

Introduction to High-Performance Computing

Session 01

Organization

Introduction to HPC

but before we begin...

Course Organisation

Contact Information

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Course Organisation

Monday	Tuesday	Wednesday
10:15 – 11:15 (SH) Introduction to HPC	10:15 – 11:15 (WT) Introduction to Parallel Programming	10:15 – 11:15 (SH) Introduction to Matlab Distributed Computing (MDCS)
11:30 – 13:00 (WT) Basic Cluster Usage	11:30 – 13:00 (WT) Introduction to OpenMp	11:30 – 13:00 (SH) Parallel Programming in Matlab
13:45 – 15:15 (SH) HPC Environment	13:45 – 15:15 (SH) Introduction to OpenMP	13:45 – 15:15 (SH) Parallel Programming in Matlab
15:30 – 17:00 (SH) Advanced Cluster Usage	15:30 – 17:00 (SH) Performance Optimization	

- times will probably change
- lectures and practical parts (on your own)
- slides and files for practical parts will be available in the Wiki, see https://wiki.hpcuser.uni-oldenburg.de/index.php?title=HPC_Introduction

Hands-on Sessions

- we will be using the local HPC clusters CARL and EDDY
- if you don't have an account yet go to <http://www.uni-oldenburg.de/fk5/wr/>
 - there are useful links to request an account and also to the HPC wiki which is the central resource for information
 - if you are not a member of a research group you can choose “student” (can be changed later if needed)

Introduction HPC

What is High-Performance Computing?

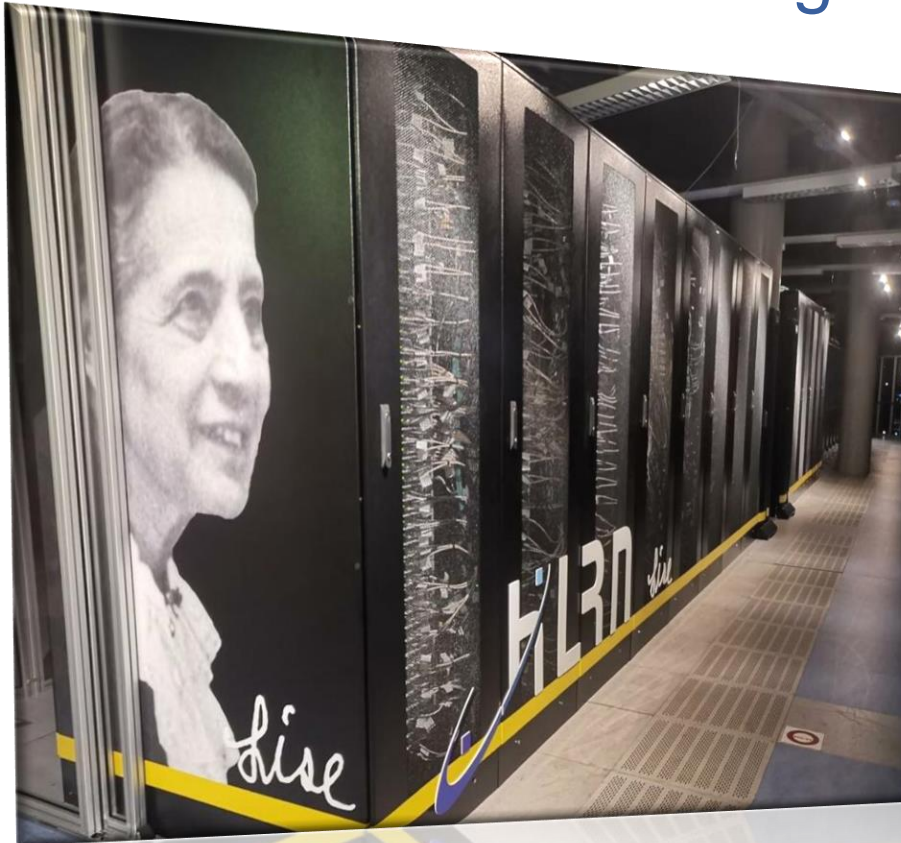
- possible answer:
 - if we ask google the first link says

“High Performance Computing most generally refers to the practice of aggregating computing power in a way that delivers much higher performance than one could get out of a typical desktop computer or workstation in order to solve large problems in science, engineering, or business.”

(<http://insidehpc.com/hpc-basic-training/what-is-hpc/>)

- in short: use a big computer (HPC cluster) to solve a big problem

What is High-Performance Computing?



Supercomputers [LISE](#) ([Lise Meitner](#)) and [EMMY](#) ([Emmy Noether](#)) @ [HLRN](#)
(ranked in places 55 and 47 in the [Top500](#) in [November 2020](#))

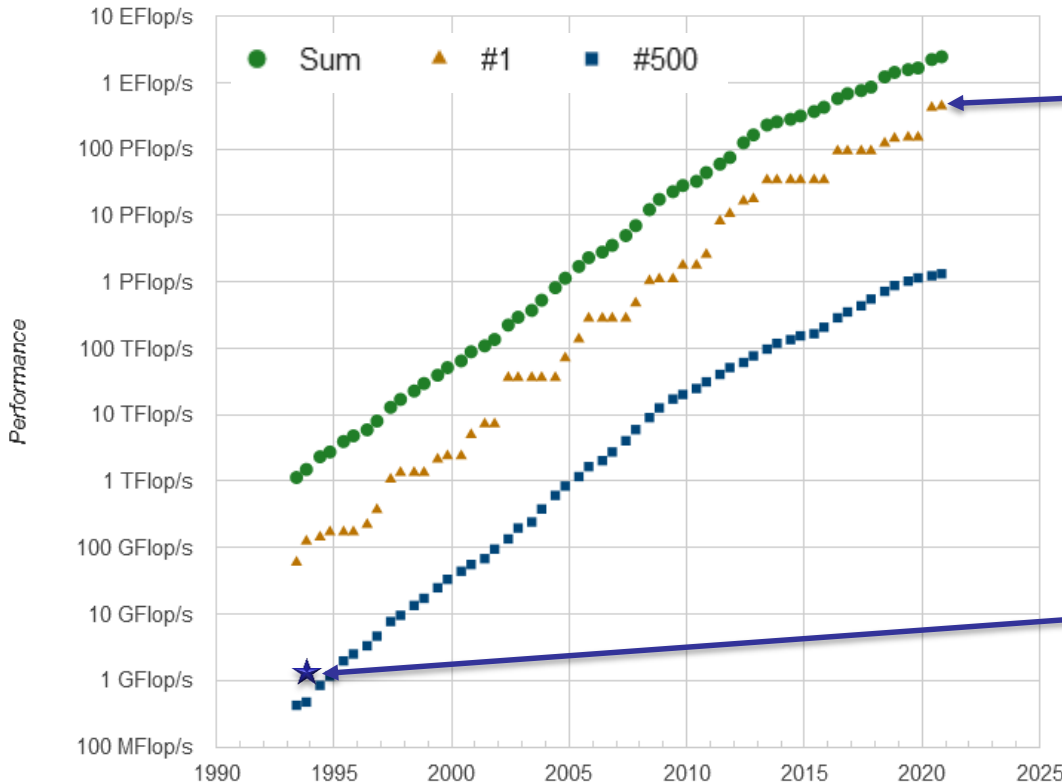
What is High-Performance Computing?

