ForWind
Center for Wind Energy Research

Introduction to HPC

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Introduction to HPC

MOTIVATION

HPC (High-Performance-Computing)

- Computing at the limit of computational resources
- Why HPC?
  - Enable to solve computational intensive problems in an optimal way
  - To increase energy efficiency
- Requirements
  - Understanding of the used computational architecture
  - Identifying the bottlenecks of the resources
  - Optimization of the algorithms w.r.t. the bottlenecks
- Typical computational resources for HPC:
  - Resources which are close to each other
    → HPC-Cluster (e.g. FLOW, HERO)
  - Distributed resources (e.g. Laptops, PC's)
    → Grid-Computing

Parallelization

- Why parallelization?
  - Enabler to solve computational intensive problems (e.g. large linear equation systems)
    - problems with high memory consumption
    - time consuming calculations

- Simple case
  - Computation of small independent problems for a huge parameter space (low memory/time consumption per parameter set)
    - Processes are independent
      → can be executed in parallel by starting them N_{proc} –times
      → e.g. 1 process per CPU core
    - Reduce simulation wall clock times
      → at best by factor 1/ N_{proc}

Parallelization

- Complex case
  - Large problem which needs parallelization, e.g. large linear equation systems (high memory/time consumption for each computation)
    - N_{proc} processes work together
      → e.g. 1 process per CPU core
    - Decrease memory usage per core
      → at best by factor 1/ N_{proc}
  - Reduce simulation wall clock times
    → at best by factor 1/ N_{proc}
  - Overhead
    - exchange/management of data
    - organization of processes
    - load imbalances

