Introduction to HPC Programming (08.128.612)

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Why you should be here

- Alternative Title: Boost your analysis
    - New or existing analysis
    - But: There is no automated way to do this.

- Main purpose of this course
    - Give you the tools at hand to boost you analysis (less theory)
    - Focus on MSc and PhD students
        - What is so special about MSc/PhD?
          (no time, credit points irrelevant, already settled analysis program)
    - Hands-on during lecture

- Alternatives to this lecture:
    - “HPC” by Bertil Schmidt (08.079.090): standard lecture with problem classes (credit points included), no hands-on, not physics-analysis orientated
    - Courses in Frankfurt or Stuttgart from PRACE community

- Motivation:

  There are some people saying, they found the use of C pointers more difficult than parallel programming with “MPI”.

Organisational issues

- Lecture times: Tuesdays, 14:15-15:45, Conference Room 1, HIM Building
- Optimised for target audience:
  - No home work or problem classes
  - No compulsory attendance (please leave me a note, when you are unable to come)
  - Learning Blocks (eg OpenMP, MPI) stretch over several lectures.
  - Universal: OpenMP and MPI can be used at any HPC computer worldwide.
- Lecture nodes get published on course webpage
  - https://www.hi-mainz.de/research/computing/lectures/
- Hands-on work:
  - 2 people share one computer (Linux, macOS, Windows)
  - Please form clusters
- Homework:
  - Set up a Computer for next week‘s session with the following software: X-Server for macOS and Linux, MobaXterm for Windows (Alternatively Putty with Xming)
  - Log into Himster 2 headnode once. Details: https://mogonwiki.zdv.uni-mainz.de/dokuwiki/access
  - Help any time: email or stop by my office.

Lecture Overview

- Typical lecture: 30’ talk + 60’ hands-on
- Up to date schedule always on course webpage

1. Introduction: (1 lecture, today)
    1. Why HPC?
    2. Setup of a HPC cluster (in general terms / Mogon2 / HIMster 2 / Clover)
2. Programming:
    1. Shared memory programming: OpenMP (3 lectures + hands on)
    2. Distributed memory programming: MPI starter (3 lectures + hands on)
3. Debugging and Performance Analysis:
    1. MPI parallel debugging with TotalView (1 lecture + hands on)
    2. OpenMP verification with Intel Inspector XE (1 lecture + hands on)
4. Effective Usage of HPC for Single Core Analysis Programs (PANDA-Root, BOSS, etc.)
5. Survey dependent:
    - 4 remaining lectures
      (h5py, advanced MPI, optimising I/O pattern, special programming languages, …)

Literature

- An Introduction to Parallel Programming, Peter Pacheco, 2011, 978-0-12-374260-5
  - Ebook freely available
- MPI-3.1: A Message-Passing Interface Standard
  - C: The standard is really readable! https://www.mpi-forum.org/docs/mpi-3.1/mpi31-report-book.pdf
  - Python: https://mpi4py.readthedocs.io/en/stable/
- Introduction to High Performance Computer for Scientists and Engineers, Hager and Wellein, 978-1-4398-1192-4
- OpenMP:
  - Eine Einführung in die parallele Programmierung mit C/C++, Springer, Hoffmann and Lienhart
  - Your favourite compiler manual

- courses at HLRS Stuttgart or Frankfurt (and more at PRACE) (https://www.hlrs.de/training/)
  - Parallel Programming (*)
  - Performance Optimization and Debugging (*)
  - Computational Fluid Dynamics and Parallelization
  - Scientific Visualization

Basic Requirements

- Basic Python or C programming skills
  - OpenMP only in C available
- Linux basics needed:
  - Bash: launch a program with different parameters, write script
  - SSH: generate a key and log into HIMster2
  - modules: list and load different modules
  - gcc: compile with different optimisations
  - (versioning with git)

- If not present, familiarise with it OR find the right team mate!

Lecture Today

- Organisational Points (10’)
- Motivation for Cluster Computing (10’)
- Cluster building blocks and our HIMster2 (10’)
- TOP 500 / Green 500
- Survey (10’)
- Guided Tour HIMster 2 (20’)

Why HPC?

Why did we gather together?

- Why HPC?

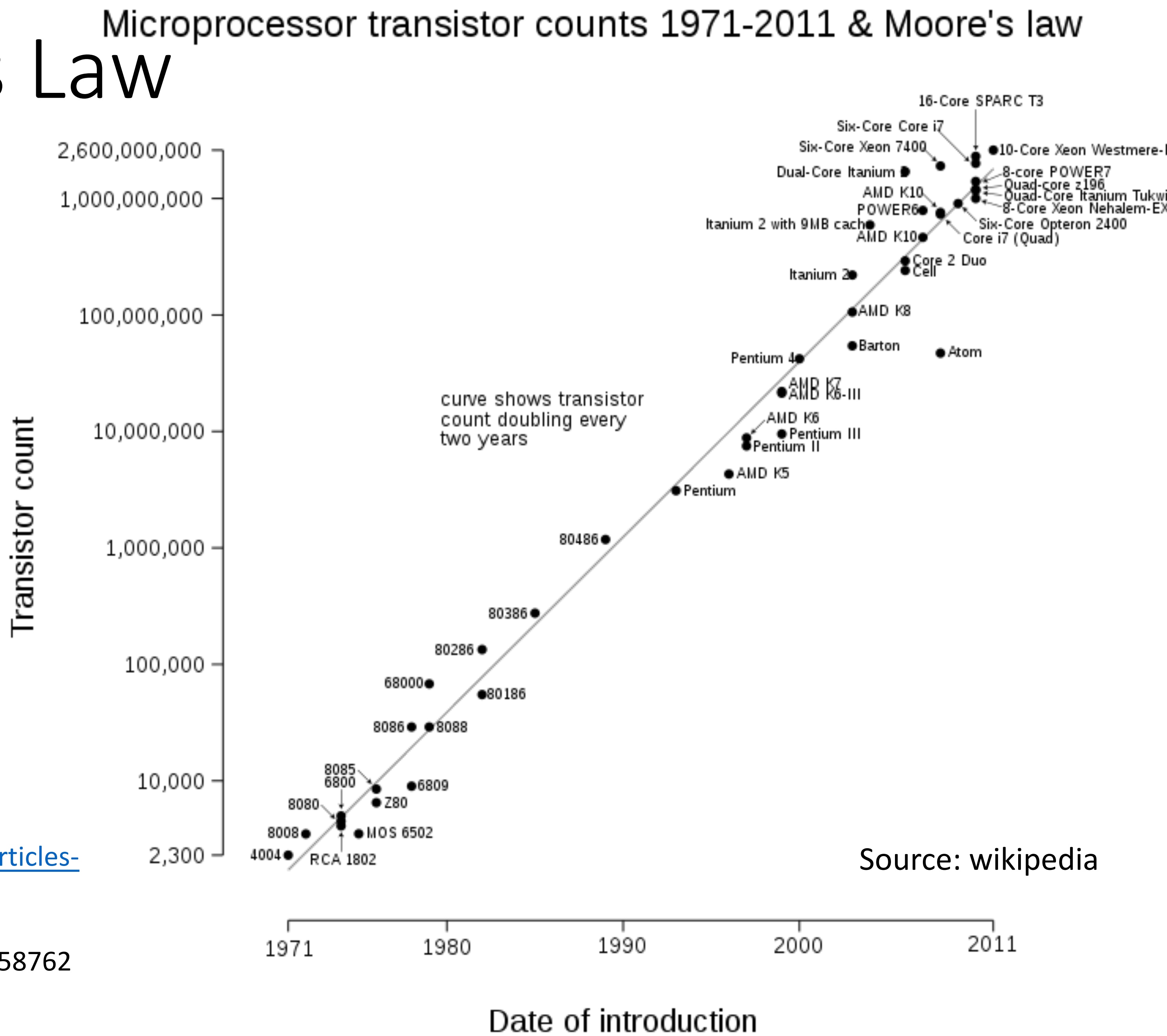
- Intense computational problem → single desktop computer not capable enough