- another answer:
 - „computing at the bottleneck“ (from G. Hager @ RRZE, see <https://www.rrze.fau.de/dienste/arbeiten-rechnen/hpc/HPC4SE/>)
 - what is the optimal performance I can achieve on a single core or a multi-core processor?
 - what is the limiting factor? e.g. CPU-speed vs. memory access

High-Performance Computing (HPC)

- why HPC?
 - enables us to solve computationally intensive problems
- requirements
 - understanding of the used computational architecture
 - identification of computing bottlenecks
 - parallelization and optimization of algorithms
- typical HPC resources
 - HPC Cluster (e.g. CARL and EDDY)
 - Grid-Computing (distributed resources, e.g. SETI@home)
 - GPUs

The Fastest Computers on Earth



#1 November 2020: [Fugaku](https://www.fugaku.jp/)
RIKEN Center for Computational Science
(442 PFlop/s, 7.3M cores, A64FX 48C
2.2GHz, Tofu interconnect D)

Expected measured Peak Performance
Current Tablet \approx 1.5 Gflop/s
would have made it into the list in 1994

http://bits.blogs.nytimes.com/2011/05/09/the-ipad-in-your-hand-as-fast-as-a-supercomputer-of-yore/?_r=1

(taken from top500.org)

The End of Moore's Law?

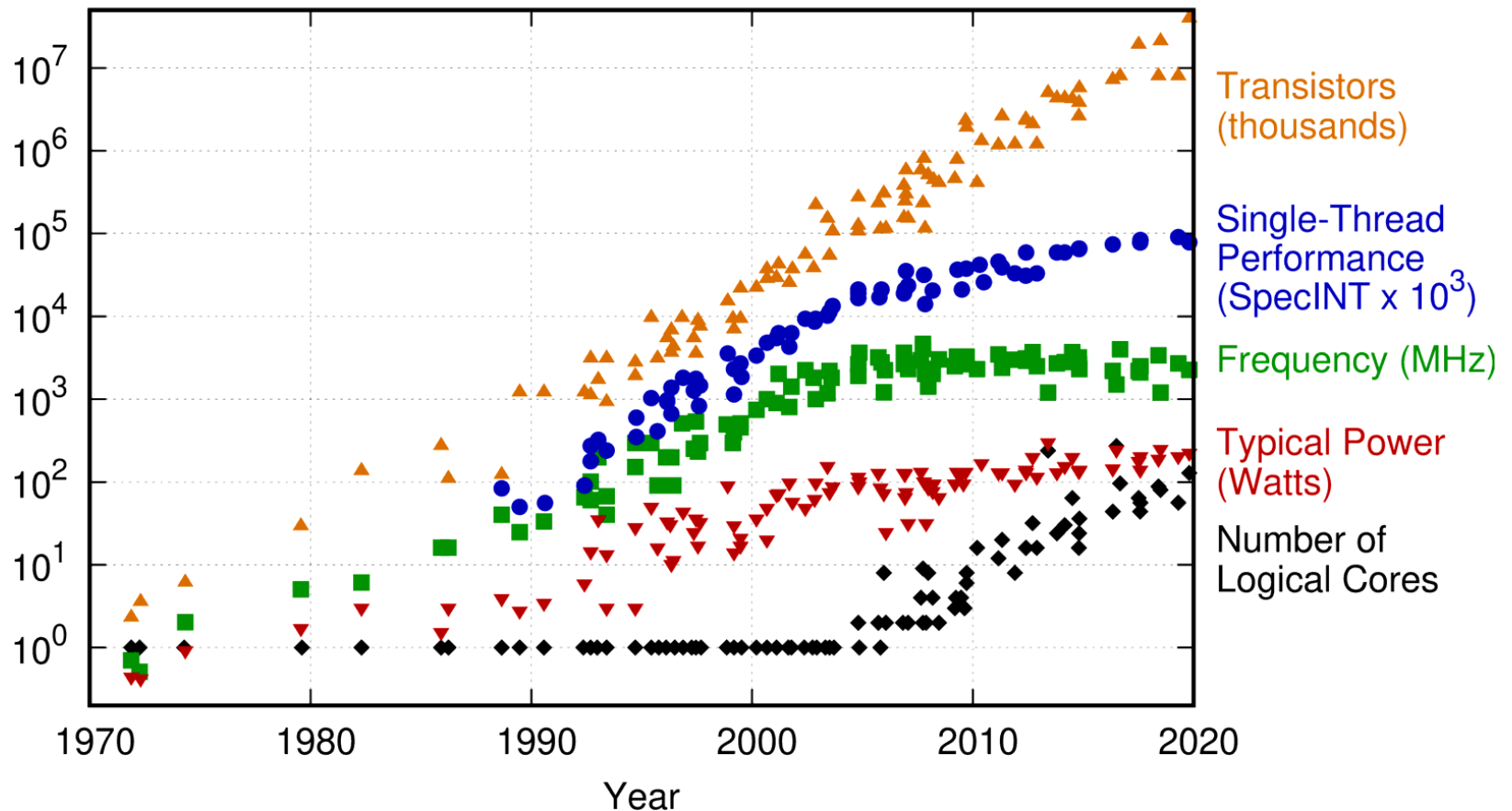
- see e.g. <http://www.nature.com/news/the-chips-are-down-for-moore-s-law-1.19338>
- it is probably not economic to shrink below a few nm
- what comes next?
 - not known yet but it will be interesting
 - one possible way is to go 3d, already seen in memory
 - quantum computer? see <https://singularityhub.com/2019/02/26/quantum-computing-now-and-in-the-not-too-distant-future> or <https://www.research.ibm.com/ibm-q/learn/what-is-quantum-computing/>

