

# High Performance Computing

ADVANCED SCIENTIFIC COMPUTING

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LECTURE 0

[in @Morris Riedel](#)

[@MorrisRiedel](#)

[@MorrisRiedel](#)

## Prologue

August 26, 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



**HELMHOLTZ**  
RESEARCH FOR GRAND CHALLENGES



HELMHOLTZ  
ARTIFICIAL INTELLIGENCE  
COOPERATION UNIT

# Outline of the Course

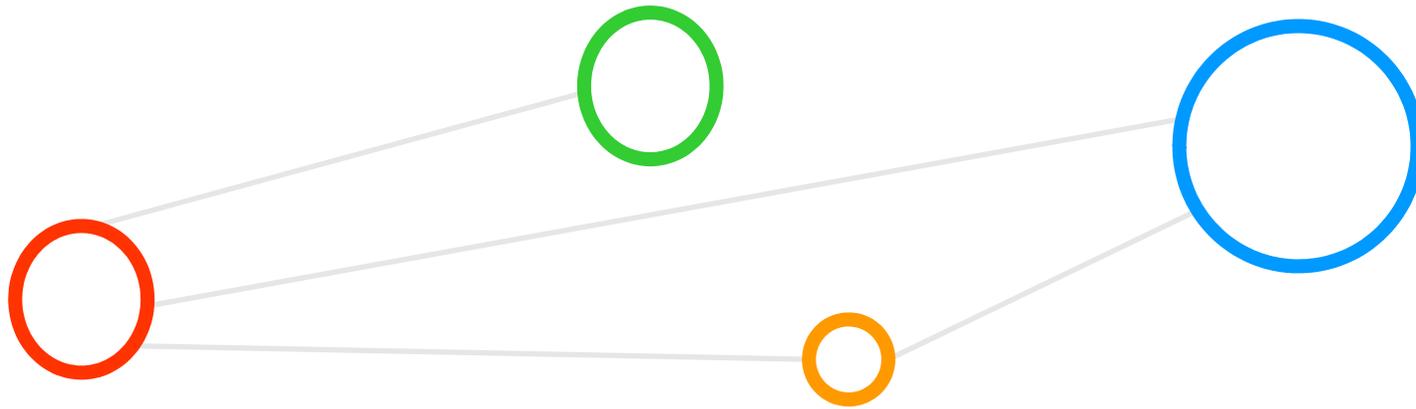
1. High Performance Computing
2. Parallel Programming with MPI
3. Parallelization Fundamentals
4. Advanced MPI Techniques
5. Parallel Algorithms & Data Structures
6. Parallel Programming with OpenMP
7. Graphical Processing Units (GPUs)
8. Parallel & Scalable Machine & Deep Learning
9. Debugging & Profiling & 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

