Introduction to
High Performance Computing

Content

W

What is High Performance Computing?
What makes it different?
What are people doing on High Performance Computers?
Which possibilities exist to access HPC-Systems?
Which systems do exist in Kaiserslautern?
Which jobs are available for HPC-Specialists?

Content

H

How do HPC systems look like?
How to access HPC facilities?
How to work on HPC systems?
How to run HPC jobs on supercomputers?

Introduction

Overview of

- supercomputers,
- application arrays,
- components,
- why they are so exciting,
- future developments.

Definitionen

Hochleistungsrechnen (englisch: *high-performance computing* – **HPC**) ist ein Bereich des computergestützten Rechnens. Er umfasst alle Rechenarbeiten, deren Bearbeitung einer hohen Rechenleistung oder Speicherkapazität bedarf.

[...], dass Rechenanwendungen, deren Komplexität oder Umfang eine Berechnung auf einfachen Arbeitsplatzrechnern unmöglich oder zumindest unsinnig macht, in den Bereich des Hochleistungsrechnens fallen.
Hochleistungsrechnen wird vor allem durch die auf parallele Verarbeitung ausgerichtete Architektur von Hochleistungsrechnern überhaupt erst möglich. [...]

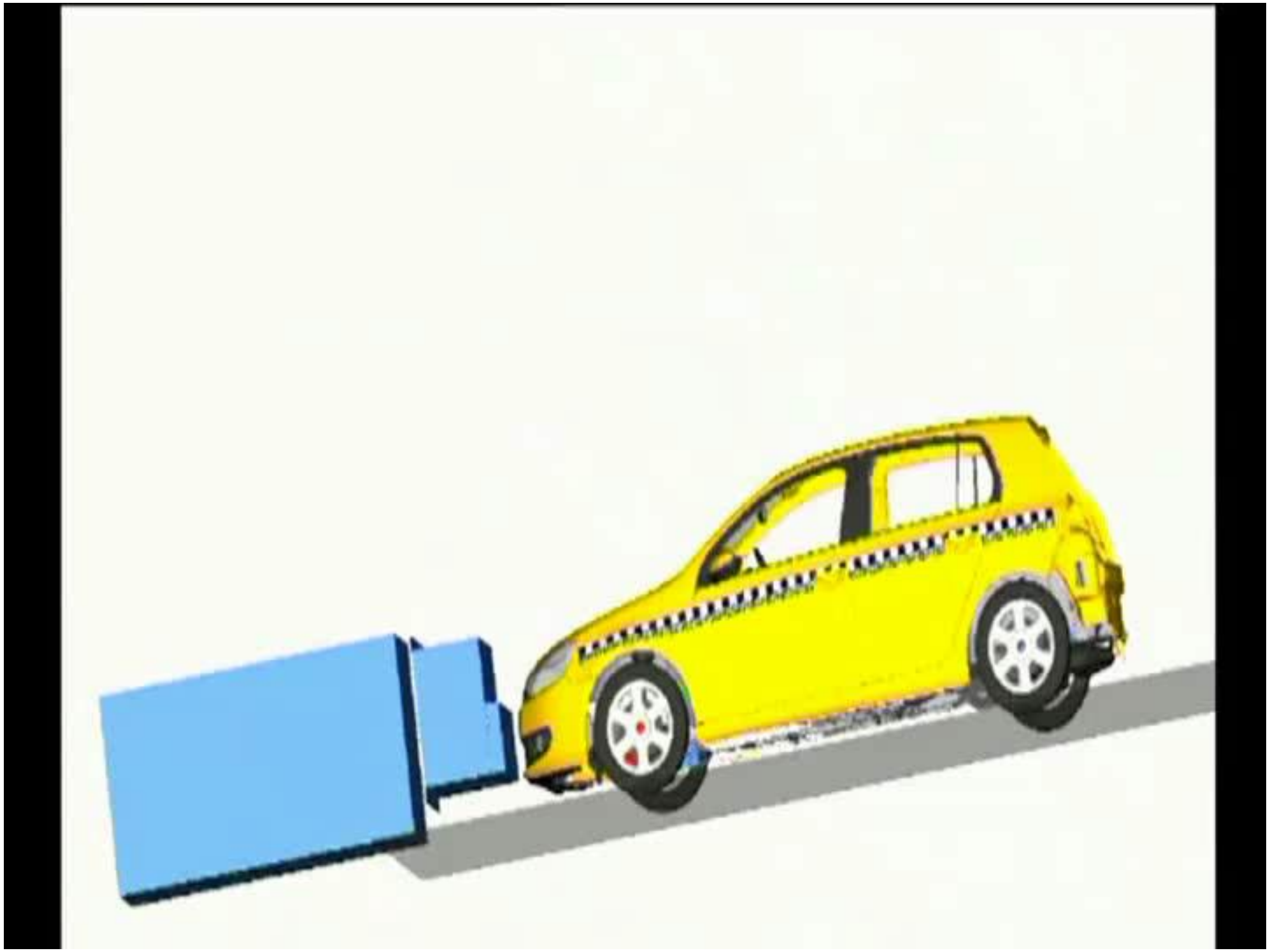
Why do we need HPC?

