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MNM TEAM
MUNICH NETWORK MANAGEMENT TEAM

lrz

In Need of Partnerships

An Essay about the Collaboration between Computational Sciences and IT Services

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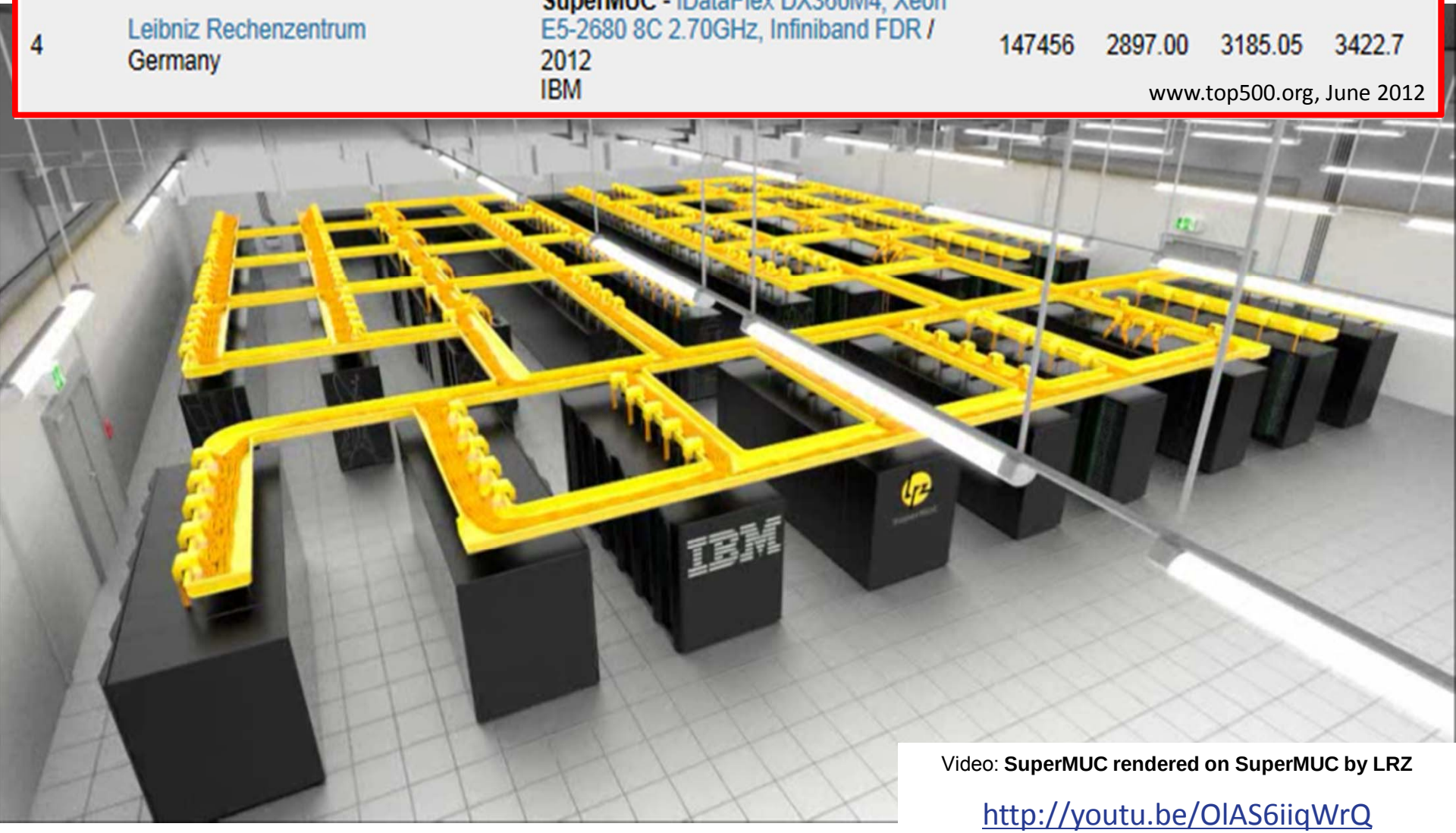
of the Bavarian Academy of Sciences and Humanities

SuperMUC @ LRZ

4	Leibniz Rechenzentrum Germany	**SuperMUC** - iDataPlex DX360M4, Xeon E5-2680 8C 2.70GHz, Infiniband FDR / 2012 IBM	147456	2897.00	3185.05	3422.7