- Run on a “super computer“
  1. <2002: fast single core super computer
  2. Since 2002: parallel systems as super computers

  → Why parallel systems?

The Era of Moore‘s Law

- Moore's law (1965) = observation number of transistors in a IC doubles every ~2a.
- Still valid, no natural law.



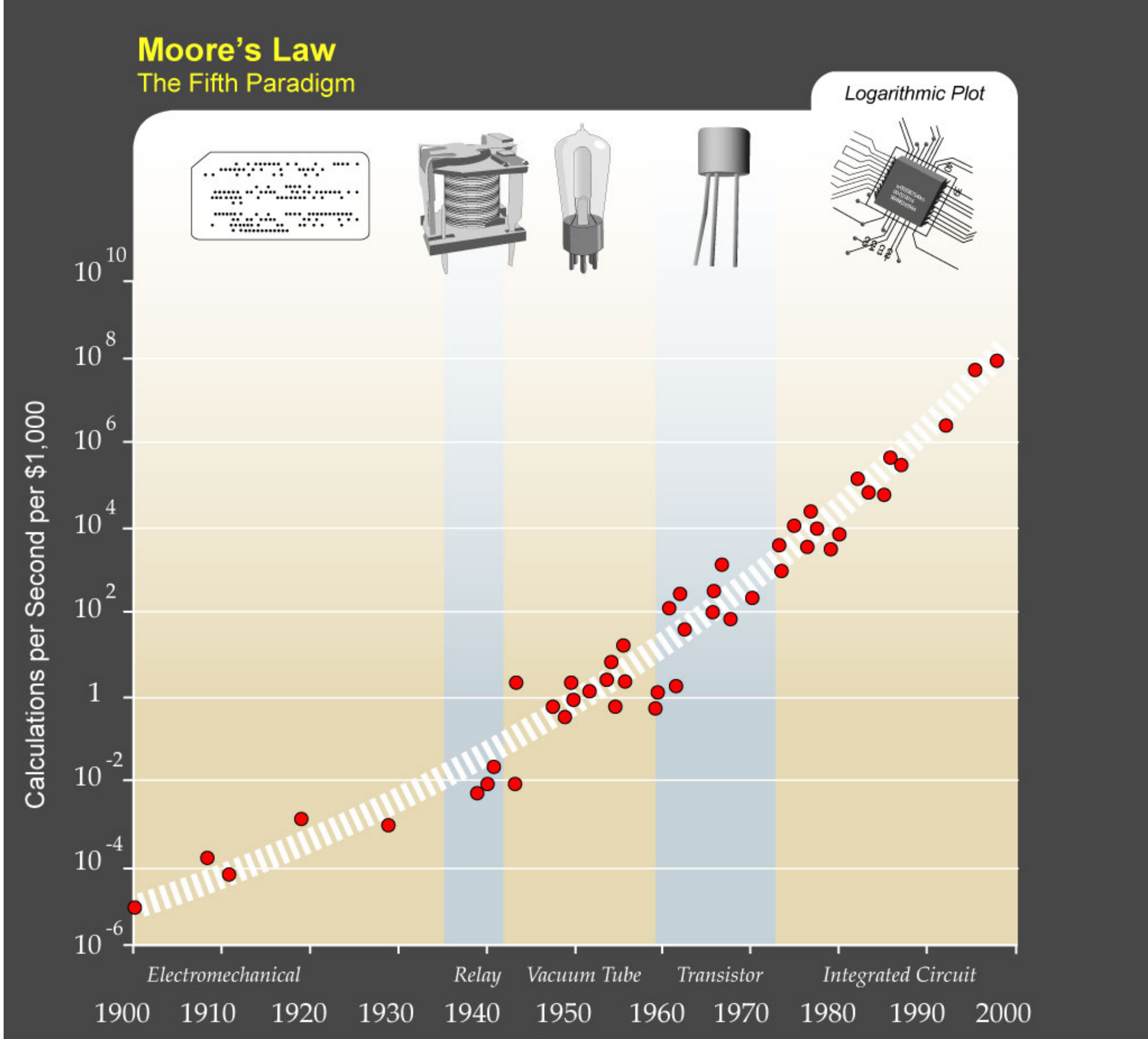
Source: wikipedia

Cramming More Components onto IC (1965):
ftp://download.intel.com/sites/channel/museum/Moores_Law/Articles-Press_Releases/Gordon_Moore_1965_Article.pdf or

