MSc Master Course – High Performance Computing

Introduction into HPC – General overview Applications, Technology, Memory Bandwidth and Locality

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How to reach us?

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- Classes:
  Tuesday, 13:30-15:15 (SI-006)
  Wednesday , 15:30-15:15 (SI-006)

Your background

- MSc CS? MSc FinTEC? MSc AI? MSc INF? Other?
- Programming experience & languages?
- Parallel programming languages?
- Operating systems?
- Working at the command line in Unix-like shells (e.g. Linux or a Mac OSX terminal)?
- Scientific libraries or mathematical libraries?
- Latex?
- Version control systems, particularly git, and the use of Github and Bitbucket repositories?

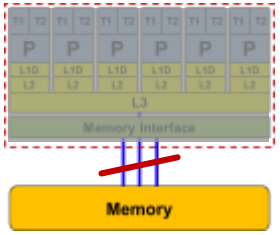
Quiz

- What does “clock frequency” mean in computers?

  The “heartbeat” of the CPU. A clock cycle is the smallest unit of time on a CPU chip. Typically < 1ns -> $f \gtrsim 1$ "GHz"

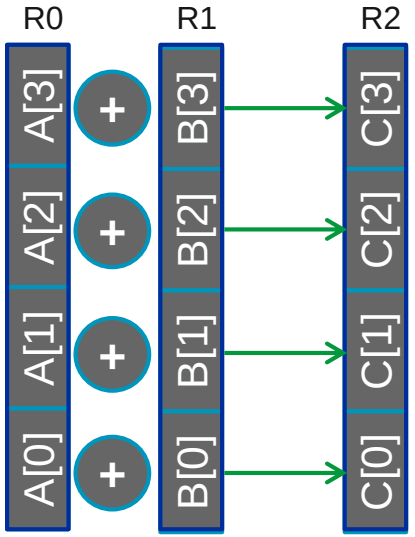
- What is “memory bandwidth”?

  Rate of data transfer between main memory (RAM) and CPU chip. Typical $b\_S \approx 10 \ldots 100$ "GB/s"

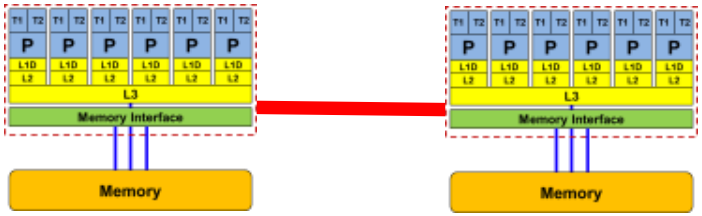


- What is SIMD vectorization?

  Single Instruction Multiple Data.
  Data-parallel load/store and execution units.



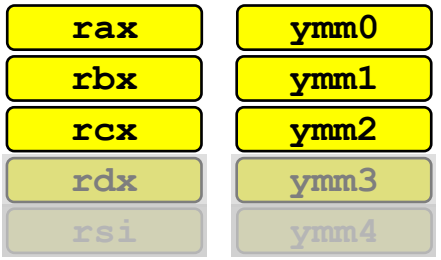
- What is ccNUMA?



Quiz

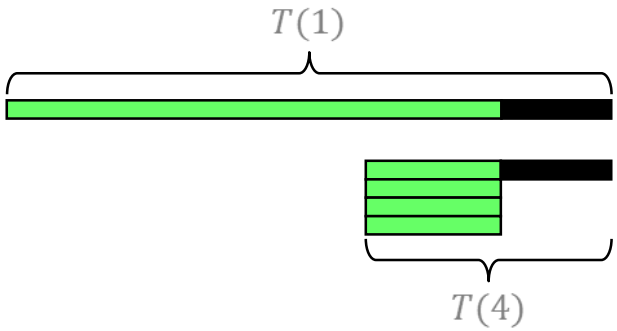
What is a register?

A storage unit in the CPU core that can take one single value (a few values in case of SIMD). Operands for computations reside in registers.



What is Amdahl's Law?

$$S_p = \frac{T(1)}{T(N)} = \frac{1}{s + \frac{1-s}{N}}$$



What is a pipelined functional unit?

An instruction execution unit on the core that executes a certain task in several simple sub-steps The stages of the pipeline can act in parallel on several instructions at once.

