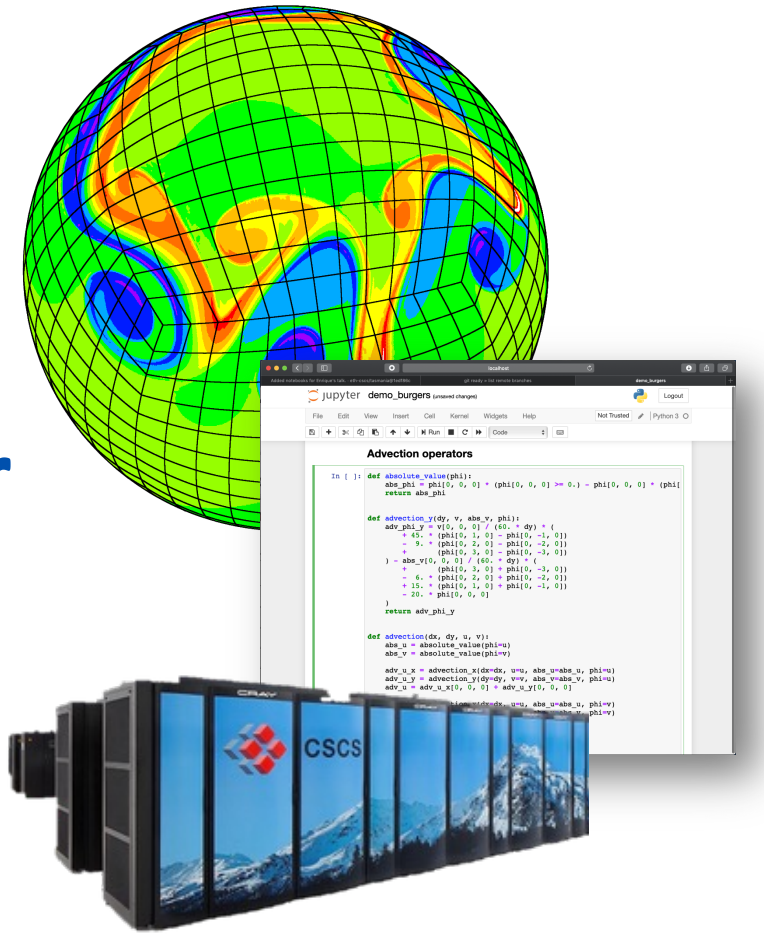
High Performance Computing for Weather and Climate (HPC4WC)

Content: Administrative
Lecturers: Oliver Fuhrer, Tobias Wicky
Block course 701-1270-00L
Summer 2023



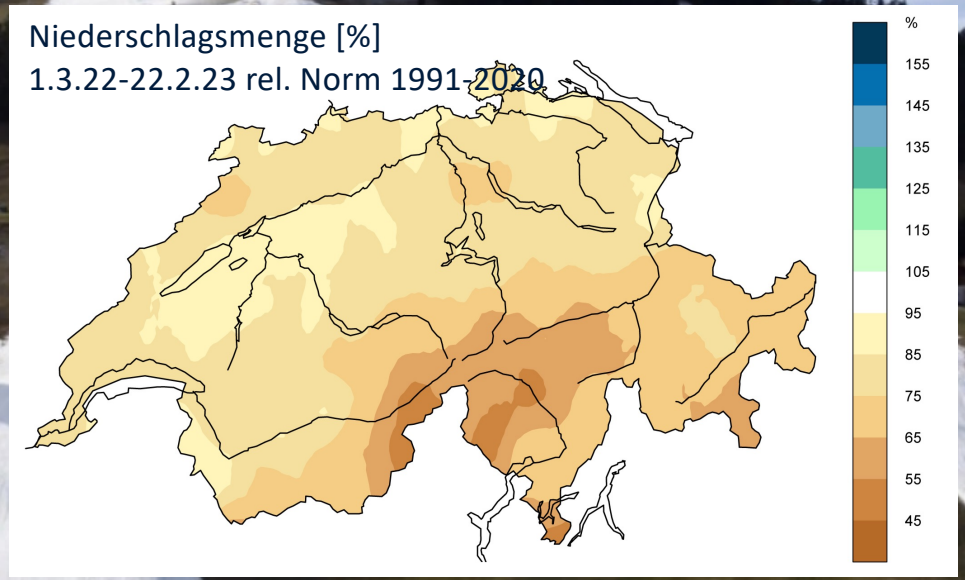
July 13, 2021 2am in the morning...