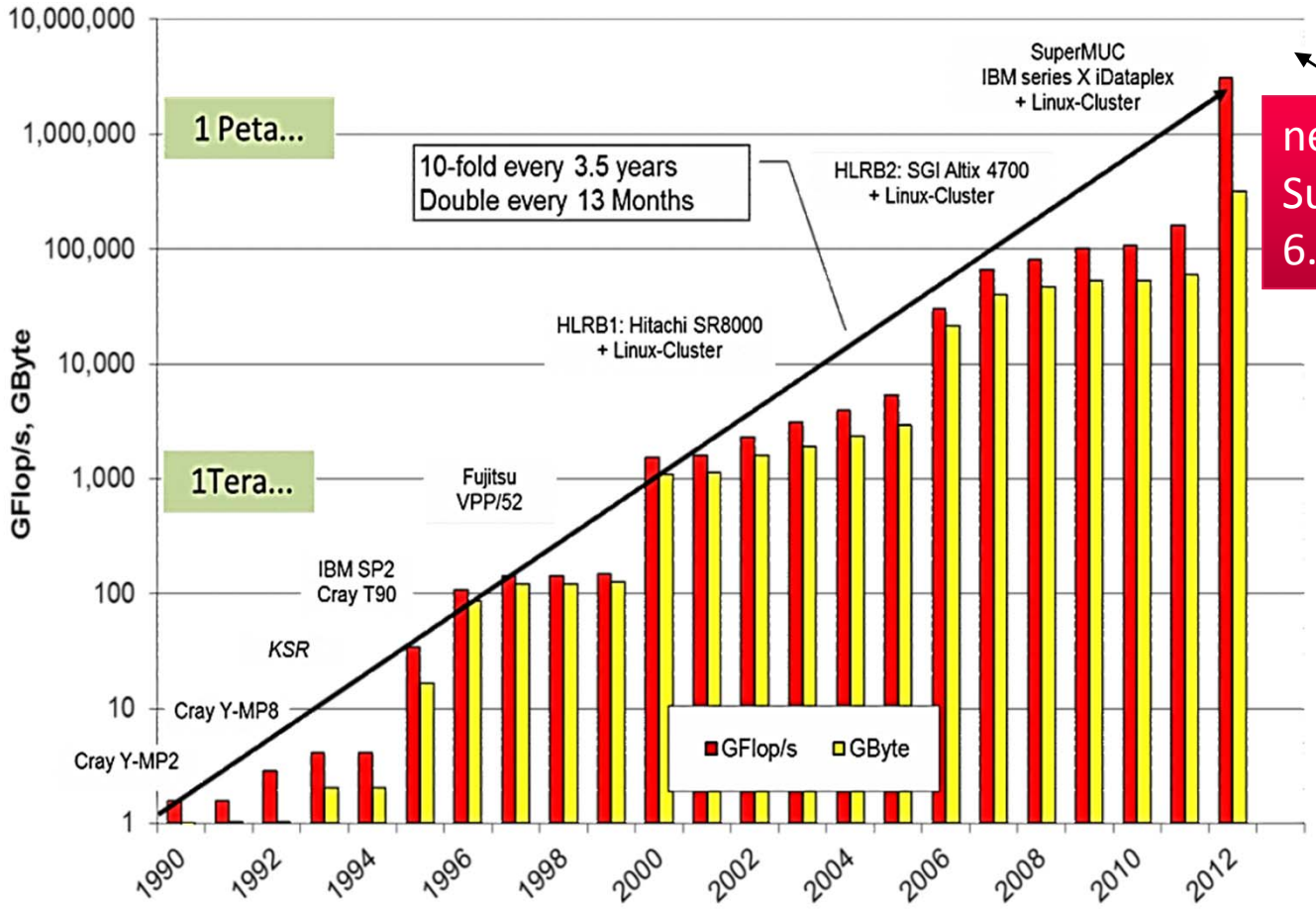
www.top500.org, June 2012



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

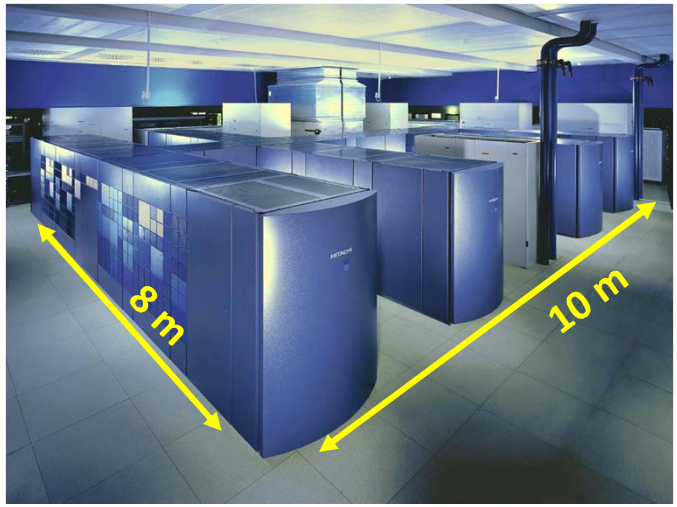
http://youtu.be/OlAS6iiqWrQ

LRZ Supercomputers