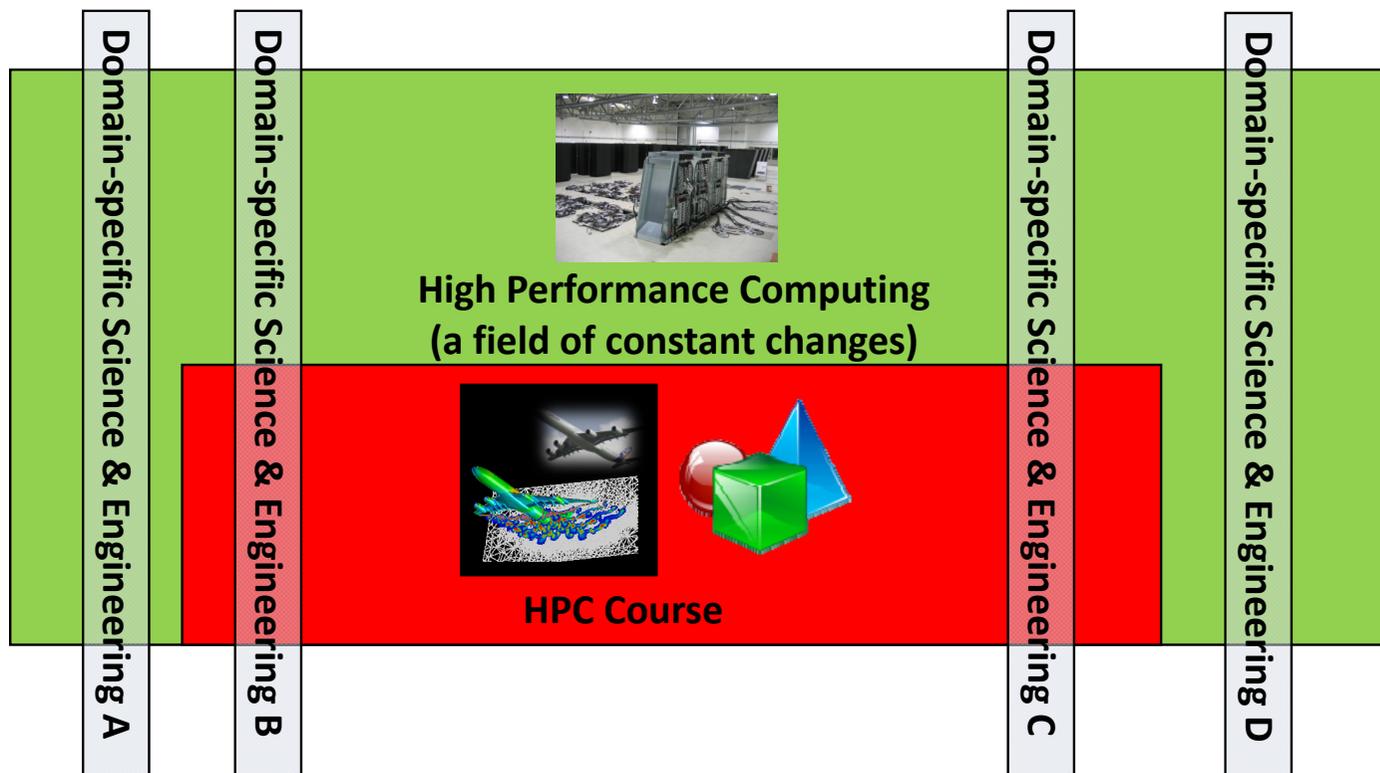
- Practical Topics
- Theoretical / Conceptual Topics

# Course Motivation & Information



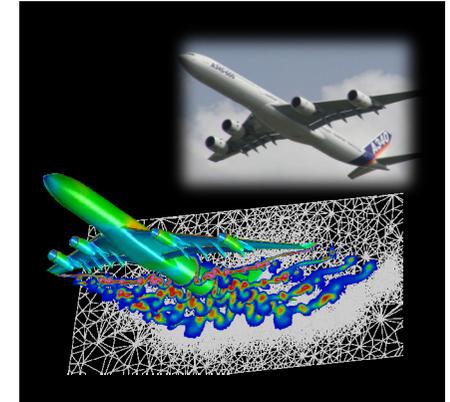
# Positioning in the Field of High Performance Computing (HPC)

- 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**



# Course Motivation

- **Parallel processing** and **distributed computing**
  - Matured over the past three decades
  - Both emerged as a well developed field in computer science
  - Still a lot of innovation, e.g. from hardware / software
- **‘Scientific computing’** with Maple, Matlab, etc.
  - Performed on small (‘serial’) computing machines like Desktop PCs or Laptops
  - Increasing number of cores enables ‘better scientific computing’ today
  - Good for **small & less complex applications**, quickly reach memory limits
- **‘Advanced scientific computing’**
  - Used with computational simulations and large-scale machine & deep learning
  - Performed on **large parallel computers**; often scientific domain-specific approaches
  - Use orders of magnitude multi-core chips & large memory & specific many-core chips
  - Enables **‘simulations of reality’** often based on known physical laws and numerical methods



# Selected Learning Outcomes

- Students understand...
  - Latest developments in **parallel processing & high performance computing (HPC)**
  - How to **create and use high-performance clusters**
  - What are **scalable networks & data-intensive workloads**
  - The importance of **domain decomposition**
  - **Complex aspects of parallel programming**
  - **HPC environment tools** that support programming or analyze behaviour
  - Different abstractions of **parallel computing on various levels**
  - Foundations and approaches of **scientific domain-specific applications**
- Students are able to ...
  - Programm and use HPC programming paradigms
  - Take advantage of innovative scientific computing simulations & technology
  - Work with technologies and tools to handle parallelism complexity



