02614

High-Performance Computing

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Course curriculum

Three modules:

- Serial tuning (week 1)
- Parallel computing with OpenMP (week 2)
- GPU computing with OpenMP (week 3)

- Three projects – one per week

Course Overview – Topics

- Hardware basics: CPU, caches, memory
- Tuning of sequential programs
- Compilers, Debuggers, Analysis Tools
- Libraries
- Parallel computers – multi-core, SMP, clusters GPGPUs, etc
- Parallel Programming with OpenMP
- GPU computing with OpenMP

Practicalities – I

- Lectures, exercises, project work, etc:
  - “*Every day*”, 9 – 17
  - on-line lectures (Zoom)
  - on-line help during labs (more details later)
- Teachers (week 1 + 2):
  - Bernd Dammann <beda@dtu.dk>
  - Martin, Sebastian, Jonas
  - members of the HPC team (Sebastian, Andrea, Hans-Henrik)

Practicalities – I (cont'd)

- more participants (week 2):
  - students from course 41391 will join us for week 2
- more teachers (week 3):
  - Hans-Henrik Sørensen <hhbs@dtu.dk>
  - Martin, Sebastian, Jonas
  - members of the HPC team (Sebastian, Andrea, Bernd)

Practicalities – II

- Lecture notes:
  - will be made available on DTU Learn
- Exercises:
  - material on DTU Learn
  - access to DTU Linux computers via SSH or ThinLinc
- On-line updates:
  - last minute info will be published on DTU Learn
  - discussions on Piazza or DTU Learn

Practicalities – IIa

Some notes about Piazza:

- Piazza is back – accessible from within DTU Learn
- usage is voluntarily
- single sign-on
- you need to accept the legal terms on the first access
- see also announcement on DTU Learn

Practicalities – III

Literature:

- Part I – Serial Tuning:
  - “Introduction to High-Performance Scientific Computing” by Victor Eijkhout, U of Texas and TACC – on-line available (also as PDF): https://theartofhpc.com/istc.html
  - “Introduction to High Performance Computing for Scientists and Engineers”, by G. Hager & G. Wellein, CRC Press (on-line via DTU Library), Chapters 1-8 relevant for this course
  - other relevant references will be made available during the course

Practicalities – III (cont'd)

Literature:

- Part II – OpenMP:
  - on-line references and articles
  - “Using OpenMP – portable shared memory parallel programming” by B. Chapman, G. Jost and R. van der Pas, MIT Press (2008)
  - “Using OpenMP – The Next Step“ by R. van der Pas, E. Stotzer and C. Terboven, MIT Press (2017) (via DTU Library)
  - “The OpenMP Common Core” by T.G. Mattson, Y. He, and A.E. Koniges, MIT Press (2019)
  - Hager & Wellein (see week 1)

Practicalities – III (cont'd)

Literature:

- Part III – GPU computing with OpenMP
  - more details in week 3

Practicalities – IV

- Three assignments:
  - Groupwork: 3-4 students/group
    - Note: 1 student is NOT a group!
  - Assignment I: Serial tuning
    - deadline: Friday, January 6, 16:00 (!!)
  - Assignment II: OpenMP
    - deadline: Friday, Jan 13, midnight
  - Assignment III: GPU computing
    - deadline: Friday, Jan 20, midnight

Practicalities – IVa

- “Individualized reports”:
  - each assignment has four sub-tasks
  - when handing in the reports, each group member has to take main responsibilty for one sub-task
  - this should be documented in an addendum to the report (we provide a template)
  - But ... remember: all group members should contribute equally to the work, and should know about all parts of the assignment!

Practicalities – V

Requirements for this course:

- Knowledge of at least one of these programming languages: C/C++ (or Fortran)
- Note: Python or MATLAB are not enough!
- Basic understanding of numerical computations
- The will to “play” with new tools and to explore new fields on your own.
- To be able to document what you have done.

Practicalities – VI

Computer usage:

- You are encouraged to use the DTU computer systems – at least for your “production runs”
- Especially needed in weeks 2 and 3, but make your first steps in week 1, already!
- Well defined environment – that is known to work
- Same environment for everybody
- Don't waste time to “roll your own”

Practicalities – VII

Lab exercises & projects:

- Please do the labs! They are the foundations for the projects/assignments
- Read the assignments carefully – and follow the instructions
- We do experiments, and our lab is the computer
- Describe your findings in a well written report – see the 'Assignment Guide' on DTU Learn

What is
High-Performance Computing?

What is HPC?

Do you want to be in low performance computing?

How do I get from A to B as fast as possible?

Vehicle A:

Vehicle B:


WIESBAUER
• Autokrane
• Schwertransporte
• Montagen
www.wiesbauer-krane.de
Rieger SPEZIALTRANSPORTE
74379 Ingersheim Tel. 07142/6867

Vehicle C:

Your choice:

A, B or C?

Road X:

Road Y:

Road Z:

Your choice:

What now?

Payload 1:

Payload 2:

Payload 3:

Payload 4:

Your choice:

Help – there are (too) many choices ...

... and what has this to do with High-Performance Computing?

How do I get from A to B as fast as possible?

... or:

How do I get from my problem (A) to a solution (B) as fast as possible?

(Large Scale) Computations

- Computers

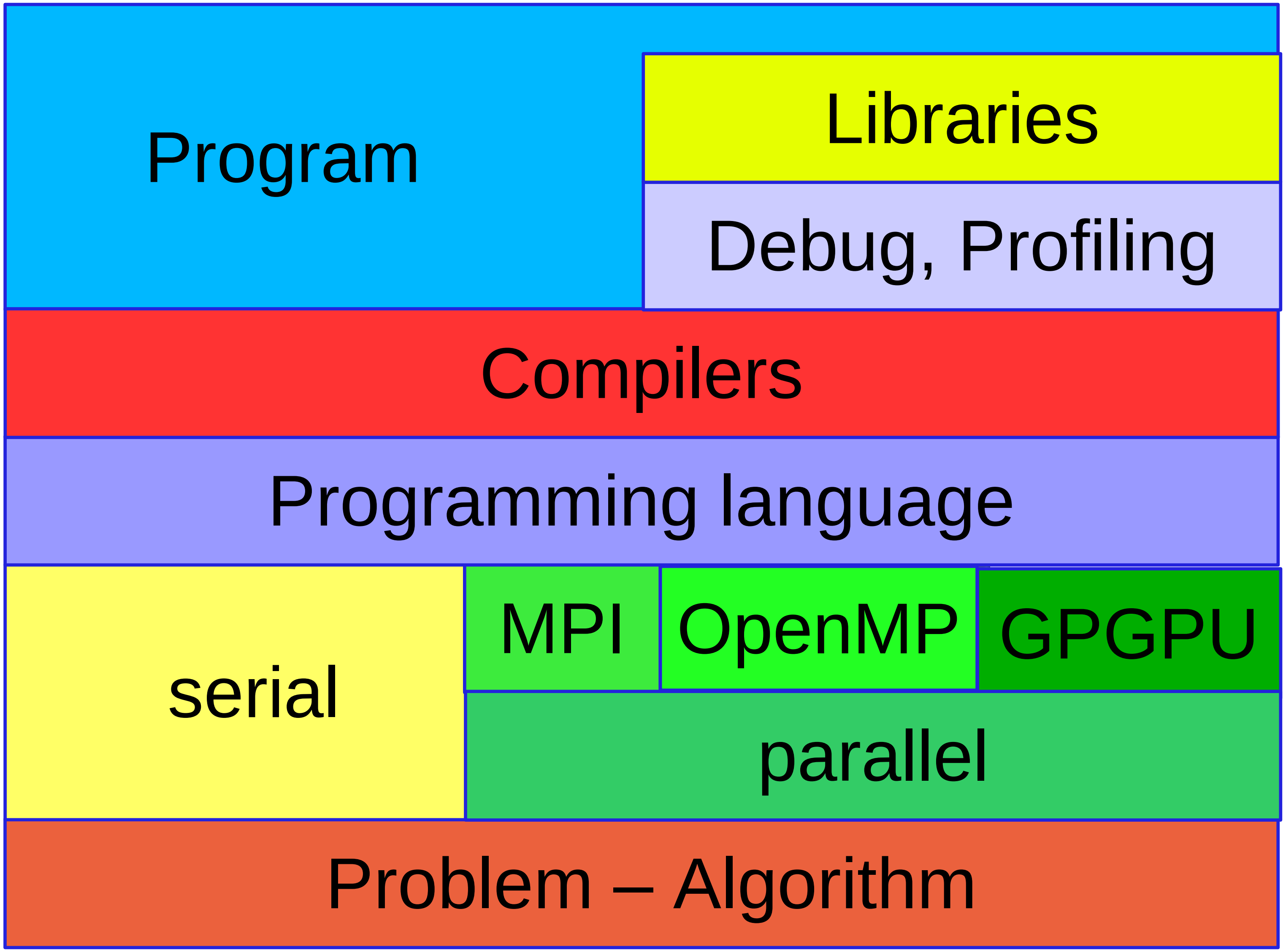
- Algorithms/ Codes

- Data

Large Scale Computations

02614 – Short Introduction

HPC's Caterpillar



… and not to forget:

Computer Simulations

- Alternative to scale models and lab experiments
  - faster and cheaper – more flexible
- Allows a variety of studies
  - isolated phenomena
  - change of one parameter at a time
- Realistic models are large
  - many model parameters
  - capture fine details – fine discretization
  - simulation over a long period of time

Scientific Computing – Examples

- **Astrophysics**
  - stellar physics
  - galaxy evolution
  - exoplanets
- **Cryptography**
  - prime numbers
- **Data mining**
  - Google's Page rank
  - BIG DATA
- **Planetary science**
  - geophysics
  - weather forecasts
  - air pollution
  - climate modeling
- **Quantum Physics & Chemistry**
  - superconductivity
  - material science
  - enzymes
- **Bio-informatics**
  - genome research
  - neuroscience
  - heart simulation
- **Engineering design**
  - fluid mechanics, turbulence
  - hydro dynamics
  - structural design
- **Finance (FinTech)**
- **Machine Learning**
- **AI**

Wind turbine design - CFD

DTU Wind Energy

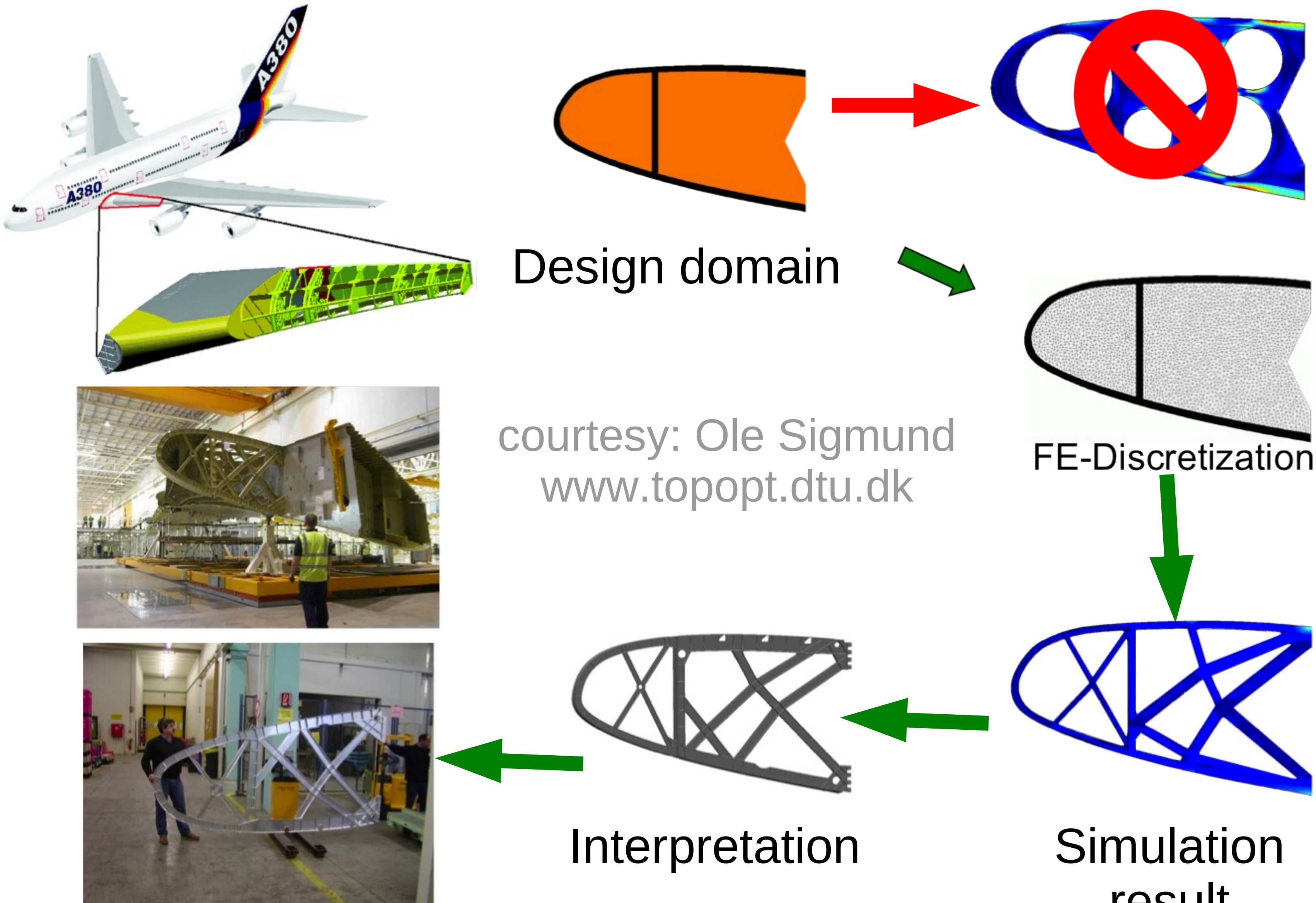
Topology Optimization

... and Materials:

safe and minimum weight structures

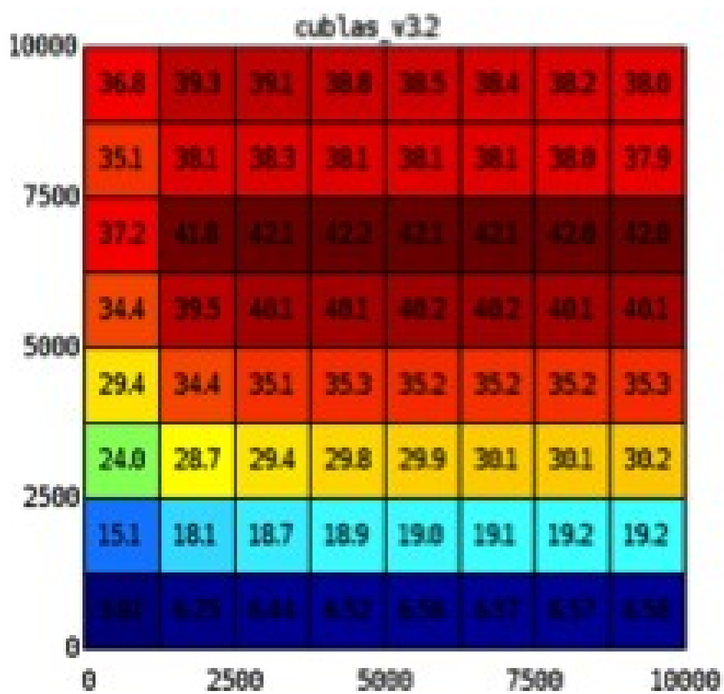
DTU Mechanical Engineering

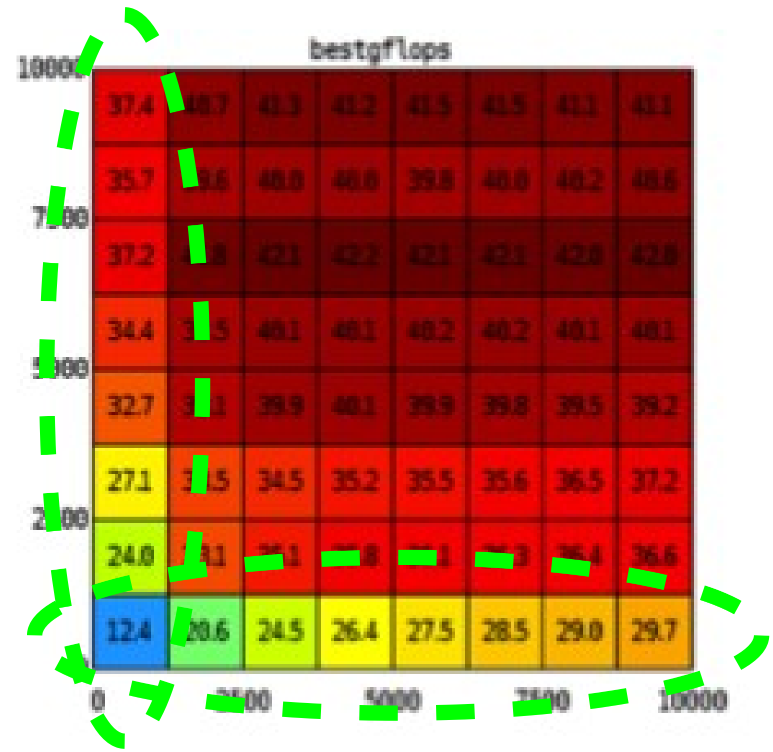
Topology Optimization



Performance Tuning – GPU

Auto-tuning Ax=y (Sgemv) on Nvidia Tesla C2050(blue = slow, red = fast)



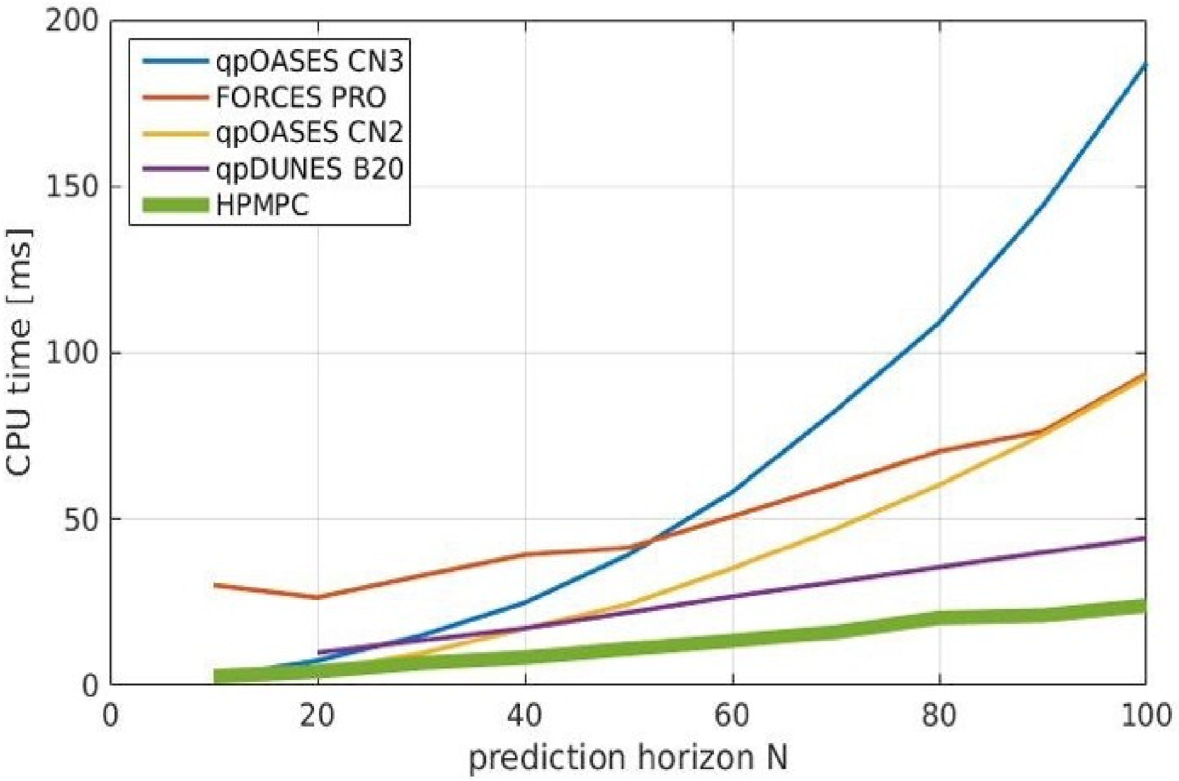


Hans-Henrik Sørensen – GPUlab, DTU Compute

Model Predictive Control (MPC)

HPMPC:

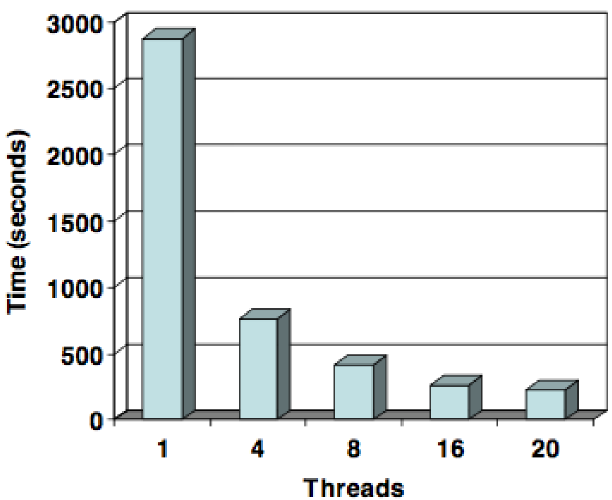
- optimized for small datasets
- “applied HPC”
- close to CPU peak performance

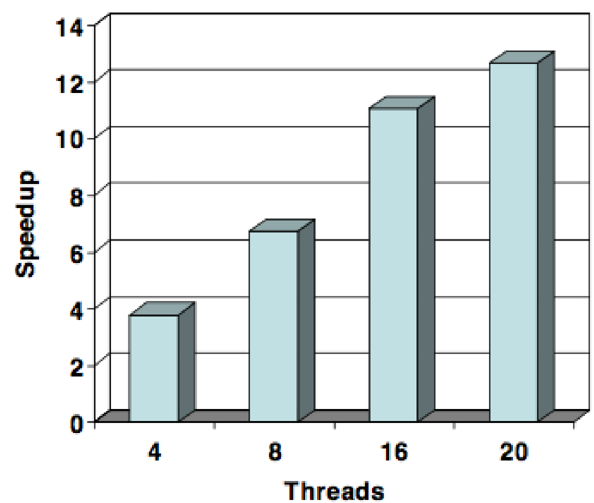


Gianluca Frison, et al – Scientific Computing, DTU Compute

Tuning & Parallelization

- Tuning and parallelization of an existing code from DTU Chemistry: Helium Scattering
- ~3000 lines of Fortran77 code
- parallelized with OpenMP





Bernd Dammann – DTU Compute

What is Performance?