Tages-Anzeiger

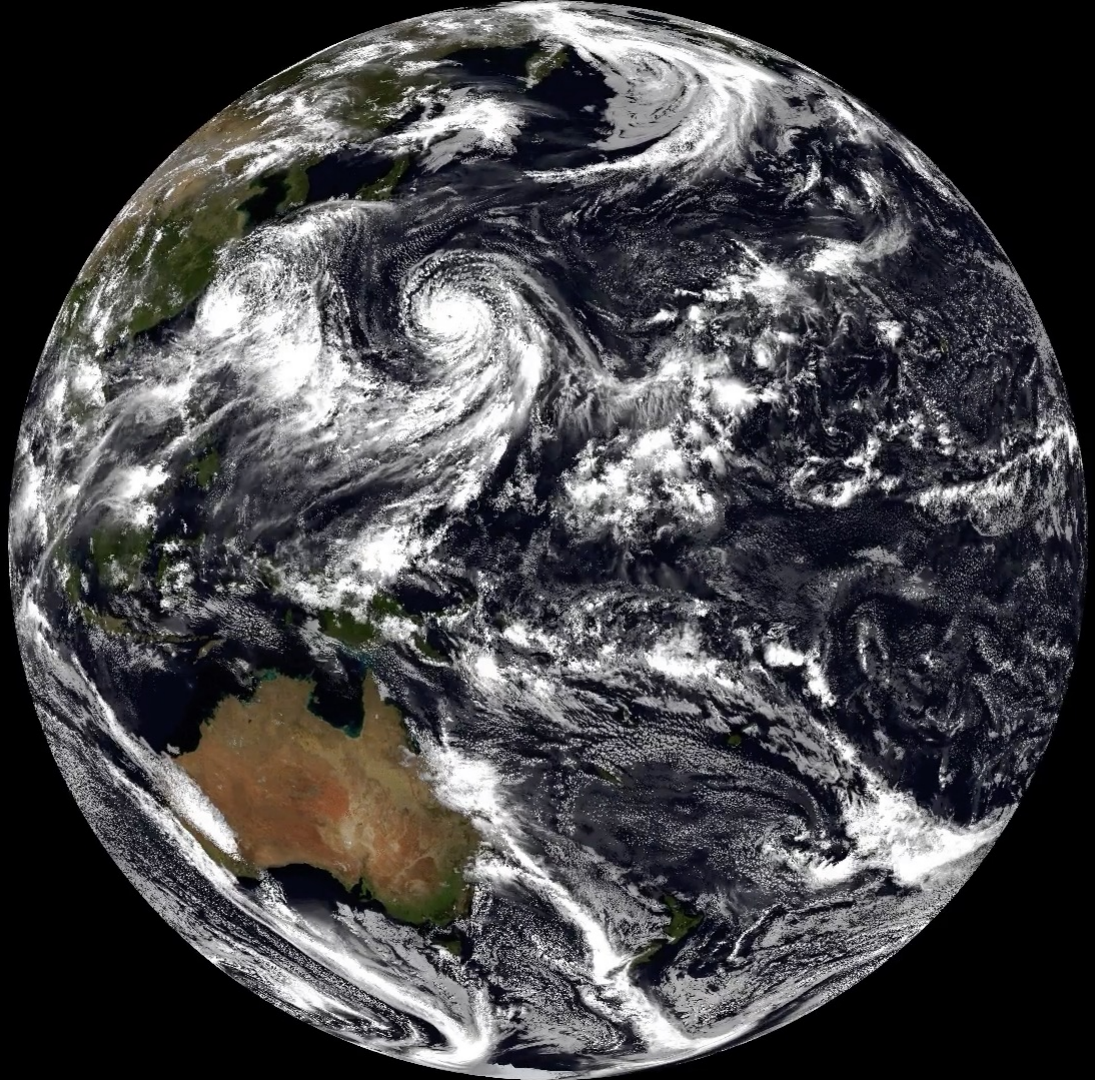
Nach dem Sturm droht Zürich jetzt Hochwasser

What's behind the warnings for such extreme events?

Winter 2022/2023



How do we know if this will be the «norm» in the future?



