High Performance Computing at TUHH

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TUHH
Technische Universität Hamburg-Harburg

Outline

TUHH

Hamburg University of Technology

Key Figures:

- Located in Hamburg-Harburg
- Founded in 1978
- ~ 6.000 students,
  15 % thereof international students,
- 13 / 29 B.Sc. / M.Sc. courses
- ~ 1.100 employees
- Budget: ~110 Mio. Euro,
  41 Mio thereof third-party funded

TUHH

Focus in teaching:

- all major engineering sciences

Focus in research:

- Energy and environment
- Biotechnology
- Medical engineering
- Maritime Systems and off-shore properties
- Aeronautical Engineering

HPC usage and users

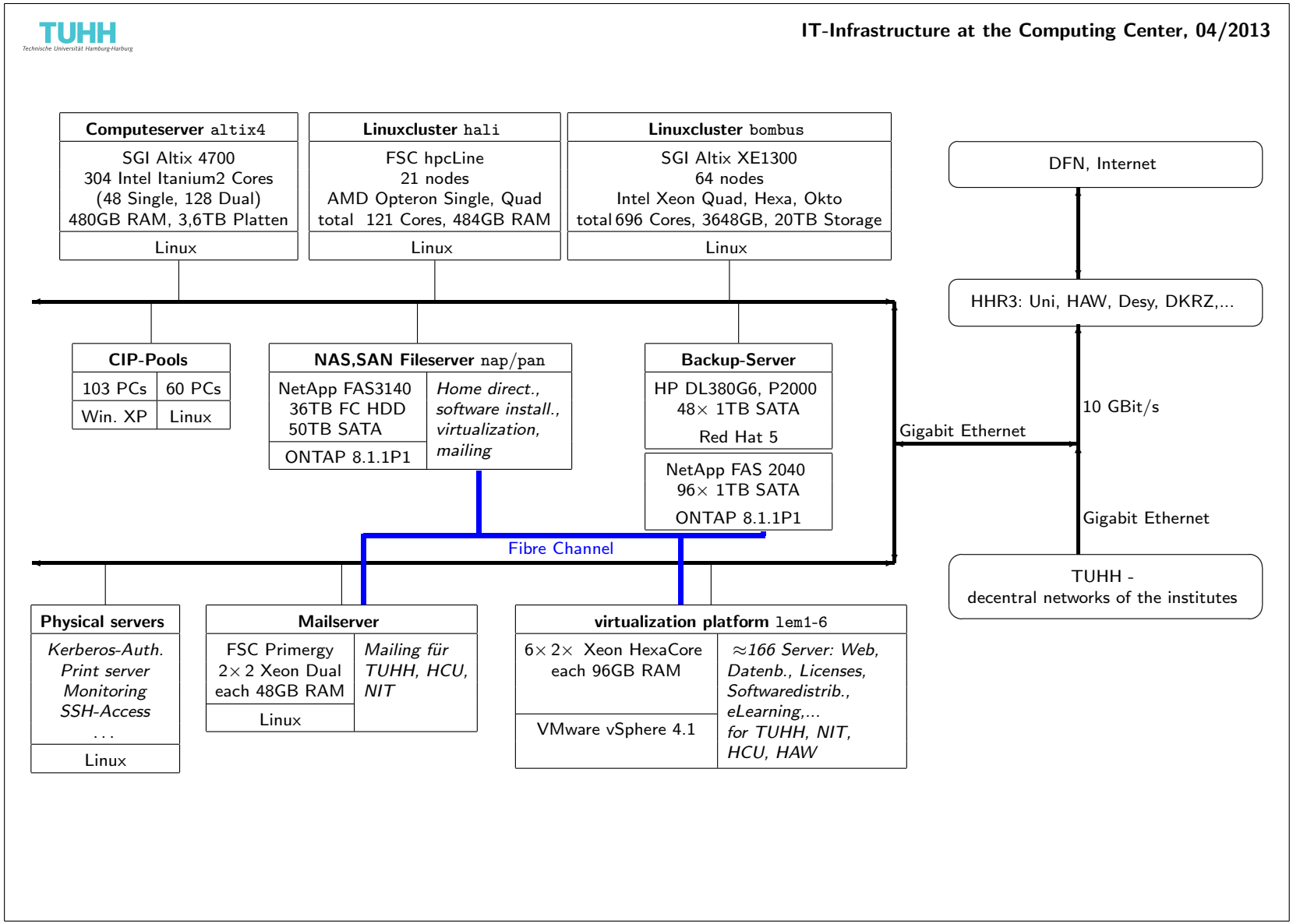
Characteristics of HPC at TUHH

- very inhomogeneous usage
- mainly commercial and open-source software packages
- little self-developed software

currently mainly in

- Chemistry (VASP, TurboMole, Gaussian)
- Fluid dynamics (OpenFOAM)
- Mechanical Engineering (Abaqus)
- Nanoelectronics (Comsol)