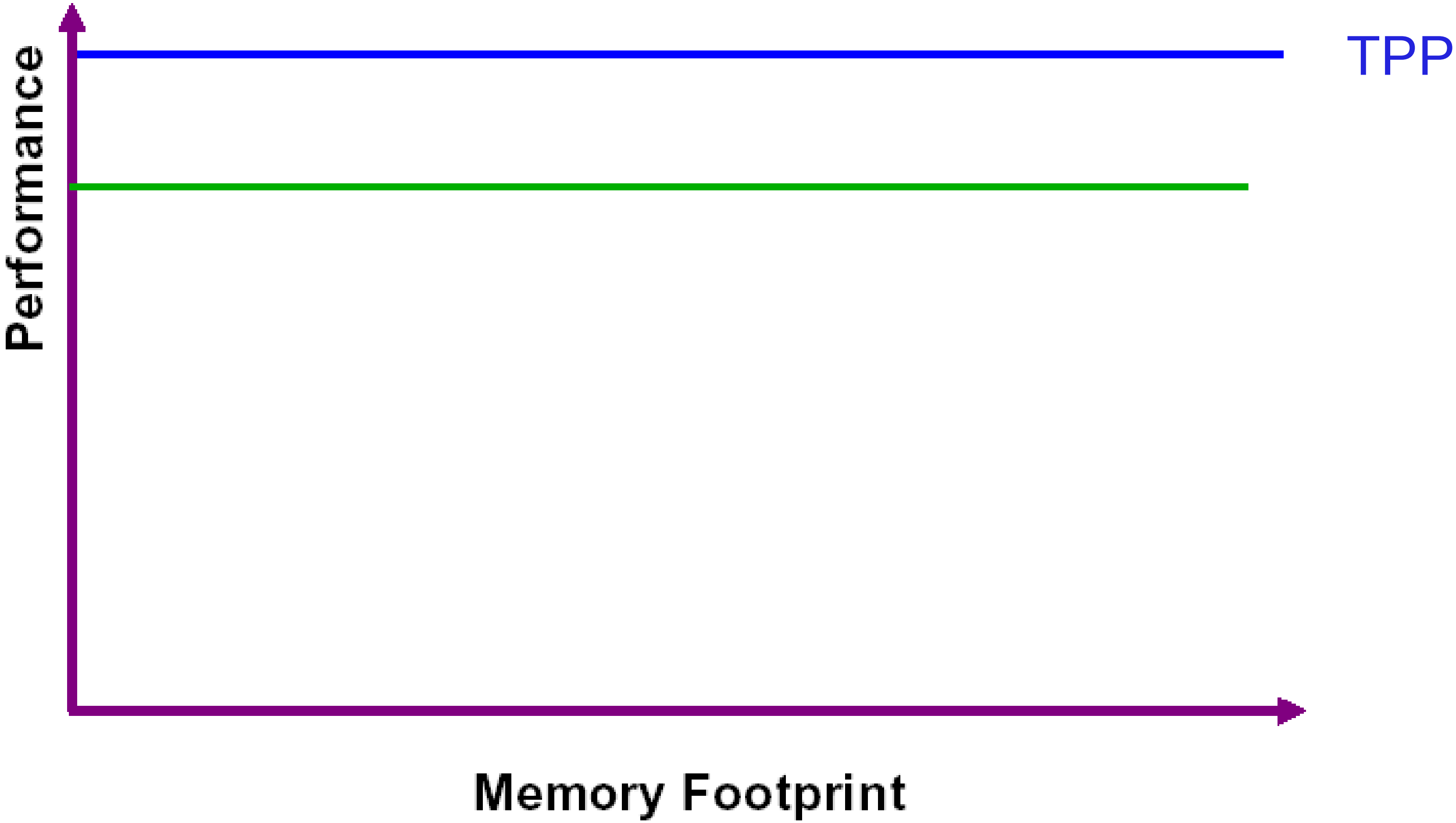
Performance of a Computer

- The performance of a computer is often expressed in Flop/s (floating point operations per second)
- How does this relate to the clock frequency of the CPU?
- Example:
  - modern Intel/AMD CPU, running at 2GHz
  - 16 Floating Point Ops per tick (double precision)
  - Performance: 32 GFlop/s

Theoretical Peak Performance!!!

Performance of a Computer

Intuitive Performance Graph for a given problem:



Live test

- Measure timings/performance of two operations, matrix multiplication and matrix times vector – for different matrix sizes
- Use either ...
  - MATLAB
  - Python
- on your own computer
- ... or on the DTU systems (via ThinLinc)
- download code from DTU Inside

Live test

- MATLAB code

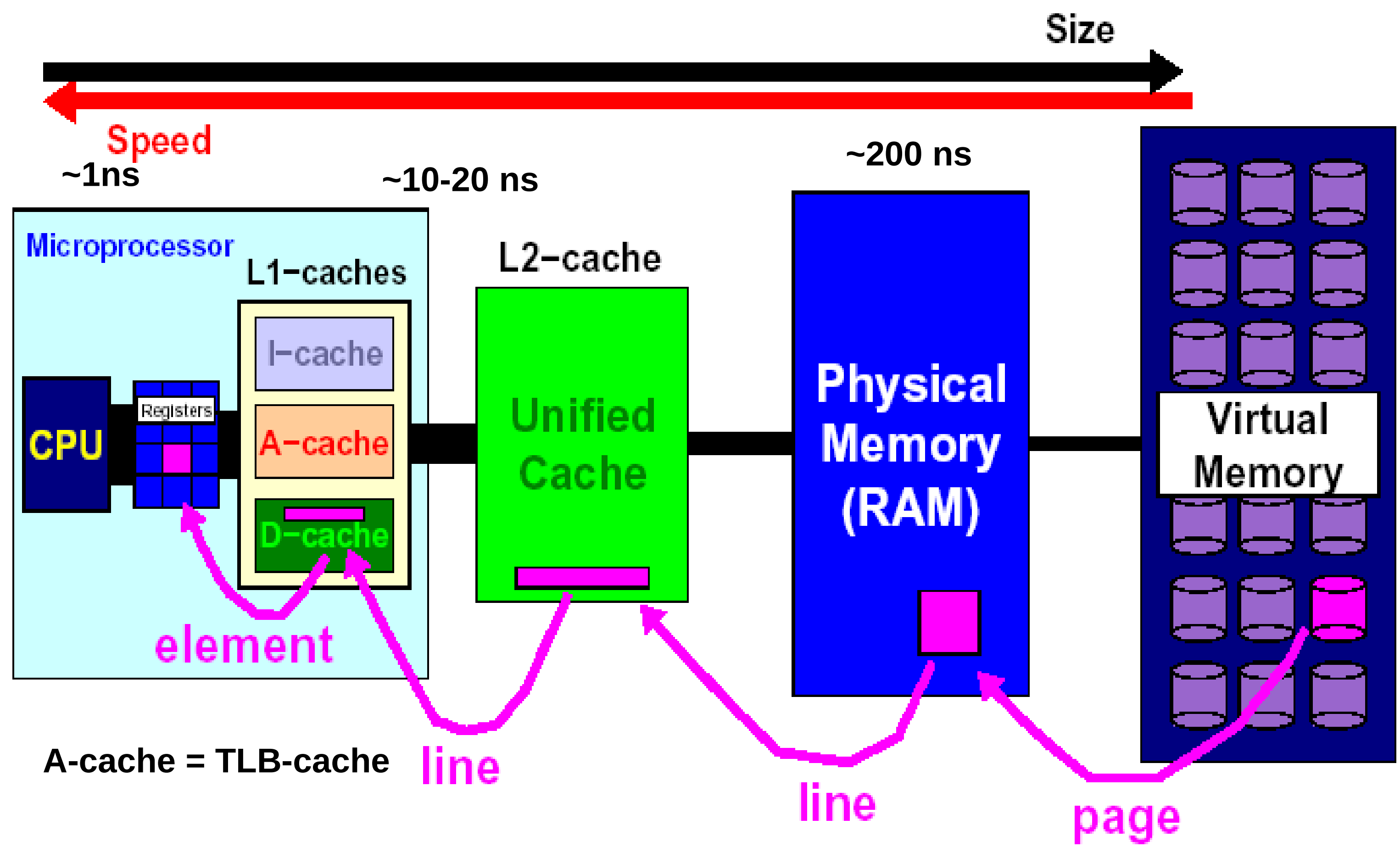
```
A = ones(n);
tic;
B = A*A;
toc
```

- Python code

```
A =np.ones((n,n))
t0 = time()
B = A @ A
dt = time() - t0
```

- do the above for different values of n (500..5000), and plot timings and performance (Mflop/s)
- use the example code from DTU Inside
- give it a try – and report results