Parallelization

- parallelization is needed if the computational power of a single computer is not enough
 - distribution of data and/or work among several computers
 - different strategies depending on the problem at hand and also the available parallel architecture
 - parallel computing is very important today and will be more important in the future
 - modern PCs have multiple core CPUs → can be utilized by parallel applications

42 Years of Microprocessor Trend Data

<https://github.com/karlrupp/microprocessor-trend-data>



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2019 by K. Rupp

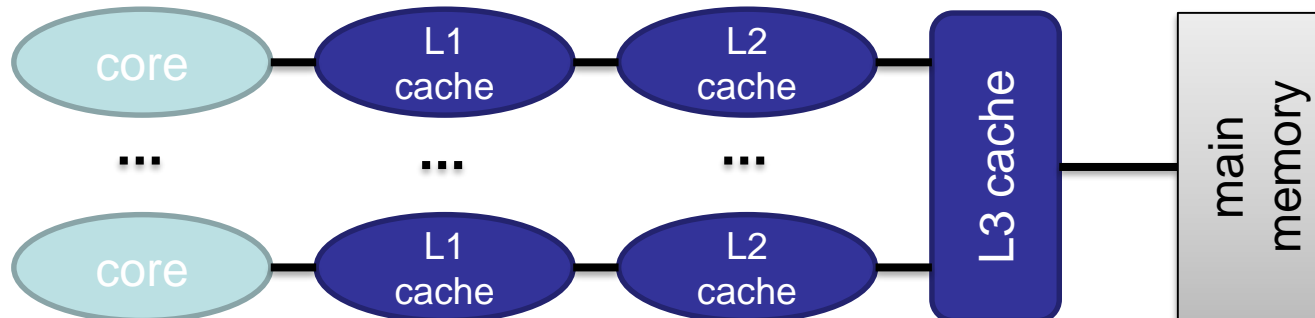
Parallel Architectures

- the knowledge of the underlying parallel architecture is important
 - allows to write more efficient code
 - avoid bottlenecks
 - understand the limiting factors for performance
- typical HPC cluster (e.g. CARL and EDDY)
 - multi-core CPU
 - multi-socket node
 - many nodes with node interconnect

Parallel Architectures

- multi-core CPU

- contains several cores (currently up to 48 or so)
- cores connected to caches for fast memory access, low latency (order of ten times faster than direct memory access)
- cache coherence



Broadwell
E5-2650

12 cores,
2.2GHz

64kB

256kB

30MB

Parallel Architectures

- how to **get** information about node architecture?
 - tools exist, e.g. hardware locality (hwloc) software, see example:

```
$ module load hwloc
$ hwloc-ls
Machine (255GB total)
  NUMANode L#0 (P#0 127GB)
    Package L#0 + L3 L#0 (30MB)
      L2 L#0 (256KB) + L1d L#0 (32KB) + L1i L#0 (32KB) + Core L#0
      L2 L#1 (256KB) + L1d L#1 (32KB) + L1i L#1 (32KB) + Core L#1
      ...
```

- how to **use** information about node architecture?
 - optimize cache usage
 - make decision about binding processes to cores

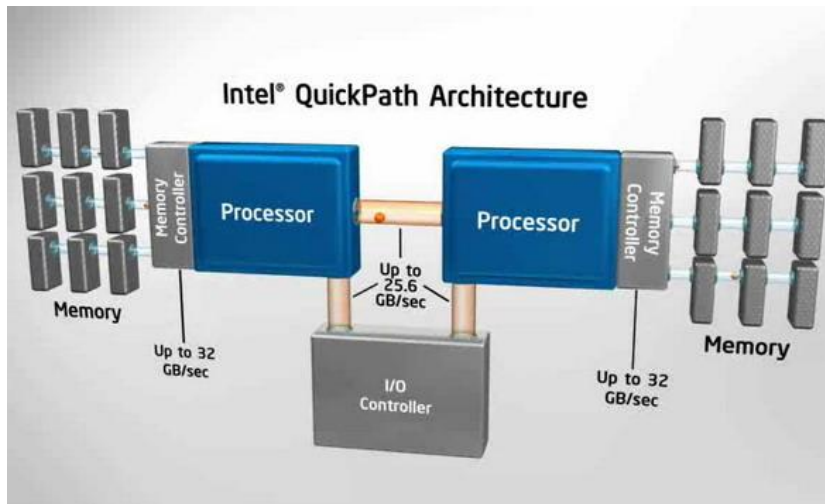
not trivial to do, best to rely on tested libraries and default settings, start to care when your application is slower than expected

Parallel Architectures

- multi-core CPU
 - number of cores increases, drives the performance increase
 - uniform memory access (UMA)
 - each core can execute single instructions on multiple data (SIMD), e.g. SSE, AVX, AVX2
 - clock frequency stagnates or even decreases (thermal effects)
 - computations can be limited by memory access (band width) or by the number of instructions per cycle

