High Performance Computing

ADVANCED SCIENTIFIC COMPUTING

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in **@Morris Riedel**   **@MorrisRiedel**   **@MorrisRiedel**

Epilogue

November 25, 2019
Room V02-156

UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES
FACULTY OF INDUSTRIAL ENGINEERING,
MECHANICAL ENGINEERING AND COMPUTER SCIENCE

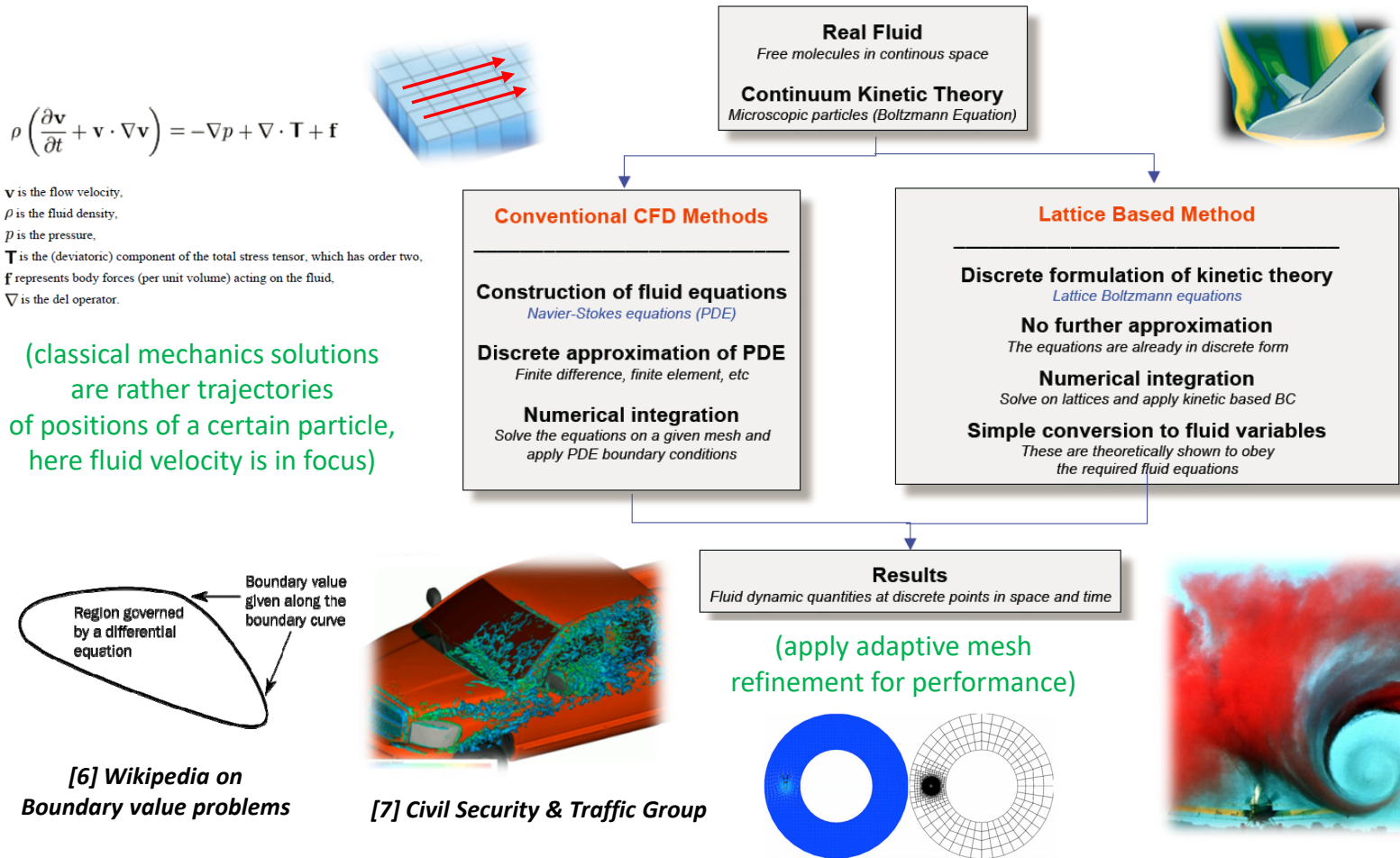JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

DEEP Projects

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

HAICU HELMHOLTZ ARTIFICIAL INTELLIGENCE COOPERATION UNIT

Review of Short Lecture 15 – Computational Fluid Dynamics & Finite Elements

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla p + \nabla \cdot \mathbf{T} + \mathbf{f}$$

$\mathbf{v}$ is the flow velocity,
ρ is the fluid density,
p is the pressure,
$\mathbf{T}$ is the (deviatoric) component of the total stress tensor, which has order two,
$\mathbf{f}$ represents body forces (per unit volume) acting on the fluid,
∇ is the del operator.