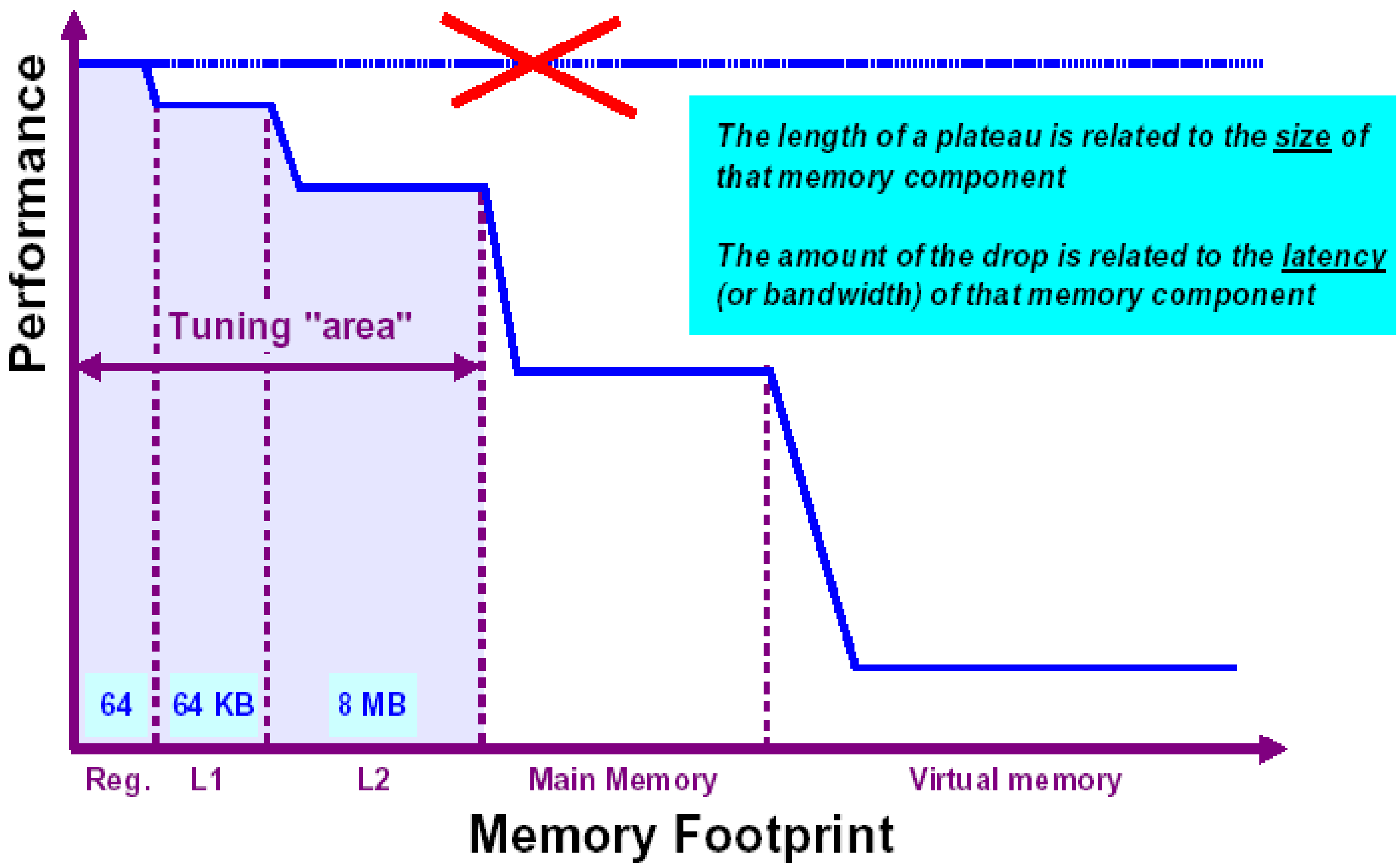
The Memory Hierarchy



Memory Optimization:
Keep frequently used data close to the processor

Performance of a Computer

Performance is not uniform:



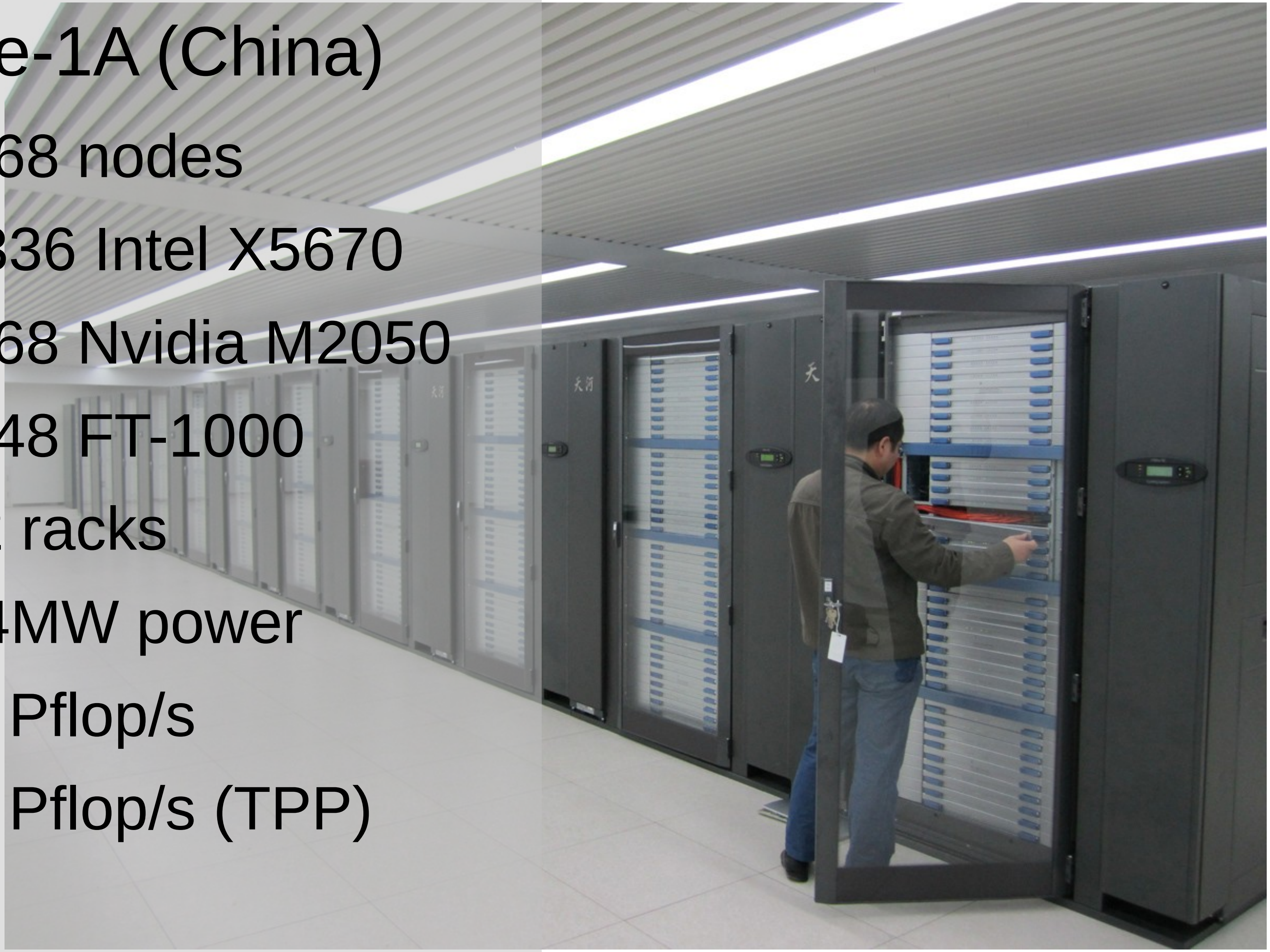
TOP500 – HPC's Formula 1

- The “fastest” computers of the world are ranked on the TOP500 list

  http://www.top500.org/

- Ranking is based on the High-Performance LINPACK (HPL) benchmark, i.e. a collection of linear algebra routines.
- Most of the top sites make use of special hardware, e.g. GPUs, i.e. hardware that is optimized to work with (dense) matrix data.