Bundesministerium
für Bildung
und Forschung

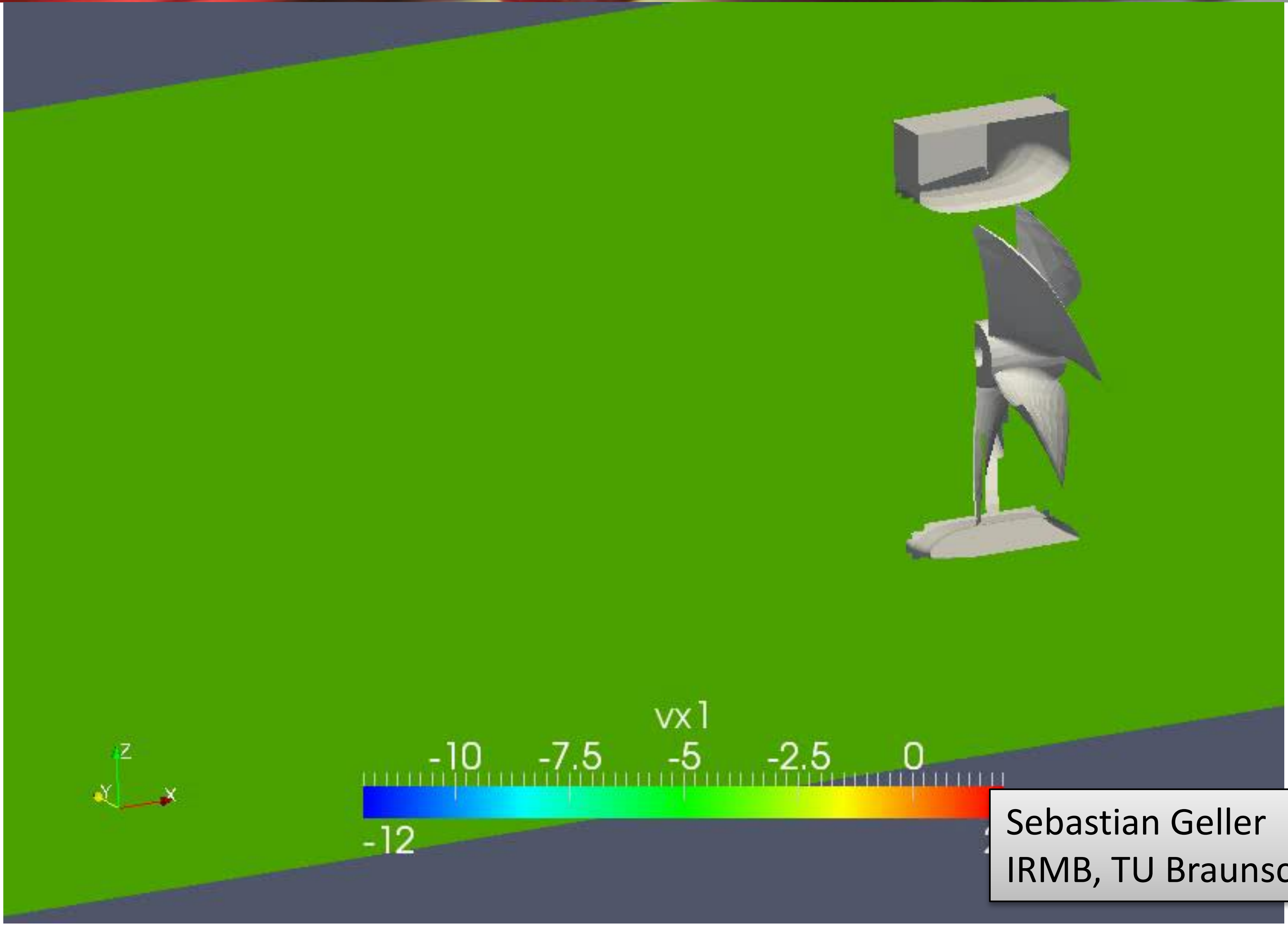
Um die gegenwärtigen Menschheitsaufgaben nachhaltig zu lösen, brauchen wir in der Forschung neben Theorien und Experimenten ausgefeilte Simulationen mit leistungsstarken Supercomputern. […] Mit ihren Berechnungen legen die Computer die Grundlagen für neue Produkte, Verfahren und Dienstleistungen.

Die Säulen des Supercomputing, BMBF 2011.