(classical mechanics solutions
are rather trajectories
of positions of a certain particle,
here fluid velocity is in focus)

Real Fluid
Free molecules in continous space

Continuum Kinetic Theory
Microscopic particles (Boltzmann Equation)

Conventional CFD Methods

Construction of fluid equations
Navier-Stokes equations (PDE)

Discrete approximation of PDE
Finite difference, finite element, etc

Numerical integration
Solve the equations on a given mesh and apply PDE boundary conditions

Lattice Based Method

Discrete formulation of kinetic theory
Lattice Boltzmann equations

No further approximation
The equations are already in discrete form

Numerical integration
Solve on lattices and apply kinetic based BC

Simple conversion to fluid variables
These are theoretically shown to obey the required fluid equations

Results
Fluid dynamic quantities at discrete points in space and time

(apply adaptive mesh
refinement for performance)

(fluid consisting of particles with a
finite number of discrete velocity values)

$$f_i^t(\vec{x}, t + \delta_t) = f_i(\vec{x}, t) + \frac{1}{\tau_f}(f_i^{eq} - f_i)$$

(Collision step)

$$f_i(\vec{x} + \vec{e}_i \delta_t, t + \delta_t) = f_i^t(\vec{x}, t + \delta_t)$$

(Streaming step)

(particles perform consecutive
propagation and collision processes
performed over a discrete lattice mesh)

(large eddy simulations
for turbulence)

Boundary value
given along the
boundary curve

Region governed
by a differential
equation

[6] Wikipedia on Boundary value problems

[7] Civil Security & Traffic Group

[5] Wikipedia on LES

[4] Wikipedia on LBM

[3] Wikipedia on Navier-Stokes

[2] Wikipedia on CFD   *[1] S. Orszag et al.*

HPC-A[dvanced] Scientific Computing (cf. Prologue) – Second Part

- Consists of techniques for programming & using large-scale HPC Systems
  - Approach: Get a broad understanding what HPC is and what can be done
  - Goal: Train general HPC techniques and systems and selected details of domain-specific applications

High Performance Computing
(a field of constant changes)