Introduction to HPC

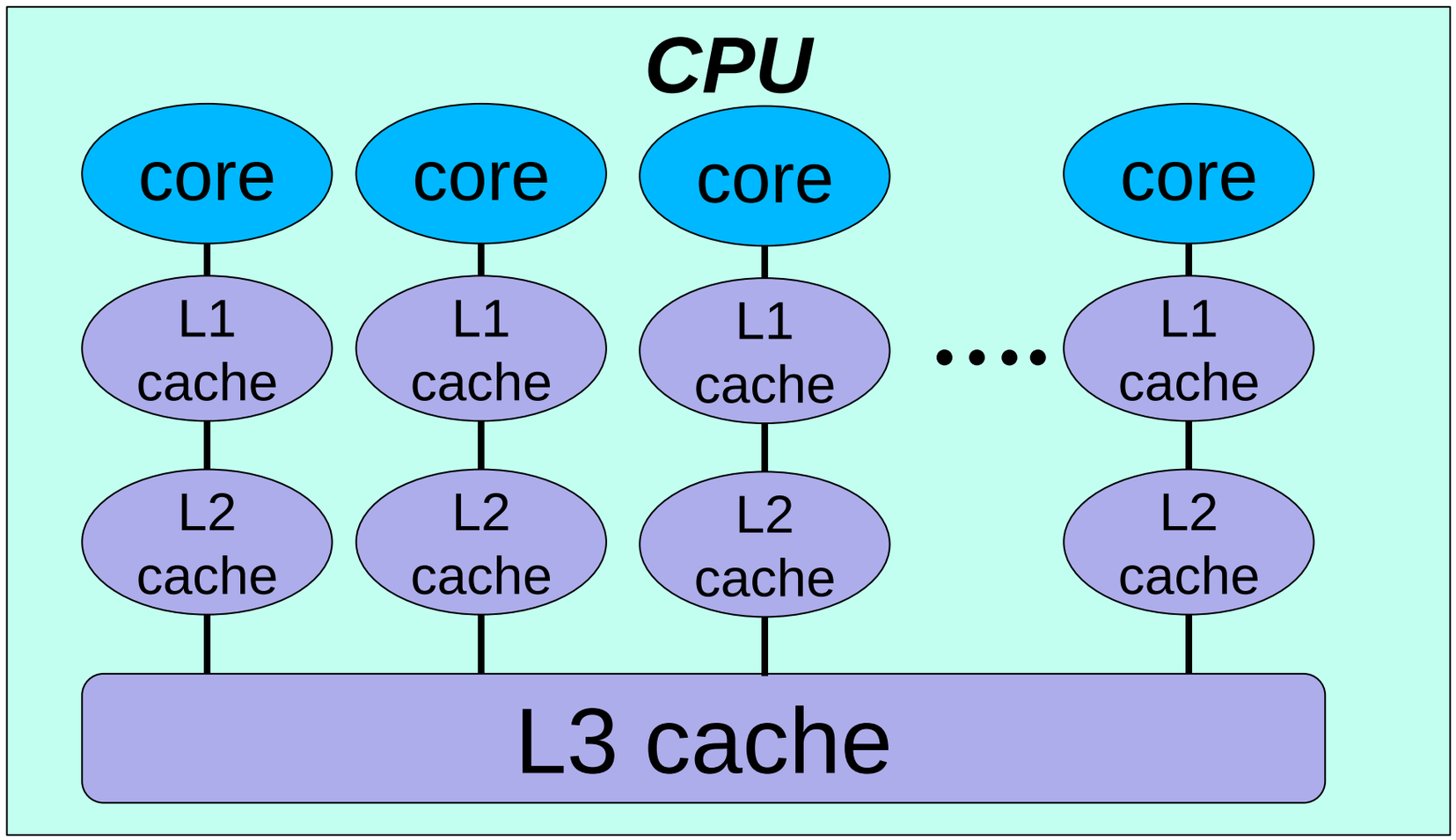
ARCHITECTURES

Architectures

- Why is knowledge about hardware architecture important?
  - To write efficient code:
    - Algorithm should fit to the architecture
      → Increase performance
  - To know the limits/bottlenecks

Central Processing Unit - CPU

- CPU (chip on a socket) contains several cores
- Cores connected to caches for fast memory access, low latency
  → O(10) faster than direct memory access
- Cache coherence



Westmere X5650

6 cores, 2,66GHz

64Kb

256Kb

12Mb

Central Processing Unit - CPU