TOP 500 No. 1 – Nov 2010



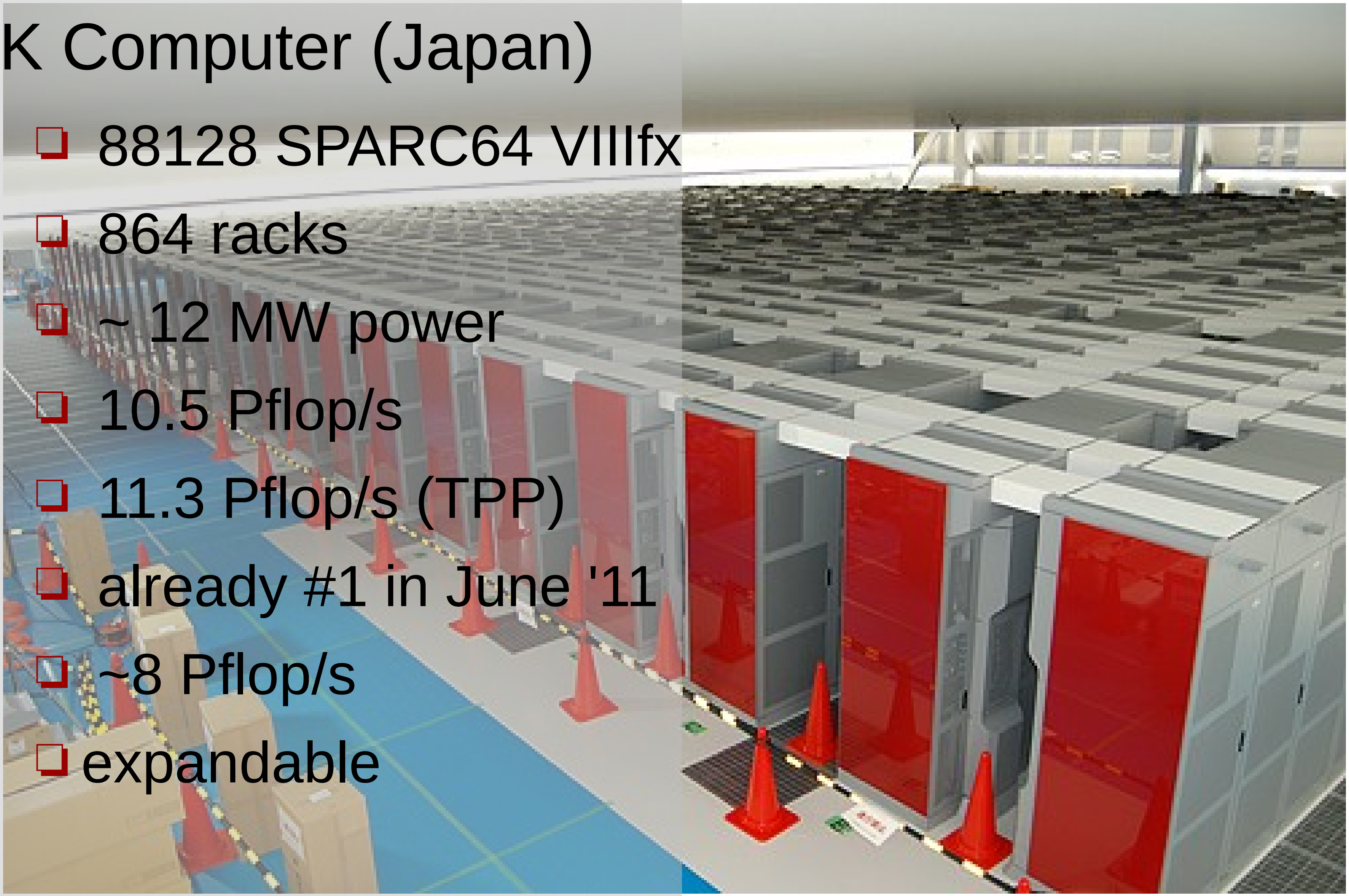
Tianhe-1A (China)

- 7168 nodes
- 14336 Intel X5670
- 7168 Nvidia M2050
- 2048 FT-1000
- 112 racks
- ~ 4MW power
- 2.5 Pflop/s
- 4.7 Pflop/s (TPP)

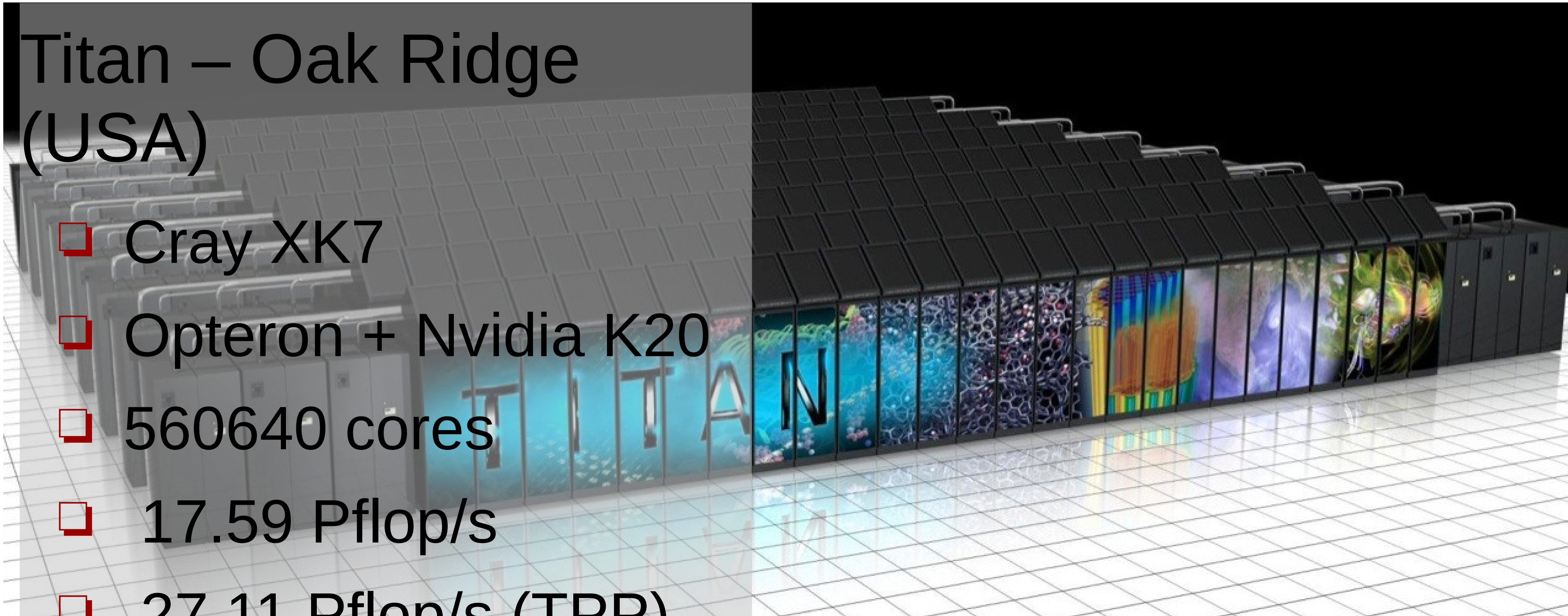
TOP 500 No. 1 – Nov 2011

K Computer (Japan)

- 88128 SPARC64 VIIIfx
- 864 racks
- ~ 12 MW power
- 10.5 Pflop/s
- 11.3 Pflop/s (TPP)
- already #1 in June '11
- ~8 Pflop/s
- expandable



TOP 500 No. 1 – Nov 2012



Titan – Oak Ridge (USA)

- Cray XK7
- Opteron + Nvidia K20
- 560640 cores
- 17.59 Pflop/s
- 27.11 Pflop/s (TPP)
- ~ 8.2 MW power