HPC Course

Domain-specific Science & Engineering A

Domain-specific Science & Engineering B

Domain-specific Science & Engineering C

Domain-specific Science & Engineering D
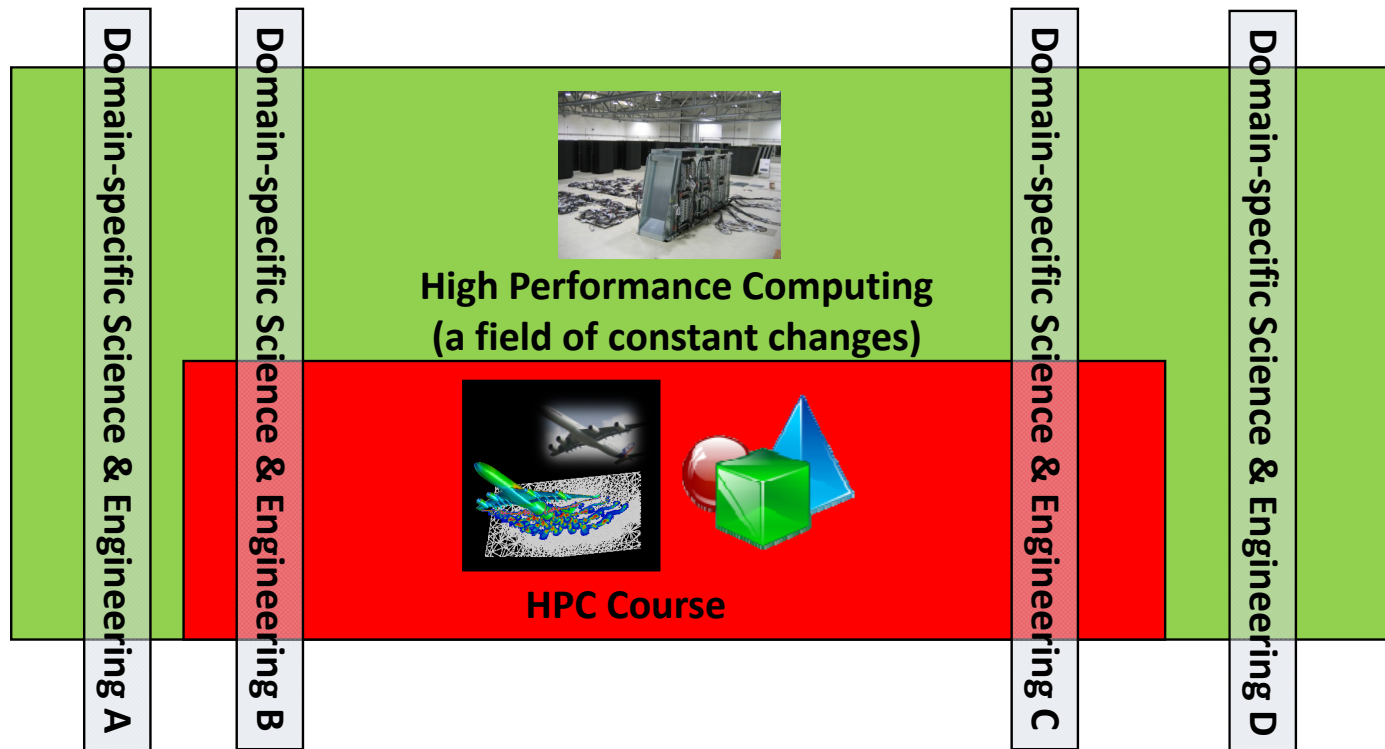
Outline of the Course

1. High Performance Computing

2. Parallel Programming with MPI

3. Parallelization Fundamentals

4. Advanced MPI Techniques

5. Parallel Algorithms & Data Structures

6. Parallel Programming with OpenMP

7. Graphical Processing Units (GPUs)

8. Parallel & Scalable Machine & Deep Learning

9. Debugging & Profiling & Performance Toolsets

10. Hybrid Programming & Patterns

11. Scientific Visualization & Scalable Infrastructures

12. Terrestrial Systems & Climate

13. Systems Biology & Bioinformatics

14. Molecular Systems & Libraries

15. Computational Fluid Dynamics & Finite Elements

16. Epilogue

+ additional practical lectures & Webinars for our hands-on assignments in context

- Practical Topics

- Theoretical / Conceptual Topics

Epilogue

- **Informal final lecture**
  - Answering remaining questions & guidance to future topics
  - Summary & preparation for final exam and quizzes debrief

- **Mindset**
  - Discussion of job offers on the market in the light of the course
  - What we have learned & how to turn knowhow into action

- **Skillset**
  - Knowledge of various HPC system techniques & parallel computing skills
  - PHD positions & Master Thesis topics HPC and/or Machine & Deep Learning

- **Toolset**
  - Knowledge of parallel programming tools & machine/deep learning libraries
  - Future Topics to study: Quantum computing, neural networks on the chip, neuromorphic computing, modular supercomputing, etc.

