High-Performance Computing

02614

High-Performance Computing

02614 – Short Introduction

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Course curriculum

Three modules:

- Serial tuning (week 1)
- Parallel computing with OpenMP (week 2)
- GPU computing with CUDA (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 CUDA (and OpenCL)

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Practicalities – I

- Lectures, exercises, project work, etc:
  - "*Every day*", 9 – 17
  - lecture room 49, building 303B
- Teachers (week 1 + 2):
  - Bernd Dammann <beda@dtu.dk>
  - Nicolai Brogaard Riis
  - members of the HPC team (Sebastian, Andrea, Hans-Henrik)

Practicalities – I (cont'd)

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

Practicalities – II

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

Practicalities – III

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Literature:

- Part I – Serial Tuning:
  - list of relevant articles, books and on-line references will be made available during the course, e.g.
  - “Introduction to High-Performance Scientific Computing” by Victor Eijkhout, U of Texas and TACC – on-line available as PDF http://tinyurl.com/EijkhoutHPC
  - “Introduction to High Performance Computing for Scientists and Engineers”, by G. Hager & G. Wellein, CRC Press (on-line via DTU Library)

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Practicalities – III (cont'd)

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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)
  - Hager & Wellein (see week 1)

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Practicalities – III (cont'd)

Literature:

- Part III – CUDA:
  - on-line references and articles
  - “CUDA by example”, by J. Sanders & E. Kandrot, Addison-Wesley (2011)
  - “Programming Massively Parallel Processors”, by David B. Kirk & Wen-mei W. Hwu, Morgan Kaufmann (2010)

Practicalities – IV

- Three assignments:
  - Groupwork: 3 students/group
    - Note: 1 student is NOT a group!
  - Assignment I: Serial tuning
    - deadline: Saturday, Jan 6, 12:00 (noon!!)
  - Assignment II: OpenMP
    - deadline: Friday, Jan 12, midnight
  - Assignment III: GPU computing
    - deadline: Friday, Jan 19, midnight
- The last assignment report is individual!!!

Practicalities – V

Requirements for this course:

- Knowledge of at least one programming language: C, C++ (or Fortran)
- 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
- Describe your findings in a well written report – see the 'Assignment Guide' on CampusNet

Where to go from here?

- Advanced courses:
  - 02616 – Large Scale Modelling (not this year!)
- MSc (or BSc) projects:
  - Scientific Computing Section at DTU Compute
  - HPC Competence Center
  - Collaboration with other DTU departments, e.g.
    - DTU Physics
    - DTU Electrical Engineering
    - DTU Mechanical Engineering
    - DTU Management Engineering

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:

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 ...

... 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?

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Large Scale Computations

- Computers

- Algorithms/ Codes

- Data

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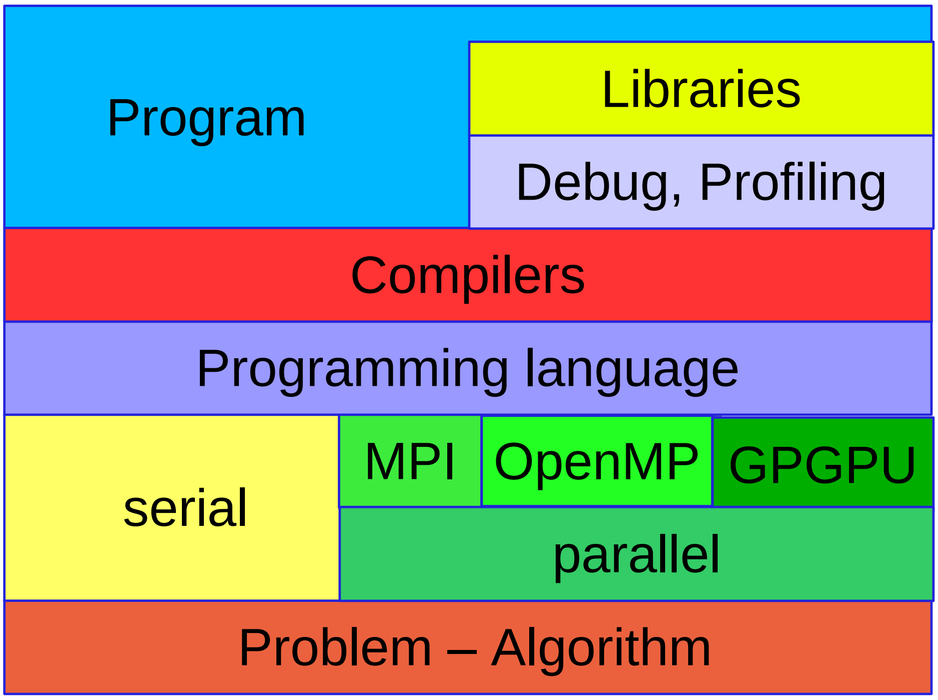
Large Scale Computations

Scientific Computing's Caterpillar



... and not to forget:

The PITAC report - 2005

President's Information Technology Advisory Committee, US

- "Computational science now constitutes what many call the third pillar of the scientific enterprise, a peer alongside theory and physical experimentation."
- "Computational science is a rapidly growing multidisciplinary field that uses advanced computing capabilities to understand and solve complex problems."