Crash Tests



Propeller



Sebastian Geller
IRMB, TU Braunschweig

Fastest Computers

Rank	Name	Country	Year	Cores	Acc Cores	Rmax	Power	Mflops/Watt
1	Tianhe-2	China	2013	3120000	2736000	33862700	17808	1901,54
2	Titan	United States	2012	560640	261632	17590000	8209	2142,77
3	Sequoia	United States	2011	1572864	0	17173224	7890	2176,58
4	K Computer	Japan	2011	705024	0	10510000	12659,9	830,18
5	Mira	United States	2012	786432	0	8586612	3945	2176,58
6	Trinity	United States	2015	301056	0	8100900	11079	731,19
7	Piz Daint	Switzerland	2012	115984	73808	6271000	2325	2697,2
8	Hazel Hen	Germany	2015	185088	0	5640170	3200	1763
9	Shaheen II	Saudi Arabia	2015	196608	0	5536990	2834	1953,77
10	Stampede	United States	2012	462462	366366	5168110	4510	1145,92
11	JUQUEEN	Germany	2012	458752	0	5008857	2301	2176,82
12	Vulcan	United States	2012	393216	0	4293306	1972	2177,13
13	Pleiades	United States	2011	185344	0	4089430	3380	1209,89
14	Abel	United States	2015	145920	0	4042460	1800	2245,81
15		United States	2015	72800	62400	3577000	1498,9	2386,42

Fastest Computers

Rang	Name	Land	Architektur	Peak	Eff.	Power	GFlops/W
1	Titan	USA	+ GPUs	27 PFlops	65 %	8,2 MW	2,14
2	Sequoia	USA	BlueGene	20 PFlops	81 %	7,9 MW	2,07
3	K Computer	Japan	SPARC64	11 PFlops	93 %	12,7 MW	0,83
4	Mira	USA	BlueGene	10 PFlops	81 %	3,9 MW	2,07
5	Juqueen	D	BlueGene	5,0 PFlops	82 %	1,9 MW	2,10
6	SuperMUC	D		3,2 PFlops	91 %	3,4 MW	0,85
7	Stampede	USA	+ Phi	4,0 PFlops	67 %	k.A.	k.A.
8	Tianhe-1A	China	+ GPUs	4,7 PFlops	55 %	4,0 MW	0,64
9	Fermi	Italien	BlueGene	2,1 PFlops	82 %	0,8 MW	2,10
10	DARPA	USA		1,9 PFlops	78 %	3,6 MW	0,42

Fastest in Germany

Jülich

München

Gauss Centre for Supercomputing

GCS
Gauss Centre for Supercomputing

HPC in Germany

Gauss Centre for Supercomputing

RWTH Aachen	HLRN (Berlin, Hannover)
ZIH Dresden	Deutscher Wetterdienst
Max-Planck-Ges.	Deutsches Klimarechenzentrum
SCC Karlsruhe	CE Darmstadt
Desy Hamburg	Rechenzentrum Erlangen
PC2 Paderborn	ZDV Mainz
CSC Frankfurt	GWDG Göttingen
Rechenzentrum Köln	

HPC in Europe

- foundet in 2010
- Grid-Infrastructure with high bandwidth
- 24 countries
- investment:
  - Germany
  - France
  - Italy
  - Spain
  - …