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

SuperMUC and its predecessors



SuperMUC and its predecessors

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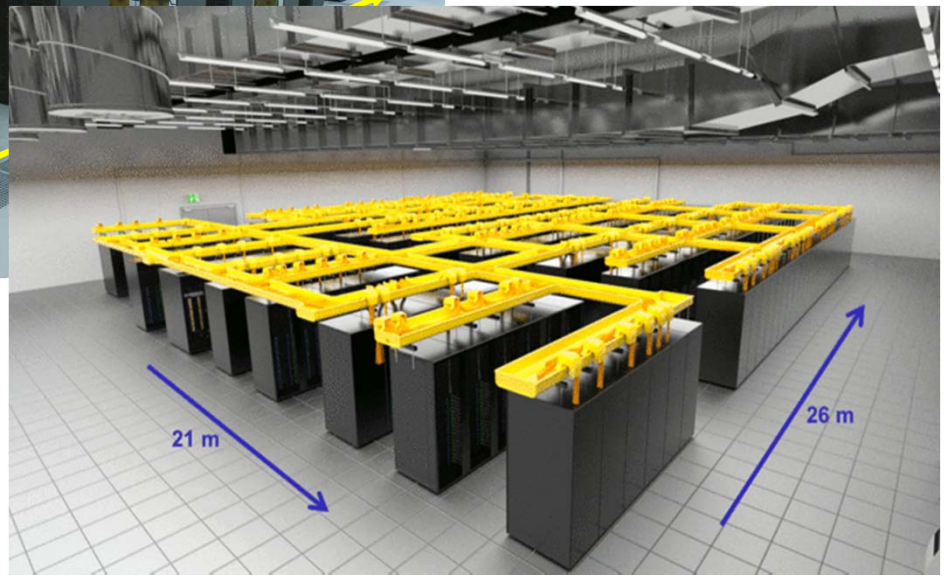


