Extreme Scaling - From Exploding Volcanos to Personalized Medicine

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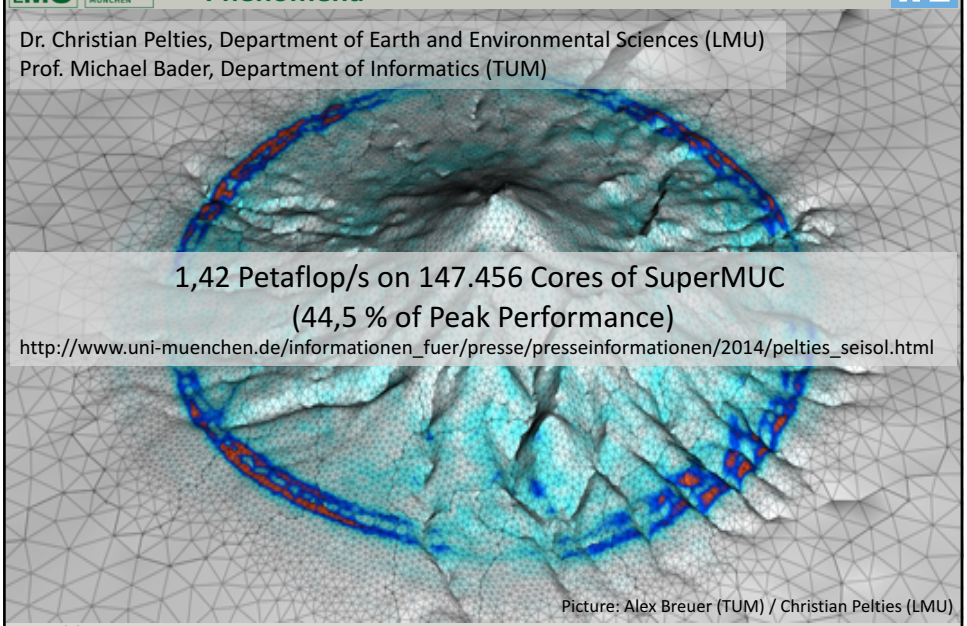
SeisSol - Numerical Simulation of Seismic Wave Phenomena

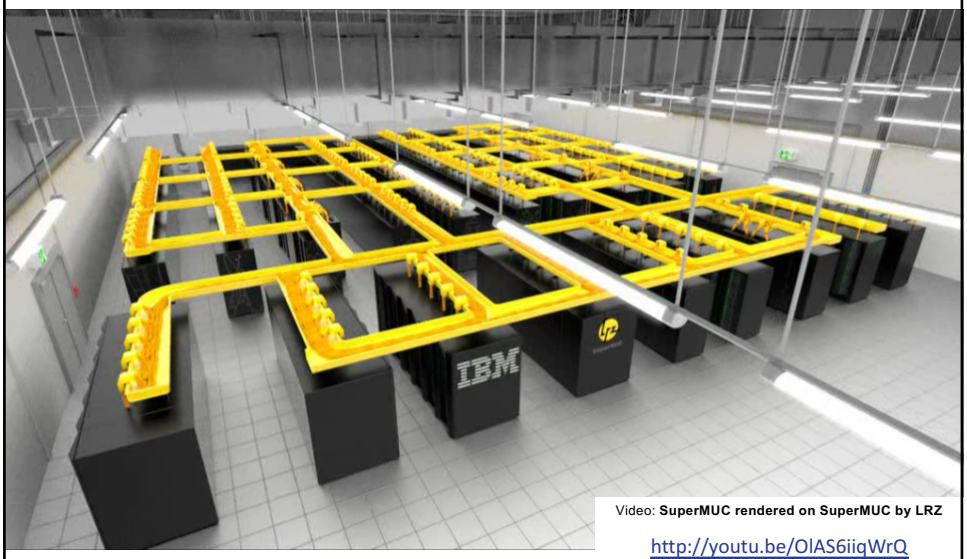
Dr. Christian Pelties, Department of Earth and Environmental Sciences (LMU)
Prof. Michael Bader, Department of Informatics (TUM)