https://ieeexplore.ieee.org/document/658762?tp=&arnumber=658762

The Era of Moore’s Law

- 1900-2000
- source: Wikipedia



Single-Core Performance

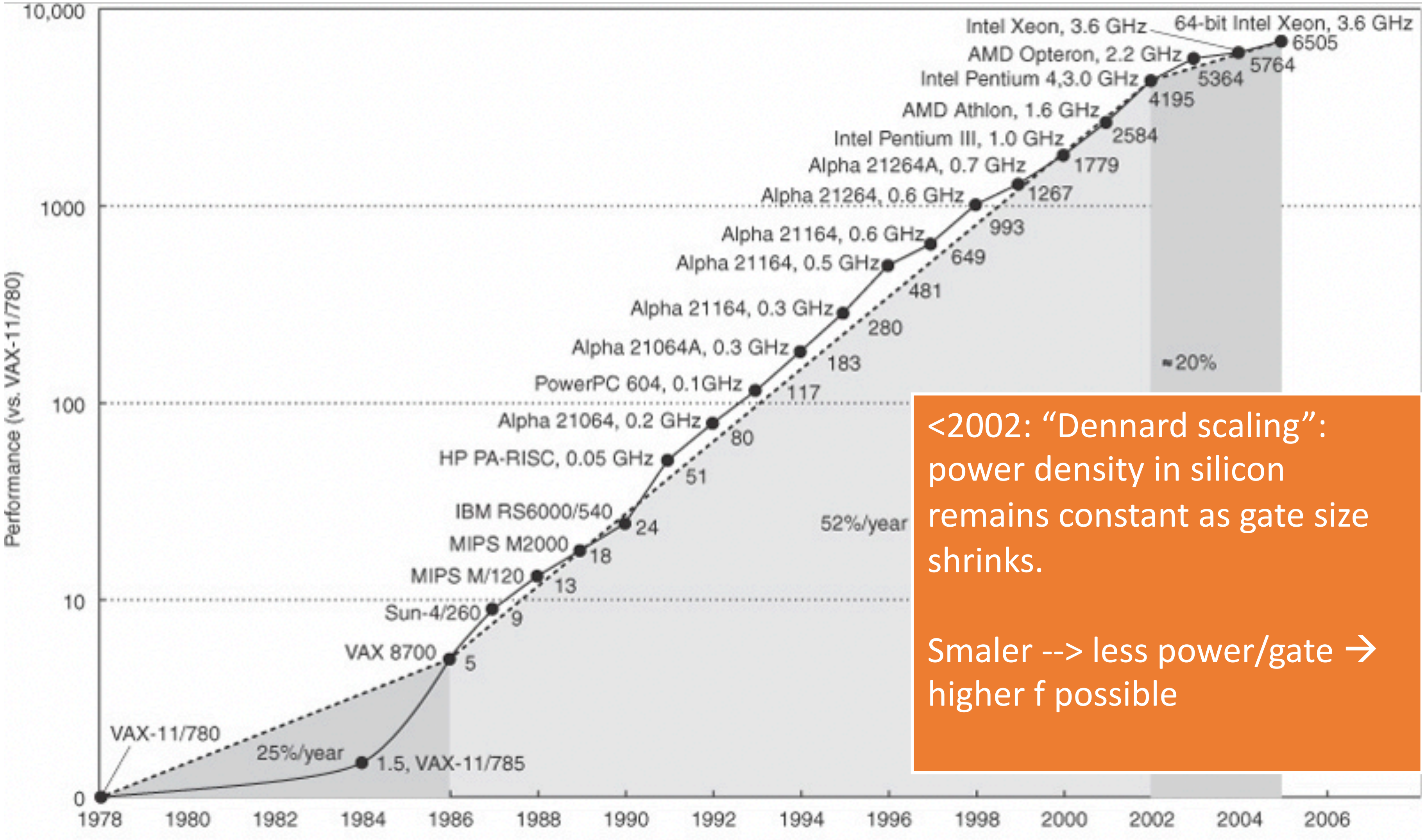
The single core-performance increased by

- <2002: 50%/a
- >2002: 20%/a

Speedup after 10a:

- <2002: ~6000%
- >2002: ~600%

Simply wait for the next CPU release is not enough any longer.

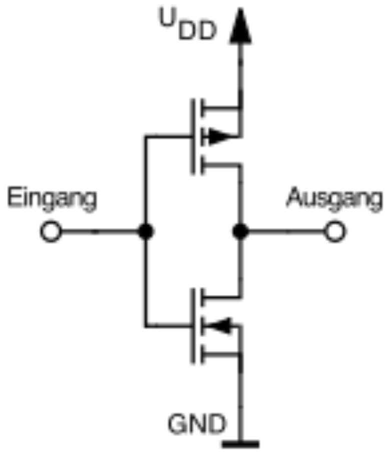


<2002: “Dennard scaling”: power density in silicon remains constant as gate size shrinks.

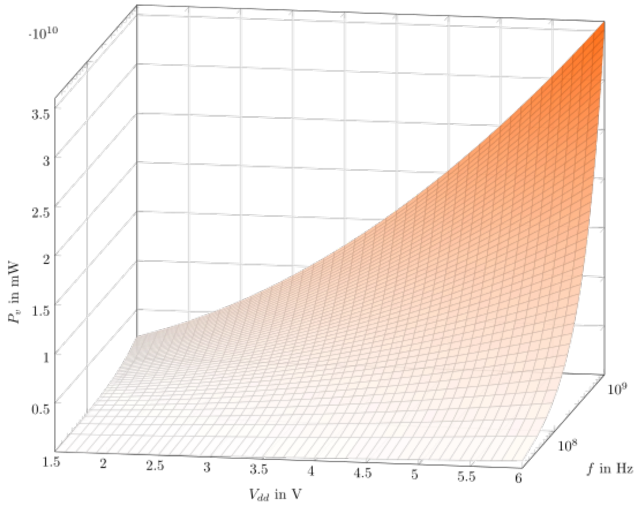
Smaler --> less power/gate → higher f possible

Why not increasing frequency?

- Core speeds topped out at 2-4 GHz
  - World record standard CPU: 8722.78 MHz with liquid nitrogen cooling (http://hwbot.org/benchmark/cpu_frequency/)
- Problem #1: cooling the chip
- Finding: "Dennard scaling" (constant power density) no longer valid
  - No longer (since 2000's) true since 90nm gate sizes (leakage current!)
- The two things that consume energy (CMOS gate):
  1. switching state (1 ⇔ 0) (10µW/MHz, prop with f^1.75)
  2. leakage current (10nW / CMOS-Gate, anti-prop with Vdd and gate size)
- Increasing f: increase in power on same area → compensate this: shrinking gate sizes and lower Vdd
  - But: smaller gates have higher leakage current. → New innovations needed. → multi-cores at fixed f to gain performance