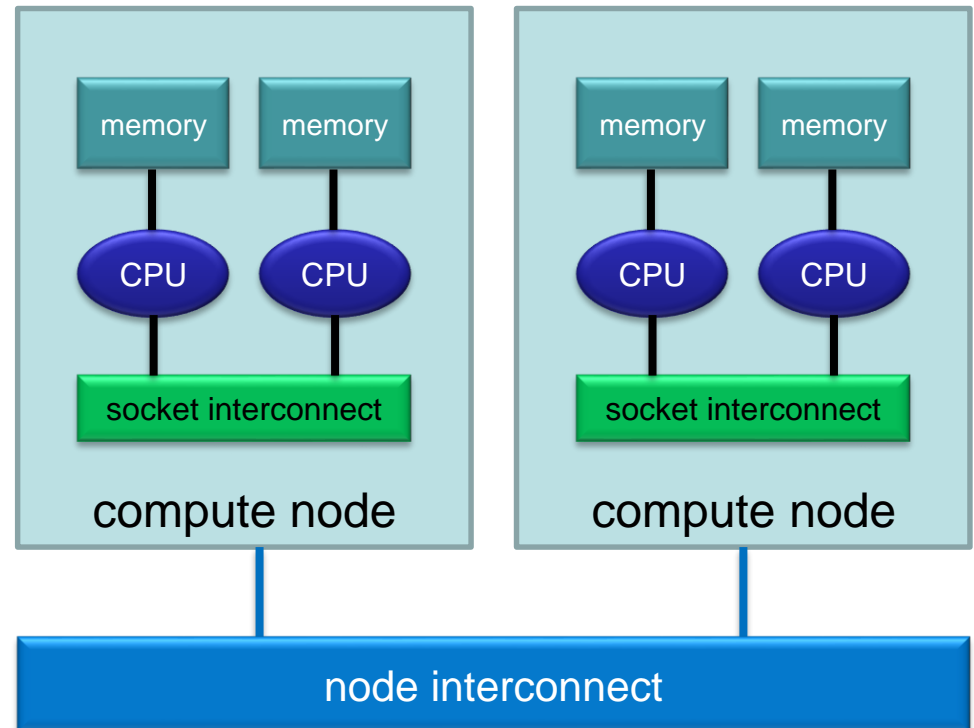
Parallel Architectures

- multi-socket node
 - several CPUs on a single main board
 - each CPU has access to its own main memory and cache levels
 - different, non-uniform memory access (NUMA)
 - with cache coherence → ccNUMA



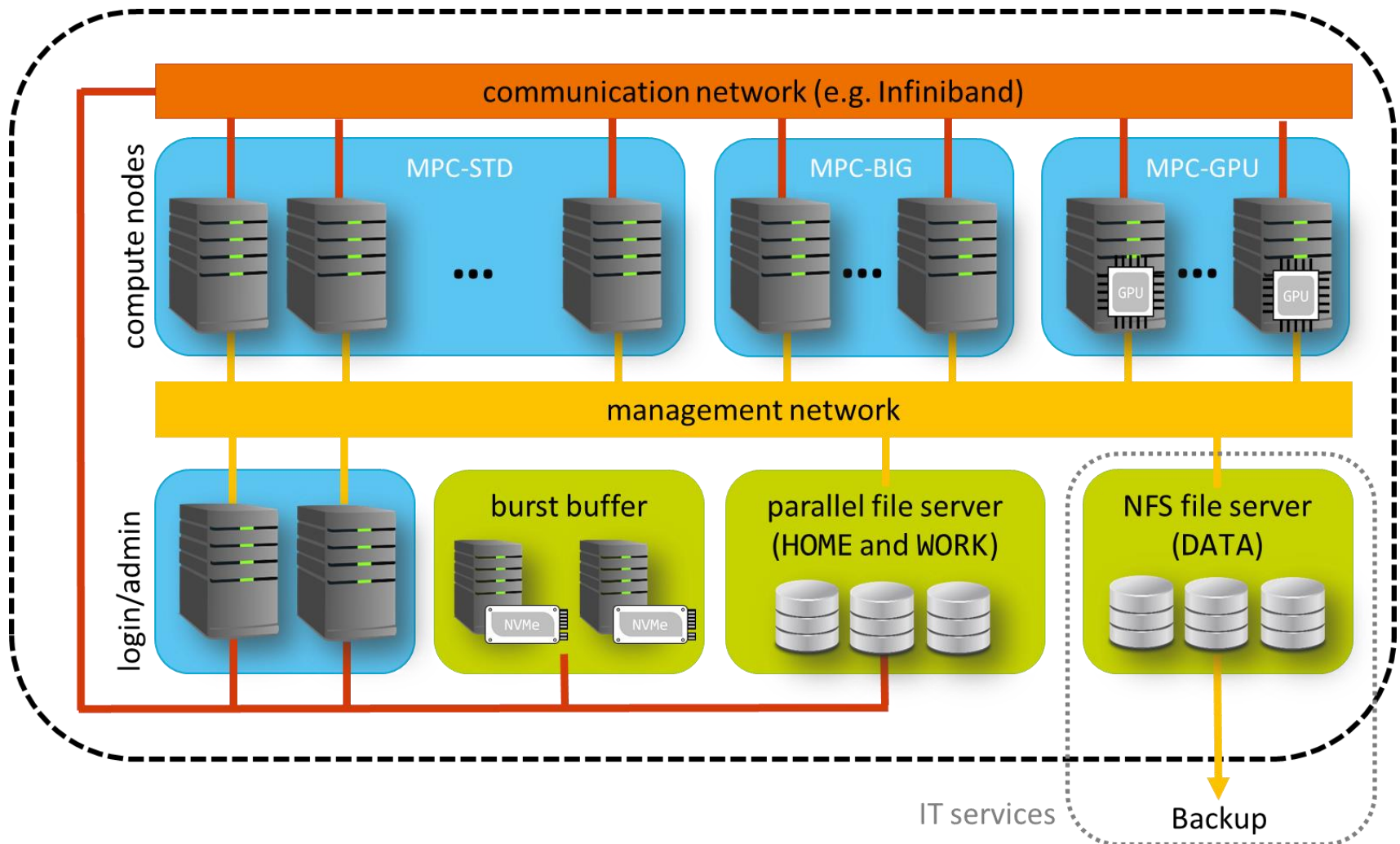
Parallel Architectures

- multi-computer
 - many (ccNUMA) nodes
 - distributed memory
 - node interconnect