Todays CPU (chip on a socket)

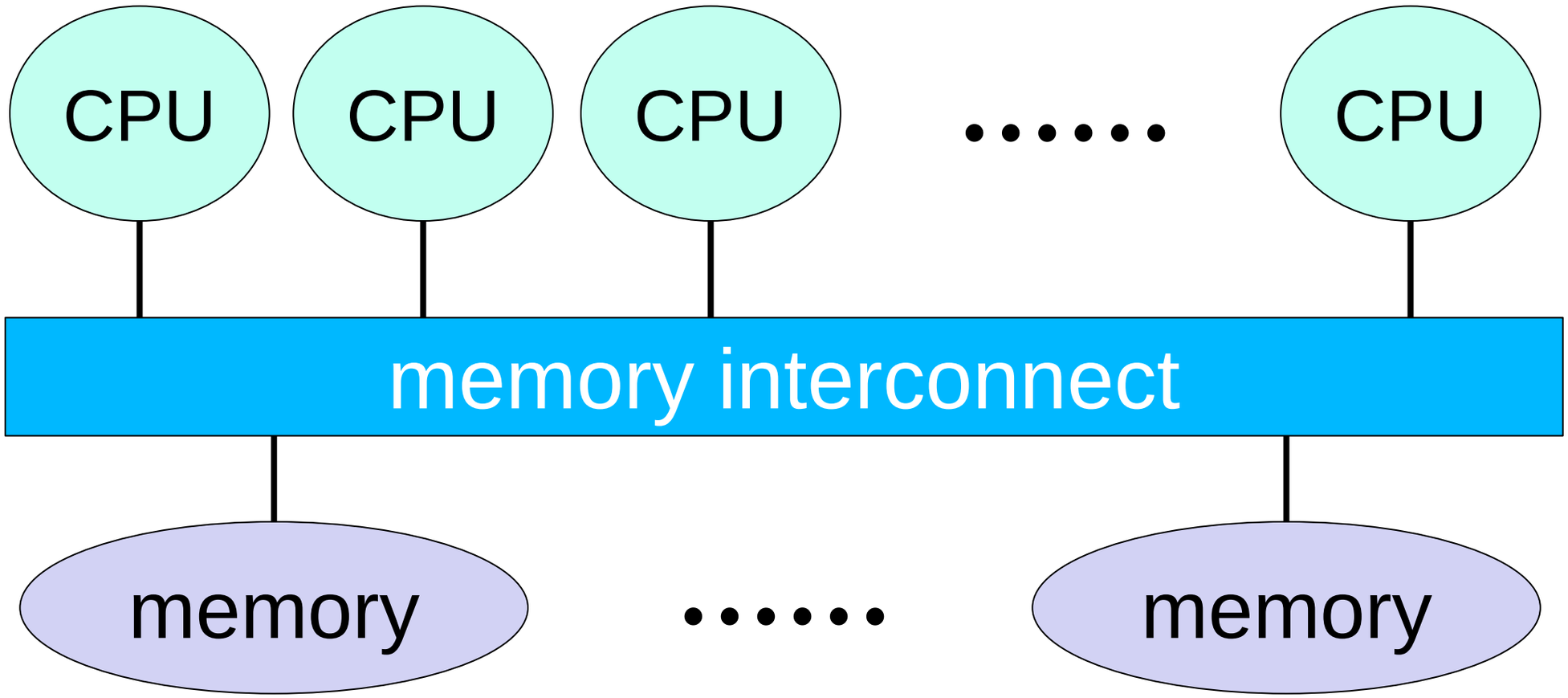
- contains several cores
  → number of cores increases, todays driver for performance increase
- several levels of caches (high transfer rates, low latency)
- execute instructions in parallel (pipelines)
- *Single Instruction, Multiple Data* (SIMD) features, e.g. SSE, AVX, AVX2,... instruction sets
  → multiple floating point/integer operations within on cycle
- clock frequency stagnates/decrease due to
  - energy efficiency
  - thermal effects (heating, leakage current,...)