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)

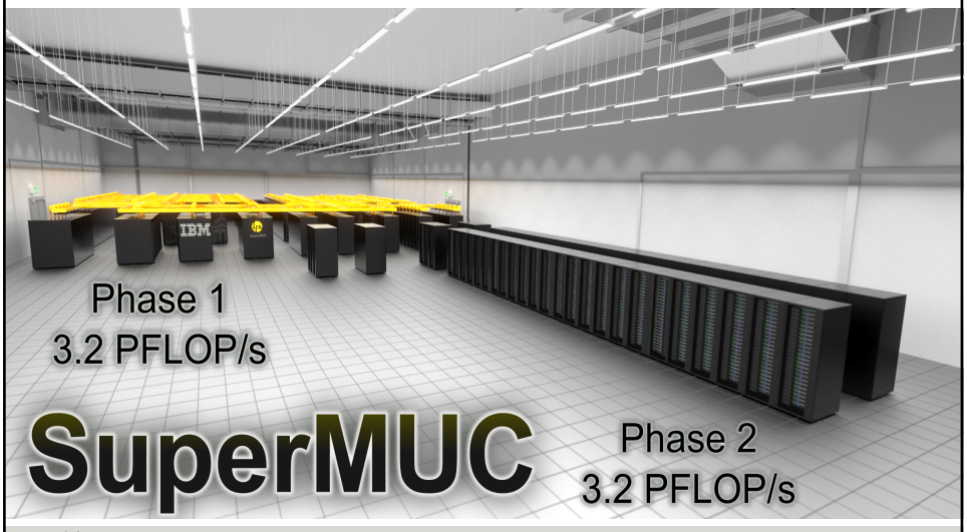
SuperMUC @ LRZ



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

http://youtu.be/OlAS6iiqWrQ

SuperMUC Phase 1 + 2



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
2015	SuperMUC Phase II	3.2 + 3.6 Pflop/s	229960

Leibniz Supercomputing Centre
of the Bavarian Academy of Sciences and Humanities

With approx. 230 employees
for more than 100.000 students and
for more than 30.000 employees
including 8.500 scientists

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

Photo: Ernst Graf

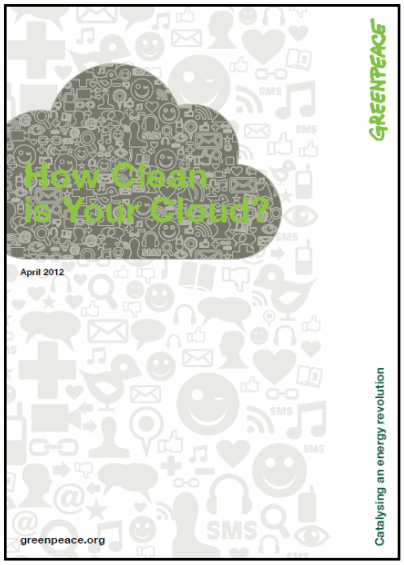
ICT and Global Warming

- CO2 emissions 2010 expected to be 30.6 Gigatons
  2010 is the year with the highest emissions to date

International Energy Agency

Picture © Flickr User johnb

Clean Energy Consumption?

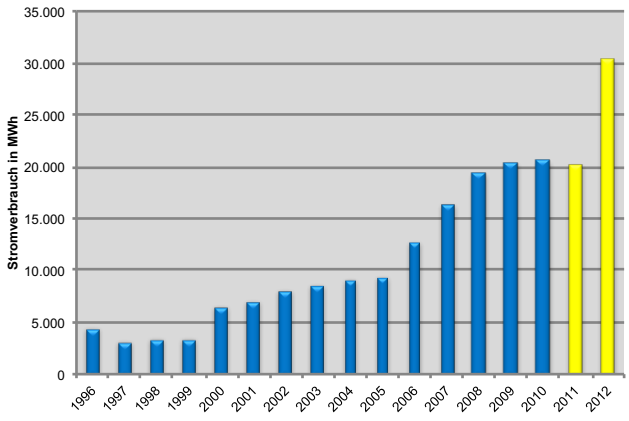


http://www.greenpeace.org/international/Global/international/publications/climate/2012/iCoal/HowCleanisYourCloud.pdf

