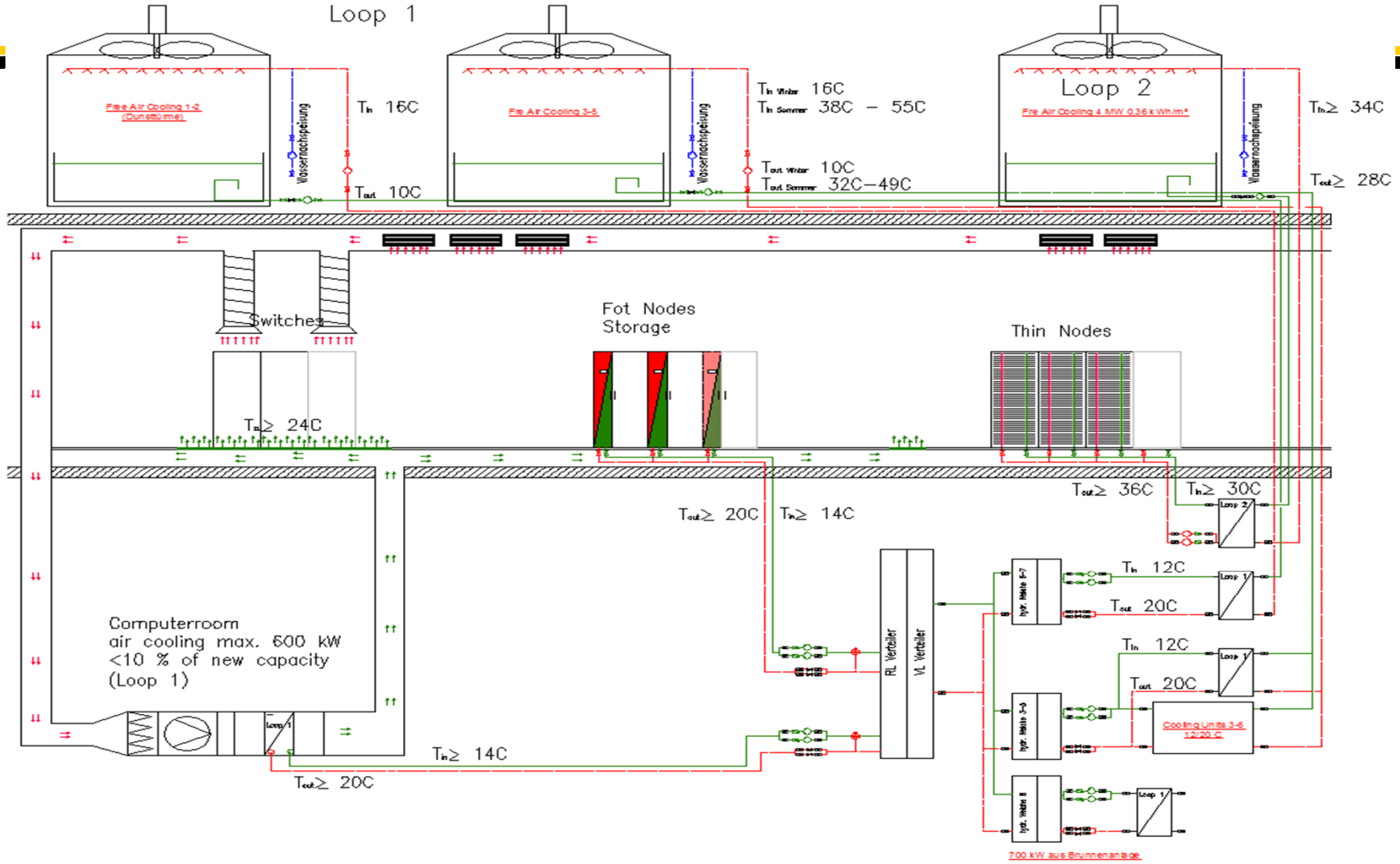
iDataplex DWC Rack
w/ water cooled nodes
(rear view of water manifolds)