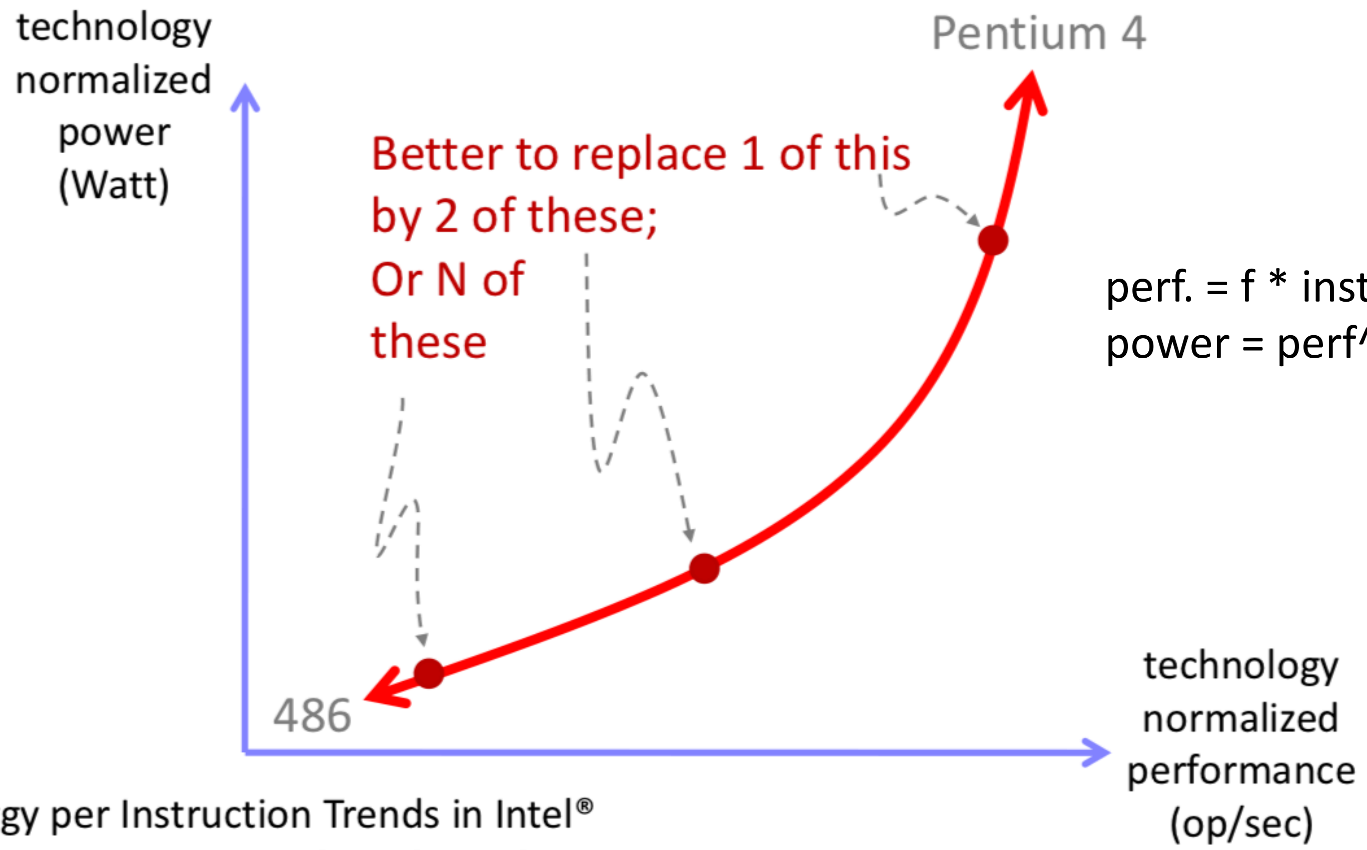


not gate



Power=P(Vdd, f)

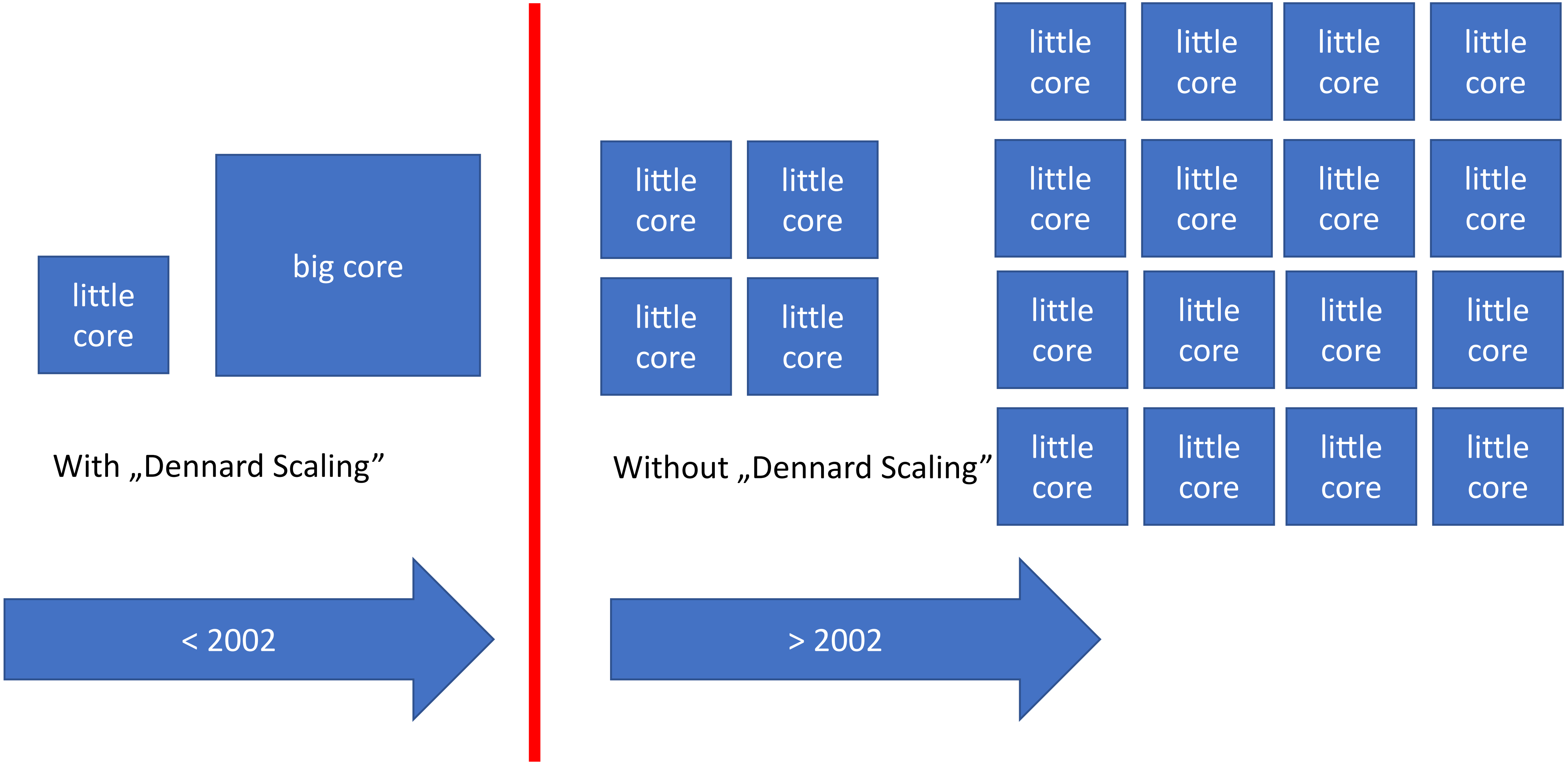
Answer: multicores



perf. = f * instr./clock
power = perf^1.75 + const.