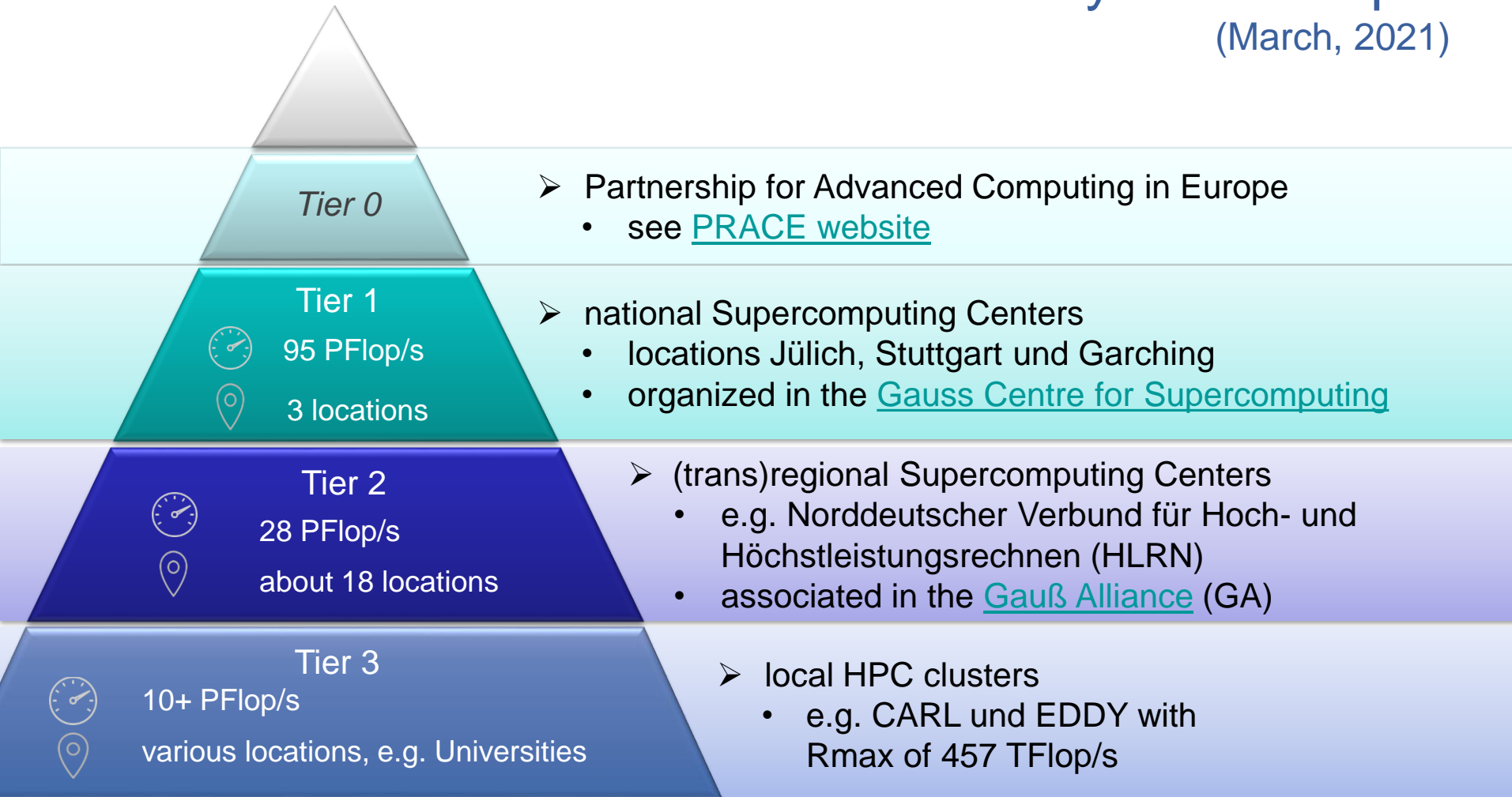
HPC cluster

HPC Cluster

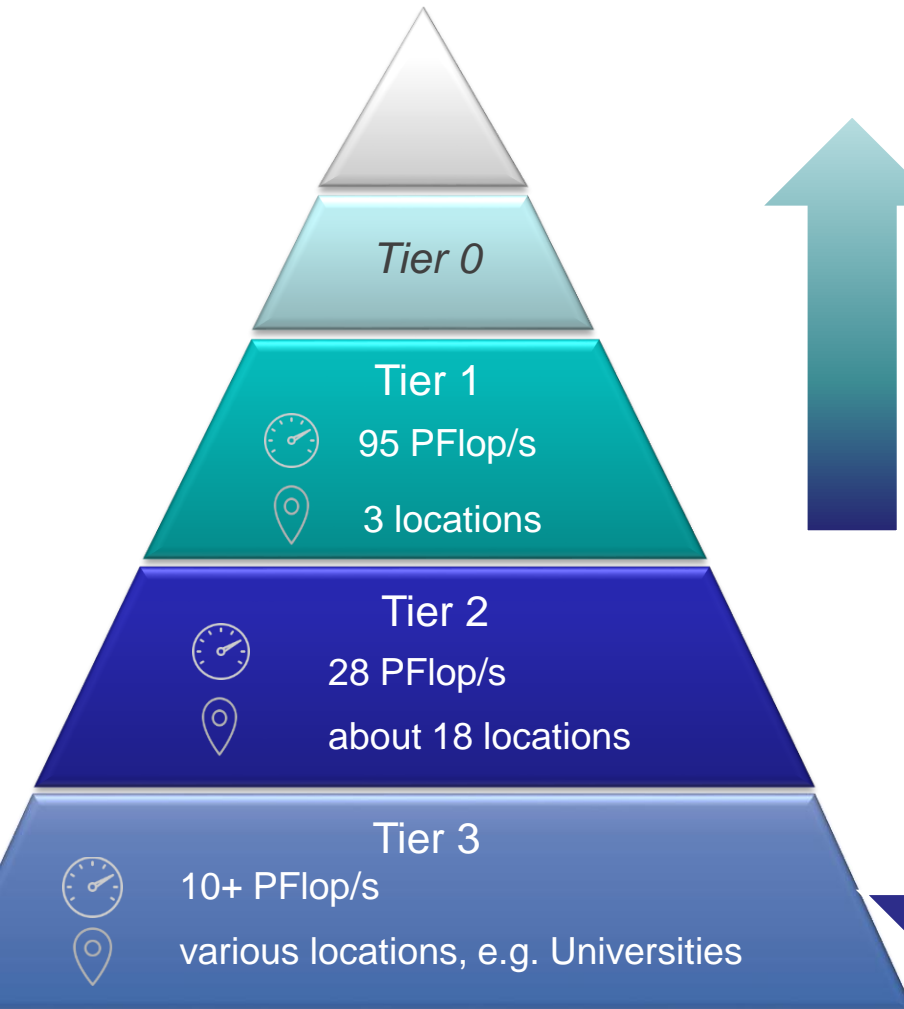


HPC Resources in Germany and Europe

(March, 2021)