Torsten Bloth, IBM Lab Services - © IBM Corporation

IBM iDataplex dx360 M4



Cooling Concept – Dedicated Free Cooling



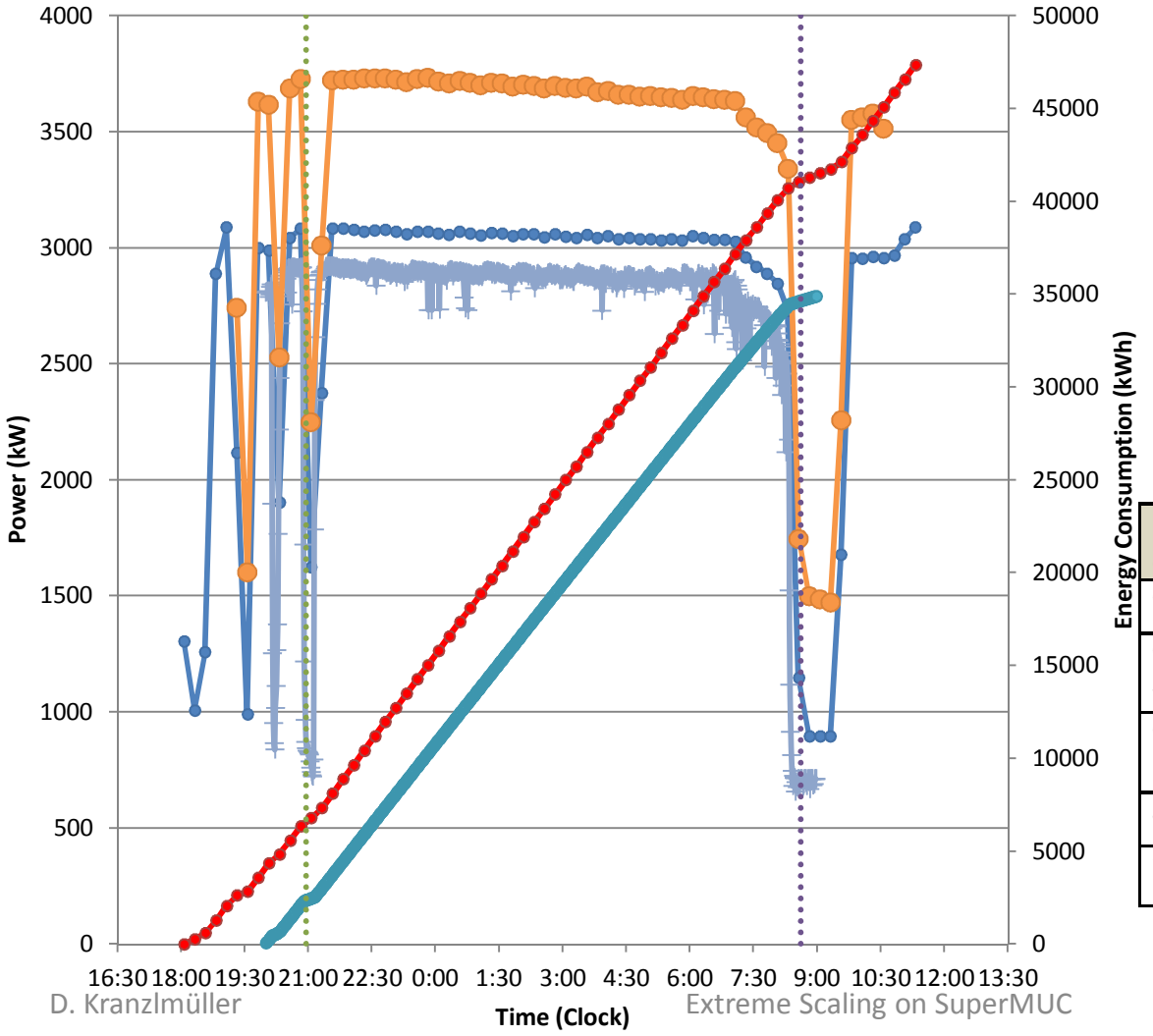
Cooling Infrastructure

Photos: StBAM2 (staatl. Hochbauamt München 2)

Cooling Infrastructure (Roof)

Photo: 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)

Extreme Scaling on SuperMUC

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