2016-08-11 18:00Z
258 Forecast Hours
FV3 3km

Visualization
Xi Chen@FV3 team

Goals of course

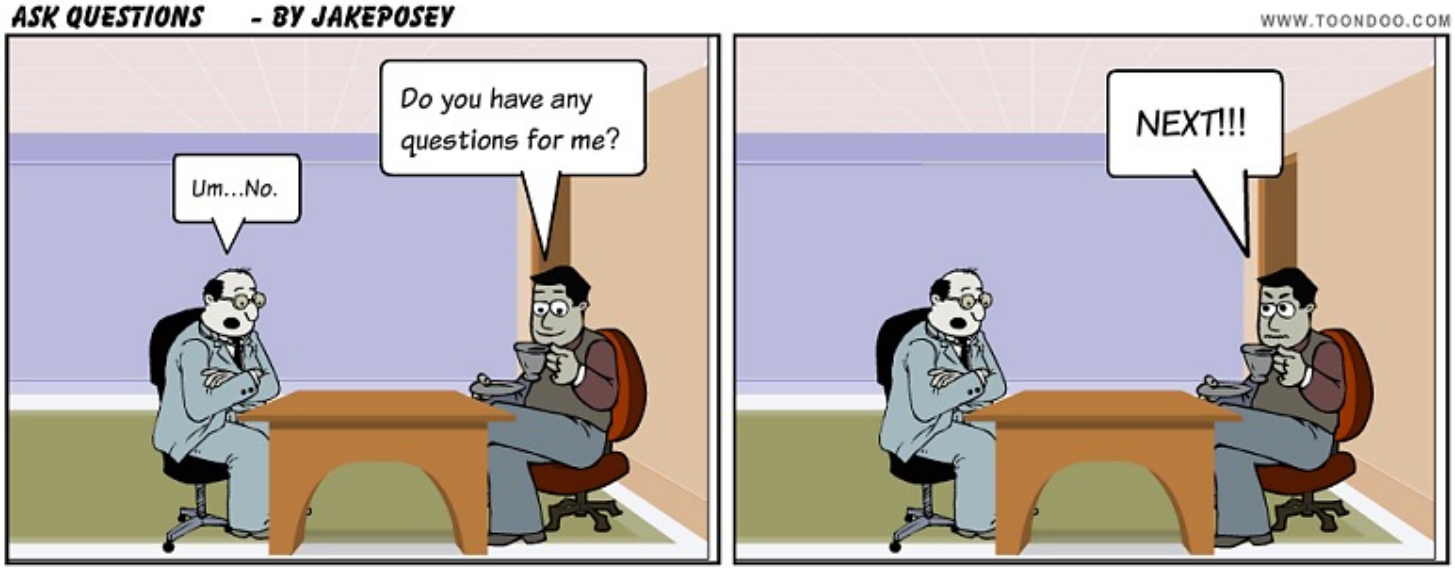
- Understand high performance computing concepts relevant for weather and climate simulations
- Able to work with weather and climate simulation codes that run on large supercomputers

Approach

> “ I ***hear***, and I forget.
> I ***see***, and I remember.
> I ***do***, and I understand. ”
>
> (chinese proverb)

- Lectures that explain concepts and give context (***hear***).
- Demonstrations of the concepts being applied (***see***).
- Practical exercises and a work project (***do***).

Questions, please!



Schedule

Monday	Motivation, stencil computations, memory hierarchy, lab environment
Tuesday	Shared memory parallelism, OpenMP, performance metrics
Wednesday	Distributed memory parallelism, domain-decomposition and halo-updates
Thursday	Hardware trends in supercomputing, GPU computing
Friday	High-level programming, domain-specific languages, wrapup

08:15 – 12:00	Morning session
12:00 – 13:30	***Lunch break***
13:30 – 17:00	Afternoon session

Currently registered students (eDoz)

MSc Atmosphere and Climate Science (USYS)	9
MSc/Bsc Computational Sciences and Engineering (MAVT)	8
MSc Environmental Science (USYS)	6
MSc Physics (PHYS)	6
PhD students (USYS, PHYS)	6
MSc Earth Sciences	2
MSc Statistics	1
MSc Mechanical Engineering (MAVT)	1
MSc Data Science	1
MSc Computer Science	1
Total	**41**