A conversation

From a student seminar on “Efficient programming of modern multi- and manycore processors”

Student: I have implemented this algorithm on the GPU, and solves a system with 26546 unknowns in 0.12 seconds, so it is really fast.

Me: What makes you think that 0.12 seconds is fast?

Student: It is fast because my baseline C++ code on the CPU is about 20 times slower.

Focus

- Focus
  - High Performance Scientific Computing (LAB)

- high emphasis on
  - numerical programming (less on theory and proofs)
  - less teaching lectures, but full-time in-class mini-projects (programming projects!)
  - new theory is explained in reading assignments, and if needed, explained in class on an individual basis.

- Essential prerequisite for this course is a solid knowledge
  - topics covered in a bachelor course on numerical methods
  - in programming experience in C/C++

Software Atelier: Supercomputing and Simulations

- Spring 2019:

  Software Atelier: Software Atelier: Simulation, Data Science & Supercomputing (6 ECTS)

CSCS - Swiss National Supercomputing Centre
Via Trevano 131
6900 Lugano

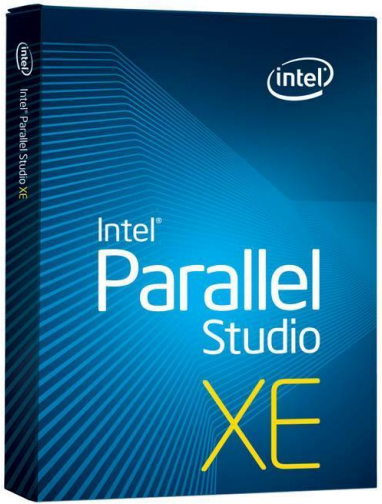
- CSCS Visit (no class for MSc students in CS/FinTEC/INF)

  TBA (13:30 to 16:00). The agenda will be
  Dr. Michele de Lorenzi (CSCS) - Overview CSCS (30 min)
  Student from USI (15 min)
  Guided Tour CSCS Server Room (60 min)

What you should get out of the lab?

In depth understanding of:

- When is parallel computing useful?
- Understanding of parallel computing hardware options.
- **Overview of programming models (software) and tools, and experience using some of them**
- Some important parallel applications and the algorithms
- Performance analysis and tuning
- Ability to implement **parallel numerical algorithms** efficiently in C/C++ using the Intel Math Kernel Library.



Three types of modern accelerators

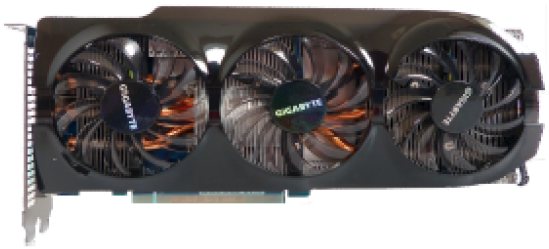
GPU: NVIDIA Tesla K20c

Kepler GK110, 28 nm

13 mp × 192 cores @ 0.71 GHz

5 GB GDDR5 @ 2.6 GHz

225W



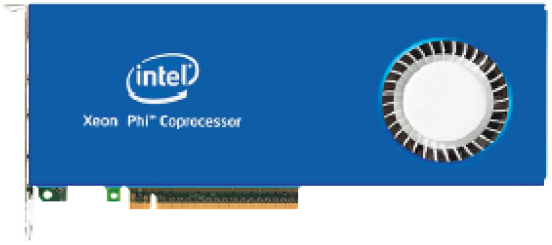
GPU: Radeon HD 7970

Graphics Core Next, 28 nm

32 mp × 64 cores @ 1 GHz

3GB GDDR5 @ 1.5 GHz

250W



MIC: Intel Xeon Phi 3120A

Knights Corner (KNC), 22 nm

57 cores @ 1.1 GHz

6GB GDDR5 @ 1.1 GHz

300W

up to 4 threads per core

512-bit vectorization (AVX-512)

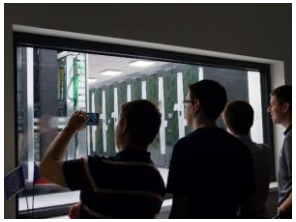
Università della Svizzera italiana | Faculty of Informatics | Institute of Computational Science ICS

Software Atelier: Simulation, Data Science & Supercomputing (Spring 2019, 6 ECTS)

Students will get the chance to work on a **software simulation project** namely to take **all the** theoretical and practical **knowledge** obtained so far and put it in use in a **real world context.**