Main limitations

- memory bandwidth (e.g. floating point operations faster then getting the number out of memory)
- limit in instruction per cycle (to many work)
- parallelization of algorithms

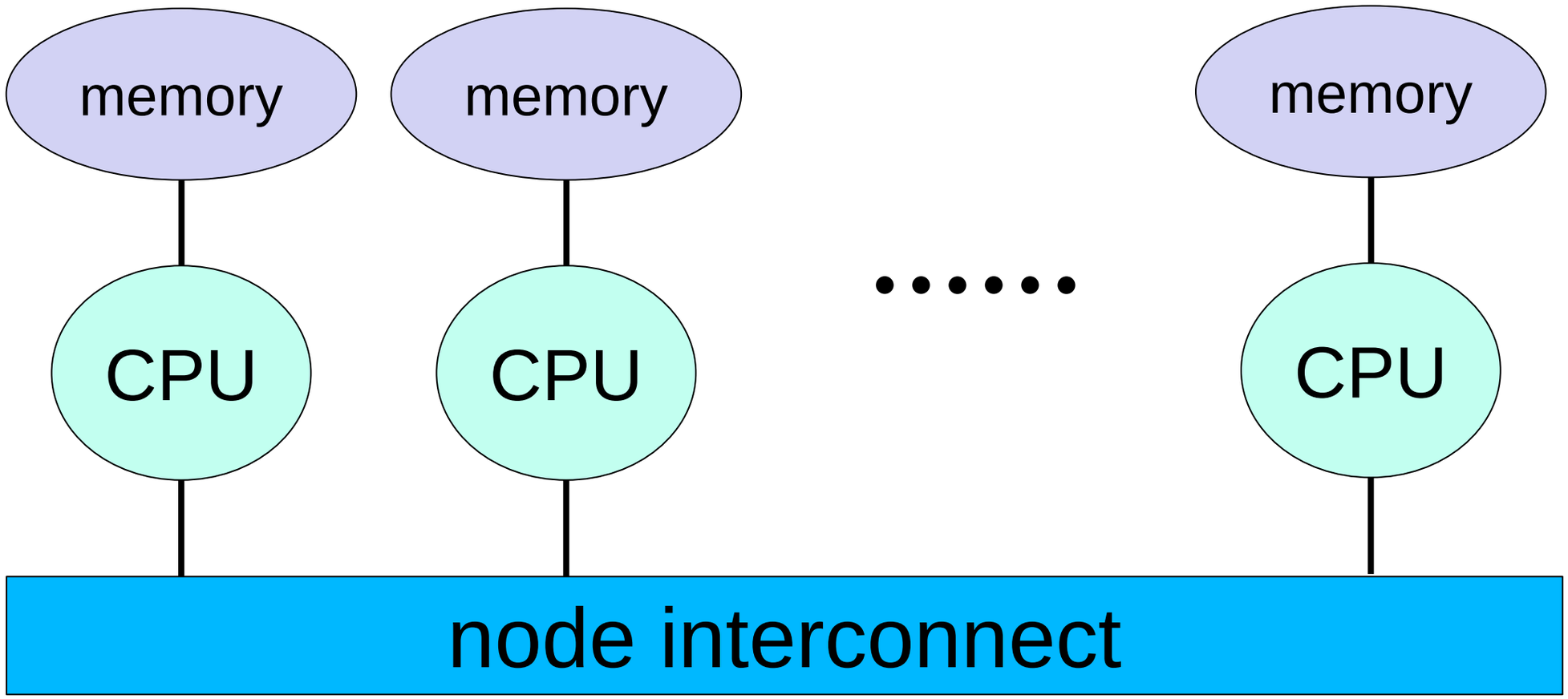
Shared memory system

- Symmetric multi-processing (smp)
- Uniform memory access (uma)
  - Same access time from every CPU



