MSc Master Course – High Performance Computing

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

Olaf Schenk

Institute of Computational Science USI Lugano September 24, 2019

How to reach us?

Prof. Olaf Schenk
 Institute of Computational Science
 Faculty of Informatics
 2nd floor, ICS Lab, USI Lugano
 Email: olaf.schenk@usi.ch

• TA: Radim Janalik, Juraj Kardos, Aryan Eftekhari Email: <u>radim.janalik@usi.ch</u>, <u>juraj.kardos@usi.ch</u>, <u>aryan.eftekhari@usi.ch</u>

• Classes:

Tuesday, 15:30-17:15 (SI-006) Wednesday, 13:30-15:15 (SI-006)

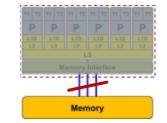
Your background

- 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?

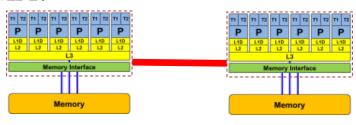
Quiz

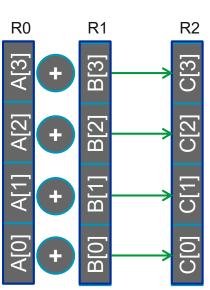
- What does "clock frequency" mean in computers?

 The "heartbeat" of the CPU. A clock cycle is the smallest unit of time on a CPU chip. Typically < 1ns → f≥1 "GHz"
- What is "memory bandwidth"?
 Rate of data transfer between main memory (RAM) and CPU chip. Typical b S≈10...100 "GB/s"



- What is SIMD vectorization?
 Single Instruction Multiple Data.
 Data-parallel load/store and execution units.
- What is ccNUMA?





Quiz



rbx

rcx

rdx

ymm0

ymm1 ymm2

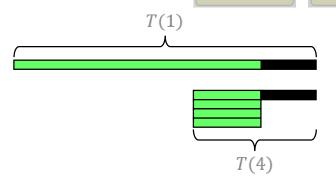
ymm3

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)

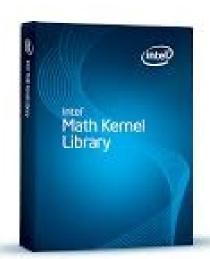
TBA (13:30 to 16:00). The agenda will be Dr. Michele de Lorenzi (CSCS) - Overview CSCS (30 min) Student from USI (15 min) Guided Tour CSCS Server Room (60 min)

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)

CSCS-USI HPC Summer School 2019 (July 15-25, 2019)

• Effective High-Performance Computing & Data Analytics with GPUs

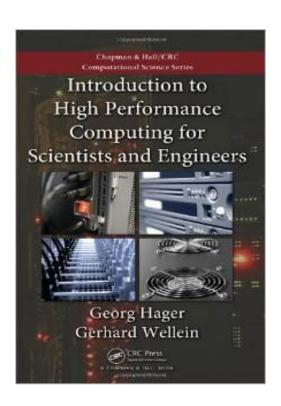


- This summer school will focus on the effective exploitation of state-of-the-art hybrid High-Performance Computing (HPC) systems with a special focus on Data Analytics.
- First week
 - GPU architectures
 - GPU programming (CUDA and OpenACC)
 - Message passing programming model (MPI)
 - Performance optimization and scientific libraries

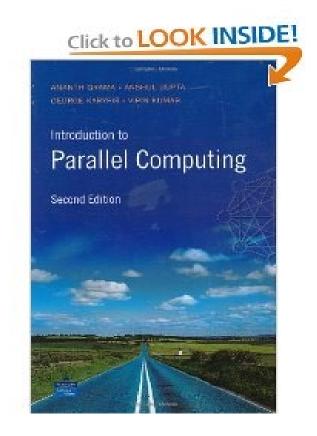
- Second week
 - Interactive supercomputing
 - Python HPC libraries
 - Introduction to Machine Learning and GPU optimized frameworks (Rapids)
 - Deep Learning on HPC platforms (TensorFlow)

Books:

Performance Computing for Scientists and Engineers by G. Wellein and G. Hager

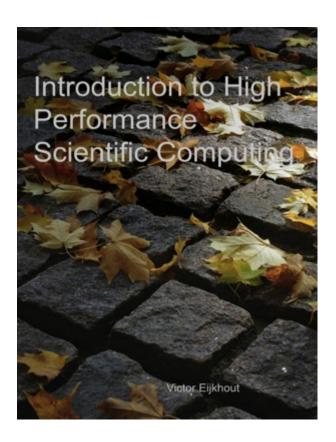


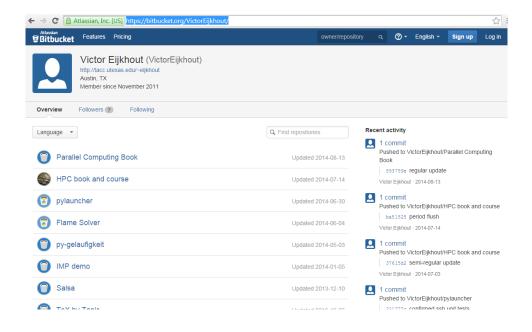
 Introduction to Parallel Computing (2nd Edition) by Ananth Grama.
 George Karypis, Vipin Kumar.
 Anshul Gupta



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 ICS 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% must be passed with a grade of at least 6/10.

- 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://www.icorsi.ch/course/view.php?id=7797
- Registration Please enroll within **until September 26** on <u>teaching.inf.usi.ch</u> and on <u>https://www.icorsi.ch/course/view.php?id=7797</u>

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://www.icorsi.ch/course/view.php?id=7797)
- 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.

Questions

• Questions?