LRZ Building Extension

Picture: Horst-Dieter Steinhöfer

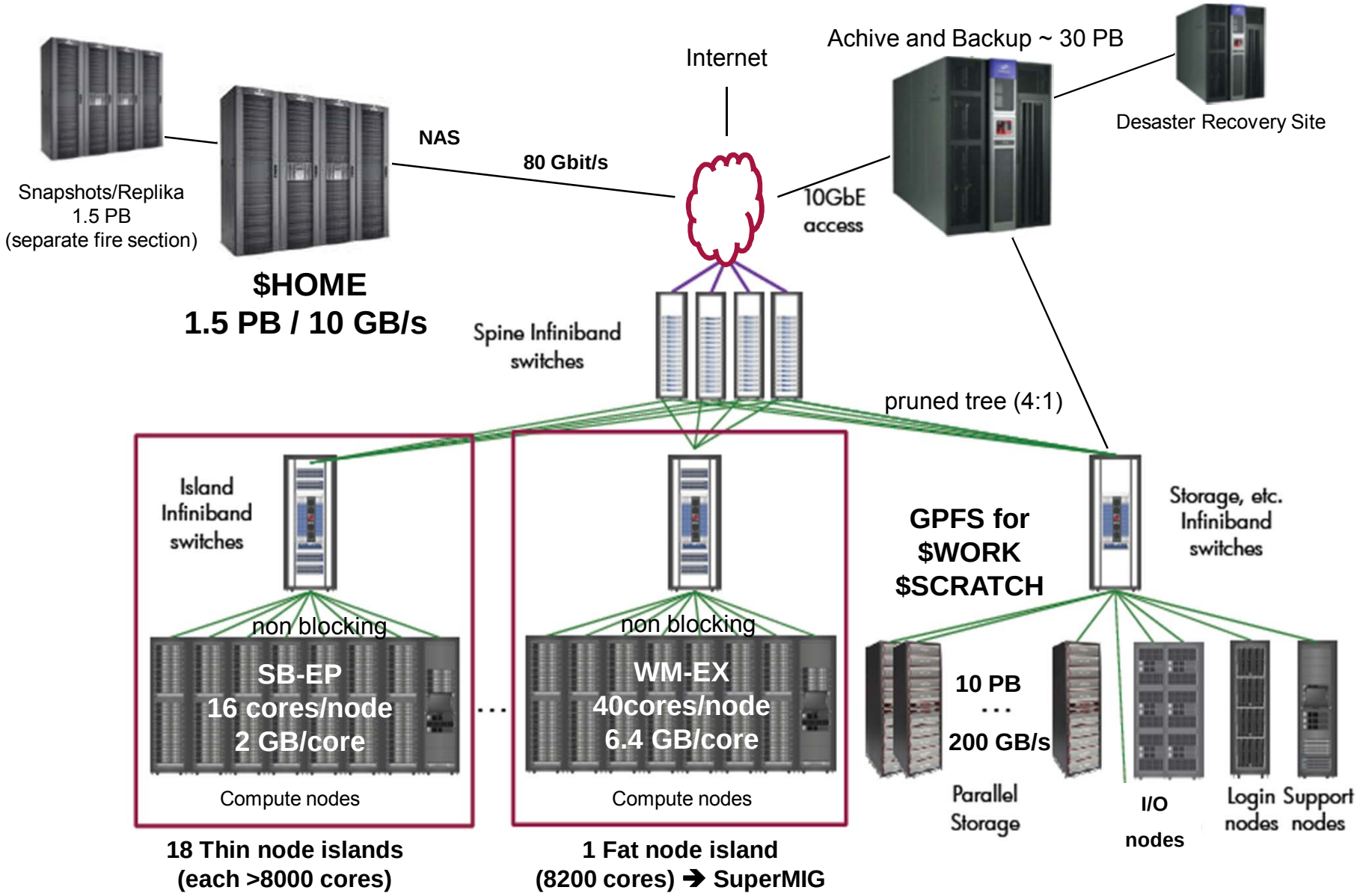
Figure: Herzog+Partner für StBAM2 (staatl. Hochbauamt München 2)

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



Questions

- How to use today‘s supercomputers?
- How to cope with the complexity?
- How to use these machines efficiently?
- How to scale applications?
- How to do I/O?
- How about resilience?
- …

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

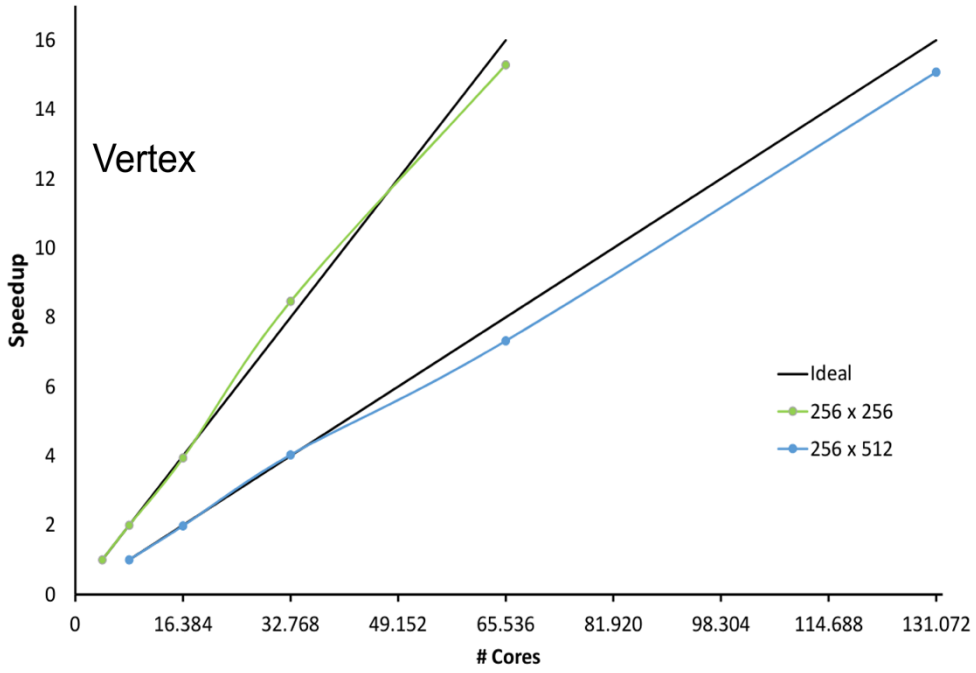
Results (Sustained TFlop/s on 128000 cores)