The US Exascale Initiative

- In the US, HPC is a matter of national importance:
  - on Jul 29, 2015, the US President issued an "*Excutive Order*" for the "National Strategic Computing Initiative (NSCI)"
- in popular words called the 'Exascale Initiative'
- for more information, see the announcement on the 'Whitehouse Blog'

Computational Science

Computational science fuses 3 distinct elements:

- Algorithms (numerical and non-numerical) and modeling and simulation software developed to solve science (e.g., biological, physical, and social), engineering, and humanities problems
- Computer and information science that develops and optimizes the advanced system hardware, software, networking, and data management components needed to solve computationally demanding problems
- The computing infrastructure that supports both the science and engineering problem solving and the developmental computer and information science

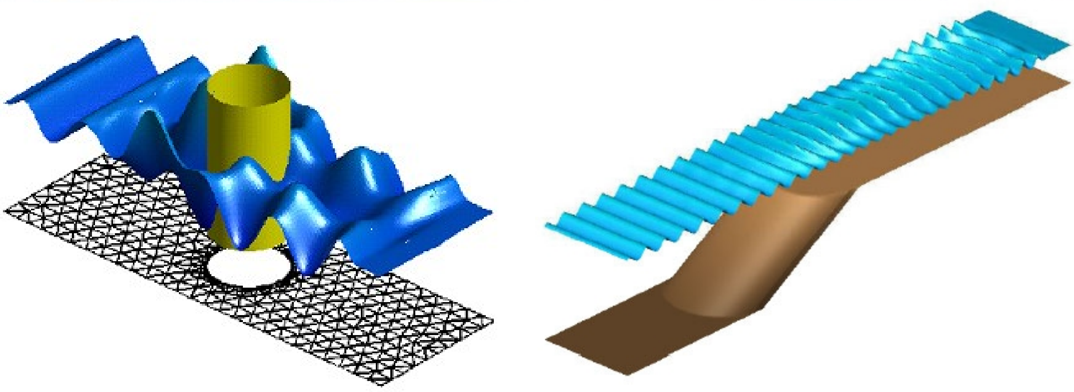
Computer Simulations

- 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

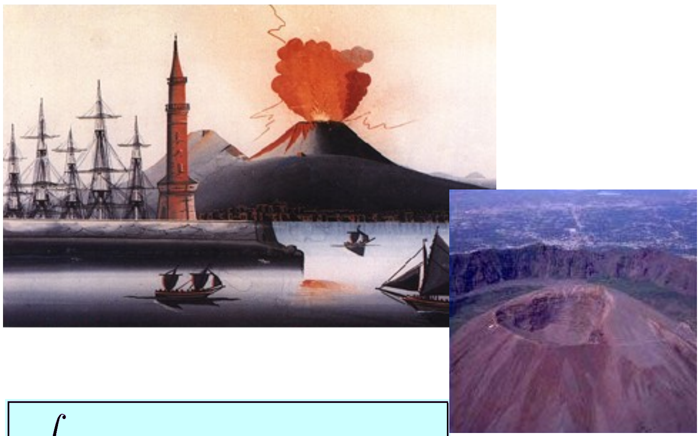
- **Astrophysics**
  - stellar physics
  - galaxy evolution
- **Cryptography**
  - prime numbers
- **Experimental mathematics**
  - fast convergent series
- **Data mining**
  - Google's Page rank
  - BIG DATA
- **Planetary science**
  - geophysics
  - weather forecasts
  - air pollution
  - climate modeling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

Breaking The Waves



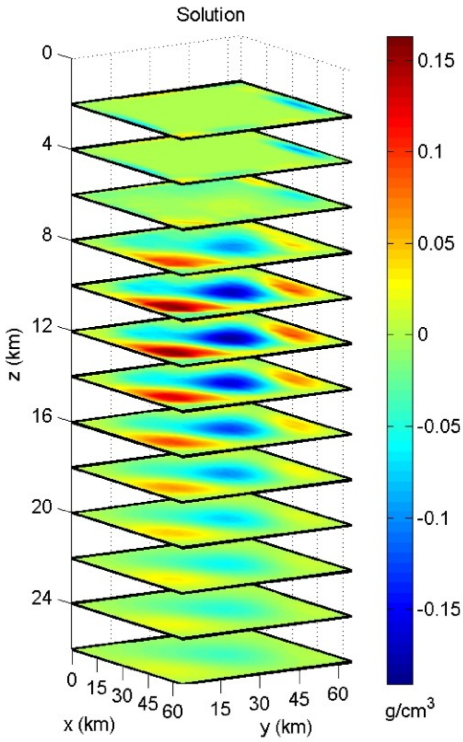
Allan Engsig-Karup – DTU Compute

Inverse Geomagnetic Problems



$$\int_{\Omega} K(\mathbf{s},\mathbf{t})\, f(\mathbf{t})\, d\Omega = g(\mathbf{s})$$

$$\begin{aligned} f(\mathbf{t}) &= \text{magnetization} \\ g(\mathbf{s}) &= \text{data (anomaly)} \\ K(\mathbf{s},\mathbf{t}) &= \text{magnetic dipole field} \end{aligned}$$



