High-Performance Computing

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High-Performance Computing

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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?

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Vehicle A:

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Vehicle B:

Vehicle C:

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Your choice:

A, B or C?

Road X:

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Road Y:

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Road Z:

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Your choice:

What now?

Payload 1:

Payload 2:

Payload 3:

Payload 4:

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Your choice:

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

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

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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?

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Large Scale Computations

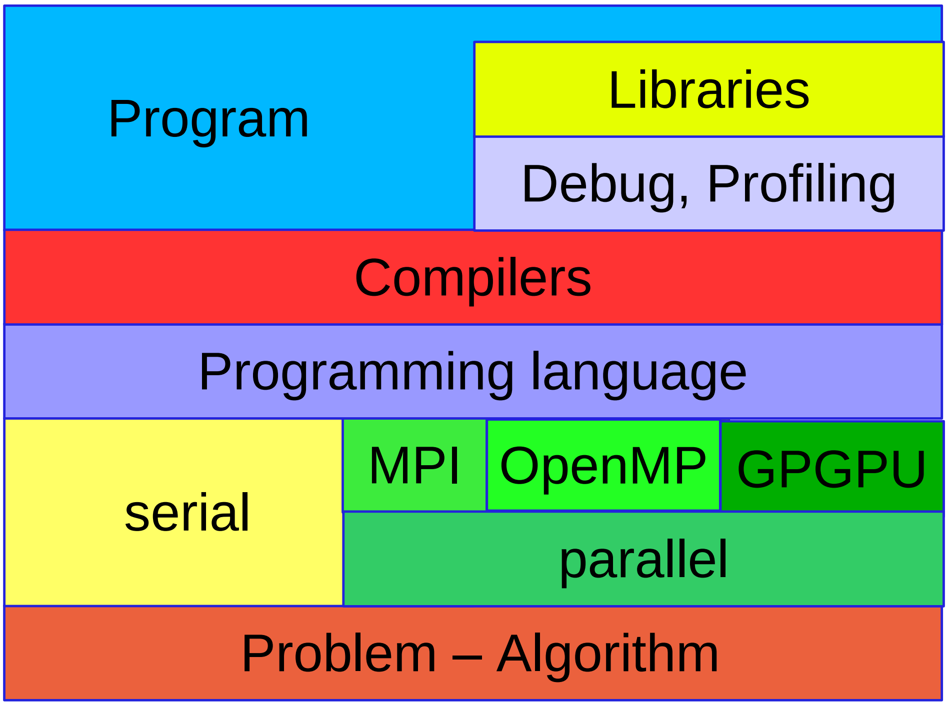
- Computers

- Algorithms/ Codes

- Data

Large Scale Computations

Scientific Computing'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

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Topology Optimization

... and Materials:

safe and minimum weight structures

DTU Mechanical Engineering

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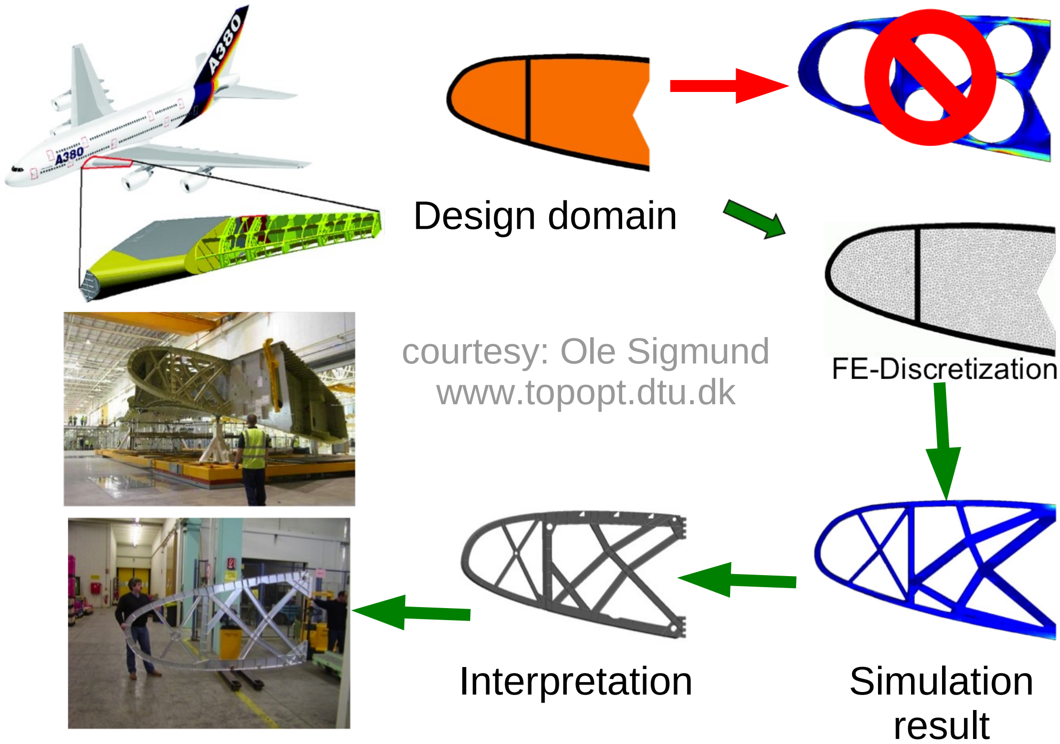
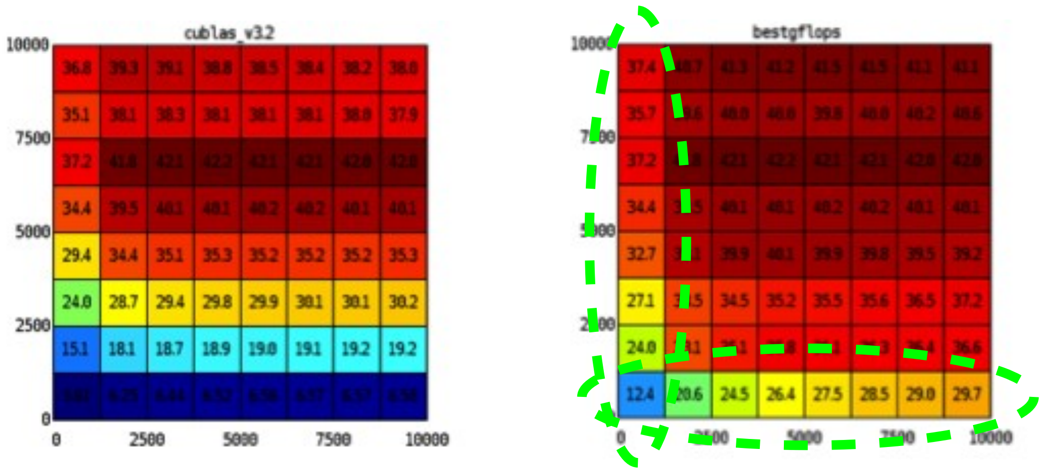
Topology Optimization



Performance Tuning – GPU

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

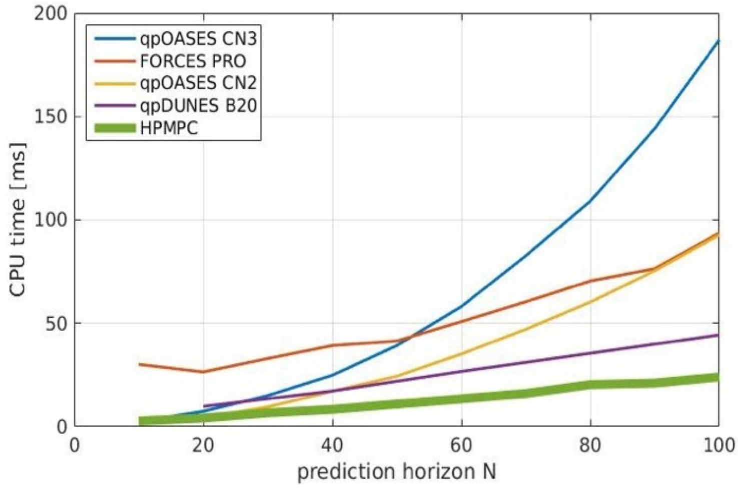


Hans-Henrik Sørensen – GPUlab, DTU Compute

Model Predictive Control (MPC)

HPMPC:

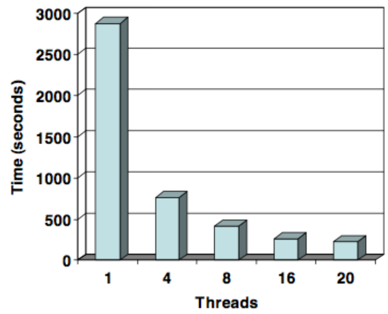
- optimized for small datasets
- "applied HPC"
- close to CPU peak performance

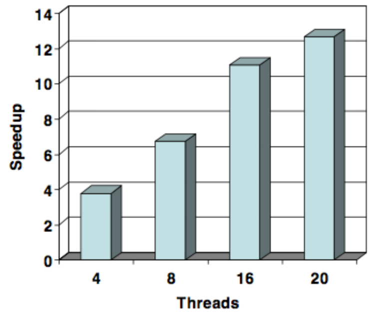


Gianluca Frison, et al – Scientific Computing, DTU Compute

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?

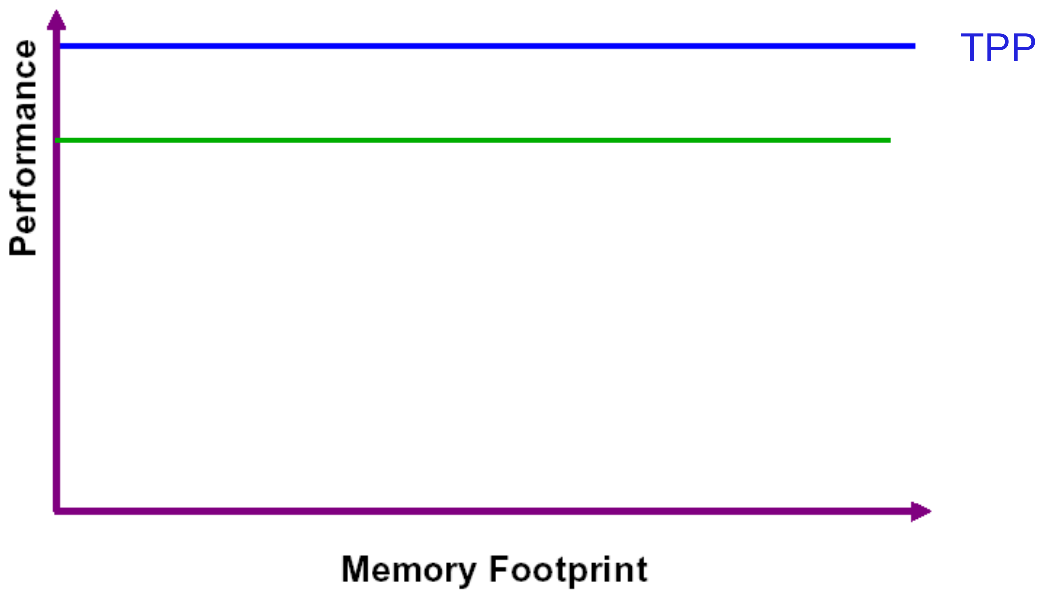
Performance of a Computer