TU Kaiserslautern

Elwetritsch

Part I, 2012

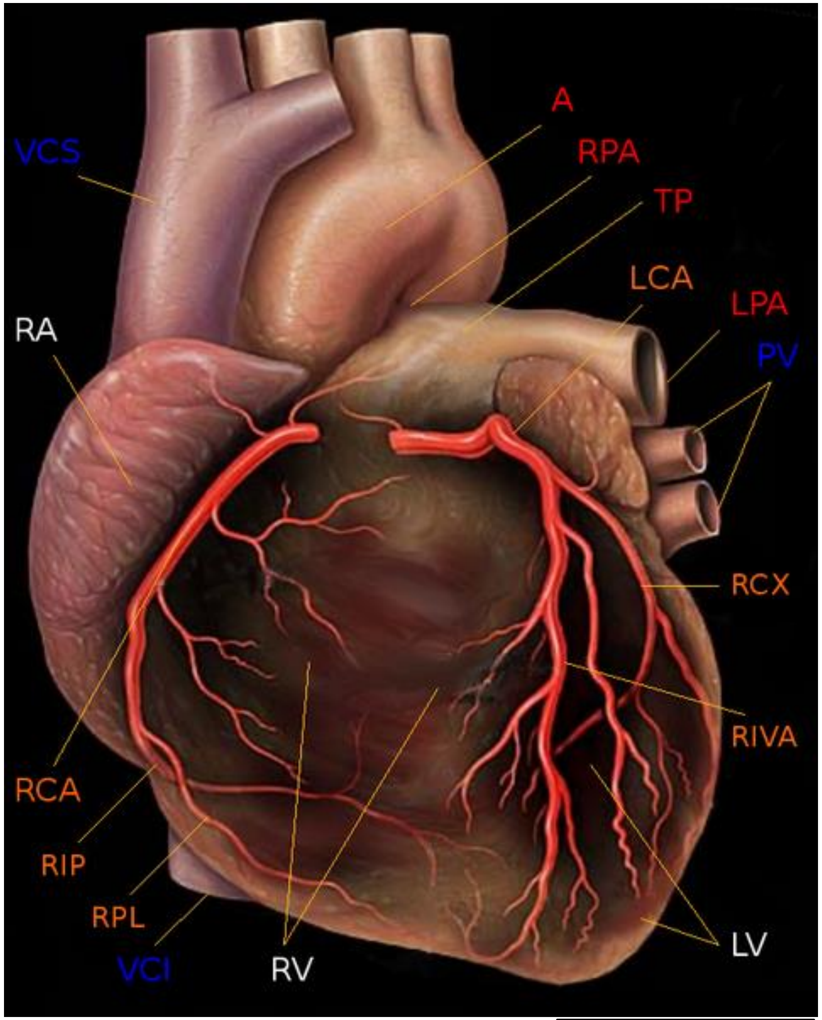
- 186 nodes
- 2944 cores

TU Kaiserslautern

Part II, 2014
- 135 nodes
- 2160 cores

Part III, 2016
- 144 nodes
- 2112 cores

Introductory Example



Quelle: Wikipedia

Which vessels require a bypass?

Location of vulnerable pieces?

- eddy induced stagnation
- danger of a thrombose
- decision before surgery

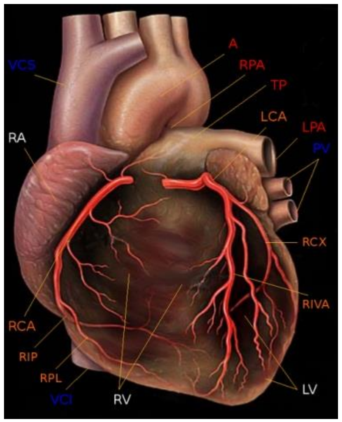
Geometry of coronary arteries from a tomogramm

Blood flow simulation

Blood flow in coronary vessels

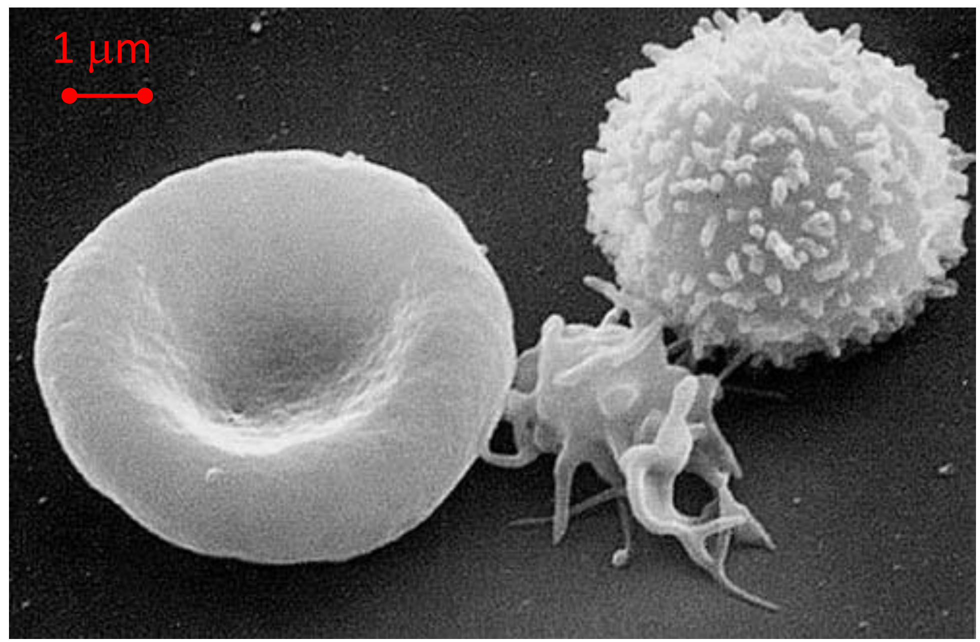
„Blut ist ein ganz besonderer Saft“

Goethe, Faust



Blood flow simulation

- simulation domain several centimeters
- dissolved particles in blood are very small
- resolution requires several billions of grid cells



From left to right:
Erythrozyt, Thrombozyt and Leukozyt

Quelle: Wikipedia

Blood flow in coronary vessels

- Simulation time requires a computer capable of 10^{15} operations per second
- CPUs spend 50% of their time handling communications (message passing)
- 4000 Graphical Processing Units with more than 1,7 Mill. of ALUs
- Effectivity of simulation: 80%

Quelle: Grinberg et al., SC11, 2011

Blood flow in coronary vessels

- Simulation time requires a computer capable of 10^{15} operations per second
  - In 10-20 years large specialized hospitals are capable to perform associated simulations before a surgery.
  - In 40-50 years this omputational power will available in Desktops and associated simulations are common praxis.