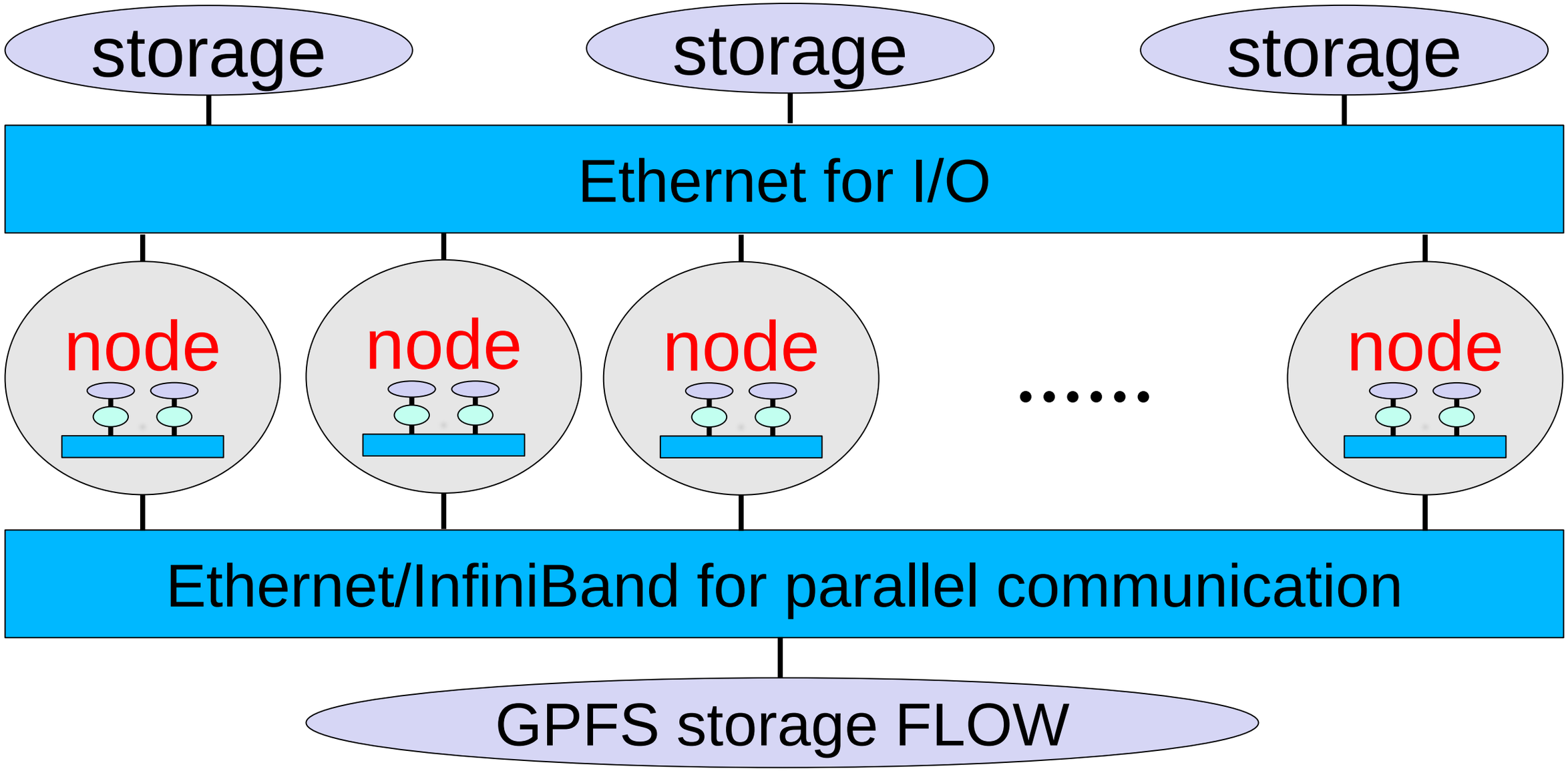
Shared memory system

- Today architecture of a node: Non-uniform memory access (NUMA)
  - Fast access to own memory, slow access to other memory
  - Cache coherence → ccNUMA
- Nodes on HERO and FLOW have ccNUMA architecture (except UV100)



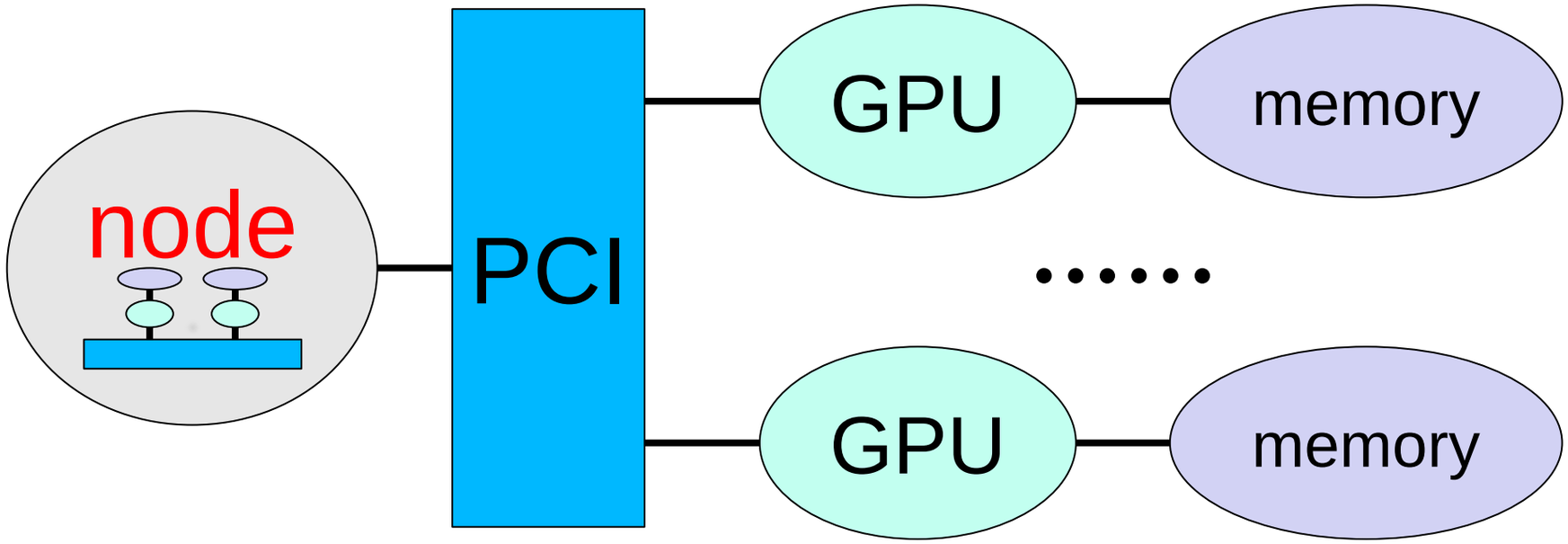
HPC-Cluster FLOW/HERO

- O(100) NUMA nodes connected by fast interconnect



Accelerators (many cores)

- Todays typical accelerators
  - General-Purpose computing on Graphics Processing Units (GPGPU), e.g. Graphic card chips with O(1000) cores
  - Intel Phi (~60 Pentium cores)



- Other
  - Field-Programmable Gate Arrays (FPGA)
  - ...