Outline

- High Performance Computing from another Perspective

- Further Readings

- Bachelor & Master Thesis Topics Available

- Cloud Computing Course Fall 2020

- Acknowledgements

High Performance Computing from another Perspective
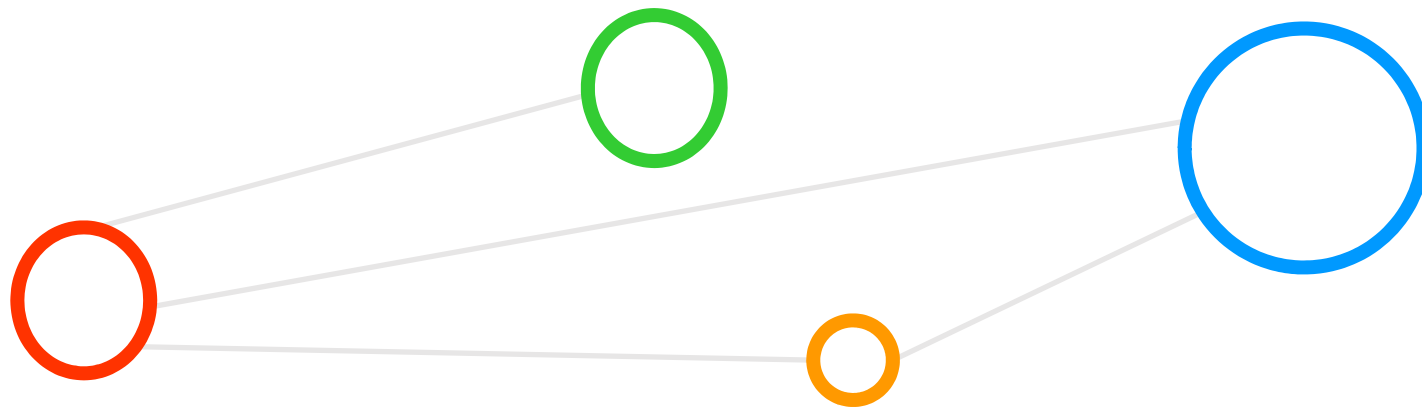
High Performance Computing from another Perspective

THEORY	TECHNIQUES	PARADIGMS
Parallel Algorithms	Message Passing Interface	High Throughput Computing
Speed-Up	OpenMP & Hybrid Programming	High Performance Computing
Weak/Strong Scaling	Network & Communication	Computational Modeling
Amdahls & Gustafson Law	Discretizations & Mesh Refinements	Machine & Deep Learning from Data
Numerical Approximation	Cloud & Grid Infrastructures	Iterative Numerical Simulations
Partial Differential Equations	Coupling & CFD & FEM	Ensembles & Monte Carlo Methods