Quelle: Grinberg et al., SC11, 2011

Blood flow in coronary vessels

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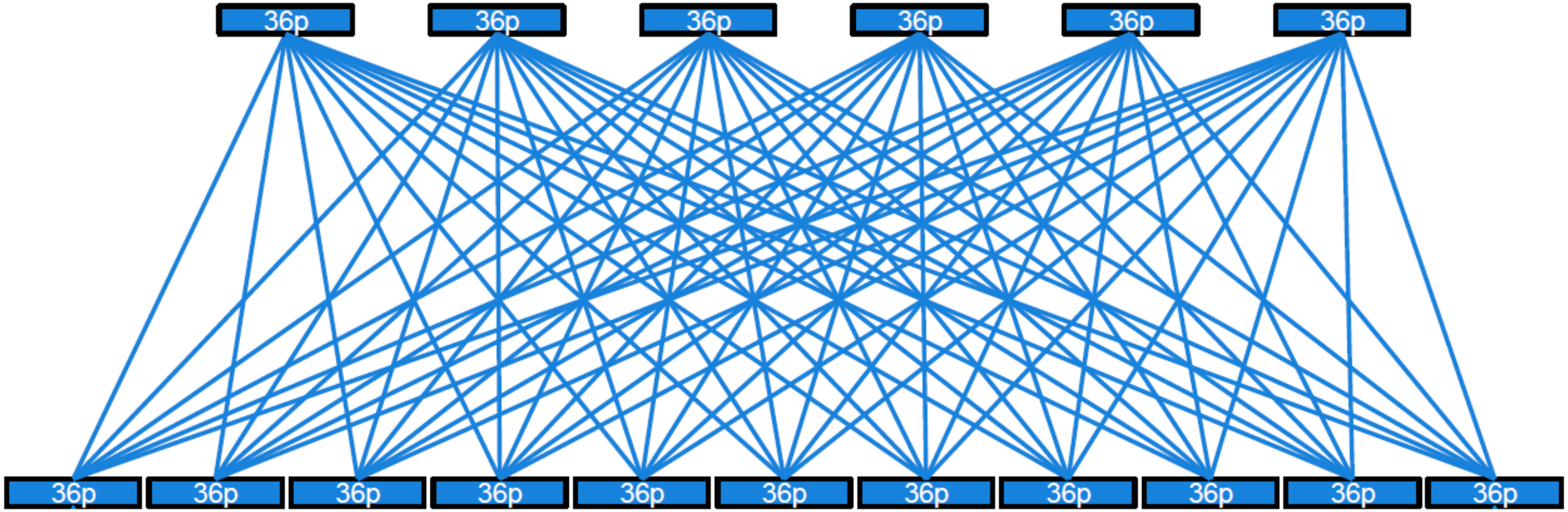
One send takes appr. 76 μ sec with 570 MB/s bandwidth
Calculating a single number from partial sums over all processes: 675 μsec

Quelle: Grinberg et al., SC11, 2011

Networks

An effective bandwidth of 570 MB/s (4.5 Gb/s) for a send of a message between two processes simultaneously to a send between all other pairs means a bandwidth of **2400 GB/s** (19,200 Gb/s) in total.



Networks

Calculating a single number from partial sums over all processes: 675 µsec

- The supercomputer may add 675 billions of numbers in 675 µsec
- This addition from 4000 processes must be effective
  - linear dependency would mean, each process gets max. 169nsec
  - light travels in 169nsec appr. 50 m – the wires in a computing center a longer!

Highest requirements on network technology.
Highest requirements on communication software.

Networks

Networks are an issue

- bandwidth of a single connection
- aggregate bandwidth
- topology of connections
- time for short messages

Blood flow in coronary vessels

- Simulation time requires a computer capable of 10^{15} operations per second
- CPUs spend 50% of their time handling communications (message passing)
- 4000 Graphical Processing Units with more than 1,7 Mill. of ALUs

Massively parallel
At everery time 1,7 Mill. operations may be executed simultaneously
Graphical Processing Units (GPUs) instead of CPUs

Lecture in winter term

Quelle: Grinberg et al., SC11, 2011

Around HPC

Grid Technology

- Computing power from the socket
- Grid and Cloud
- Computing power, storage as a service, software as a service

GRIDCORE

SABALCORE
[WHERE DATA BECOMES DISCOVERY]