Prerequisites

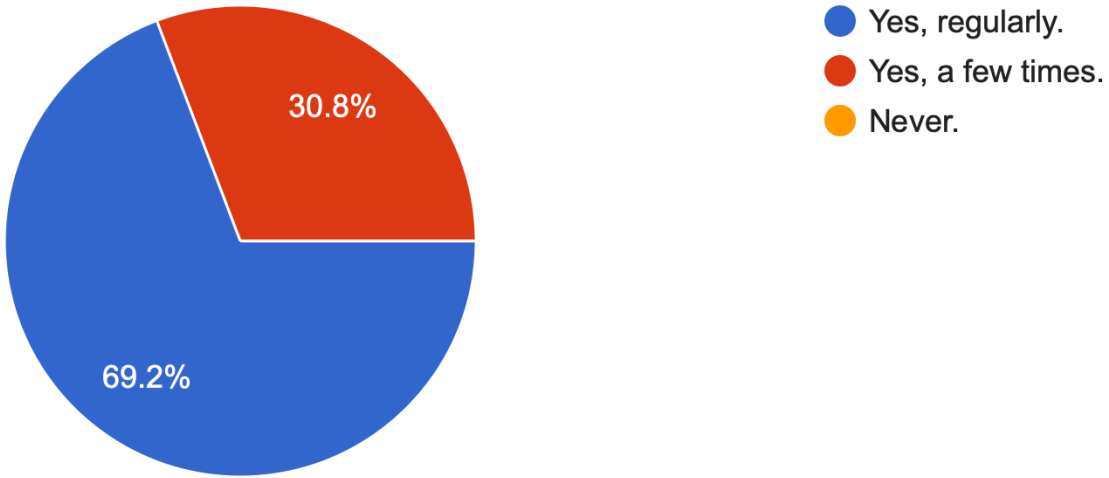
- **Fundamentals of numerical analysis and atmospheric modeling**
  - Basic partial differential calculus and finite difference methods.
  - e.g. ETH course "Numerical methods in environmental physics" or "Weather and climate models"
- **Experience in a programming language (C/C++, Fortran, Python, …)**
  - We will read and write Fortran, C++ and Python in this course.
- **Experience using command line interfaces in *nix environments (e.g., Unix, Linux)**
  - Familiar with work in the command line shell and the most commonly used shell commands.
  - Can logon to linux system via ssh and can work remotely on that system.
  - We will work on the Piz Daint supercomputer at the Swiss National Supercomputing Center (CSCS) in Lugano in this course.

If you think this course might not be suitable for you, talk to us!

Questionnaire (Work environment)

Have you worked with Jupyter Notebooks before?

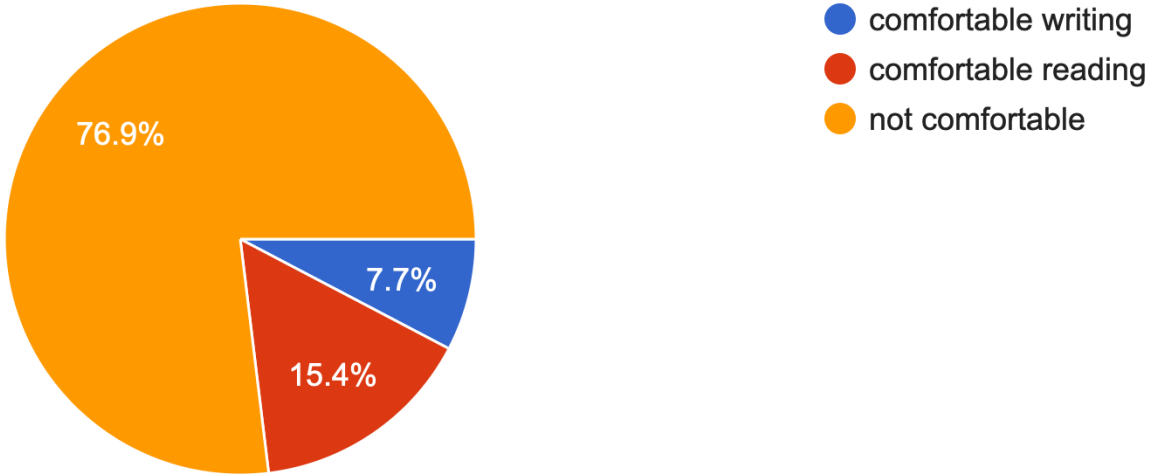
26 responses



Questionnaire (Programming)

How comfortable are you with this code example (CUDA)?