Software Atelier: Supercomputers used in 2016 and 2017

- Local CUB Cluster at ICS

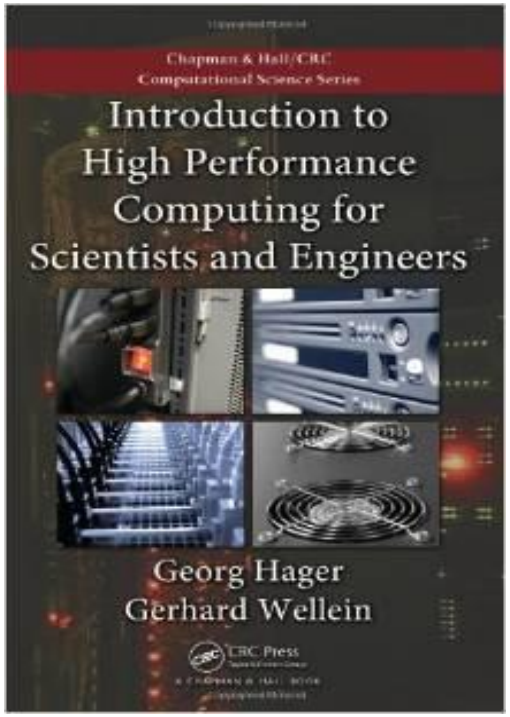


- The Salomon cluster at Czech Supercomputer Center
- **Largest Intel Xeon Phi Installation in Europe**
- 2 Pflop/s theoretical peak performance.
- 1,008 compute nodes, up to **24,192 cores**
- 129TB RAM

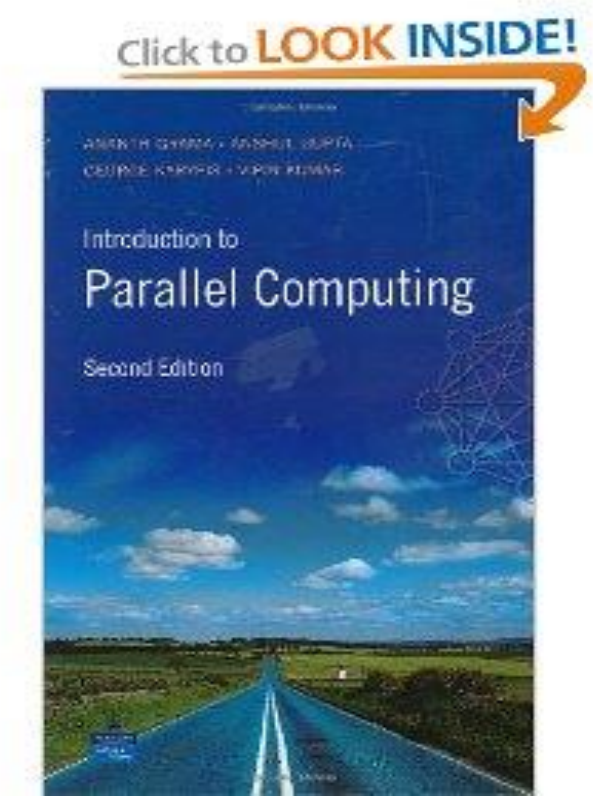
- Piz Daint Cluster at CSCS:
- User Lab for Swiss Scientists
- 25.3 Pflop/s theoretical peak performance.
- Ranking - TOP500: 6th, as of June 2018.
- 5,272 compute nodes, **129,108 cores** - 672 TB of RAM, 5,320 NVIDIA P100 GPUs
- Intel Haswell node
- 6PB local disks

Books:

- Introduction to High Performance Computing for Scientists and *Engineers by G. Wellein and G. Hager*