amazon web services

Future

Sustainability

- Software control of resources and their power consumption

- Green Hosting – website hosting based on sun and wind energy

- Ranking of energy-efficient supercomputers

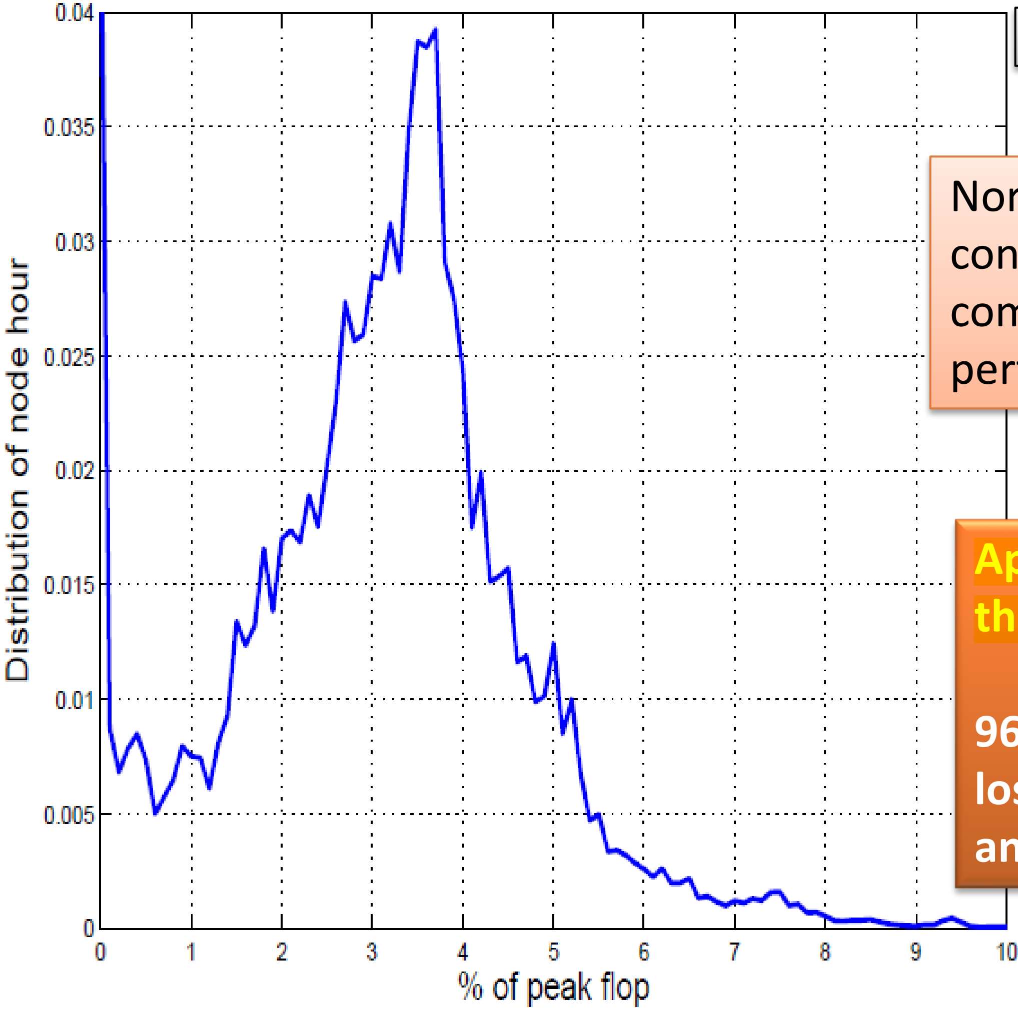
Future

By the end of this decade the Department of Energy of the United States requires exascale computing systems to satisfy critical national security mission requirements and to accelerate discovery science for the economic health of the Nation. [..]

Panel Discussion, SC11, Seattle 2011

Exascale: Next generation computer, capable of 10^{18} operations per second – as much as 3000 soccer field full of people with connected laptops.

Effectivity



Quelle: Vento et al., SC11, 2011

Normed distribution of the consumed processor performance compared to their peak performance.

Applications use in most cases less than 4% of the peak performance.

96% of the power consumption is lost by poor programming style and languages.