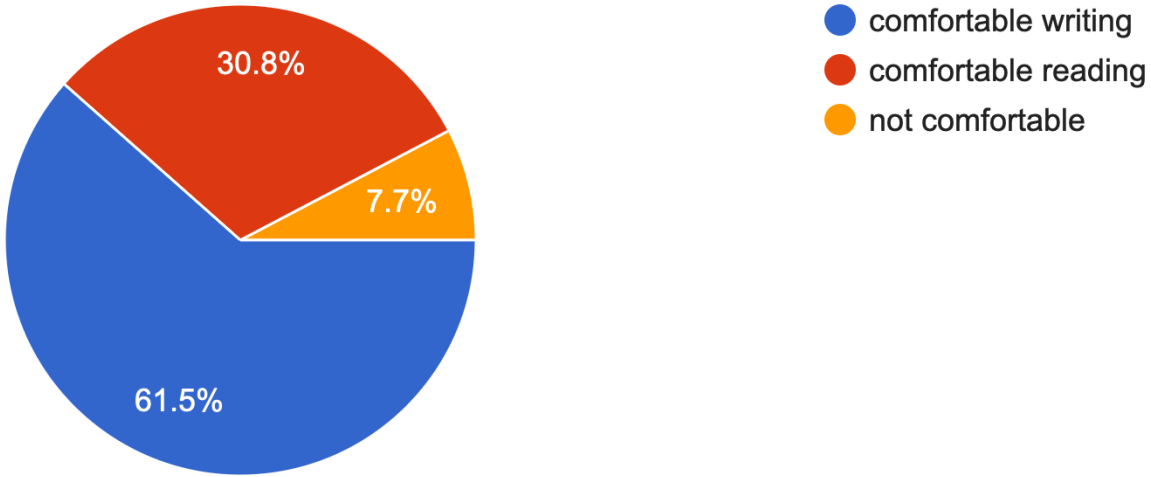
26 responses



Questionnaire (Weather and Climate Modeling)

How comfortable are you with this code example (discretized PDE in Python)?

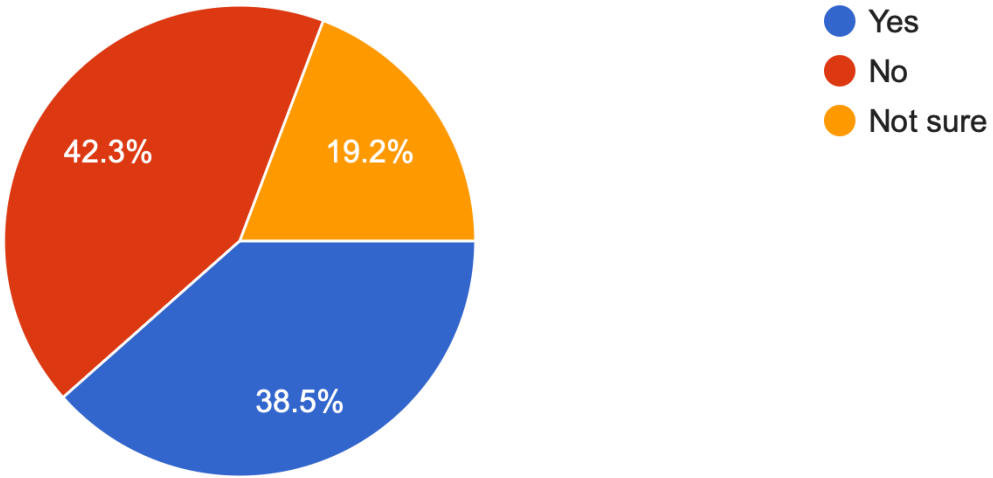
26 responses



Questionnaire (High Performance Computing)

Have you seen a program deadlock due to bad communication patterns?