TOP 500 No. 1 – Jun 2016

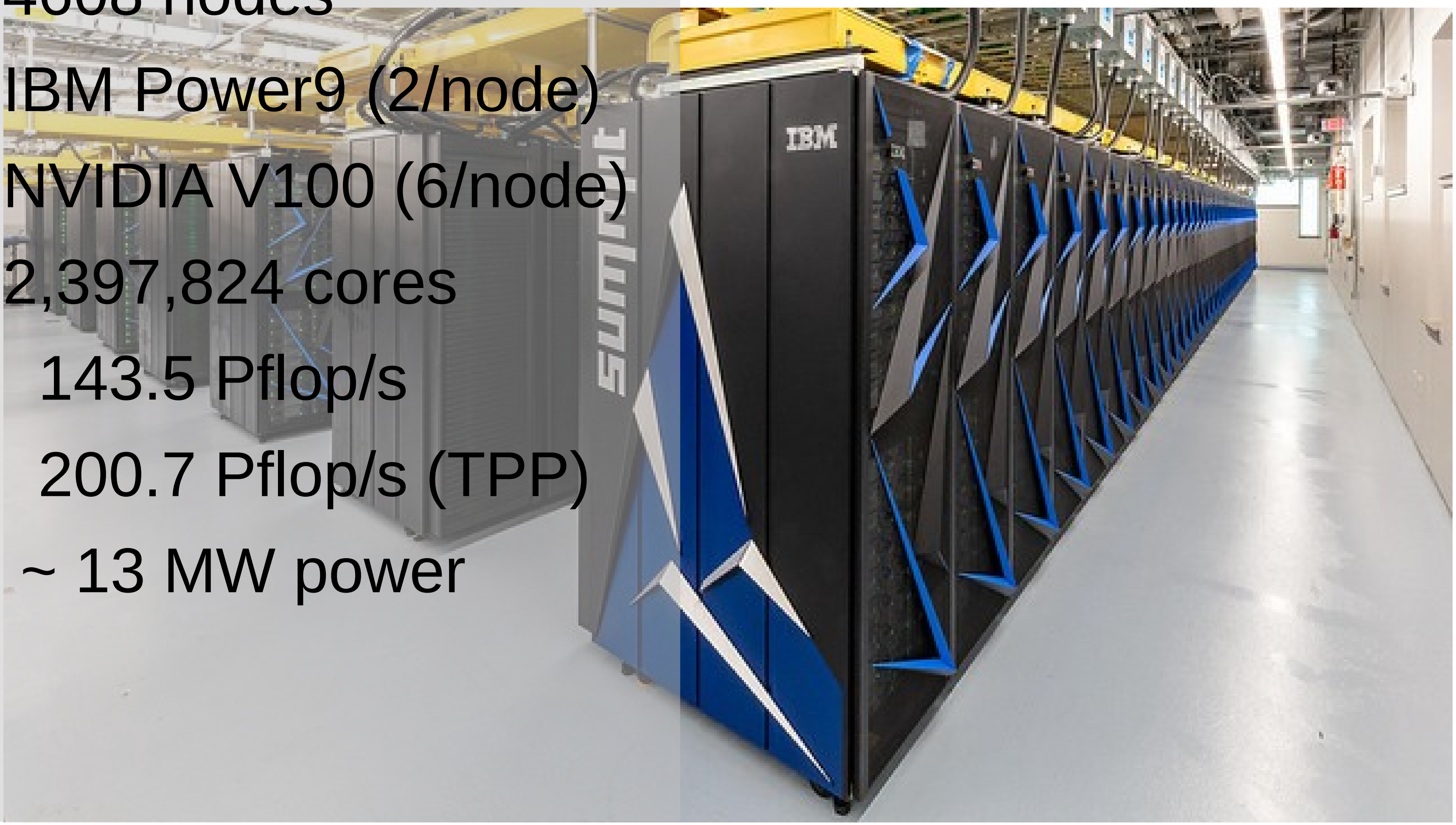
Sunway TaihuLight (China)

- Sunway SW26010 260C 1.45GHz
- 10,649,600 cores
- 93 Pflop/s
- 125 Pflop/s (TPP)
- ~ 15.4 MW power

TOP 500 No. 1 – Nov 2018

Summit (USA)

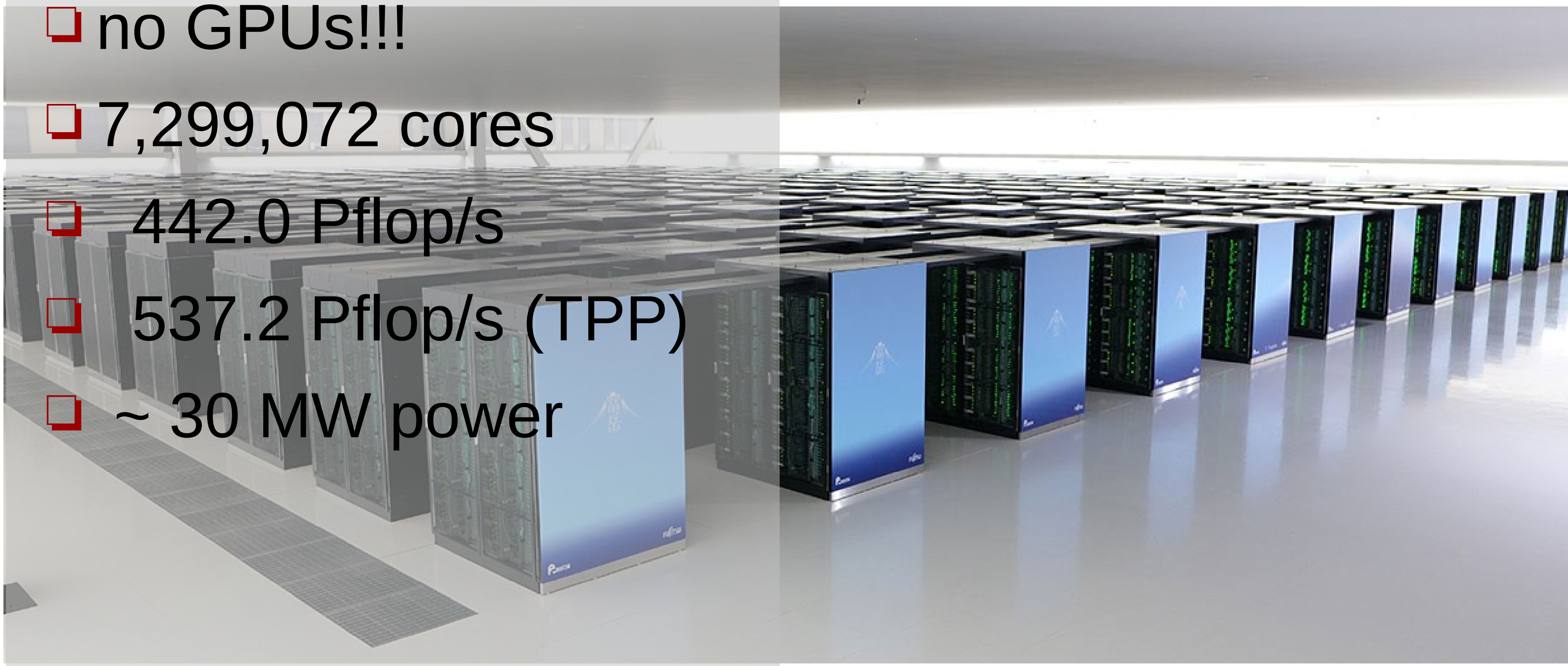
- 4608 nodes
- IBM Power9 (2/node)
- NVIDIA V100 (6/node)
- 2,397,824 cores
- 143.5 Pflop/s
- 200.7 Pflop/s (TPP)
- ~ 13 MW power



TOP 500 No. 1 – Jun 2020

Fugaku (Japan)

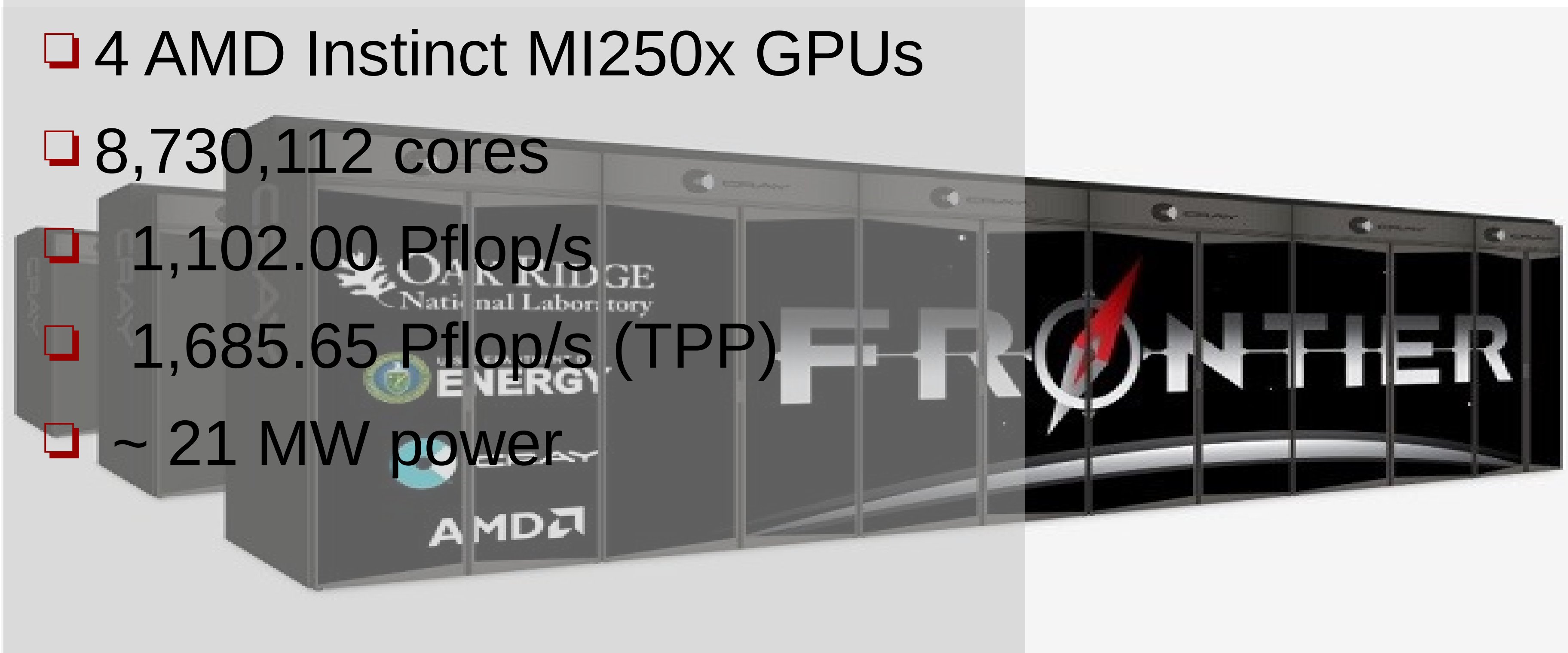
- 158,976 nodes
- ARM A64FX (48 cores)
- no GPUs!!!
- 7,299,072 cores
- 442.0 Pflop/s
- 537.2 Pflop/s (TPP)
- ~ 30 MW power