Energy per Instruction Trends in Intel®
Microprocessors, Grochowski et al., 2006

Moore‘s Law scaling with cores



little core

big core

With „Dennard Scaling”

< 2002

little core

little core

little core

little core

Without „Dennard Scaling”

little core

little core

little core

little core

little core

little core

little core

little core

little core

little core

little core

little core

little core

little core

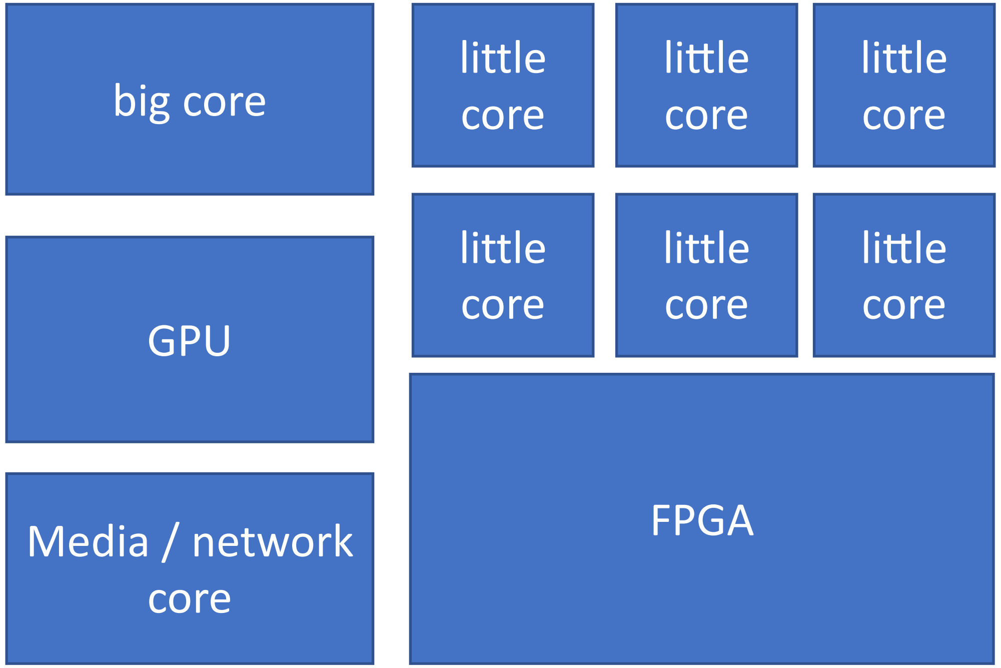
little core

little core

> 2002

Future

- All about performance/watt and performance/€



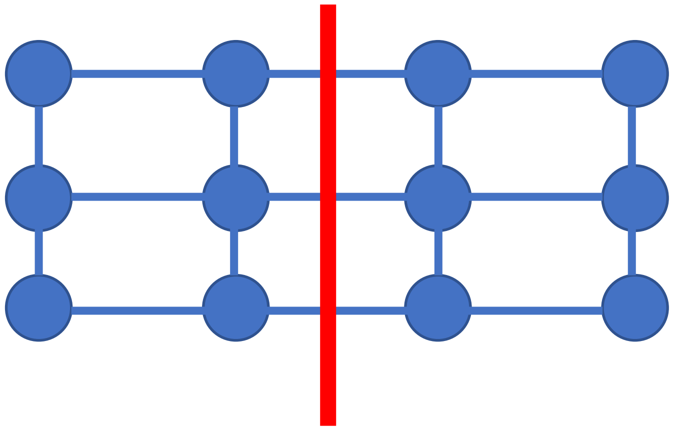
Finally: Why specialised?

Comparison with distributed office computers at HIM

- FLOPS / computer (floating-point operation per second):
  - FLOPS = f × N_{cores} × $N_{instr\ per\ cycle}$
  - Intel E5-2670 (2,6 GHz, 8 cores): 2,6GHz × 8 × 8 = 166,4 GFLOPS
- $N_{computers}$: 25 offices / floor, 4 floors, 2 people / office, 1 computer / person = 200.
- 33TFLOPS (Clover = 106TFLOPS, HIMster2/Mogon2: 2801TFLOPS) cluster “for free”

Drawbacks:

- OS: Windows (20%), MacOS (20%), Linux (50%) other (10%) – all on a different version level
- Temperature in office rooms, closed window, 15th July: 0W = 29°C, with 400W = 50°C
- Network: 1GBit/s, Backbone 10GBit/s (HIMster2: 100GBit/s)
  - 10GBit/s / 200 computers / 8 cores = 780kByte/s
  - Compare bisection bandwidth (minimal accumulated bandwidth between any bisections of the network): fat tree ⇔ binary tree
- Storage?
- No node checks, difficult to maintain, reduced availability



bisection bandwidth

Basic concepts

Parallel Programs: Worked out example (1)

Large task: grading 100 exams, 5 questions each

- Approaches:
    - task-parallelism (grading exam questions: one core = one task = one question)
    - data-parallelism (grading exam: one core = one exam = data)

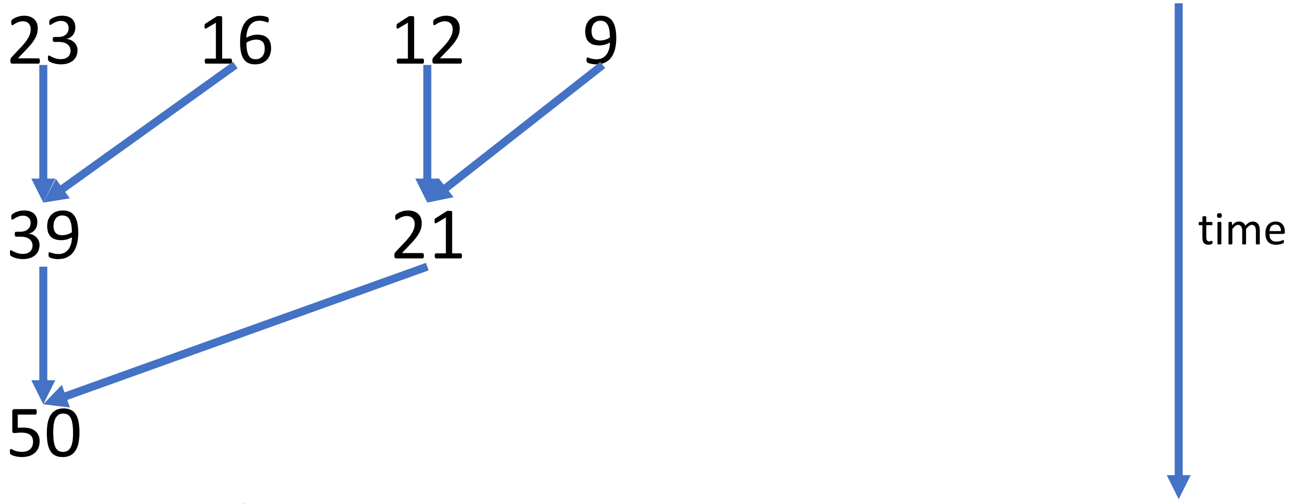
- Check, Coordination of work:
    - Load balancing (assign all cores with equal load) (⇔ your brain while coding)
    - Communication (⇔ Storage, Interconnect)
    - Regular synchronisation (waits!) (⇔ MPI, OpenMP)

- We will write explicitly parallel programs:
    - C language with extensions (OpenMP and MPI) or Python (MPI)

Parallel Programms: Worked out example (2)

- Task: calculate a large sum of numbers (eg for integration)

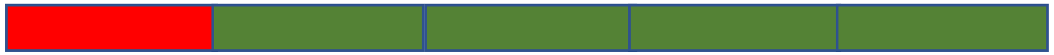
- 6,8,9 core 0 3,5,8 core 1 9,1,2 core 2 2,3,4 core 3
- local sums: 23 16 12 9
- collection: 39 21
- final sum: 50



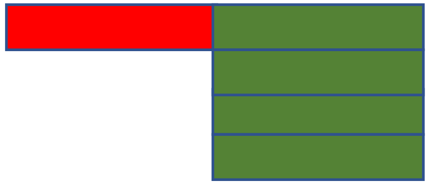
Always check the scaling of your program.