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)



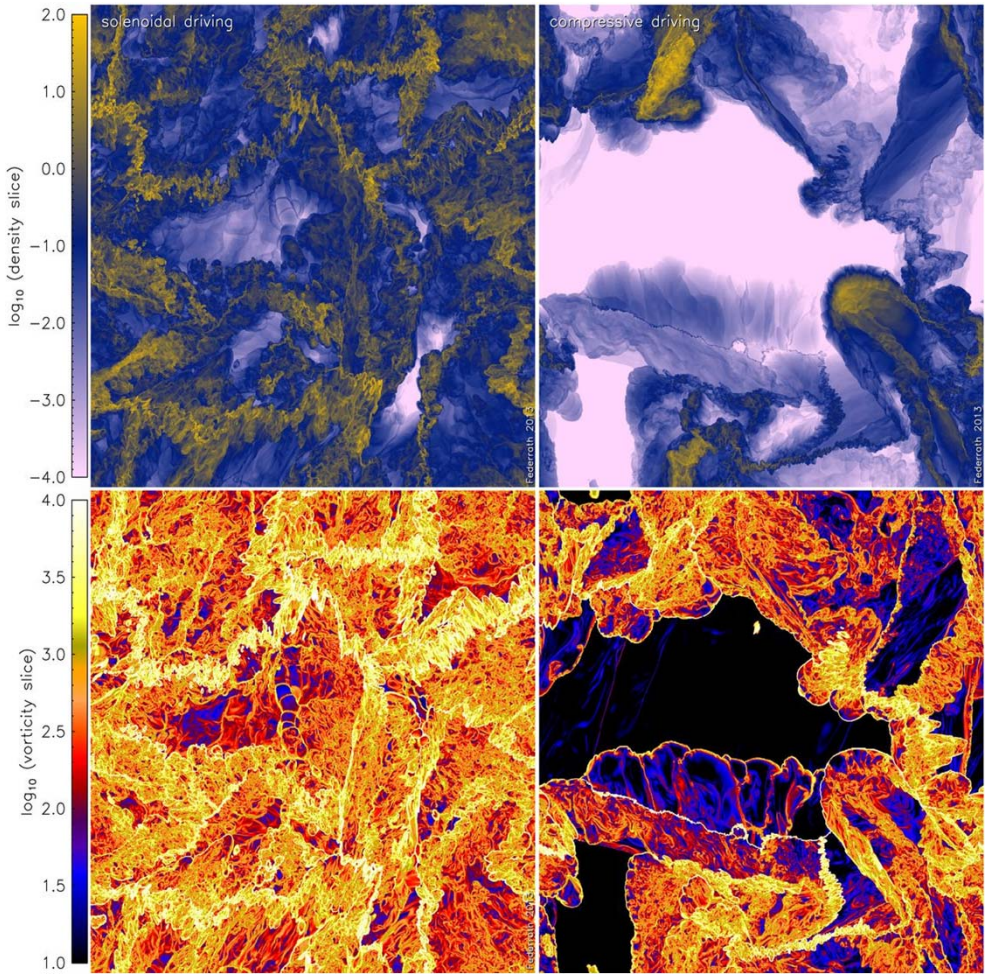
Lessons learned – Technical Perspective

- 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.