Further Readings
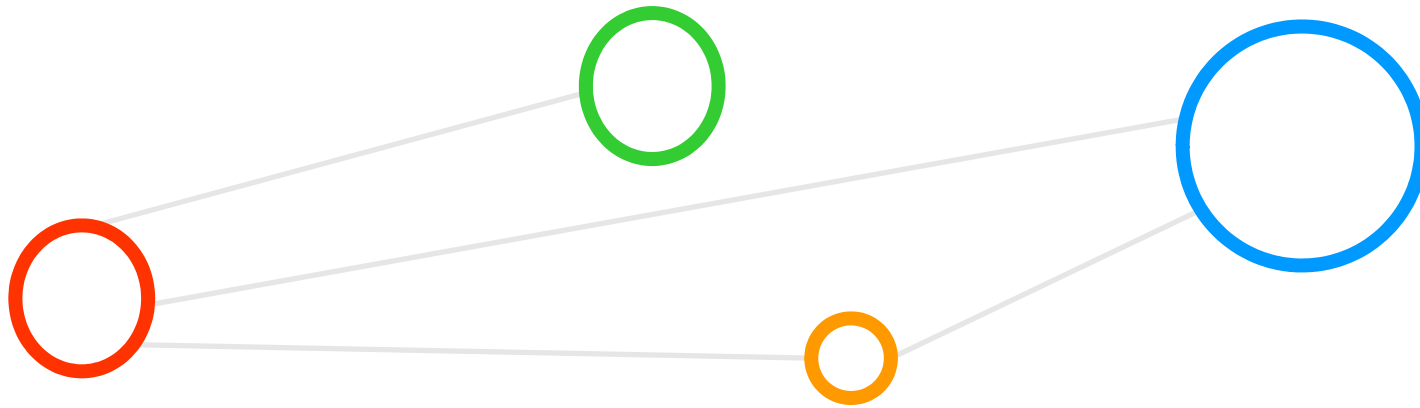
PRACE Training Portal

Search training materials

Browse by category tree

- Debugging, Profiling and Optimization Tools (11)
  - Compiler Suites (0)
  - Debugging Techniques (1)
  - Debugging Tools (0)
  - Optimization Tools (2)
  - Parallel Debugging (0)
  - Testing Methodologies (0)
- Hardware architecture (10)
- Parallel I/O and Fault Tolerance (0)
  - Checkpoint/Restart implementation (0)
  - Parallel I/O implementation (2)
- Parallel Programming Paradigms (12)
  - GPU Programming (29)
  - HPC architectures (21)
  - HPC principles (2)
  - Mixed-mode (hybrid) OpenMP-MPI (14)
  - MPI (10)
  - OpenMP (17)
- Performance analysis (20)
- Programming environments (0)
- Programming Languages (1)
  - C / C++ (0)
  - Fortran (1)
  - Java (0)
  - Matlab / R (0)
  - Next-gen languages (4)
  - PGAS languages (11)
  - Scripting Languages (4)
- Programming Tools and Libraries (3)
  - Batch Job Systems (0)
  - Grid Middleware (0)
  - Numerical Libraries (7)
  - PETSc (0)
  - Source Code Documentation Tools (0)
  - Version Control Systems (0)
- Scientific Visualisation Tools (10)
  - AVS (0)
  - EnSight (0)
  - OpenDX (0)
  - Paraview (1)
  - VisIT (0)
- Visualisation (11)

[8] PRACE Training Portal

Sessional Teacher with Supervision of Courses

1. **Introduction to Deep Learning Models**, Training Course organized by the DEEP-EST Project, Juelich Supercomputing Centre, Germany, May 21 – 23, 2019, Juelich, Germany

   [MORE]

2. **PRACE Tutorial: Parallel and Scalable Machine Learning**, PRACE Advanced Training Center, Juelich Supercomputing Centre, Germany, February 25 – 27, 2019, Juelich, Germany

   [MORE]

3. **DEEP-EST Tutorial: Machine Learning and Modular Supercomputing**, HiPEAC – European Network on High Performance and Embedded Architecture and Compilation Conference, January 21 – 23, 2019, Valencia, Spain

   [MORE]

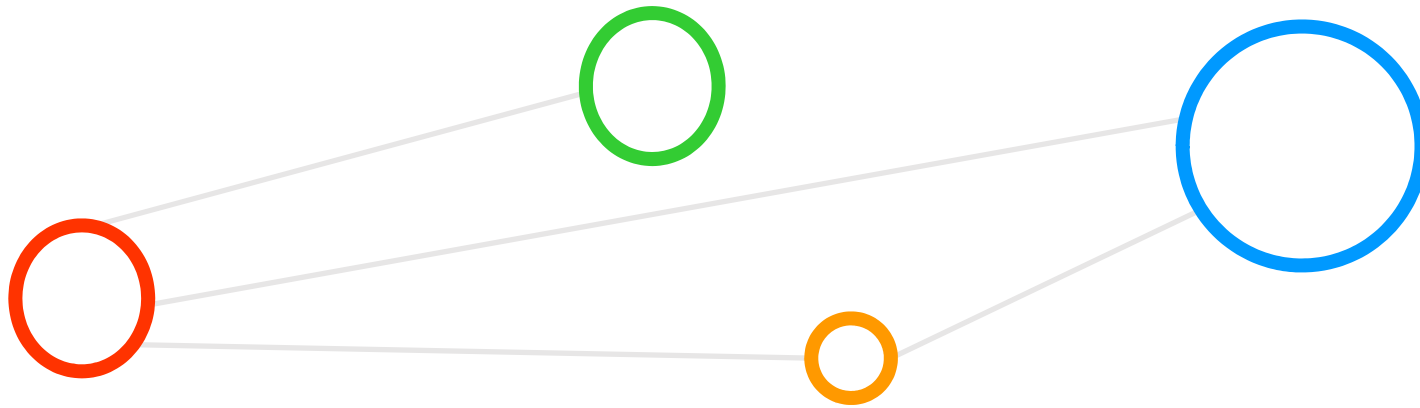*[9] Morris Riedel Teaching Web Page*

Associated Literature

Introduction to High Performance Computing for Scientists and Engineers,

Georg Hager & Gerhard Wellein,
Chapman & Hall/CRC Computational Science,
ISBN 143981192X, English, ~330 pages, 2010