ICT and Global Warming

- 2-3% of the world wide CO2 emissions from computing centres
  U.S. Department of Energy
- Energy consumption 2008 in Germany: 616,6 TWh
- Energy consumption in HPC & Data Centres: 10,1 TWh
  ➔ approx. 1.6% - 6.4 Millionen Tonnen CO2
  Bundesministerium für Wirtschaft und Technologie
- ICT of fundamental importance for measuring and optimizing energy efficiency in all areas, including ICT
  Stephan Scholz, CTO Nokia Siemens Networks

Power Consumption at LRZ



Energy Consumption and CO2

- Driving from LRZ Garching to HLRS Stuttgart: 230 km with my little Audi (average consumption: 6,7 l Diesel/100 km)

➔ 40,8 kg CO2-Emission

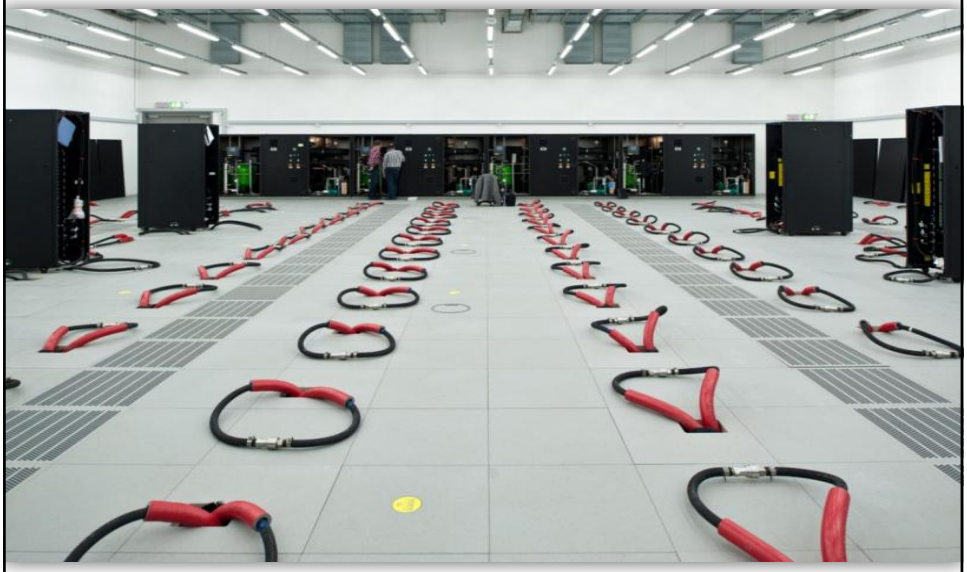
(177,50 g/km)
http://www.dekra-online.de/co2/co2_rechner.html

- Average power consumption of SuperMUC: 3 MWatt / hour

➔ ca. 1605 kg CO2/Std

(1 kWh Power 2015: approx. 535 g/kWh)
http://www.umweltbundesamt.de/themen/klima-energie/energieversorgung/strom-waermeversorgung-in-zahlen?sprungmarke=Strommix

Cooling SuperMUC



SuperMUC Phase 2 @ LRZ

Photos: Torsten Bloth, Lenovo

High Energy Efficiency

- ✓ Usage of Intel Xeon E5 2697v3 processors
- ✓ Direct liquid cooling
  - 10% power advantage over air cooled system
  - 25% power advantage due to chiller-less cooling
- ✓ Energy-aware scheduling
  - 6% power advantage
  - ~40% power advantage
  - Total annual savings of ~2 Mio. € for SuperMUC Phase 1 and 2