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
- Second LRZ Extreme Scaling Workshop ➔ 2-5 June 2014
- Initiation of the LRZ Partnership Initiative πCS

Astrophysics: world's largest simulations of supersonic, compressible turbulence



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

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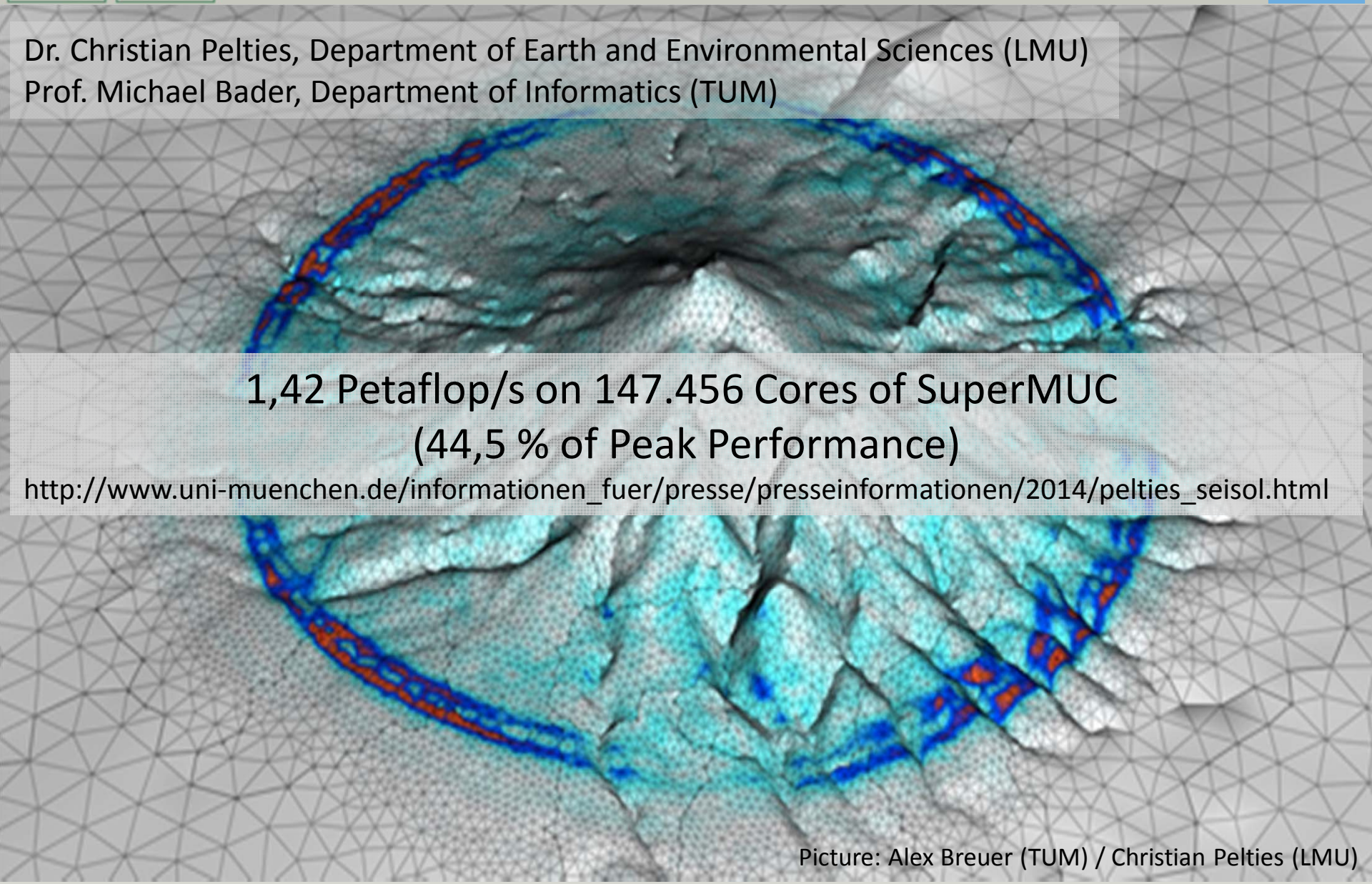
SeisSol - Numerical Simulation of Seismic Wave Phenomena

Dr. Christian Pelties, Department of Earth and Environmental Sciences (LMU)
Prof. Michael Bader, Department of Informatics (TUM)