Amdahl’s Law

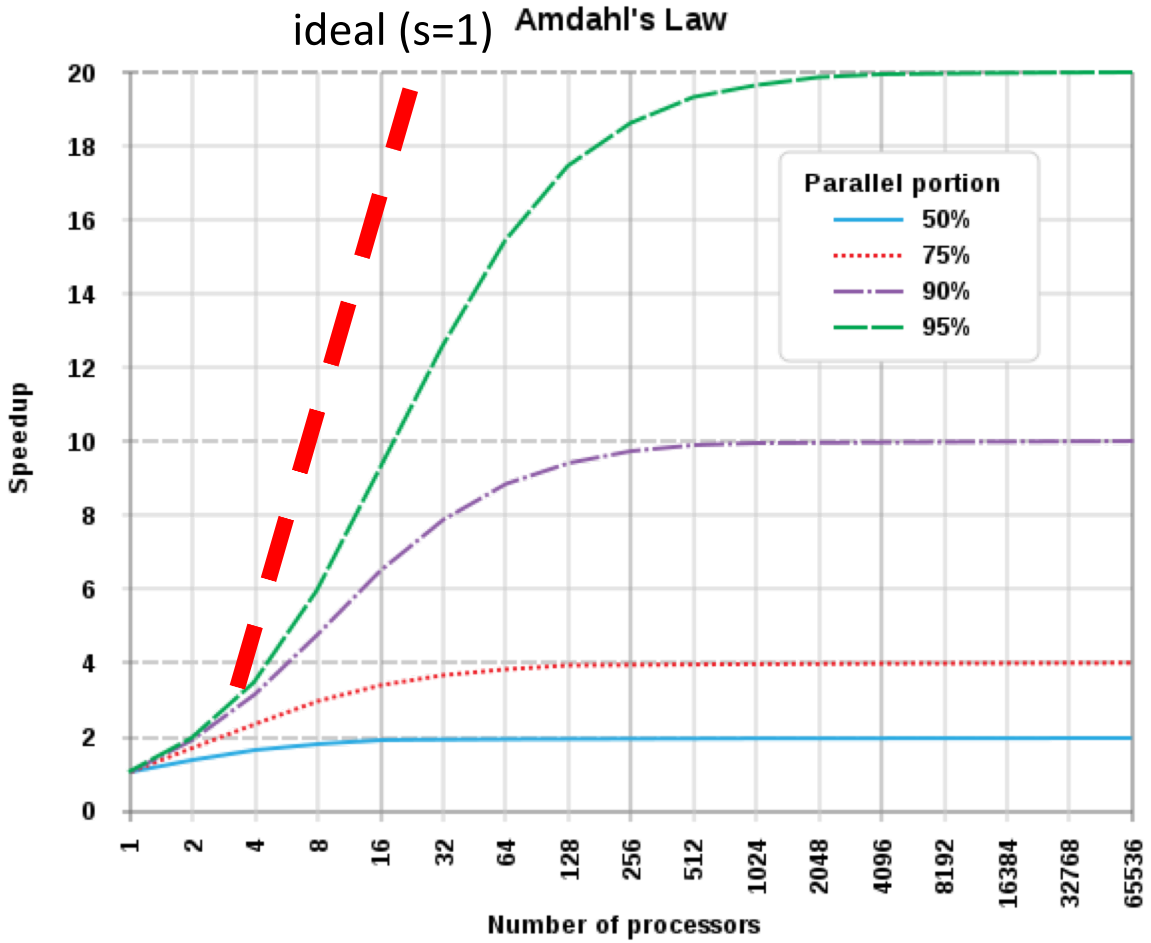
- Given a program consisting of a non-parallelisable and a perfectly parallelisable part



- Fraction s of the non-parallelisable part: $T(p)=T_{seq} + T_{par}(p) = T(1) * s + T(1) * (1-s)/p$



- Speed-up: $S(p) = (1+(1-s)/p)^{-1}$
  - p → inf: $S(p) = 1/s$
  - If $S(p) > 1/s$ → “super-scaler speedup”, problem fit’s into CPU cache.



More Conventions

- Concurrent computing
  - Single program, inside: multiple tasks can be *in progress* at any time.
- Parallel computing
  - Single program, inside: multiple tasks *cooperate closely*
  - tasks run on cores with a very high-speed interconnect, like inside a CPU
- Distributed computing
  - Many programs. These may need to cooperate with each other
  - “loosely coupled”, but in reality: None of these programs may crash.

Shared System: Why two C extensions?

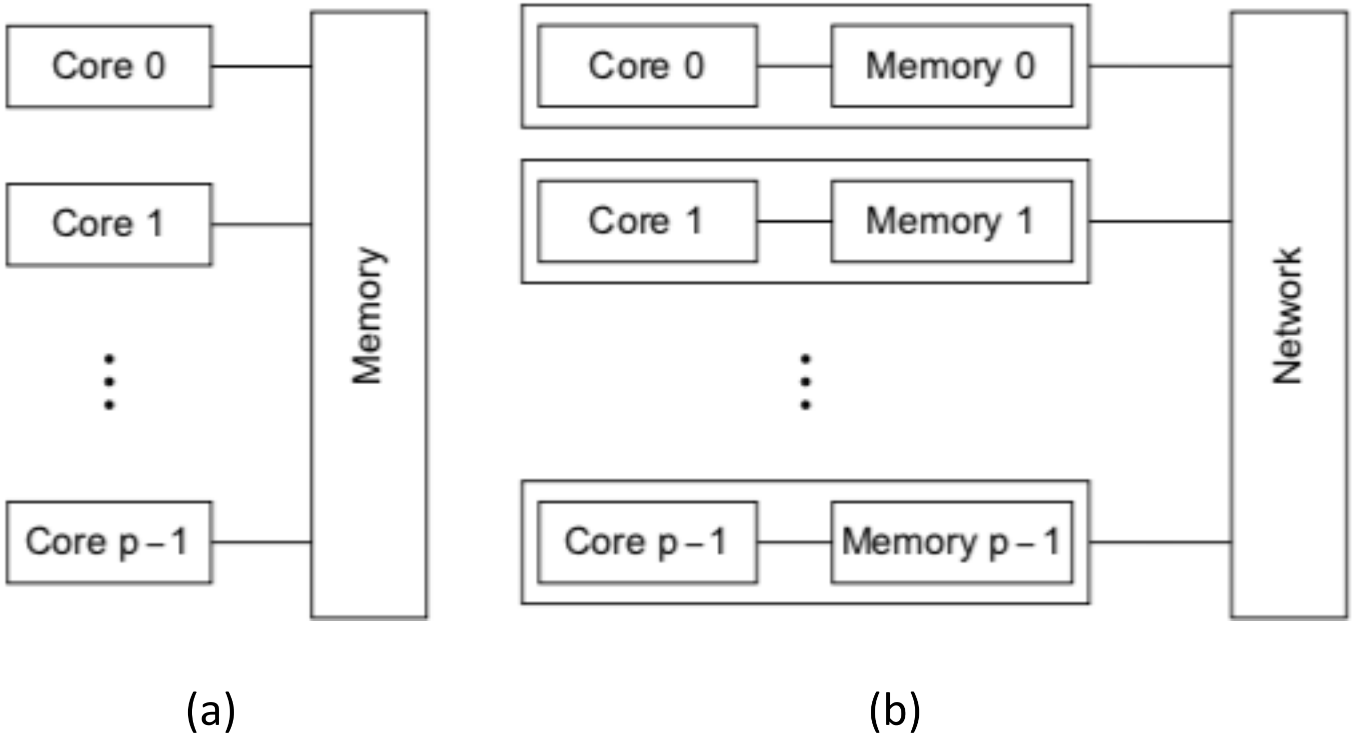
(a) Shared-Memory system:

- Each core can read/write each memory location
- Coordination of cores via shared-memory locations
- Use OpenMP
- Small projects. HIMster2: up to 32 cores/node

(b) Distributed-Memory system:

- Each core has private memory
- Cores explicitly sending messages for data exchange and coordination
- MPI
- Several nodes of a cluster

- Hybrid-Programming:
  - OpenMP+MPI



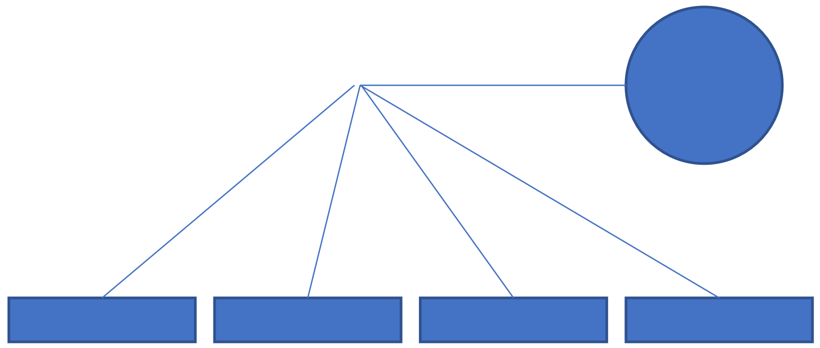
Trivial vs full usage of HPC

- Trivial parallelisation:
  - Run your analysis several times (with different parameters)
  - Out of the box with any non-interactively linux program
  - Outcome / speedup unclear, but works very good for 10-100 jobs in parallel

- Full usage:
  - No automated process to convert a single-core to a multi-core program
  - Write parallel code: This is the content of this lecture starting next week.
  - Use parallel programs: We can discuss such cases.

Building Blocks of a High Performance Computer (HPC)

- Basic building blocks are:
  1. compute nodes
  2. fast interconnect
  3. parallel file system



- Usage remotely, non interactively, through head node

Our HPC: HIMster II. Specs

- 320 Compute Nodes (252 theory, 64 experiment, 4 dev) in 8 racks
  - dual socket Intel 6130 @ 2.1GHz (à 16 cores)
  - 3GB RAM /core
  - OmniPath 100 Gbit/s interconnect
  - 400 GB local SSD scratch
  - https://mogonwiki.zdv.uni-mainz.de/dokuwiki/nodes
- Parallel File System: 747TB Lustre volume (more is ordered)
- Software
  1. organized in modules
     - eg: module avail; module load devel/MariaDB/5.5.52-clientonly
     - See: https://mogonwiki.zdv.uni-mainz.de/dokuwiki/setting_up_environment_modules
  2. More via nfs mount: /cluster (no cvmfs)
  3. Job Scheduler: SLURM (https://slurm.schedmd.com)

HIMster II and Mogon II

- HIMster II and Mogon II form a compound state
  - share login nodes, maintenance servers
  - interconnect: OmniPath (100GBit/s)
- situated in the institute's basement computing room, 750kW
- 2PFlops Linpack (20% contributes HIMster II)
- although calculation on all clusters is possible, use HIMster II
- account registration via PI of HIM or it@him.uni-mainz.de.
  University of Mainz account is mandatory (→ HIM Admin will contact you).
- ssh pbotte@miil01-miil04 (only ssh-key login possible, login Mogon I first via password)
- home directory: Shared with Mogon I, quota 300 GB
- More info: https://mogonwiki.zdv.uni-mainz.de/dokuwiki/ssh_from_outside
- Rules apply: https://www.en-zdv.uni-mainz.de/regulations-for-use-of-the-data- center/

Comparison with its predecessor / do’s

- Per core memory bandwidth
  - HIMster II = 5.6 GByte/sec
  - HIMster = 3.8 GByte/sec
- More memory per core
- HIMsterII has Skylake CPUs (eg AVX512 avail.)
- Storage / Parallel File system:
  - NO BACKUP of data
  - Try to use large files: Source code should be in /home/
  - Try not to put too many files into one directory on LUSTRE (less than 1k)
  - Try to avoid too much metadata load:
    - DO NOT DO ls –l unless you really need it
    - In your scripts avoid excessive tests of file existence (put in a sleep statement between two tests say 30 secs)
    - Use lfs find rather than GNU tools like find
    - Use `O_RDONLY | O_NOATIME` (readonly and no update of access time)