- 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

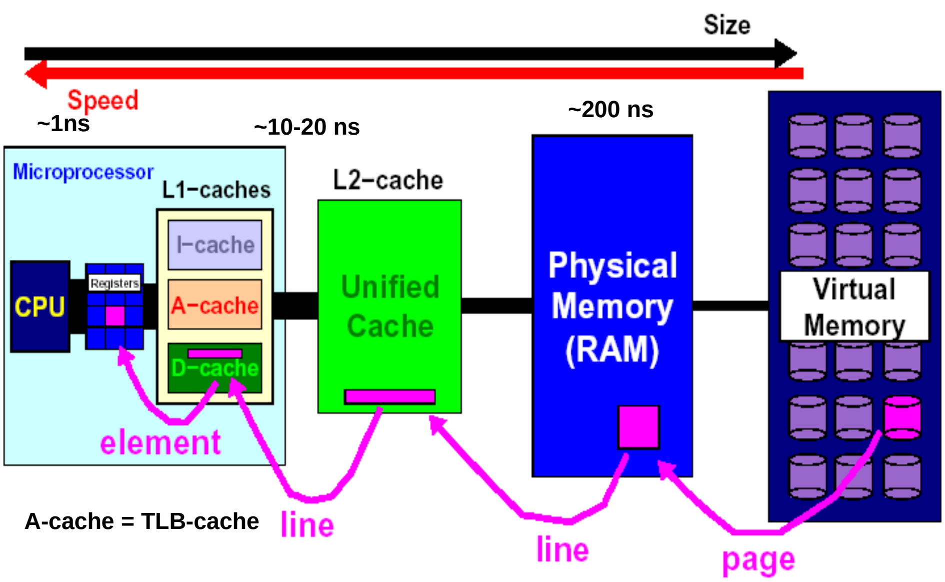
```
A = ones(n);
tic;
B = A*A;
toc
```

- 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

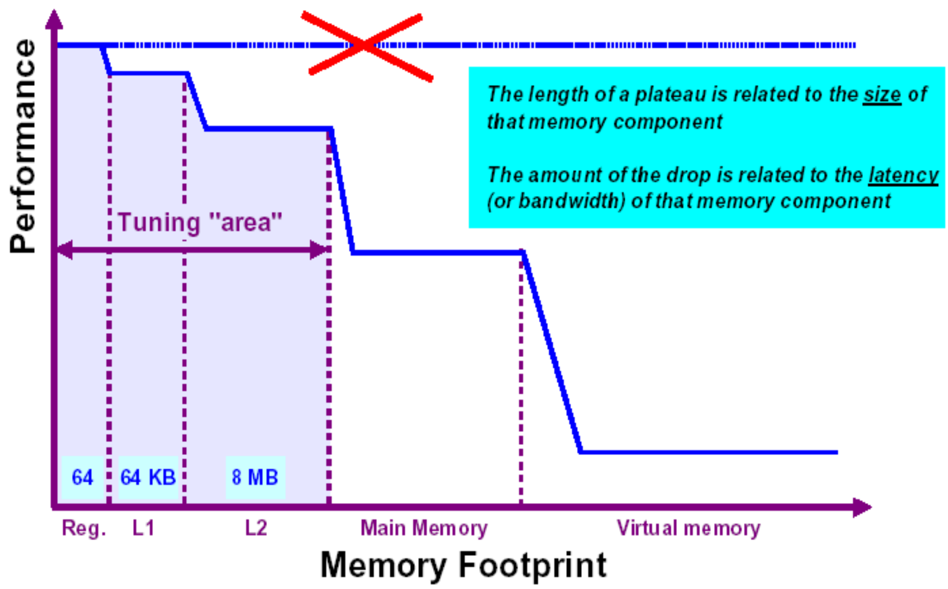
The Memory Hierarchy



Memory Optimization:
Keep frequently used data close to the processor

Performance of a Computer

Performance is not uniform:



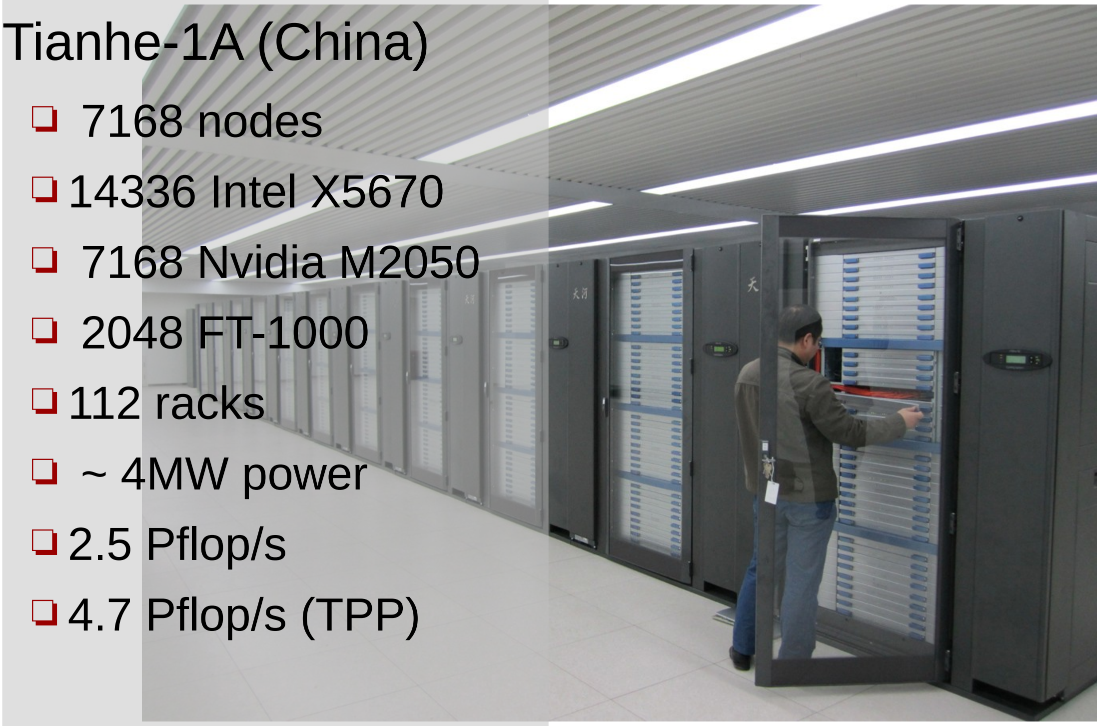
TOP500 – HPC's Formula 1

- 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.

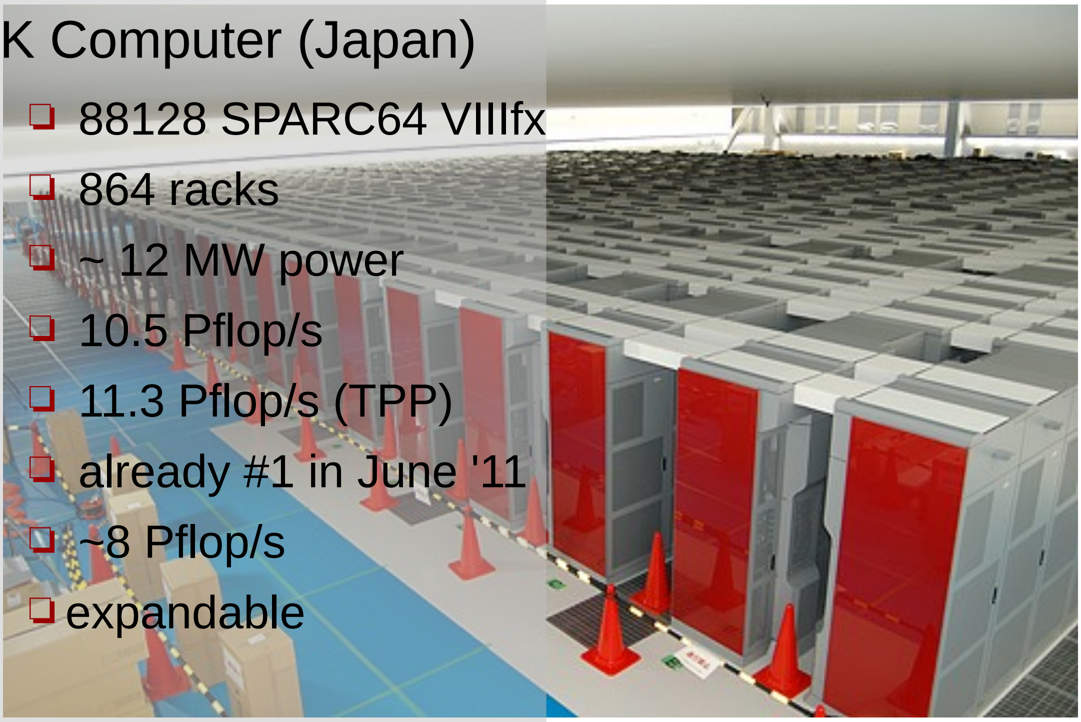
TOP 500 No. 1 – Nov 2010



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)