Conclusions

- **Energy Efficiency** is an important aspect to maximize scientific throughput
- Efficient computational science needs to be an integral part of teaching domain scientists
  - Learn how to get access to HPC infrastructures and use them efficiently
  - Learn how to program HPC infrastructures with increasing complexity, heterogeneity and scalability – efficiency, reliability, portabiliy
- The LRZ Partnership Initiative Computational Science (piCS) tries to improve user support

http://www.sciencedirect.com/science/article/pii/S1877050914003433

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

Challenges on Extreme Scale Systems

- Size: number of cores > 100.000
- Complexity/Heterogeneity
- Reliability/Resilience
- Energy consumption as part of Total Cost of Ownership (TCO)
  - Execute codes with optimal power consumption (or within a certain power band) ➔ Frequency scaling
  - Optimize for energy-to-solution ➔ Allow more codes within given budget
  - Improved performance ➔ (in most cases) improved energy-to-solution

1st LRZ Extreme Scale Workshop

- July 2013:

  1st LRZ 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

1st 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

Extreme Scaling Continued

- Lessons learned ➔ Stability and scalability
- 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
- 2nd LRZ Extreme Scaling Workshop ➔ 2-5 June 2014
  - Full system production runs on 18 islands with sustained Pflop/s (4h SeisSol, 7h Gadget)
  - 4 existing + 6 additional full system applications
  - High I/O bandwidth in user space possible (66 GB/s of 200 GB/s max)
  - Important goal: minimize energy*runtime (3-15 W/core)
- 3rd Extreme Scale-Out with new SuperMUC Phase 2

Extreme Scale-Out SuperMUC Phase 2

- 12 May – 12 June 2015 (30 days)
- Selected Group of Early Users

- Nightly Operation: general queue max 3 islands
- Daytime Operation: special queue max 6 islands (full system)

- Total available: 63,432,000 core hours
- Total used: 43,758,430 core hours (Utilisation: 68.98%)

Lessons learned (2015):

- Preparation is everything
- Finding Heisenbugs is difficult
- MPI is at its limits
- Hybrid (MPI+OpenMP) is the way to go
- I/O libraries getting even more important

4th Extreme Scale Workshop 2016

- 4 Day Workshop (29 February – 3 March 2016)
- 13 Projects:

	Application	Field	Institution	PI
1	INDEXA	CDF	TU München	M. Kronbichler
2	MPAS	Climate Science	KIT	D. Heinzeller
3	Inhouse	Material Science	TU Dresden	F. Ortmann
4	HemeLB	Life Science	UC London	P. Coveney
5	KPM	Chemistry	FAU Erlangen	M. Kreutzer
6	SWIFT	Cosmology	U Durham	M. Schaller
7	LISO	CFD	TU Darmstadt	S. Kraheberger
8	ILDBC	Lattice Boltzmann	FAU Erlangen	M. Wittmann
9	Walberla	Lattice Boltzmann	FAU Erlangen	Ch. Godenschwager
10	GASPI	Framework	ITWM Kaiserslautern	M. Kühn
11	GADGET	Cosmology	LMU München	K. Dolag
12	VERTEX	Astrophysics	MPI for Astrophysics	T. Melson
13	PSC	Plasma	LMU München	K. Bamberg

- 147,456 cores in 9216 Nodes
- 14.1 Mio CPUh
- Max Time per Job 6h
- Daily and nightly operation mode

VERTEX: Simulation Code for Supernove Explosions (plasma + neutrino dynamics)

A. Marek and Team (Max Planck-Institute for Astrophysics, Garching)

SuperMUC System @ LRZ

Phase 1 (IBM System x iDataPlex):

- 3.2 PFlops peak performance
- 9216 IBM iDataPlex dx360M4 nodes in 18 compute node islands
- 2 Intel Xeon E5-2680 processors and 32 GB of memory per compute node
- 147,456 compute cores
- Network Infiniband FDR10 (fat tree)