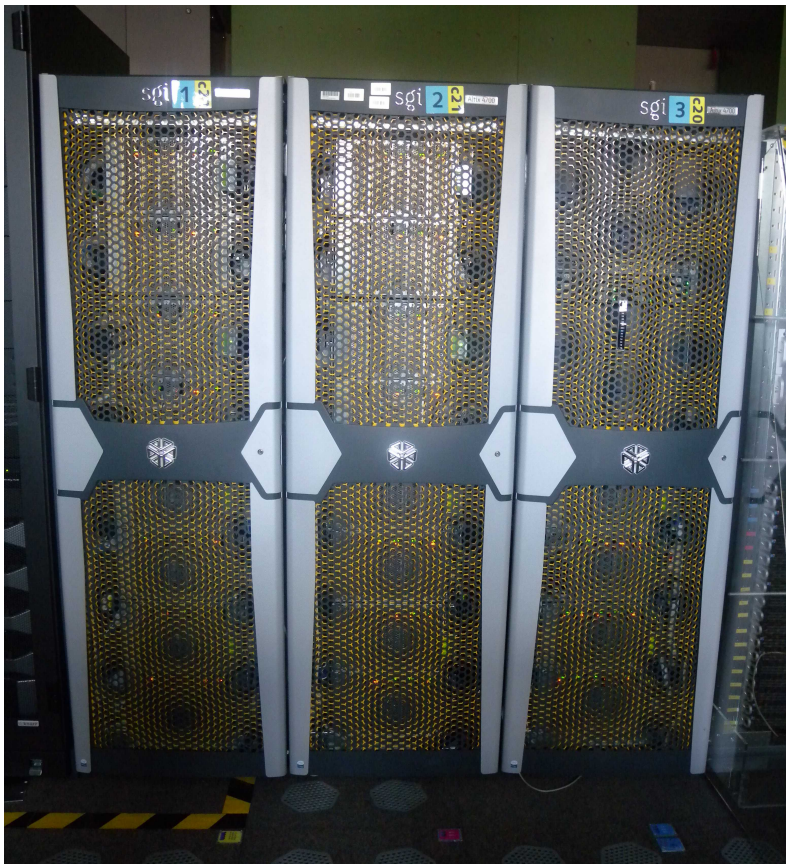
General IT-Infrastructure



Altix 4700

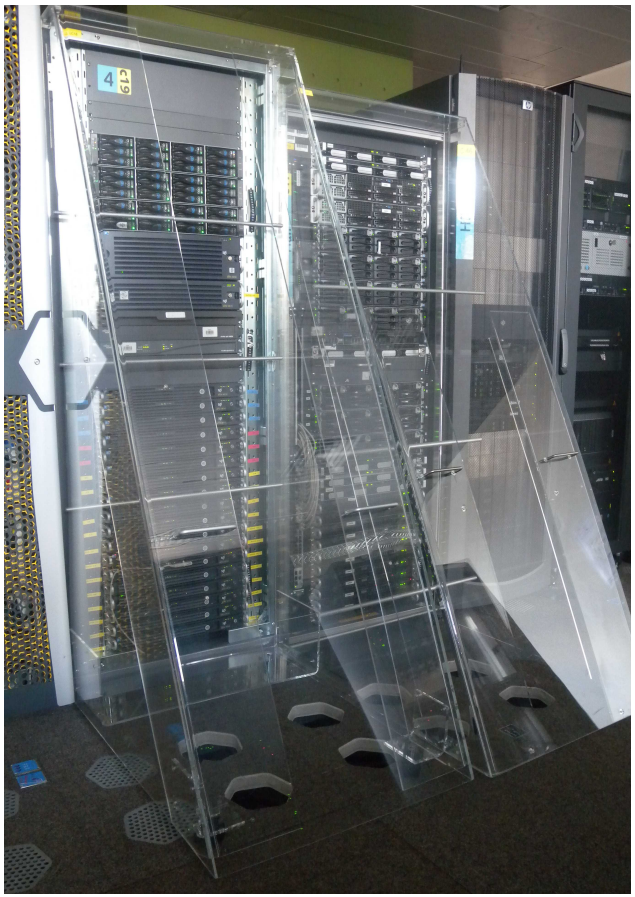
SMP machine **`altix`**: Still used for quantum chemistry calculations