[10] Introduction to High Performance Computing, 2010

Bachelor & Master Thesis Topics Available

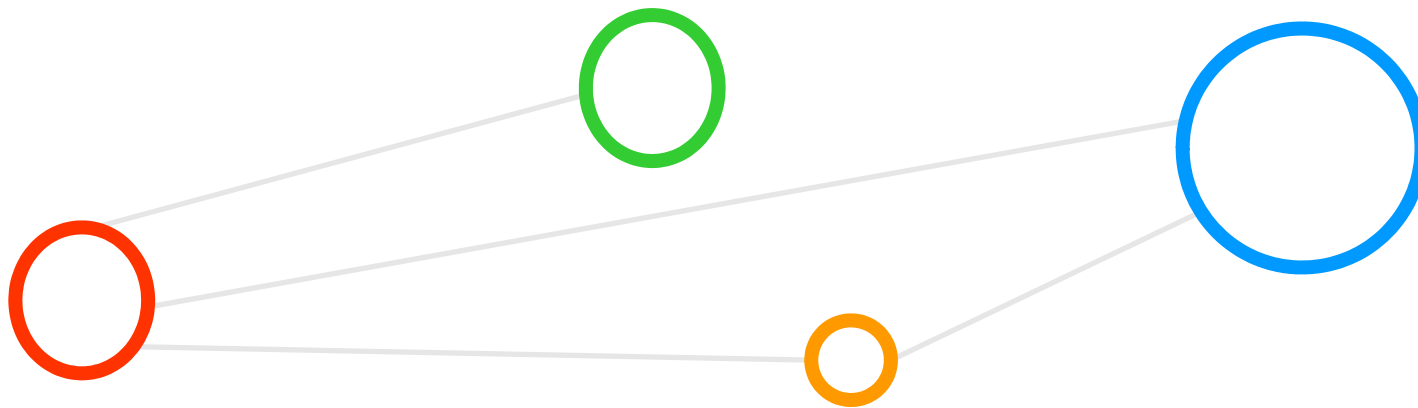# Cloud Computing Course Fall 2020

Cloud Computing Course Fall 2020 – Check Topics from 2018

Teaching Experience

[9] Morris Riedel Teaching Web Page

Adjunct Lecturer, Lecturer, Senior Lecturer or Professor

1. University Course: **High Performance Computing – Advanced Scientific Computing**, REI105M, School of Engineering and Natural Sciences, University of Iceland, Iceland, Fall 2019

   [MORE]

2. University Course: **Cloud Computing and Big Data – Parallel and Scalable Machine Learning and Deep Learning**, REI504M, School of Engineering and Natural Sciences, University of Iceland, Iceland, Fall 2018
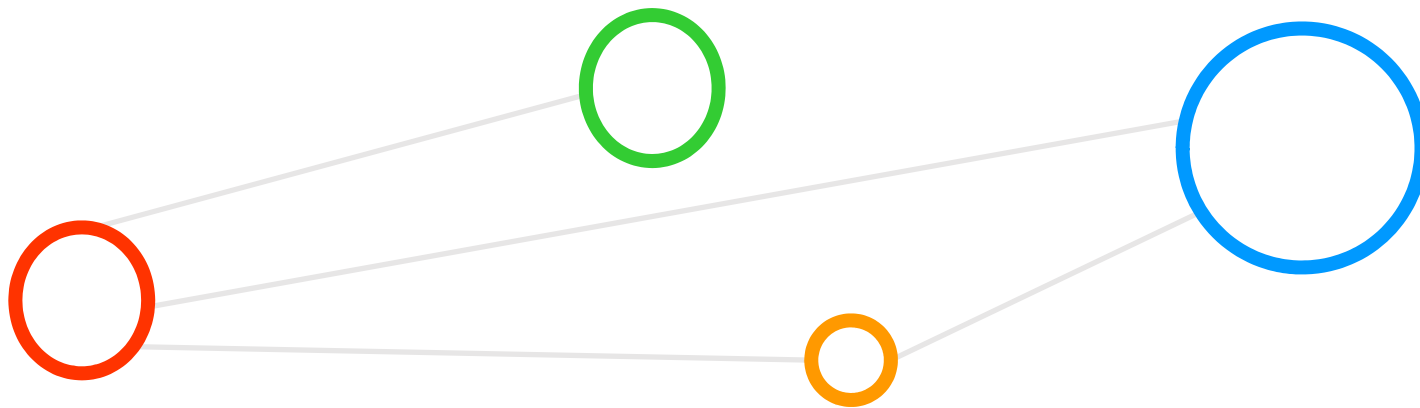
   [MORE]