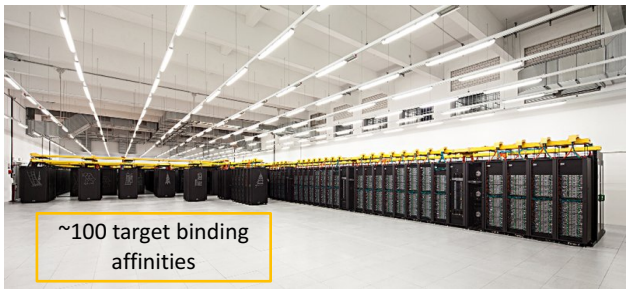
Phase 2 (Lenovo NeXtScale WCT):

- 3.6 PFlops peak performance
- 3072 Lenovo NeXtScale nx360M5 WCT nodes in 6 compute node islands
- 2 Intel Xeon E5-2697v3 processors and 64 GB of memory per compute node
- 86,016 compute cores
- Network Infiniband FDR14 (fat tree)

Common GPFS file systems with 10 PB and 5 PB usable storage size respectively
Common programming environment
Direct warm-water cooled system technology

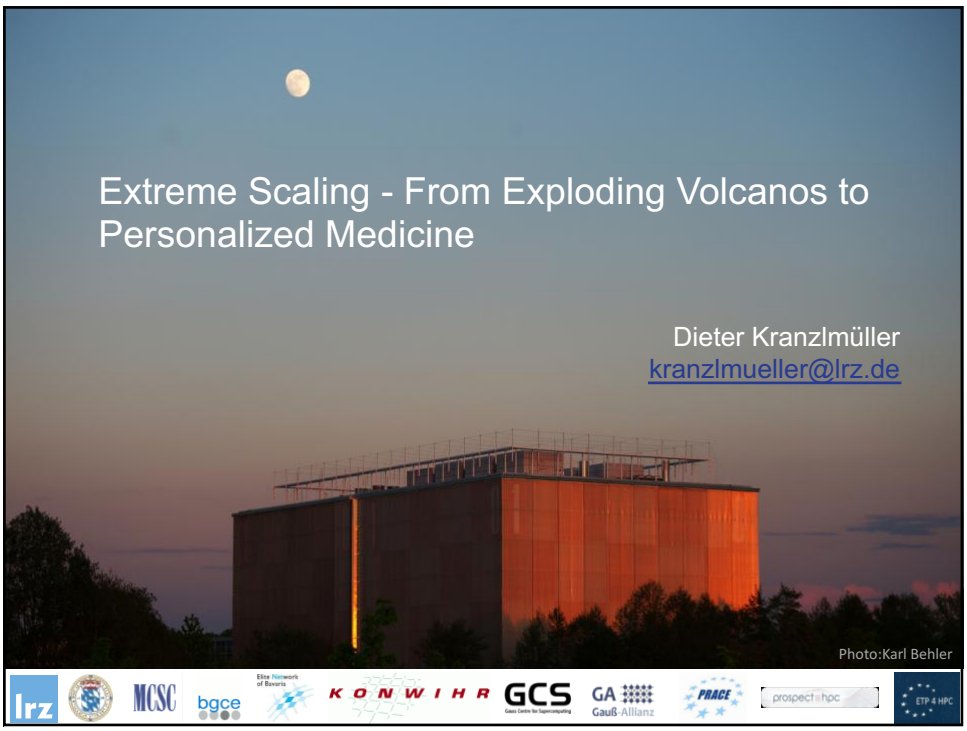
Molecular Simulation for Personalized Medicine

- Running on all cores of SuperMUC Phase1+2



- Docking simulation of potentials drugs for breast cancer
- 37 hours total run time
- 241,672 cores
- 8.900.000 CPU hours
- 5 Terabytes of data produced

EU Projects COMPAT and MAPPER
http://www.compat-project.eu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