- 304 cores on 176 processors
- 480 GB RAM
- 3,6 TB Storage system
- NUMA Interconnect
- Suse Linux Enterprise 10



Linux-Cluster

Linux Cluster **bombus** / **hali**: General purpose HPC cluster



- 800 cores on 164 processors on 80 compute nodes
- 3,5 TB RAM
- Local storage on SATA disks
- Ethernet Interconnect
- Red Hat Linux Enterprise 5 / 6

Central HPC Storage on File server

- NFS connected
- 20 TB Storage for I/O intensive applications

Software configuration

- Current Linux System on local hard disks
- Application software provided via NFS
- Modules
- Batch system: PBS Pro
- Data handling: home directories, local hard disks, scratchspace
- Monitoring: Ganglia, Spong

Common workflow for the users of the HPC systems

Graphical preprocessing on local workstation

⇓

Login to the HPC systems (via ssh/putty)
and copy input files (via scp/WinSCP)

⇓

Check current status of batch systems with qstat (when indicated)

⇓

Submit job by qsub

⇓

Check performance or characteristics of running job on compute nodes
(when indicated)

⇓

Receive mail when job is finished and fetch results (via scp/WinSCP)

⇓

Graphical postprocessing on local workstation

Planned Systems

Planned Infiniband-Cluster at the TUHH computing center

- Currently in review process at DFG
- Installation planned in two phases in 2013/2015.

Architecture:

- 152 dual-socket compute nodes
- 128 / 256 GB RAM on each node
- Infiniband QDR and Gigabit Ethernet interconnect
- Local storage on 500GB SATA disks
- 3 File servers and 1 Meta-data server for Fraunhofer Parallel Cluster File System

Ansys

Most common Ansys license features available at TUHH:

- `aa_t_a`
- `aa_r_cfd`
- `aa_r`
- `aa_r_hpc`
- some more features for meshers, pre & post processing and special solvers

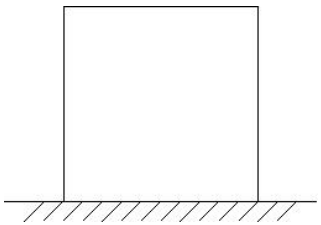
mostly used by

- Institut für Fluiddynamik und Schiffstheorie
- Institut für Konstruktion und Festigkeit von Schiffen
- Institut für Baustoffe, Bauphysik und Bauchemie

General observed properties of Ansys:

- Ansys is CPU- and I/O-bound
- For CFD simulations, Ansys (Fluent) scales well

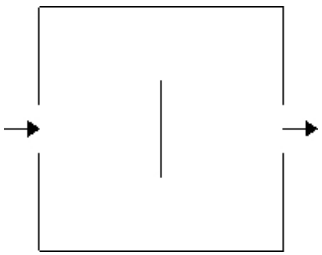
Benchmark I: Ansys (Mechanical)



- eigenfrequency analysis of a two-dimensional square
- discretization: 1 million dof
- test machines: two-socket servers with Intel Octo Core, SandyBridge CPUs

Cores	Machines	Wallclock Time	Efficiency
1	1	100%	100%
2	1	82%	61%
4	1	63%	40%
8	1	50%	25%
16	1	42%	15%
32	2	31%	10%

Benchmark II: Ansys (CFD)



- stationary air flow inside a two-dimensional square
- discretization: 1 million dof
- test machines: two-socket servers with Intel Octo Core, SandyBridge CPUs

Cores	Machines	Wallclock Time	Efficiency
1	1	100	100%
2	1	51%	98%
4	1	26%	95%
16	1	7.4%	85%
32	2	4.0%	77%
64	4	2.2%	70%

Thank you for your attention !