26 responses



Practicalities

- **All course material on GitHub repository** (slides, notebooks, codes, …)
  https://github.com/ofuhrer/HPC4WC/
- **Questions related to course and projects in dedicated Slack workspace**
  https://join.slack.com/t/hpc4wc-workspace/shared_invite/zt-1a0hd2f2s-X9oOK2DtpdcgIroQPtfQAw
  - Generally, try to use public channels for questions since others probably have the same questions.
- **Lectures are not recorded**

How to earn credits (3 ECTS)

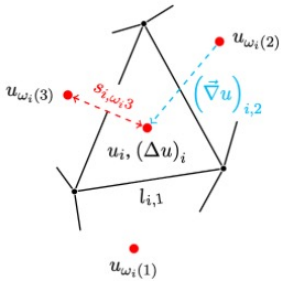
- **Attend the block course** (and participate actively!)
- **Work project**
  - Choose group and topic
  - Hand in working source code and report (max. 10 pages)
  - Projects will be graded
  - **Deadline: 31. August 2023**
- Credits are awarded if course attended and grade of work project ≥ 4.0
- Same rules apply for BSc, MSc, and PhD students

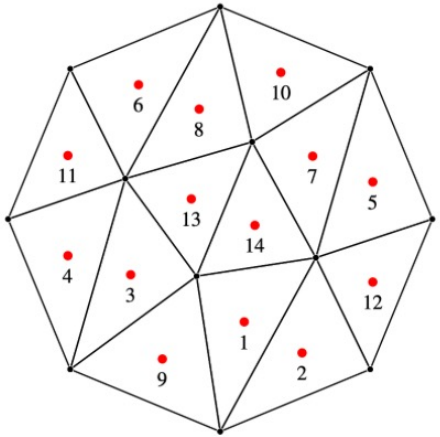
Work project

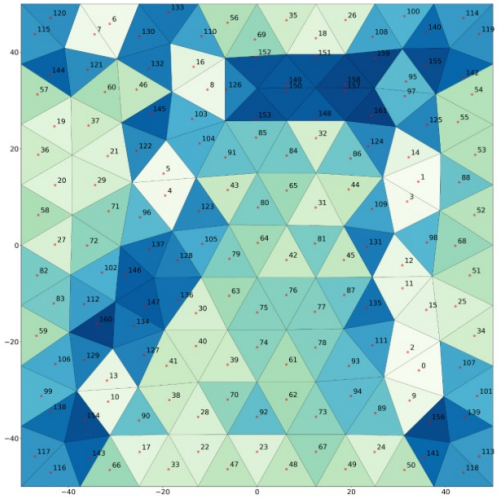
- **Work in groups of 2-3** (individual projects are strongly discouraged)
  - Programming is not a solitary art!
- **Topics will be presented on Thursday**
  - If you prefer to choose your own, you are required to discuss with us beforehand
  - Each project must have a software development and performance evaluation part and has to be related to course material
- **Grading**
  - 25% correctness (compiles & runs, results correct, no bugs)
  - 25% quality (structure, clean code, comments, naming, tests, error handling)
  - 25% performance (depending on work project)
  - 25% report (maximum 10 pages)
- **See last year's projects for examples**

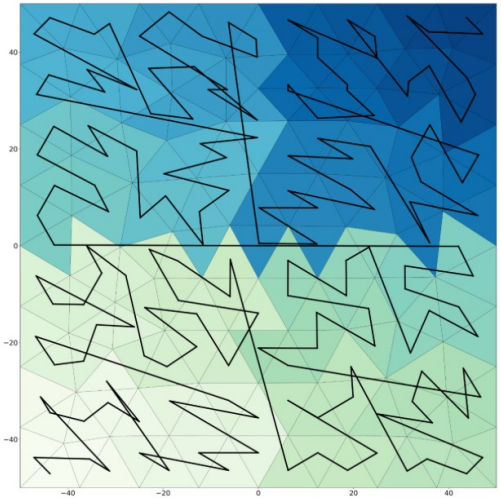
Example: Unstructured grid

$$(\Delta u)_i := \left(\vec{\nabla} \cdot \vec{\nabla} u\right)_i \approx \frac{1}{|\Omega_i|} \sum_{j=1}^{N} l_j \left(\vec{\nabla} u\right)_{i,j} \cdot \vec{n}_j \approx \frac{1}{|\Omega_i|} \sum_{j=1}^{N} l_j \frac{u_{\omega_i(j)} - u_i}{s_{i,\omega_i(j)}}$$