Per Chr. Hansen – DTU Compute

Wind turbine design - CFD

DTU Wind Energy

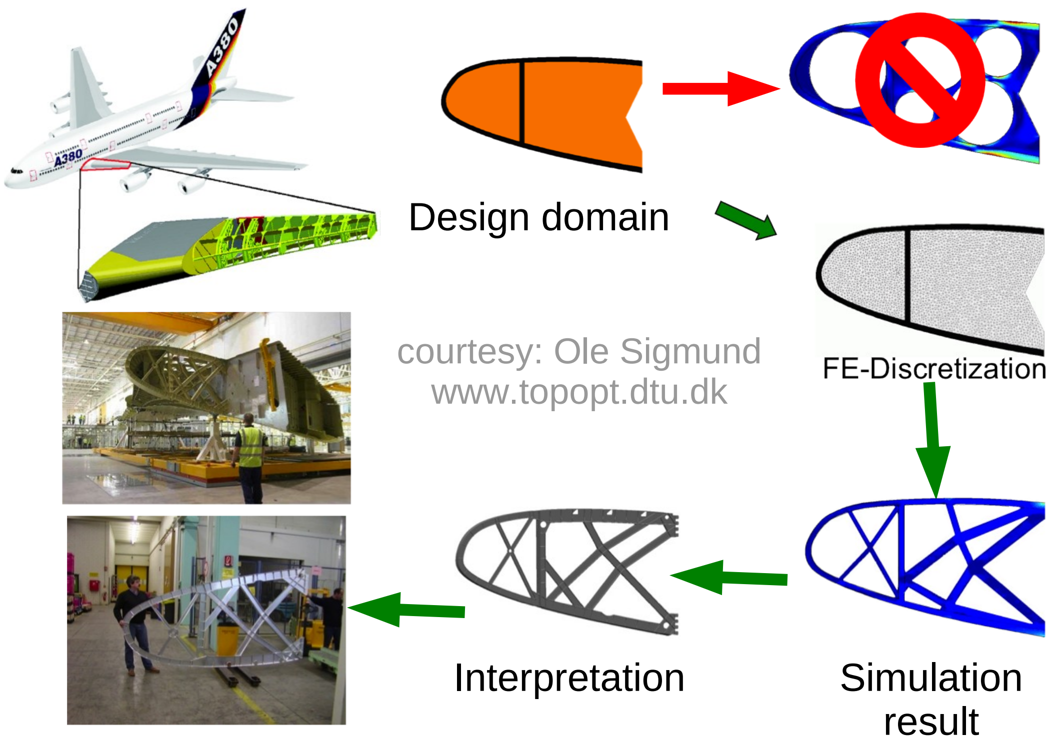
Topology Optimization

... and Materials:

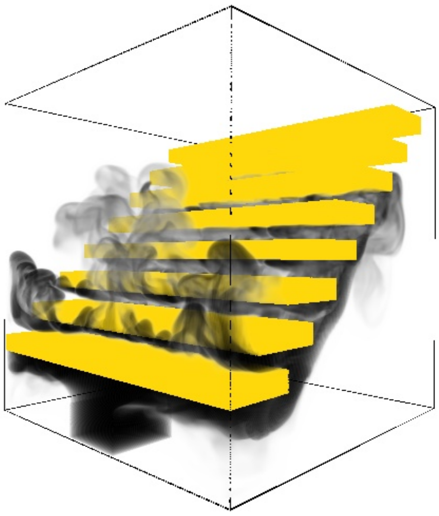
safe and minimum weight structures

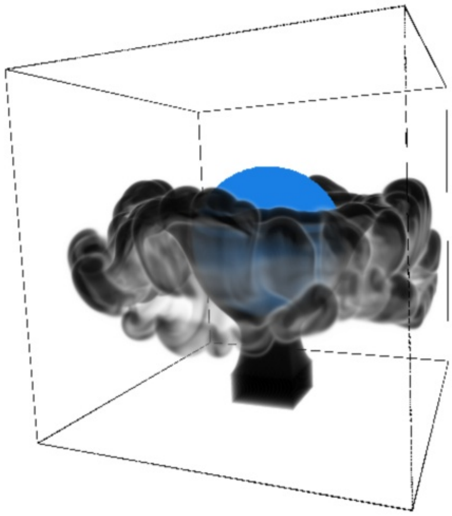
DTU Mechanical Engineering

Topology Optimization



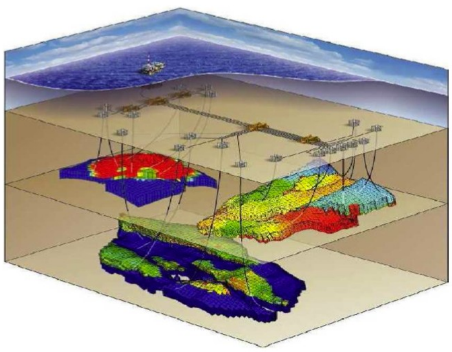
Smoke Simulations



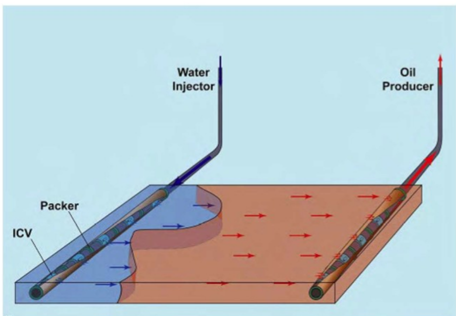


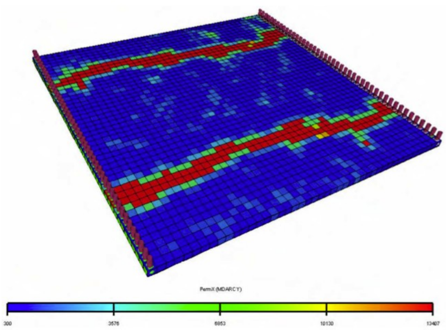
Stefan Glimberg – GPUlab, DTU Compute

Reservoir Production Optimization



Carsten Völcker,
John Bagterp Jørgensen –
DTU Compute





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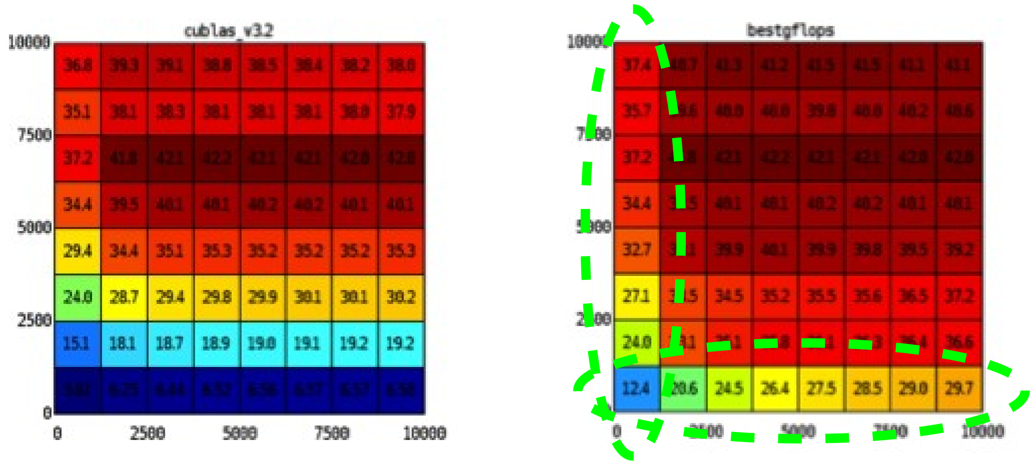
Performance Tuning – GPU

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



Hans-Henrik Sørensen – GPUlab, DTU Compute

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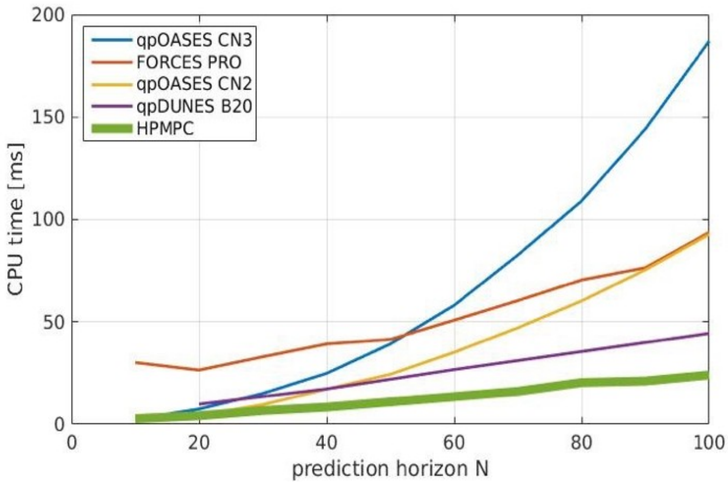
Model Predictive Control (MPC)

HPMPC:

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



Gianluca Frison, et al – Scientific Computing, DTU Compute

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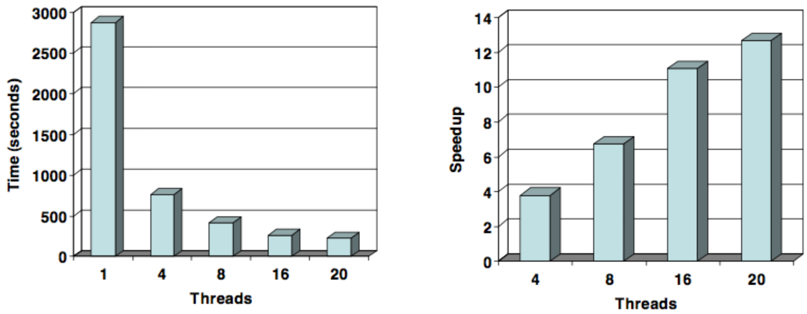
Tuning & Parallelization

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



Bernd Dammann – DTU Compute

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Other examples from DTU

- Bioinformatics
- Theoretical Atomic-scale Physics
- Computational Chemistry
- Photonics
- Nanotechnology
- ... and ... “Big Data”

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What is Performance?