HPC Performance Pyramid



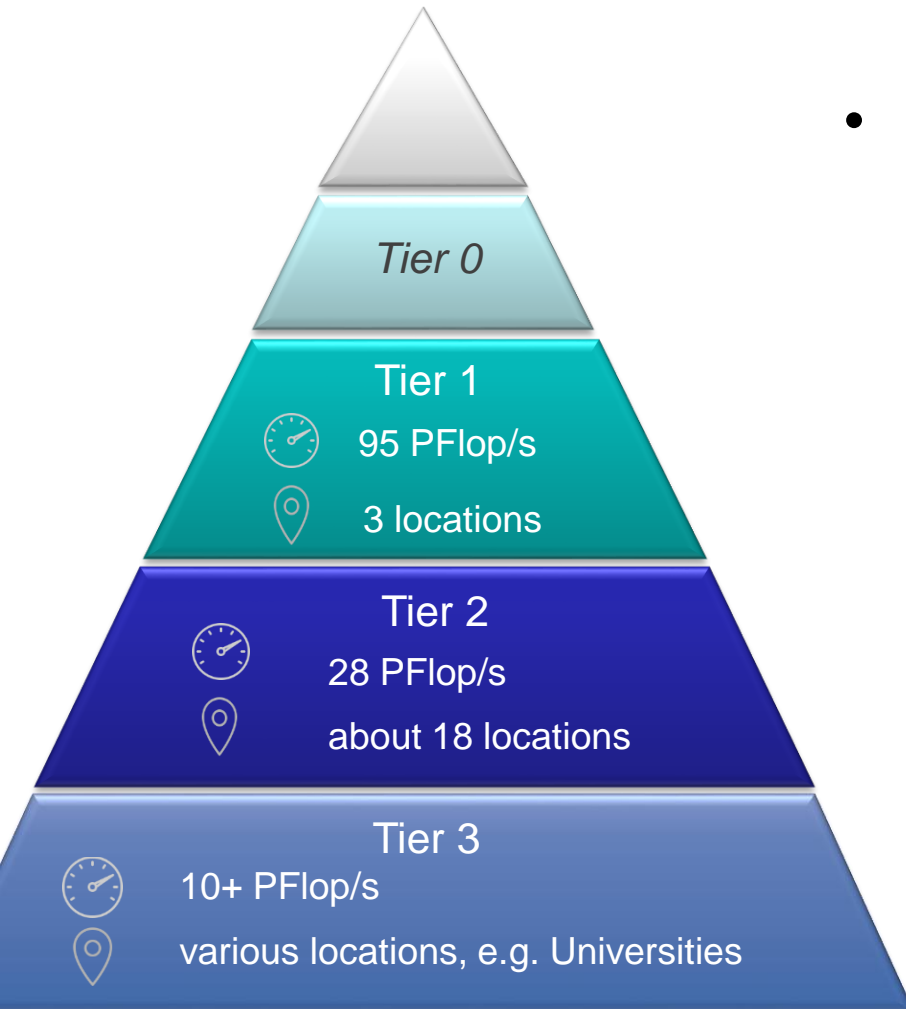
„capability computing“

- using massively parallel computing power to solve a problem in minimal time

„capacity computing“

- using cost-efficient computing power to solve a large number of smaller problems

HPC Performance Pyramid



- permeability between the levels
 - preparation of projects on the lower levels
 - development of algorithms on the lower levels („capability test computing“)
 - transfer of knowledge in both directions
 - special requirements can be better fulfilled in the lowest tier
 - education and training from the bottom to the top

Accessing HPC Resources

- researchers at UOL can always use CARL and EDDY
- for larger projects you can apply for compute time at
 - HLRN
 - one of the Tier 1 centers
 - PRACE
- in 2020 NHR-grants have been awarded to eight supercomputing centers
 - a new HPC infrastructure will be created to improve access to HPC resources
 - eventually you will be allowed to apply for compute time at all NHR centers

North German Supercomputing Alliance (HLRN)

NORRDEUTSCHER VERBUND FÜR HOCH- UND HÖCHSTLEISTUNGSRECHNEN

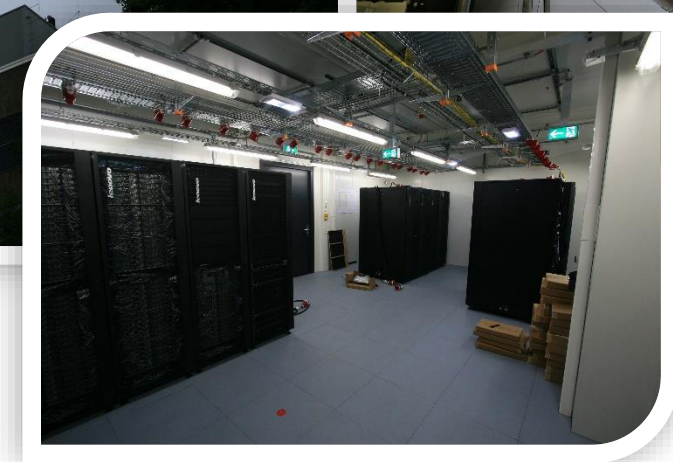
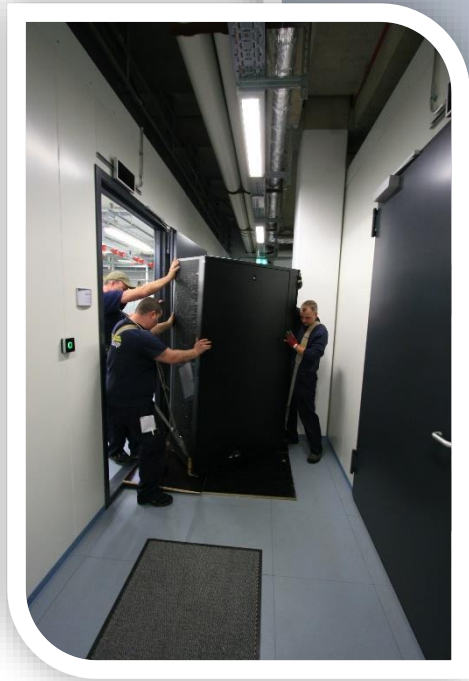
- supercomputing centers at two locations (Berlin and Göttingen)
 - two of the eight NHRs
 - large (25+) network of consultants for scientific computing and HPC
- two HPC clusters – EMMY and LISE
 - fourth generation (HLRN-IV) became operational in 2019/20, total peak performance of more than 16 PFlop/s
 - EMMY: 974 compute nodes (2x Intel Cascade Lake, 48C @ 2.3 GHZ, 384+ GB RAM, OmniPath)
448 compute nodes (2x Intel Skylake, 20C @ 2.4 GHZ, 384+ GB RAM, OmniPath)
 - LISE: 1270 compute nodes (2x Intel Cascade Lake, 48C @ 2.3 GHZ, 384+ GB RAM, OmniPath)
- accessing HLRN (see <https://zulassung.hlrn.de/>)
 - request a user account (to prepare project proposal, valid for 9 months)
 - submit project proposal (dead-lines 28th of January, April, July, October)
 - compute time is allocated for one year (in form of NPLs per quarter)