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HPC AT THE UNIVERSITY OF OLDENBURG

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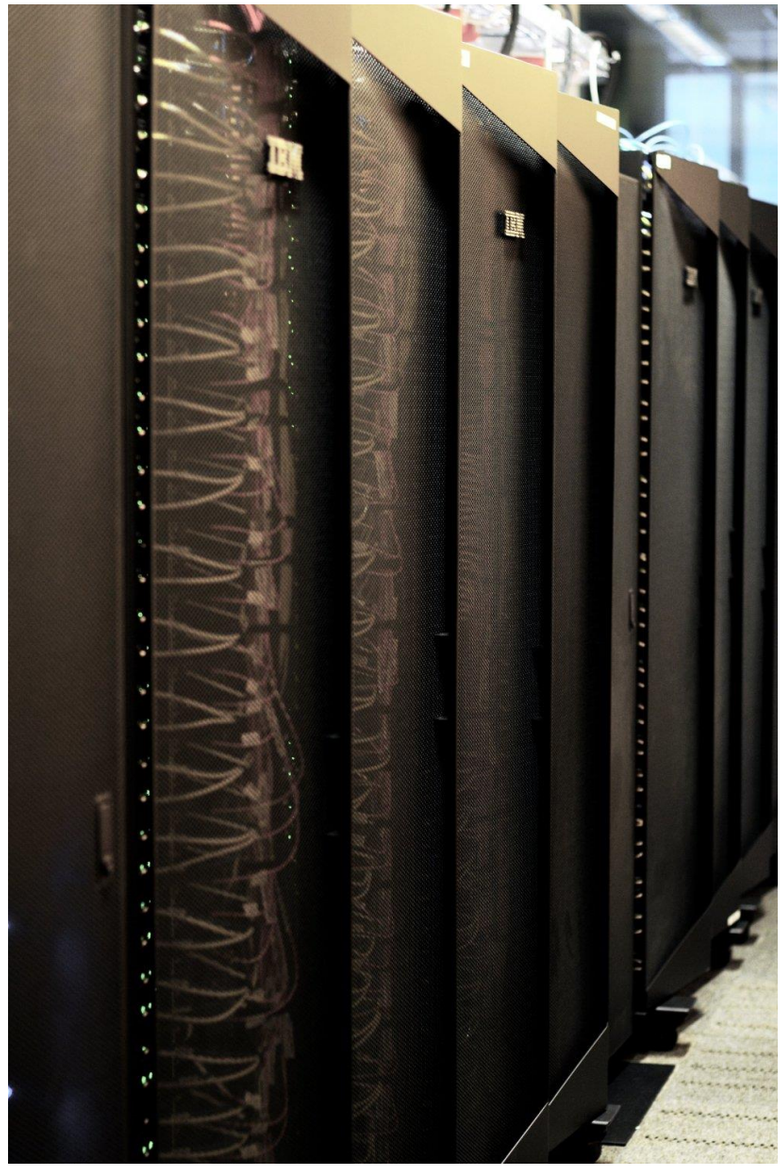
FLOW –
Facility for Large-Scale Computations in Wind Energy Research

- 122 "low-memory" compute nodes: 2x6 cores per node, 24Gb, diskless (host names cfdl001..cfdl122)
- 64 "high-memory" compute nodes: 2x6 cores per node, 48Gb, diskless (host names cfdh001..cfdh064)
- 7 compute nodes: 2x4 cores per node, 32Gb (host names cfdx001..cfdx007)
- QDR InfiniBand interconnect (fully non-blocking)
- Gigabit Ethernet for File-I/O etc.
- High-performance IBM GPFS storage system, 130TB connected by InfiniBand
- 160 TB NAS storage shared with HERO
- Theoretical peak performance: 24 TFlop/s (Flop/s – Floating Point Operations per second)