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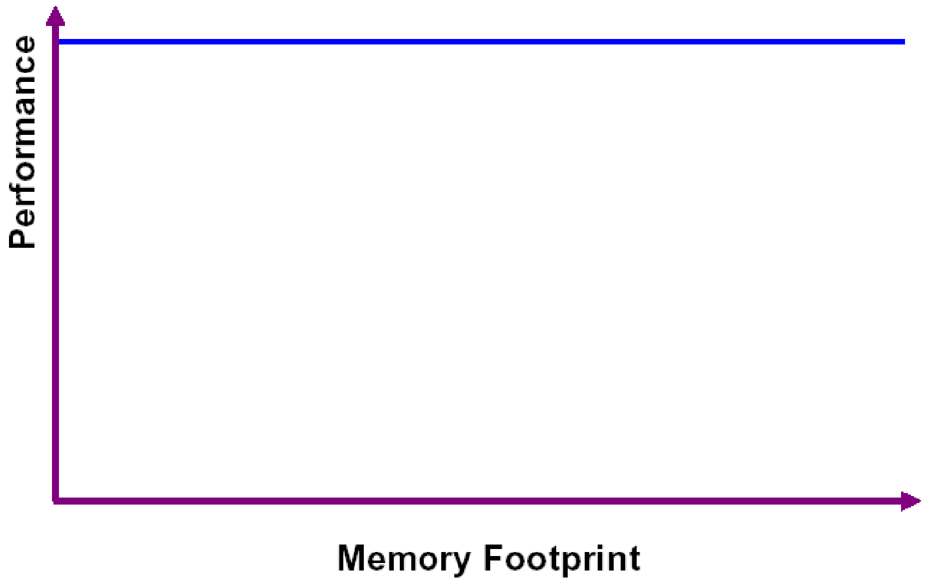
Performance of a Computer

- 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:
  - US-IV+ CPU @ 1800 MHz
  - superscalar chip: 2 Floating Point Ops per tick
  - Performance: 3600 MFlop/s

Theoretical Peak Performance!!!

Performance of a Computer

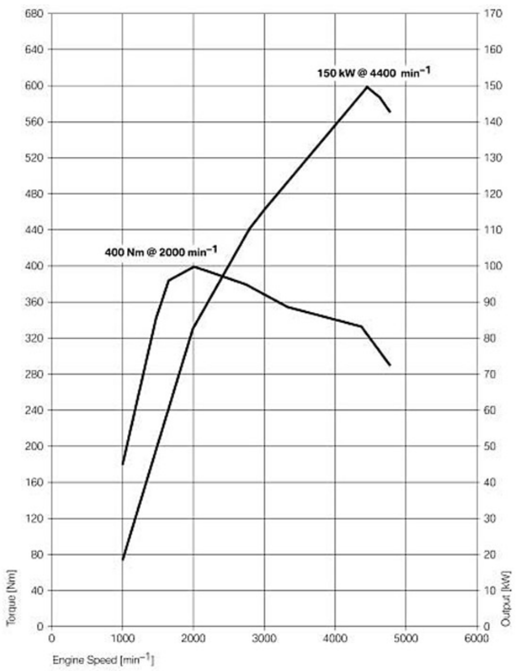
Intuitive Performance Graph for a given problem:



Performance of a Car

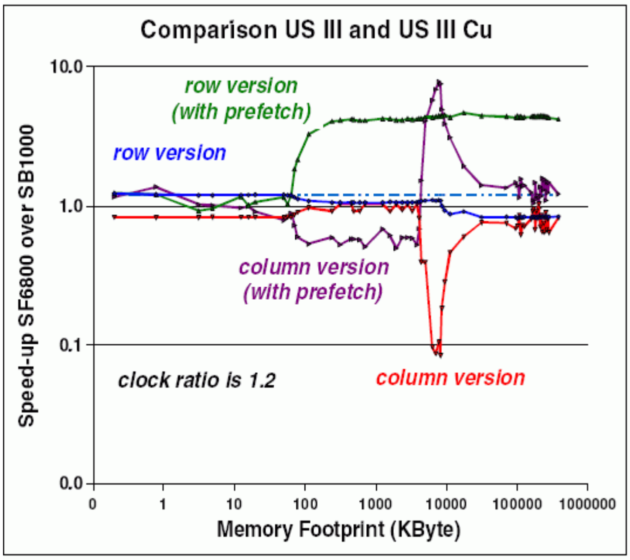
- Two ways to measure the performance of a car:
  - horsepower [kW]
  - torque [Nm]