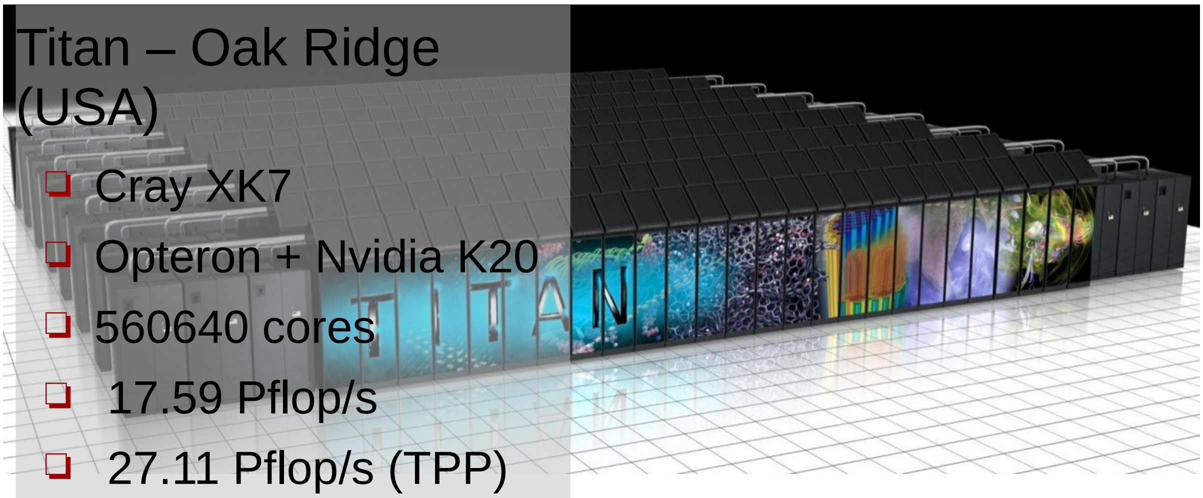
TOP 500 No. 1 – Nov 2011



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

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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

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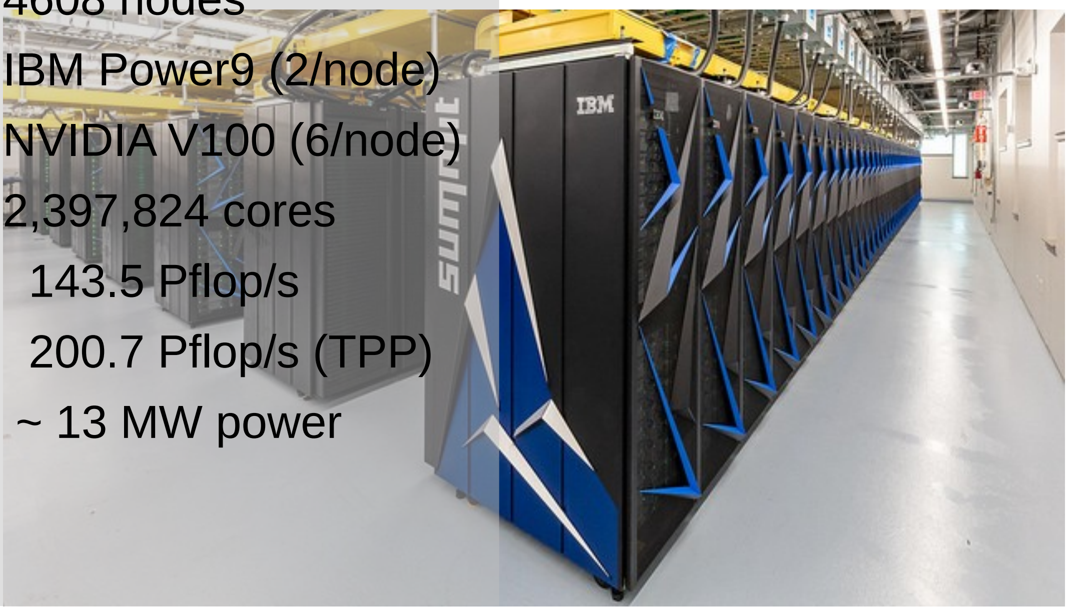
TOP 500 No. 1 – Nov 2018