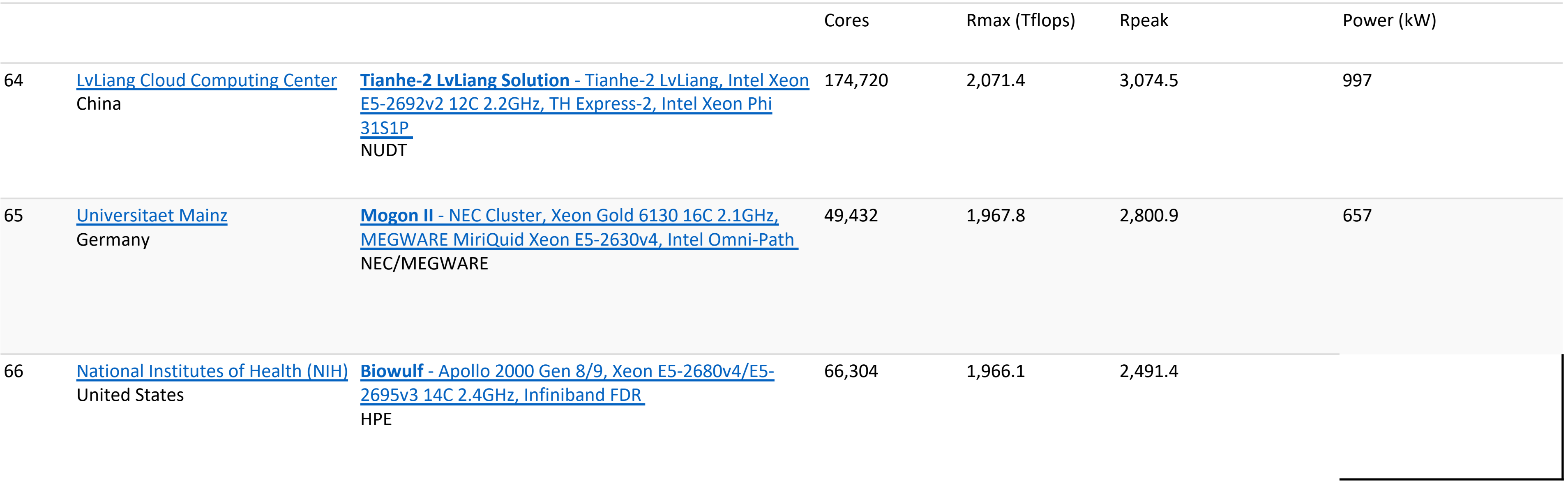
Batch System: SLURM. A quick start

- Introduction and docu:
  - https://mogonwiki.zdv.uni-mainz.de/dokuwiki/slurm_submit
  - https://slurm.schedmd.com/tutorials.html

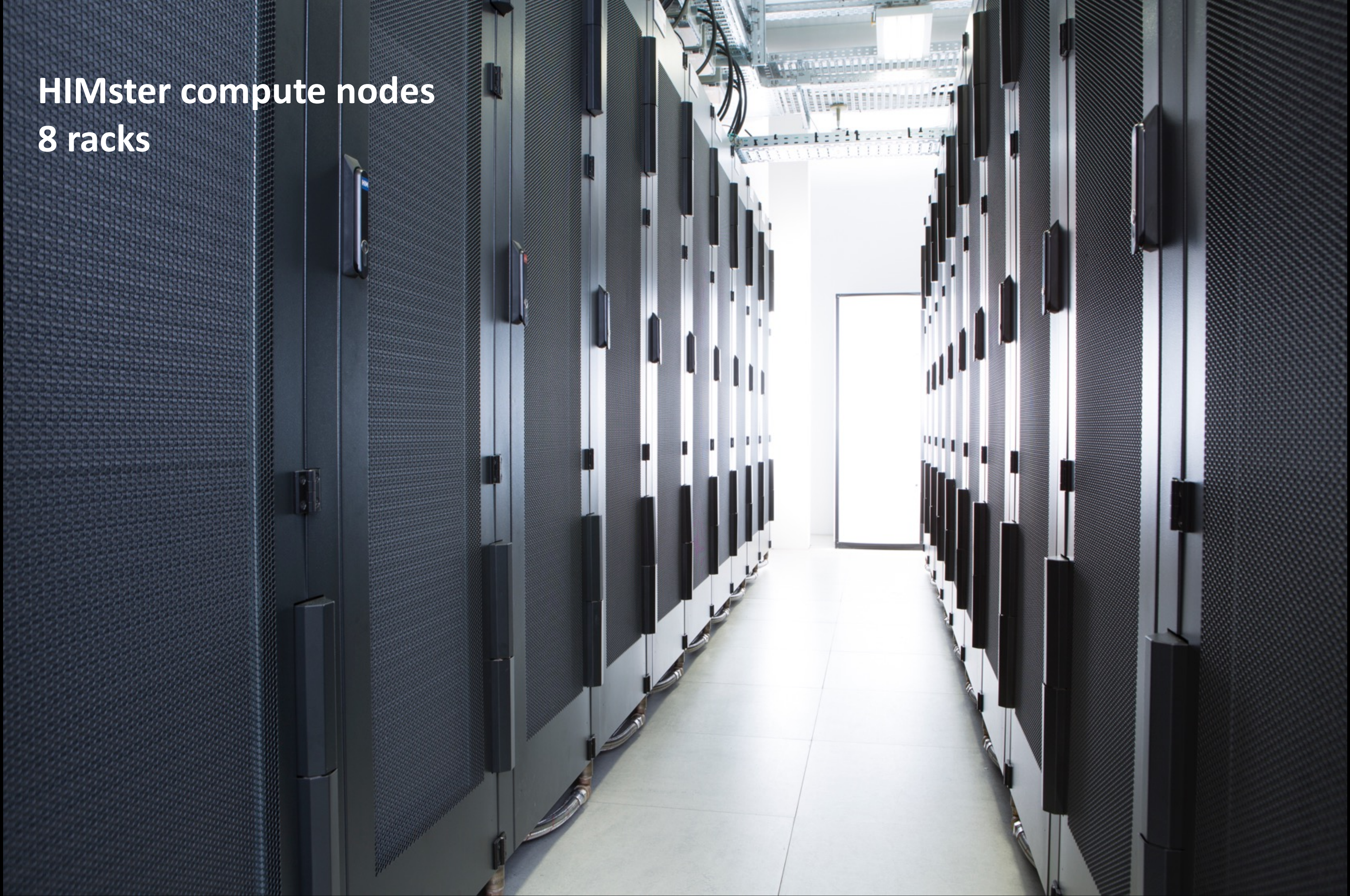
- account to use: m2_himkurs
- Reservation: himkurs
- Submit into partition "parallel" and get an interactive shell:
  - srun --pty -p parallel -A m2_himkurs --reservation kurstest bash -i
- Check what is running: squeue -h | grep pbotte
  - 1184615_79 parallel N203r001 **pbotte** R 1:00:40 52 z[0367-0386,0403-0413,0430-0450]
  - SSH login into your occupied nodes possible: eg ssh z0367

TOP500 and Green500

- https://www.top500.org
- List of all supercomputers with their measured peak performance



			Cores	Rmax (Tflops)	Rpeak	Power (kW)
64	LvLiang Cloud Computing Center China	**Tianhe-2 LvLiang Solution** - Tianhe-2 LvLiang, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	174,720	2,071.4	3,074.5	997
65	Universitaet Mainz Germany	**Mogon II** - NEC Cluster, Xeon Gold 6130 16C 2.1GHz, MEGWARE MiriQuid Xeon E5-2630v4, Intel Omni-Path NEC/MEGWARE	49,432	1,967.8	2,800.9	657
66	National Institutes of Health (NIH) United States	**Biowulf** - Apollo 2000 Gen 8/9, Xeon E5-2680v4/E5-2695v3 14C 2.4GHz, Infiniband FDR HPE	66,304	1,966.1	2,491.4	



HIMster compute nodes
8 racks

Cooling power
for up to 750kW

Power and OmniPath Interconnect

Survey

- Your Name:
- University Username (not email address)
- Workgroup (if applicable, otherwise state your semester)
- Programming Language(s) (state your favourite first, then in descending order)
- Current Use Case (eg. Master/PhD thesis, give some short description)
- Your Programming Skills? (beginner, expert, parallel code written?)
- Why are you attending this course?