"Horsepower sells cars,
torque wins races."
Caroll Shelby
(Formula 1 driver 1958/9)



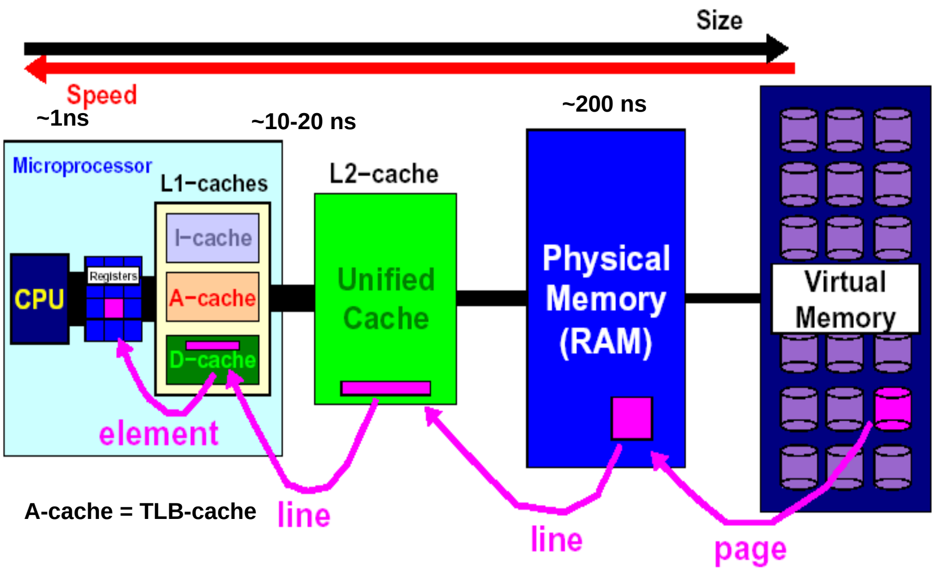
What is computer performance?

- Matrix summation in two ways
- Compare two generations of the US-III chip:



- *Compare the same version on the two different systems*
- *Very often we do not see the clock ratio ....*
- *It is either higher or lower*
- *The column version takes advantage of the larger TLB capacity of the US III Cu processor*

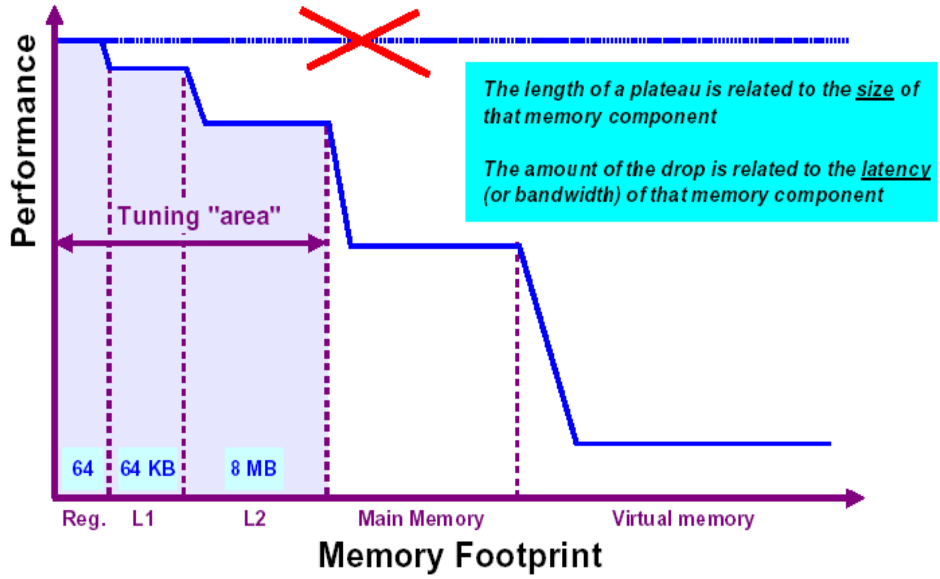
The Memory Hierarchy



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.