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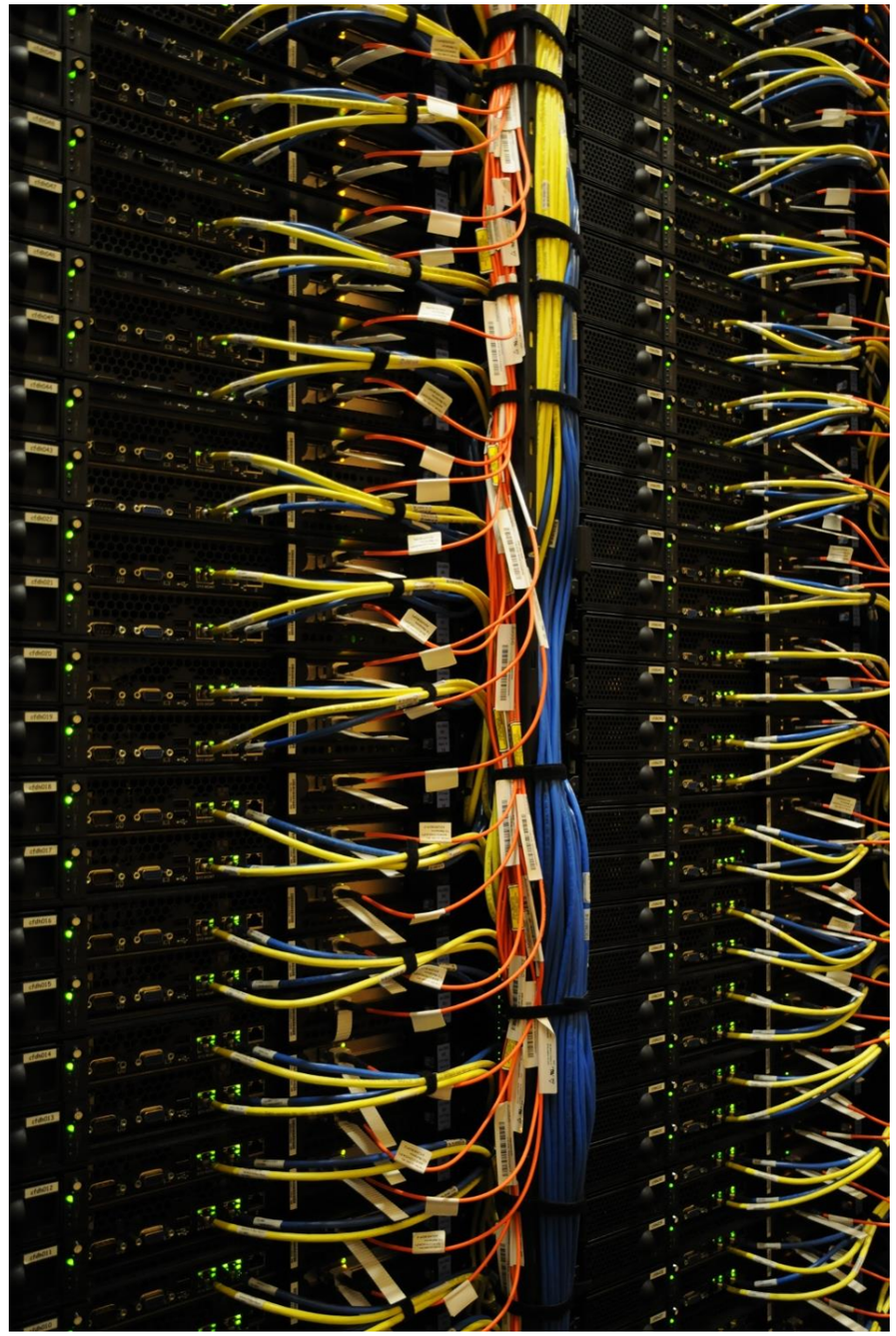
HERO - High-End Computing Resource Oldenburg