TOP 500 No. 1 – Jun 2022

Frontier (USA)

- 9,248 nodes
- 1 AMD EPYC (64 cores)
- 4 AMD Instinct MI250x GPUs
- 8,730,112 cores
- 1,102.00 Pflop/s
- 1,685.65 Pflop/s (TPP)
- ~ 21 MW power



TOP 500 – November 2020

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,730,112	1,102.00	1,685.65	21,100
2	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
3	**LUMI** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	2,220,288	309.10	428.70	6,016
4	**Leonardo** - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, Atos EuroHPC/CINECA Italy	1,463,616	174.70	255.75	5,610
5	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148.60	200.79	10,096

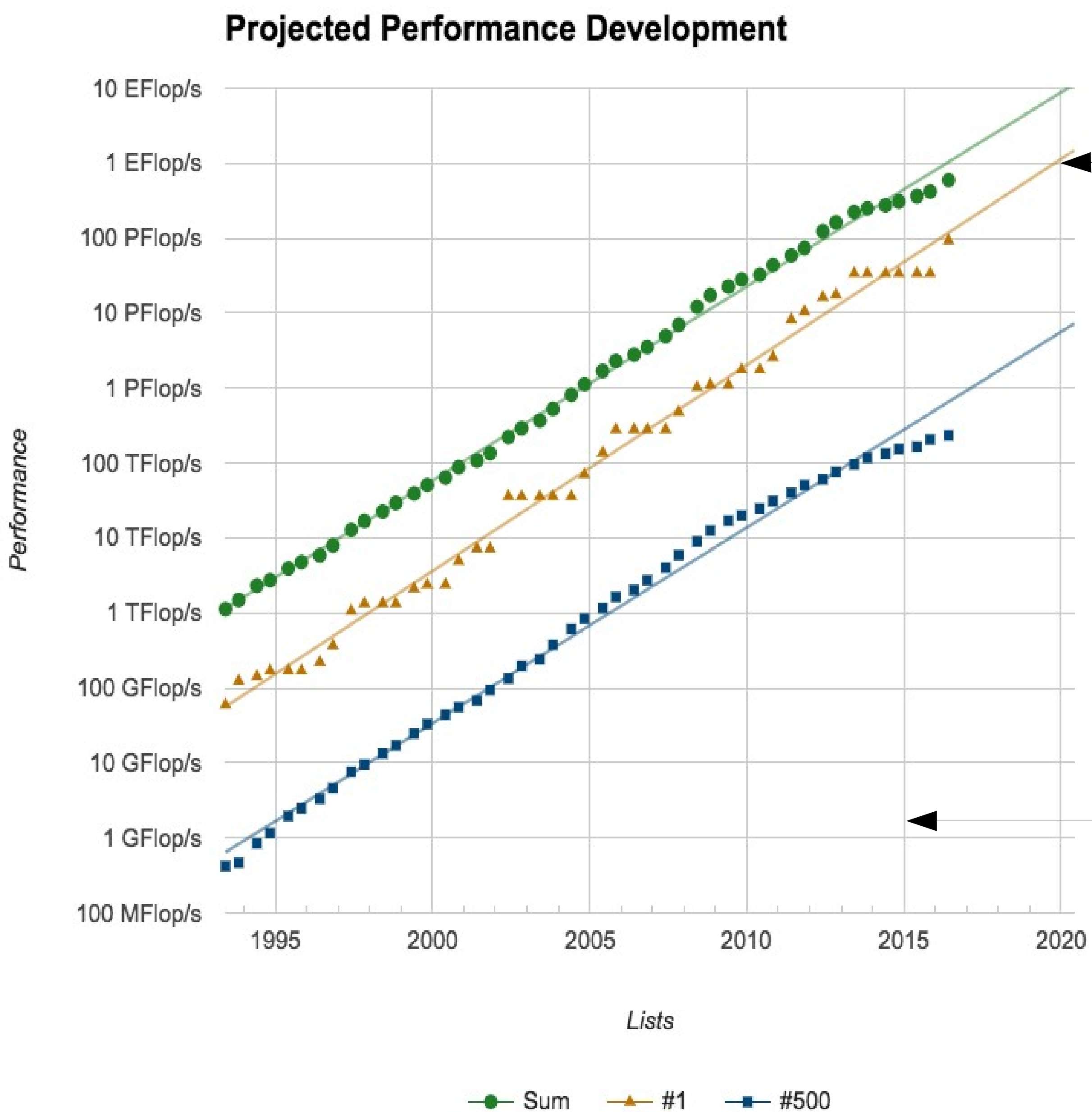
TOP500 – and where is Denmark?

- two entries on the TOP500 list as of June 2017:

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
441	**Vestas1** - Lenovo NeXtScale nx360M5, Xeon E5-2680V3/Xeon E5-2680v4 14C 2.4GHz, Infiniband FDR , Lenovo Vestas Wind Systems A/S Denmark	16,848	481.8	522.5	
459	**Abacus 2.0** - Lenovo NeXtScale nx360M5, Xeon E5-2680v3 12C 2.5GHz, Infiniband FDR, NVIDIA Tesla K40 , Lenovo University of Southern Denmark Denmark	17,928	462.4	836.6	187.5

- since then, DK is not on the list any longer!
- there are probably more powerful installations in DK, but they did not “want” to be on the list
- Denmark owns a share of LUMI (no. 3 on the list)

TOP500 – history and outlook (2017)



the next big step:
1 Exaflop/s

your smartphone

TOP500 – HPC's Formula 1

- Some remarks:
  - not always applicable to 'real world' problems
  - (sometimes) difficult to program
  - huge installations ➔ power issues
    - The TOP500 no. 2 (Fugaku) uses about 29-30 MW
- An alternative list – Green500:
  - http://www.green500.org/
  - measures the power efficiency: Mflop/s / W
  - number 1 on the Green500 list is number 405 on the TOP500 (TOP500 no. 1 ➔ Green500 no. 6)

TOP500 – the Exaflop/s challenge

- first projections said, that the world will see the first Exaflop/s machine around 2018
- since then, it has been postponed several times – the current prediction says ~2022
- Challenges:
  - power consumption (goal: max 20MW!)
  - memory technologies
  - ...
- but there are always surprises, e.g. new CPU designs and/or other technologies, like GPUs

The HPC landscape is changing ...

HPC methods are penetrating all areas of computing

- embedded systems based on multi-core
- use of GPUs as accelerators on desktop and laptop systems
  - mainly driven by AI and Machine Learning
- “Big Data” - HPC methods for high-performance data analytics and visualization

The HPC landscape is changing ...

There are currently discussions about a new and updated benchmark for the TOP500 list

- the current HPC Linpack is not very realistic (dense matrices)
- add more realistic scenarios, e.g. sparse matrix calculations
- add power consumption or a power envelope
- more ...

High-Performance Computing


ESORO
swiss energy
Continental