3. University Course: **High Performance Computing – Advanced Scientific Computing**, REI105M, School of Engineering and Natural Sciences, University of Iceland, Iceland, Fall 2017
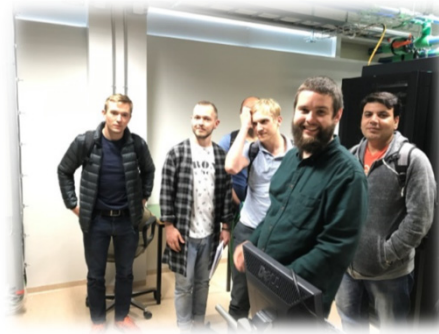
   [MORE]
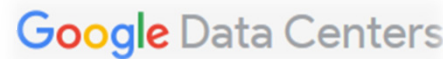
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  - Máni Maríus Viðarsson

- Organization / Management with HI
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  - Helmut Neukirchen
  - Matthias Book
  - Olafur Petur Palsson

- Discussions around Statistical Data Mining & Parallelization
  - Tomas Philipp Runnarson
 - Steinn Guðmundsson

- **Finally – Thanks to all of you!**

Morris Riedel @MorrisRiedel · Oct 8, 2018
Last week teaching on Practical Lecture 5.1 Amazon Web Services & Elastic Map Reduce in our Big Data & Cloud Computing course @Haskoli_Islands @uisens @uni_iceland @fzj_jsc @fz_juelich & HPC Expert
Máni Viðarsson @manimarius showed our real racks – slides: morrisriedel.de/teaching

Máni Maríus

Optional tours checking out our Jötunn cluster available on request
- course is too big to go alltogether this time

[12] DEEP Projects Web Page

The DEEP projects DEEP, DEEP-ER and DEEP-EST have received funding from the European Union's Seventh Framework Programme for research, technological development and demonstration under grant agreement no ICT-610476 and no ICT-287530 as well as the Horion2020 funding framework under grand agreement no. 754304.

[Video] Join our HPC Community & History
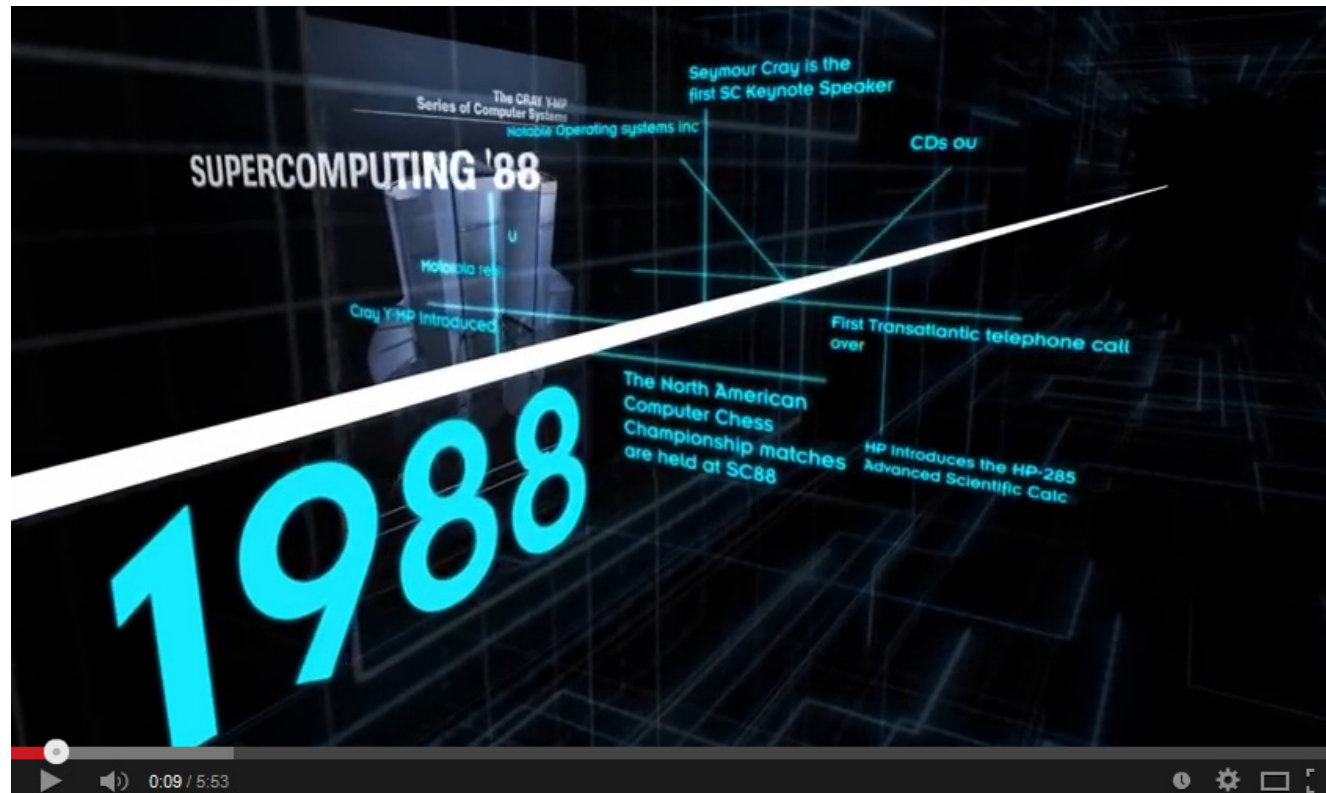
[16] YouTube Video, SC2013 – 25 years