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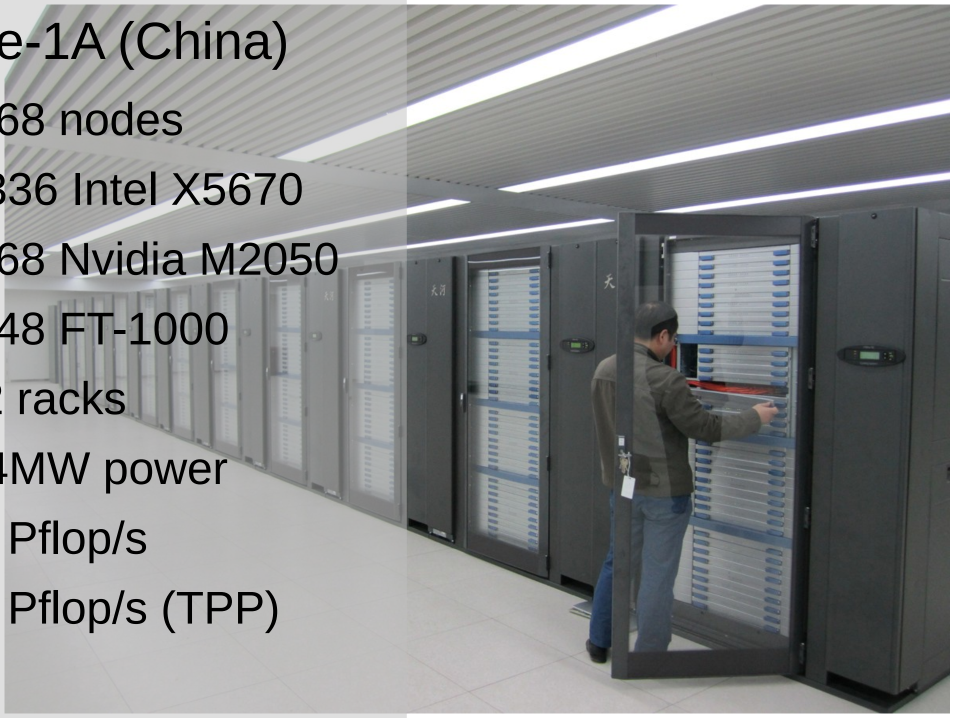
TOP 500 No. 1 – Nov 2010



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)

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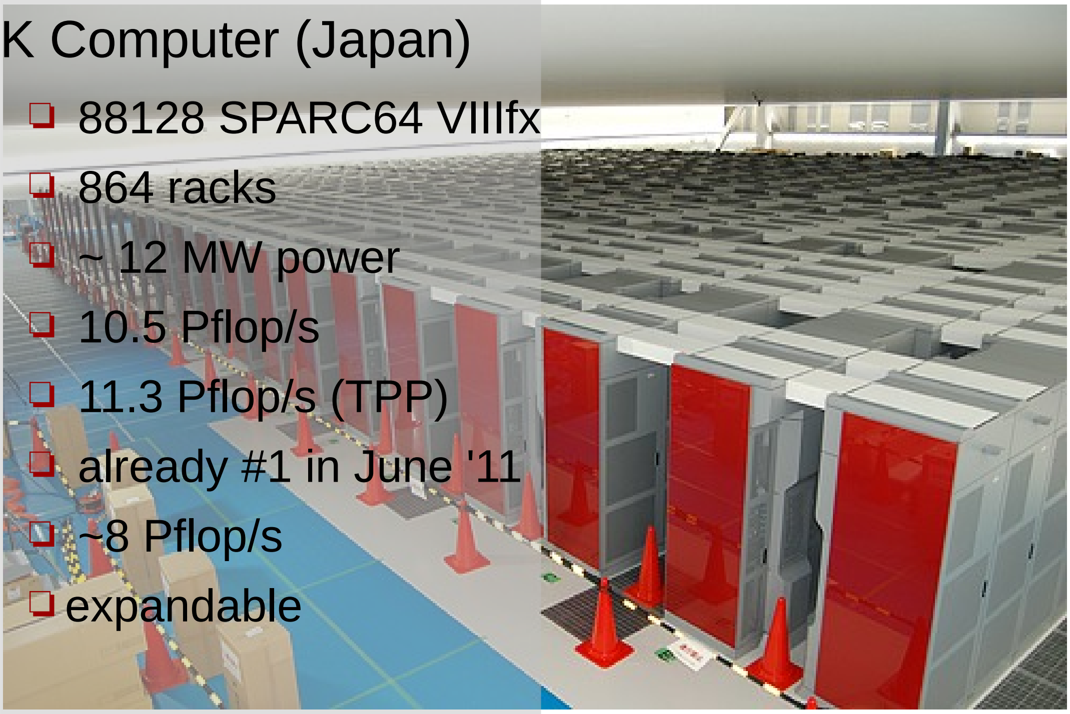
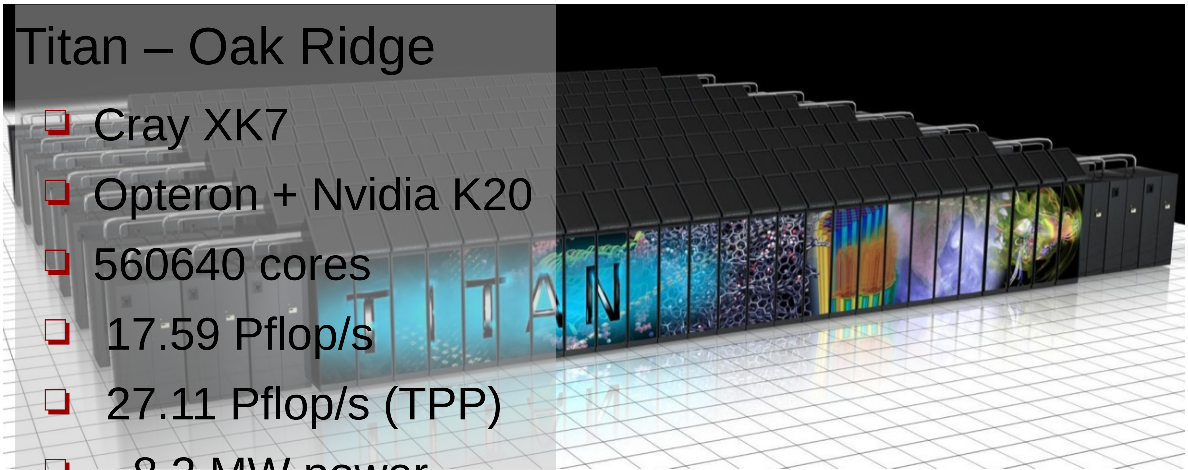
TOP 500 No. 1 – Nov 2011