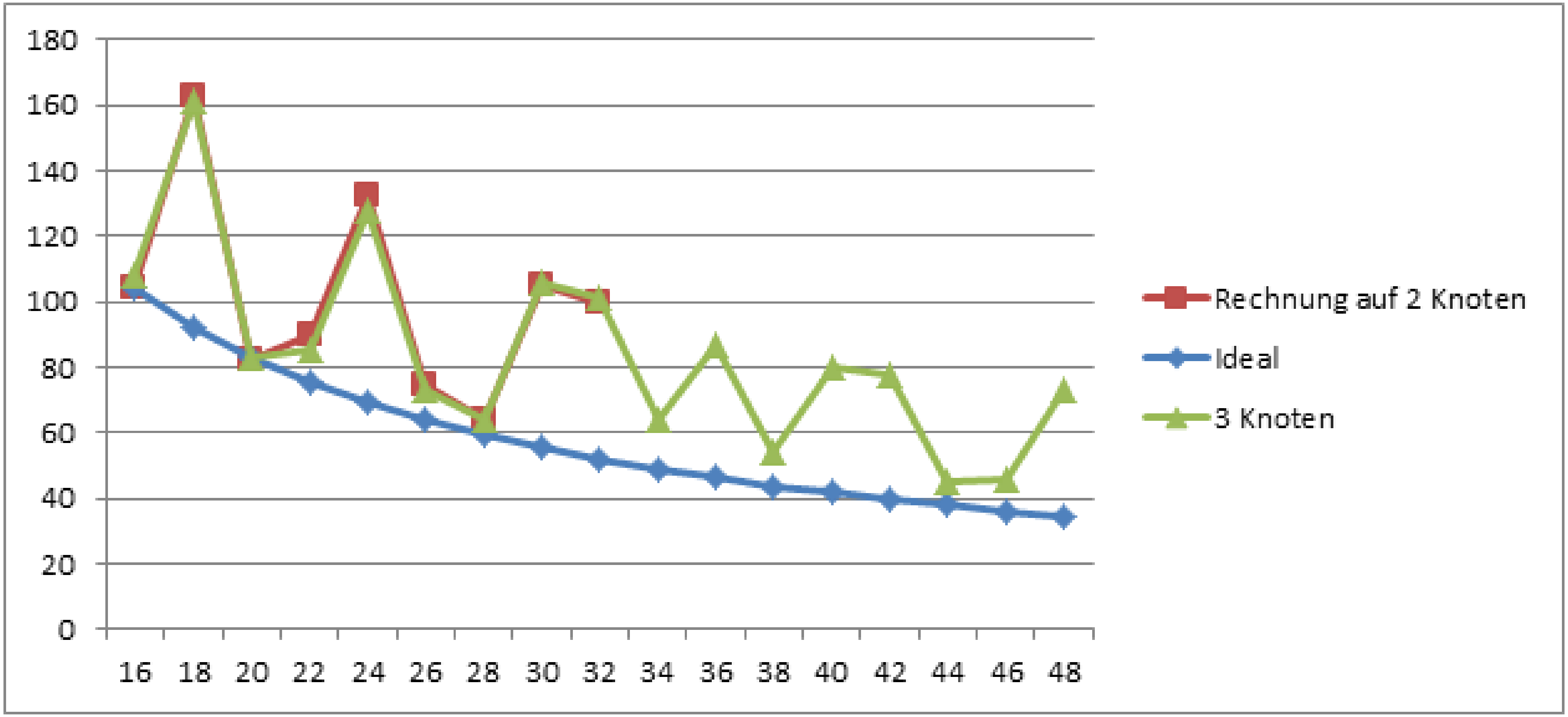
Energy awareness

Profile of the parallel execution

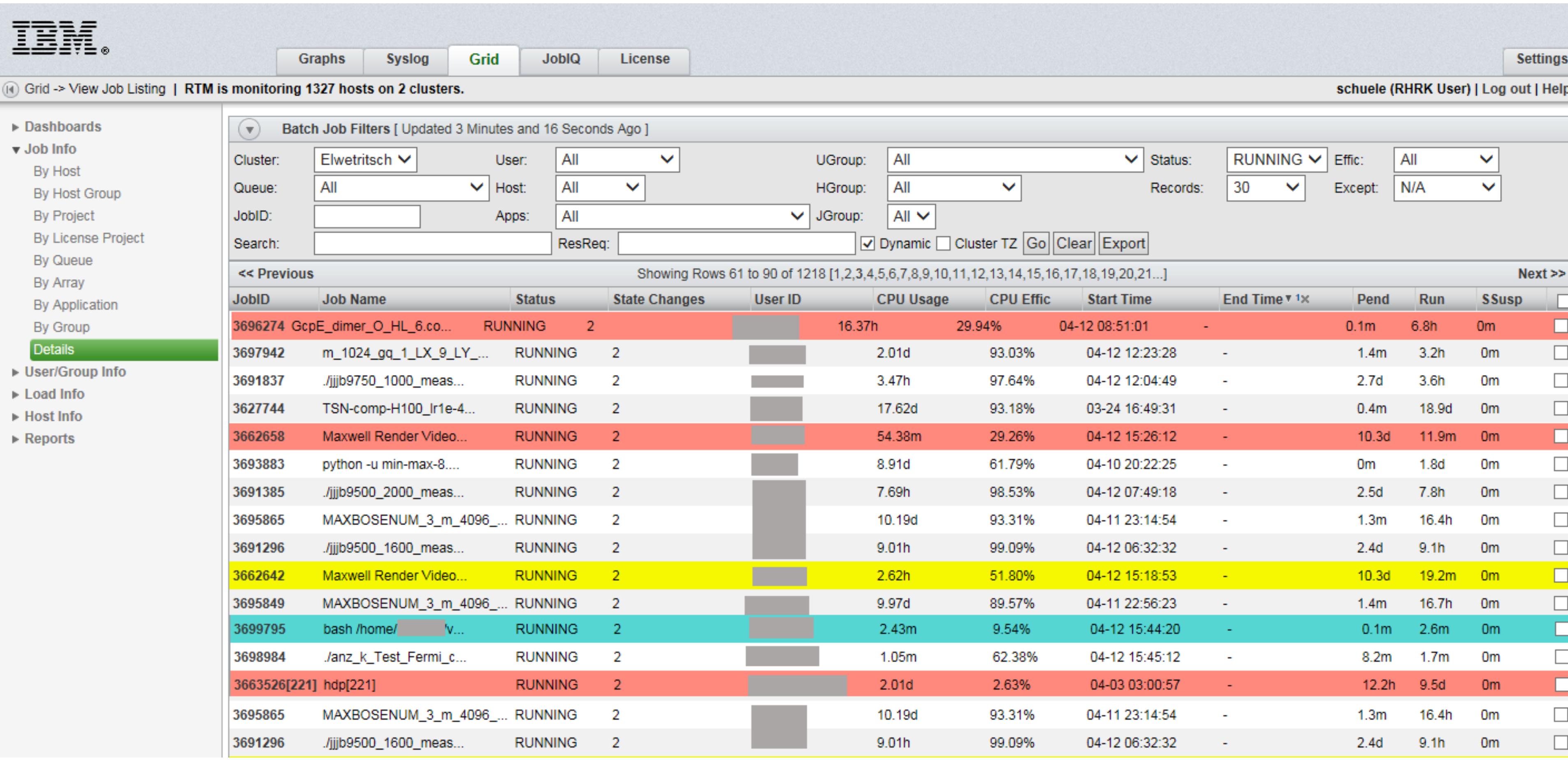
Finished last
All others wait for processor 8