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

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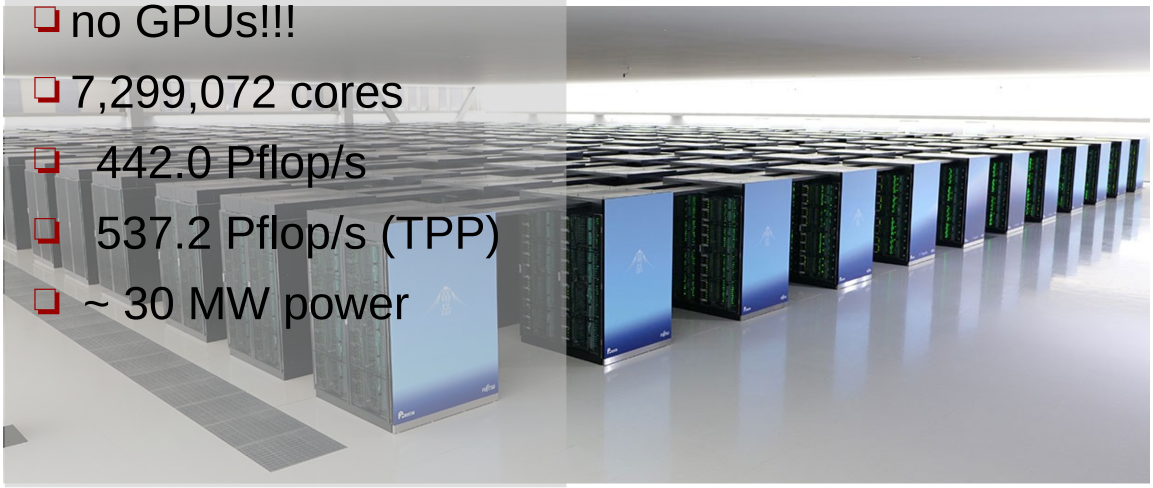
TOP 500 No. 1 – Jun 2020

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



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TOP 500 – November 2020

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442,010.0	537,212.0	29,899
2	**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	148,600.0	200,794.9	10,096
3	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	125,712.0	7,438
4	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway, NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	125,435.9	15,371
5	**Selene** - NVIDIA DGX A100, AMD EPYC 7742 64C 2.25GHz, NVIDIA A100, Mellanox HDR Infiniband, Nvidia NVIDIA Corporation United States	555,520	63,460.0	79,215.0	2,646

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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

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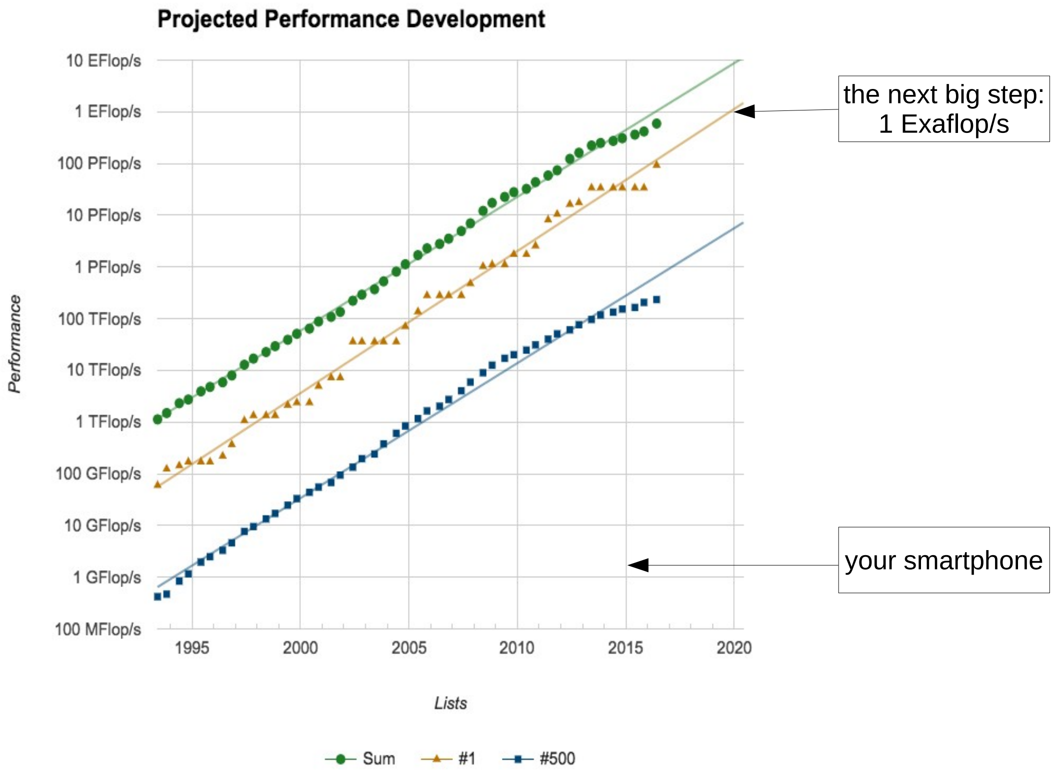
TOP500 – history and outlook



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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. 1 (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 170 on the TOP500 (TOP500 no. 1 → Green500 no. 10)

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 ~2023
- 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 ...

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