HPC Cluster at the University Oldenburg

- the new hardware was delivered Aug 22nd, 2016

Delivery Day



<http://www.uni-oldenburg.de/fk5/wr/aktuelles/artikel/art/neue-hochleistungsrechner-fuer-die-universitaet-oldenburg-2380/>

Overview New Hardware

- **CARL**
 - multi-purpose cluster as a basic computing resource
 - funded by the University/MWK and the DFG under grant number INST 184/157-1 FUGG (Forschungsgroßgerät nach Art. 91b GG)
- **EDDY**
 - CFD cluster for wind energy research
 - funded by the BMWi under grant number 0324005
- **used as a shared HPC cluster**
 - common infrastructure is shared (e.g. file systems, network)
 - shared administration

http://wiki.hpcuser.uni-oldenburg.de/index.php?title=Acknowledging_the_HPC_facilities_2016

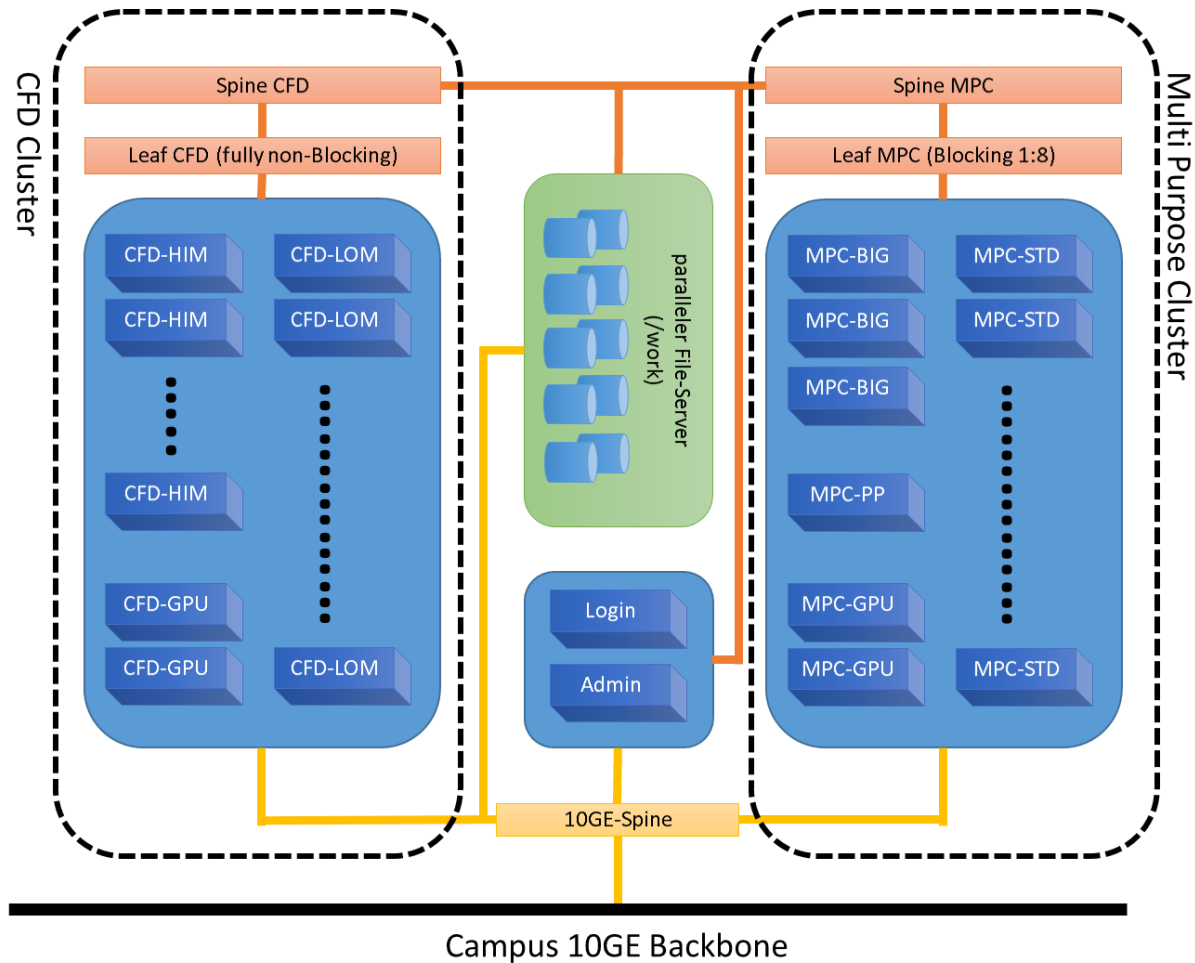
HPC Facilities @ University Oldenburg

- shared HPC cluster CARL/EDDY
 - close to 600 compute nodes
 - 4 login and 2 administration nodes
 - Infiniband FDR interconnect for parallel computing
 - 10/1GE network
 - parallel file system (GPFS) with 900TB capacity
 - NFS mounted central storage