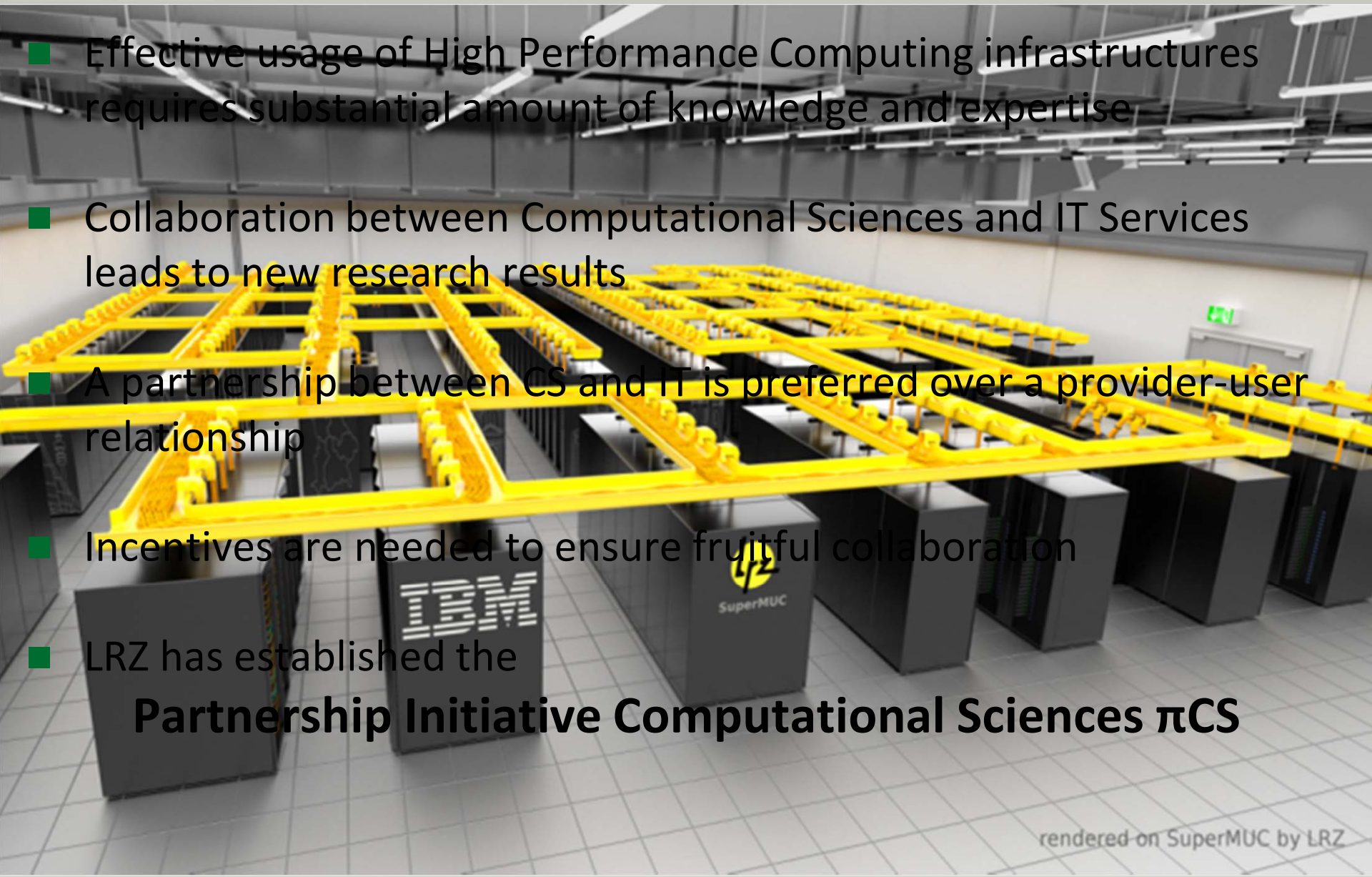


1,42 Petaflop/s on 147.456 Cores of SuperMUC
(44,5 % of Peak Performance)

http://www.uni-muenchen.de/informationen_fuer/presse/presseinformationen/2014/pelties_seisol.html

Picture: Alex Breuer (TUM) / Christian Pelties (LMU)

Summary and Conclusions



- Effective usage of High Performance Computing infrastructures requires substantial amount of knowledge and expertise
- Collaboration between Computational Sciences and IT Services leads to new research results
- A partnership between CS and IT is preferred over a provider-user relationship
- Incentives are needed to ensure fruitful collaboration
- LRZ has established the

  Partnership Initiative Computational Sciences πCS

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