Lecture Bibliography
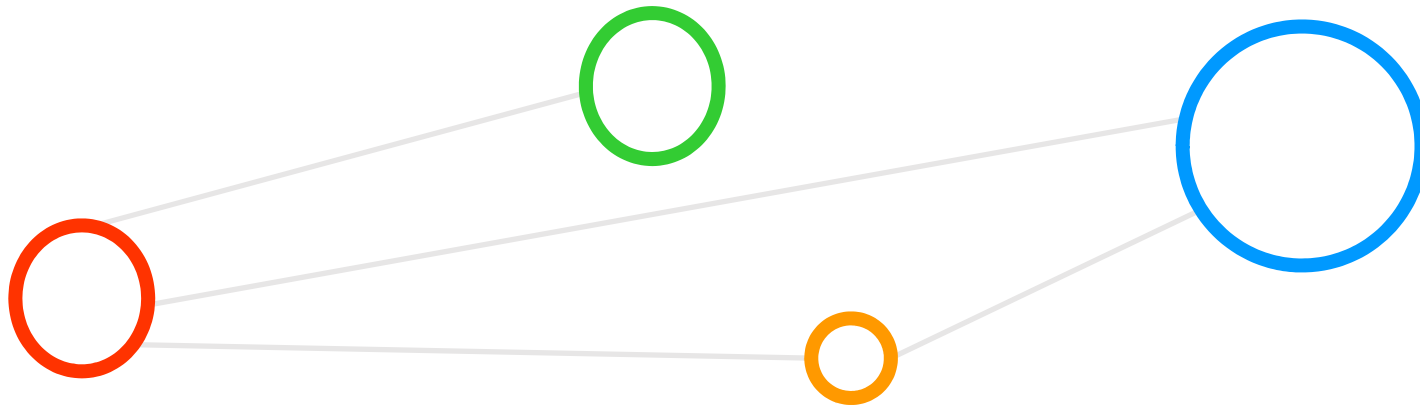
Lecture Bibliography

- [1] Steven Orszag et al., 'Lattice Boltzmann Methods for Fluid Dynamics', Online:
http://physics.wustl.edu/nd/event/qmcd09/Presentations/qmcd09Talks/orszag.pdf
- [2] Wikipedia on 'Computational Fluid Dynamics', Online:
http://en.wikipedia.org/wiki/Computational_fluid_dynamics
- [3] Wikipedia on 'Navier-Stokes', Online:
http://en.wikipedia.org/wiki/Navier%E2%80%93Stokes_equations
- [4] Wikipedia on 'Lattice Boltzmann Methods', Online:
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- [6] Wikipedia on 'Boundary Value Problems', Online:
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- [7] Civil Security & Traffice Group, Online:
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- [9] Morris Riedel Teaching Web Page, Online:
http://www.morrisriedel.de/teaching
- [10] Introduction to High Performance Computing for Scientists and Engineers, Georg Hager & Gerhard Wellein, Chapman & Hall/CRC Computational Science, ISBN 143981192X, English, ~330 pages, 2010, Online:
http://www.amazon.de/Introduction-Performance-Computing-Scientists-Computational/dp/143981192X
- [11] YouTube Video, 25 Years of HPC, Online:
http://www.youtube.com/watch?v=Q5VAMJn7tHA
- [12] DEEP Projects Web Page, Online:
https://www.deep-projects.eu/