 - Linux (RHEL) as OS
 - many scientific applications and libraries available
 - Job Scheduler (SLURM)

https://wiki.hpcuser.uni-oldenburg.de/index.php?title=HPC_Facilities_of_the_University_of_Oldenburg_2016

Schematic View of HPC Cluster



Summary CARL & EDDY

Feature	CARL	EDDY	Total
Nodes	327	244	571
Cores	7.640	5.856	13.496
RAM	77 TB	21 TB	98 TB
GPFS	450 TB	450 TB	900 TB
local disks	360 TB	-	360 TB
Rpeak (nominal)	271 Tflop/s	201 Tflop/s	482 Tflop/s
Rpeak (AVX2)	221 Tflop/s	164 Tflop/s	385 Tflop/s
Rmax			457.2 Tflop/s

Rank 363 in Top500

<https://www.top500.org/system/178942>



TOP 500 CERTIFICATE
The List.

CARL - Lenovo NeXtScale nx360M5, Xeon E5-2650v4 12C 2.2GHz, Infiniband FDR

Carl von Ossietzky University of Oldenburg, Germany

is ranked


No. 363

among the World's TOP500 Supercomputers

with 457.23 Tflop/s Linpack Performance

in the 48th TOP500 List published at SC16, Salt Lake City, UT on November 14th, 2016.


Congratulations from the TOP500 Editors



Erich Strohmaier
NERSC/Berkeley Lab



Jack Dongarra
University of Tennessee

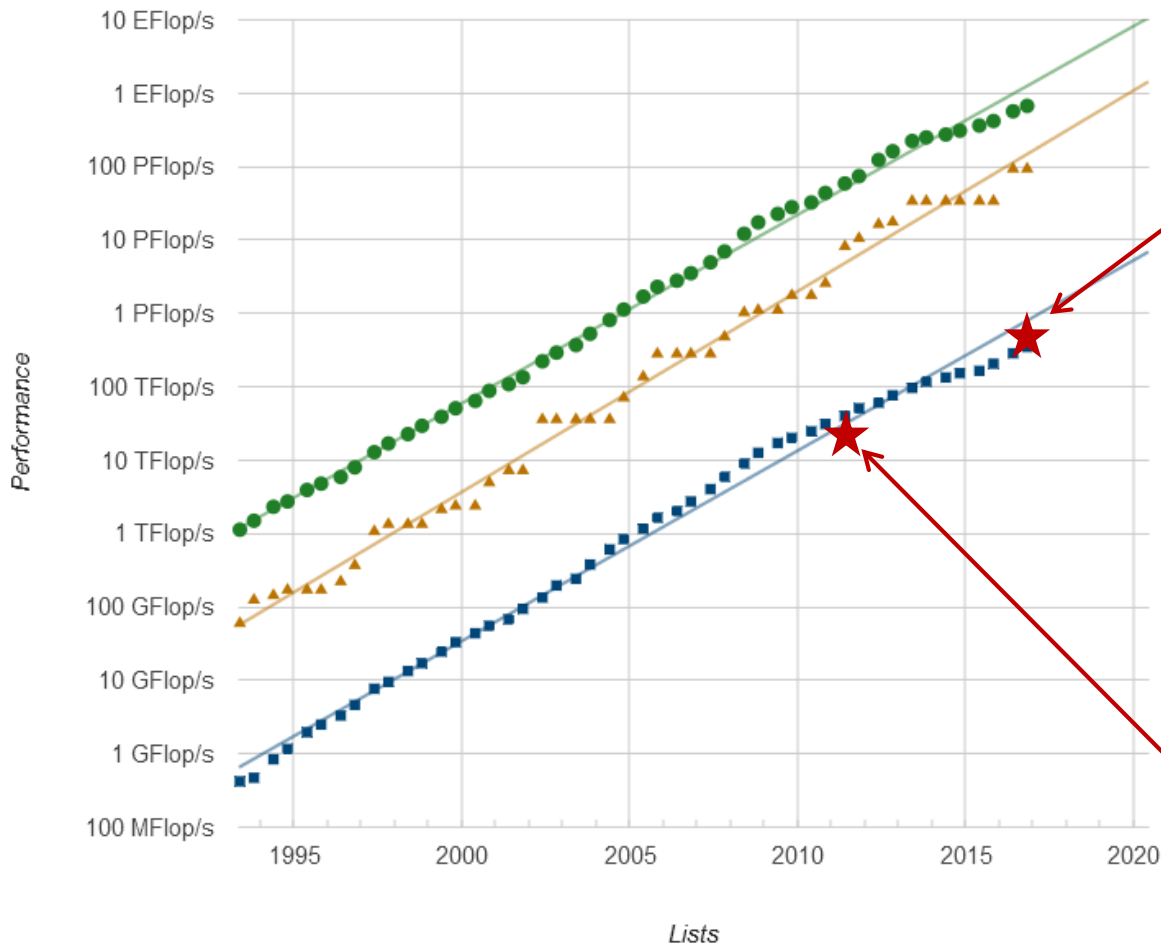


Horst Simon
NERSC/Berkeley Lab



Martin Meuer
Prometheus

Top500 Performance Development



CARL/EDDY

- Rmax 457.2 Tflop/s
- Rank 363
- 571 nodes
- 13,500 cores
- 100 TB RAM



17x Rmax
1.6x nodes
3.3x cores
10x RAM



HERO/FLOW

- Rmax 27.2 Tflop/s
- not ranked
- 350 nodes
- 4,000 cores
- 10 TB RAM

Racks in Server Room



Login to the HPC Cluster

<http://wiki.hpcuser.uni-oldenburg.de/index.php?title=Login>

- Linux
 - use ssh as before with **carl** or **eddy** as login nodes
`ssh -X abcd1234@carl.hpc.uni-oldenburg.de`
- Windows
 - use MobaXterm (recommended) or PuTTY
- login host names
 - `hpc100[1-4].hpc.uni-oldenburg.de`
 - can be used instead of **carl** or **eddy** (for login to specific node)
 - no difference between **carl** and **eddy** as login
- from outside of the campus network use VPN connection
 - see instructions at <http://www.itdienste.uni-oldenburg.de/21240.html>