Vampirtrace

Scalability



HPC - Elwetritsch



JobID	Job Name	Status	State Changes	User ID	CPU Usage	CPU Effic	Start Time	End Time	Pend	Run	SSusp
3696274	GcpE_dimer_O_HL_6.co...	RUNNING	2		16.37h	29.94%	04-12 08:51:01	-	0.1m	6.8h	0m
3697942	m_1024_gq_1_LX_9_LY_...	RUNNING	2		2.01d	93.03%	04-12 12:23:28	-	1.4m	3.2h	0m
3691837	./jjjb9750_1000_meas...	RUNNING	2		3.47h	97.64%	04-12 12:04:49	-	2.7d	3.6h	0m
3627744	TSN-comp-H100_lr1e-4...	RUNNING	2		17.62d	93.18%	03-24 16:49:31	-	0.4m	18.9d	0m
3662658	Maxwell Render Video...	RUNNING	2		54.38m	29.26%	04-12 15:26:12	-	10.3d	11.9m	0m
3693883	python -u min-max-8....	RUNNING	2		8.91d	61.79%	04-10 20:22:25	-	0m	1.8d	0m
3691385	./jjjb9500_2000_meas...	RUNNING	2		7.69h	98.53%	04-12 07:49:18	-	2.5d	7.8h	0m
3695865	MAXBOSENUM_3_m_4096_...	RUNNING	2		10.19d	93.31%	04-11 23:14:54	-	1.3m	16.4h	0m
3691296	./jjjb9500_1600_meas...	RUNNING	2		9.01h	99.09%	04-12 06:32:32	-	2.4d	9.1h	0m
3662642	Maxwell Render Video...	RUNNING	2		2.62h	51.80%	04-12 15:18:53	-	10.3d	19.2m	0m
3695849	MAXBOSENUM_3_m_4096_...	RUNNING	2		9.97d	89.57%	04-11 22:56:23	-	1.4m	16.7h	0m
3699795	bash /home/ v...	RUNNING	2		2.43m	9.54%	04-12 15:44:20	-	0.1m	2.6m	0m
3698984	./anz_k_Test_Fermi_c...	RUNNING	2		1.05m	62.38%	04-12 15:45:12	-	8.2m	1.7m	0m
3663526[221]	hdp[221]	RUNNING	2		2.01d	2.63%	04-03 03:00:57	-	12.2h	9.5d	0m
3695865	MAXBOSENUM_3_m_4096_...	RUNNING	2		10.19d	93.31%	04-11 23:14:54	-	1.3m	16.4h	0m
3691296	./jjjb9500_1600_meas...	RUNNING	2		9.01h	99.09%	04-12 06:32:32	-	2.4d	9.1h	0m

RTM Monitoring, Cluster Elwetritsch

HPC - Elwetritsch

GcpE_dimer_O_HL_6.co...	16.37h	29.94%	0.1m	6.8h
m_1024_gq_1_LX_9_LY_...	2.01d	93.03%	1.4m	3.2h
./jjjb9750_1000_meas...	3.47h	97.64%	2.7d	3.6h
TSN-comp-H100_lr1e-4...	17.62d	93.18%	0.4m	18.9d
Maxwell Render Video...	54.38m	29.26%	10.3d	11.9m
python -u min-max-8....	8.91d	61.79%	0m	1.8d
./jjjb9500_2000_meas...	7.69h	98.53%	2.5d	7.8h
MAXBOSENUM_3_m_4096_...	10.19d	93.31%	1.3m	16.4h
./jjjb9500_1600_meas...	9.01h	99.09%	2.4d	9.1h
Maxwell Render Video...	2.62h	51.80%	10.3d	19.2m
MAXBOSENUM_3_m_4096_...	9.97d	89.57%	1.4m	16.7h
bash /home/[redacted]/v...	2.43m	9.54%	0.1m	2.6m
./anz_k_Test_Fermi_c...	1.05m	62.38%	8.2m	1.7m
hdp[221]	2.01d	2.63%	12.2h	9.5d
MAXBOSENUM_3_m_4096_...	10.19d	93.31%	1.3m	16.4h
./jjjb9500_1600_meas...	9.01h	99.09%	2.4d	9.1h

Parallelization rather poor. 8 cores use CPU only for 16.37h in real 6.8h – optimal would be 6.8*8=54.4h

Starting phase – running since 2.6 minutes

programing language - java

RTM Monitoring, Cluster Elwetritsch

Einführung in das Hochleistungsrechnen

Introduction to High Performance Computing

VIELEN DANK
THANK YOU