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

- 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 – June 2016

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	National Supercomputing Center in Wuxi China	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway NRCPC	10,649,600	93,014.6	125,435.9	15,371
2	National Super Computer Center in Guangzhou China	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7	54,902.4	17,808
3	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0	27,112.5	8,209
4	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2	20,132.7	7,890
5	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705,024	10,510.0	11,280.4	12,660

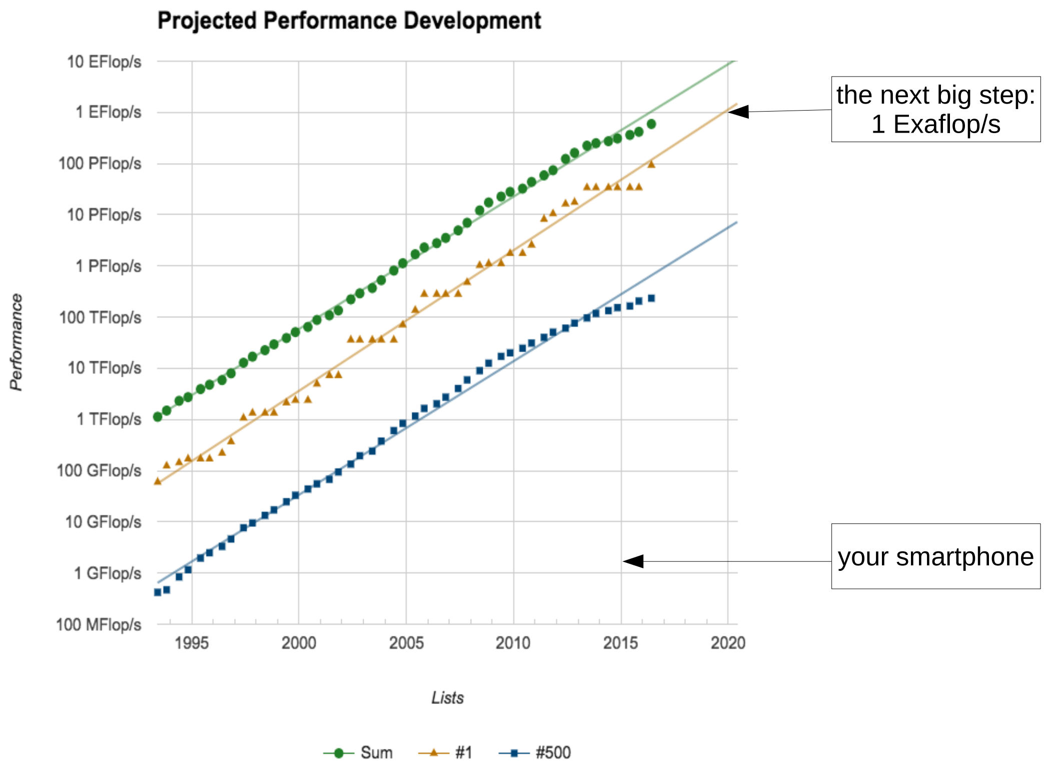
TOP500 – and where is Denmark?

- two entries on the TOP500 list as of June 2016:

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
258	University of Southern Denmark Denmark	**Abacus 2.0** - Lenovo NeXtScale nx360M5, Xeon E5-2680v3 12C 2.5GHz, Infiniband FDR, NVIDIA Tesla K40 Lenovo	17,928	462.4	836.6	187.5
315	Center for Biological Sequence Analysis - DTU Denmark	**Computerome** - Apollo 6000 XL230a, Xeon E5-2683v3 14C 2GHz, Infiniband FDR Hewlett-Packard	15,120	410.8	483.8	

- there are probably more powerful installations in DK, but they did not “want” to be on the list

TOP500 – history and outlook



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 (Tianhe-2) uses about 17-18 MW
- An alternative list – Green500:
  - http://www.green500.org/
  - measures the power efficiency: Mflop/s / W
  - number 1 on the Green500 list is number 253 on the TOP500 (TOP500 no. 1 → Green500 no. 168)

GREEN 500 No. 1 – Nov 20XX

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. the current no. 1

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
- “Big Data” - HPC methods for high-performance data analytics and visualization
- and not to forget ...

The HPC landscape is changing ...

NSA data center in Bluffdale, Utah (65 MW or more)

TheHPC 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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swiss energy
Continental