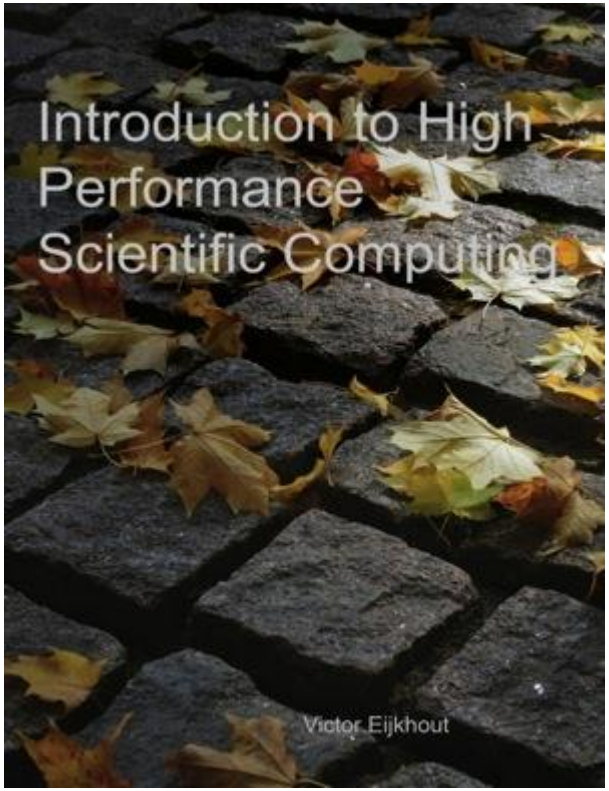


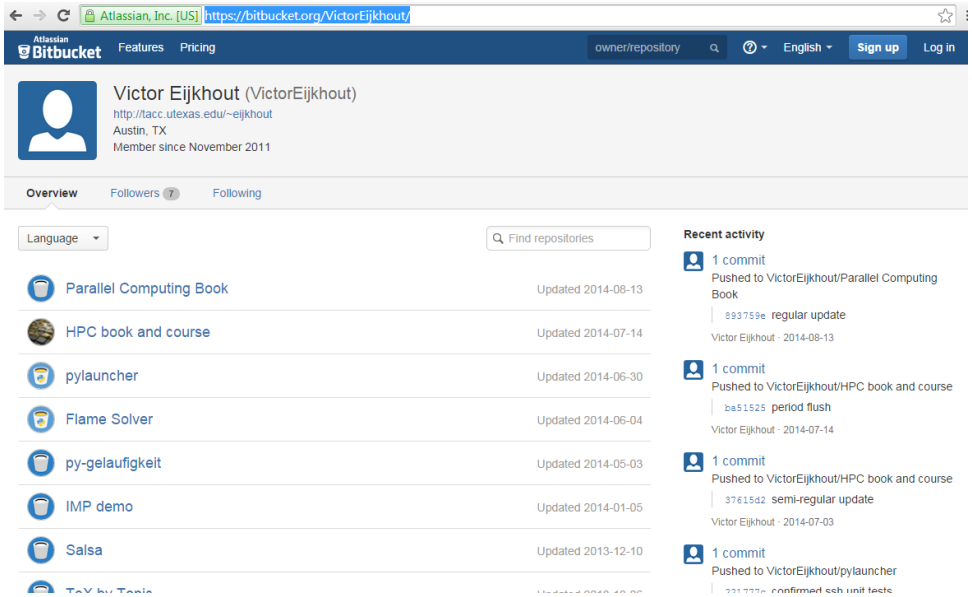
- Introduction to Parallel Computing (2nd Edition) by *Ananth Grama. George Karypis, Vipin Kumar. Anshul Gupta*



Two books from Victor Eijkout

- Introduction to High-Performance Scientific Computing by *Victor Eijkout*
- Parallel Computing Book by *Victor Eijkout*
- Both books are available on https://bitbucket.org/VictorEijkhout/





Schedule

- **Lectures** and **in-class exercises** on CUB cluster (please always bring your laptop to the class).

- 7 to 9 mini-projects & **reading assignments** (discussion in class)

- Course grading
  - 7 to 9 mini-projects 60%
  - no midterm (but much more emphasis on scientific programming)
  - Final written exam 40%, the final exam must be passed with a grade of at least 6/10.

- Course Webpage: https://www2.icorsi.ch/course/view.php?id=6851

- Registration - Please enroll within **until September 26** on teaching.inf.usi.ch and on https://www2.icorsi.ch/course/view.php?id=6851

Mini-Projects & Reading Assignments

- 7 to 9 mini-projects (including reading assignments)
- The mini-projects sheets will be uploaded on the course webpage
- The exercise should be solved until the deadline which is given on assignment (Please upload your code and solution in electronic form on https://www2.icorsi.ch/course/view.php?id=6851)
- We only accept submissions using our Latex template and C/C++ code.

- You are allowed to discuss such questions with anyone you like; however:
  - Your submission must list anyone you discussed problems with.
  - You must write up and summarize your submission independently.

Installation

- Slides from Radim Janalik