Lab exercises

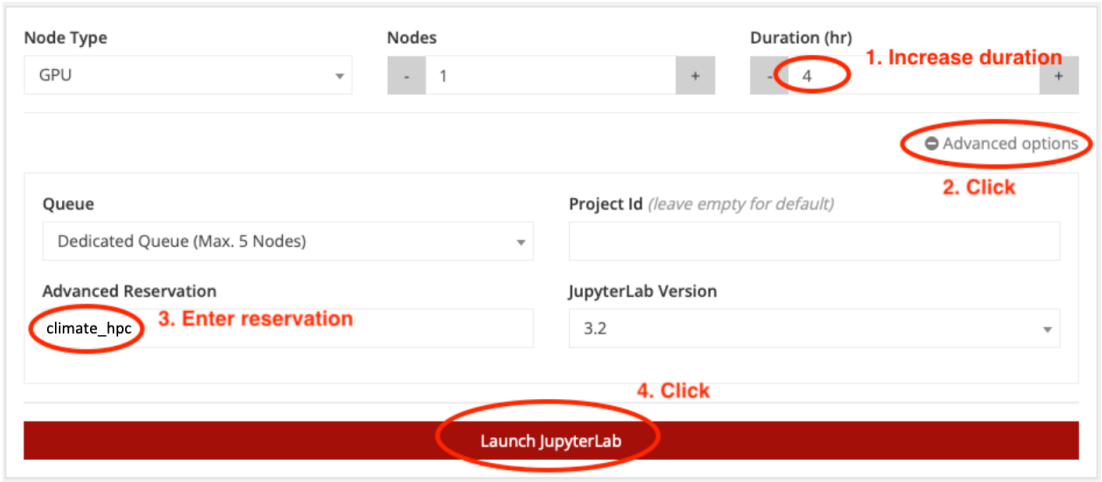
- Swiss National Supercomputing Centre https://www.cscs.ch/
- Piz Daint supercomputer (#28 on list of 500 largest supercomputers worldwide)

CSCS Accounts

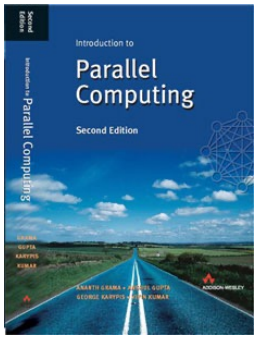
- Everybody has a unique user name (classXXX) and password.
- **Do not share you login / pwd with anybody else.** Accounts with suspicious activities will be closed down by CSCS immediately.
- **Change your password** immediately upon your first login to CSCS using the `passwd` command in a Terminal (see instructions).
- We have a shared quota of 3000 node hours for using the CSCS supercomputers for this block course.
  - Do not launch jobs with more than 1 node without checking with us first.
  - Do not leave your JupyterHub Server running if you don't need it.
- **Do not contact CSCS first** if you have trouble. Ask us or use the Slack workspace to get your issues resolved.
- Take a look at the **CSCS Code of Conduct**

JupyterHub

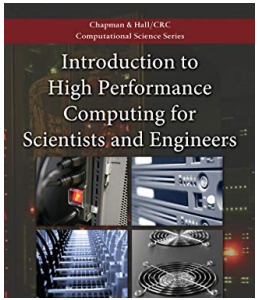
- Lab exercises will all be conducted on https://jupyter.cscs.ch/, the JupyterHub portal of CSCS.
- Interactive development and computing environment.
- If things get stuck or go wrong, it's always possible to "Stop Server" and "Lauch Server" again.
- Jupyter notebooks auto-save and *almost* certainly no work will be lost.



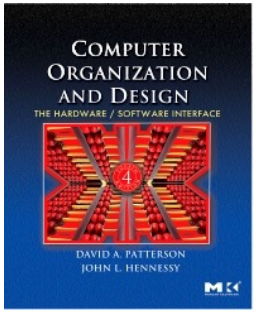
Literature & Links



Introduction to High Performance Computing for Scientists and Engineers, G. Hager and G. Wellein, CRC Press, 2011 (available online at ETH)



Parallel Computing, A. Grama, A. Gupta, G. Karypis, V. Kumar (available free online)



Parallel Programming in MPI and OpenMP, V. Eijkhout (Link to course)

Computer Organization and Design, D.H. Patterson and J.L. Hennessy (available online at ETH)