- 130 "standard" nodes: 2x6 cores, 24 GB, 1 TB disk (host names mpcs001..mpcs130)
- 20 "big" nodes: 2x6 cores, 48 GB, RAID 8 x 300 GB SAS (host names mpcb001..mpcb020)
- Gigabit Ethernet II for communication of parallel jobs
- Second, independent Gigabit Ethernet for File-I/O
- SGI Altix UV 100 shared-memory system: 10x6 cores, 640 GB, RAID 20 x 600 GB SAS (host uv100)
- 160 TB NAS storage shared with FLOW
- Theoretical peak performance: 19.2 TFlop/s (Flop/s – Floating Point Operations per second)



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HPC CLUSTER USAGE

Login

- Login nodes of FLOW and HERO
  - `flow.hpc.uni-oldenburg.de` (to access `flow01` or `flow02`)
  - `hero.hpc.uni-oldenburg.de` (to access `hero01` or `hero02`)
- Login from terminal by ssh, e.g.
  ```
  ssh -XY abcd1234@flow.hpc.uni-oldenburg.de
  ```
- Terminal programs
  - Windows
    - Putty (`http://www.putty.org/` , no X-Window support)
    - MobaXterm (`http://mobaxterm.mobatek.net/`, including X-Window support)
  - Linux/Mac: Terminal included
- Copy of data sftp/scp, e.g. from your host
  ```
  scp FILENAME abcd1234@flow.hpc.uni-oldenburg.de:TARGET_DIR
  ```
- Note: Direct login on computational nodes is forbidden
- To login from outside or University WLAN you need a special VPN connection (see HPC-WIKI)

File systems

- two directories for storage
  - home directory `/user/<user_group>/<user_name>`
    - place for long term storage
    - fully backed up
    - limited size (usually 110 Gb per user)
    - usage can be determined by the command iquota
  - working directory `/data/work/<user_group>/<user_name>`
    - place for data used or produced during the computations
    - not backed up
    - huge (limited) size (usually 3.5 Tb per user)
    - size of usage weekly per mail
- both no parallel file systems (temporal delays possible, max. 30s files, max. 60s directories)
- both mountable via CIFS on your workstation (HPC-Wiki)

File systems

Home directory has *snapshot* functionality

- hidden directory `.snapshot` exists (not visible with `ls`, but `cd .snapshot` possible)
- within that directory a list of different snapshots exist

```
hpc_user_daily_2013-06-28_01-00
hpc_user_daily_2013-06-29_01-00
...
hpc_user_daily_recent
hpc_user_hourly_2013-07-03_20-00
...
hpc_user_hourly_recent
hpc_user_weekly_2013-06-10_02-00
...
hpc_user_weekly_recent
```

- Within these subdirectories the file-structure of the current parent directory was stored (at that point in time where the particular snapshot was taken at)

File systems

Additional high performance GPFS file system on FLOW

- `/data/work/gpfs/<user_group>/<user_name>`
- place for data used or produced during the computations
- high transfer rates (about 4 times higher than the other file system)
- parallel file system
- not backed up
- huge size, up to now no quota (110Tb)
- only mountable via sshfs (SFTP) on your workstation (see HPC Wiki)

User environment

- Most of the programs (e.g. compilers, MPI,...) not available per default
- Use command `module` to load the needed environment
  - Show available modules
    ```
    module av [NAME]
    ```
    (e.g. `module av intel` to see all Intel products)
  - Module name convention: lower case letters
  - More information about a module
    ```
    module help MODULE_NAME
    module show MODULE_NAME
    ```
- Load module (make Software available)
  ```
  module load MODULE_NAME
  ```
  (e.g. `module load ics/2013_sp1.3.174/64` to load Intel Cluster Studio 2013 SP1
- Unload module (disable Software)
  ```
  module unload MODULE_NAME
  ```

Available development tools

- Compiler (C, C++,Fortran)
  - Intel Cluster Studio
  - GNU compiler
  - PGI Accelerator Suite
  - Open64
  - CLang
- MPI implementation
  - OpenMPI
  - Intel MPI
- Libraries
  - BLAS/LAPACK in MKL
  - LEDA
  - FFTW
  - NetCDF, HDF5
  - NAG
  - ...
- Other languages
  - Python
  - R
  - Matlab, Octave

and many more....

Thanks!

Please visit our HPC-Wiki

http://wiki.hpcuser.uni-oldenburg.de