## Lecturer Morris Riedel (since ~2004 in HPC)

- Holds [PhD in Computer Science](#) (from Karlsruhe Institute of Tech.)
  - MSc in data visualization and steering of HPC & Grid applications
- Over the time several Positions at Juelich Supercomputing Centre
  - OS, Grid divisions; later deputy division leader federated systems and data
  - Currently: Research Group Leader – High Productivity Data Processing
- [Selected other recent activities](#)
  - Working with CERN & LHC & Grid/Cloud (Strategic Director of EU Middleware)
  - Architect of Extreme Science and Engineering Discovery Environment XSEDE (US HPC Infrastructure)
  - Co-Design of European Data Infrastructure (EUDAT), Research Data Alliance Big Data (Analytics) Chair, DEEP-EST HPC designs, steering group of Helmholtz Artificial Intelligence Cooperation Unit (HAICU)
- University courses
  - [University of Iceland Courses: HPC A / B, Statistical Data Mining, Cloud Computing & Big Data](#)
  - [Slides from previous years available under teaching of instructors personal Web page](#)

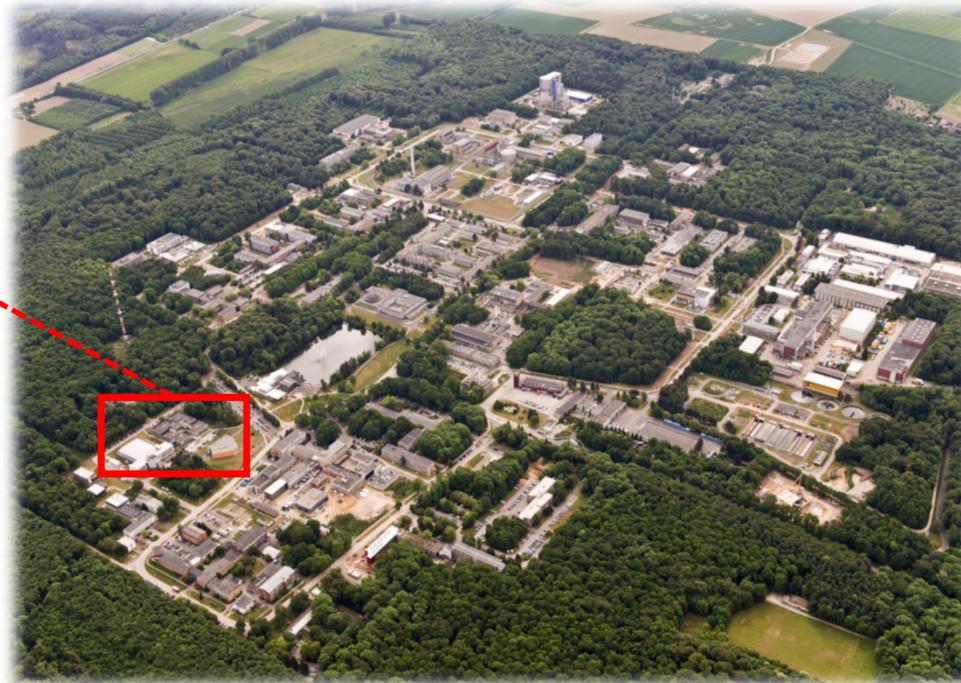


[3] Morris Riedel Web page

# Juelich Supercomputing Centre of Forschungszentrum Juelich – Germany

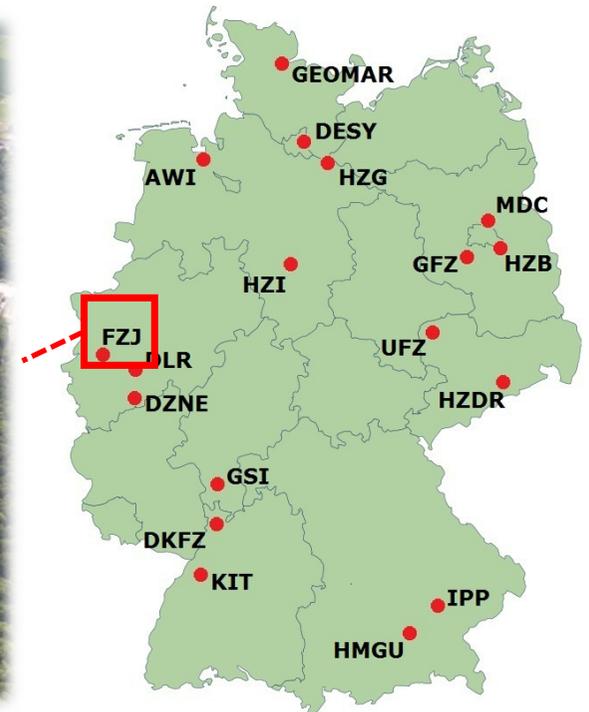


[5] Forschungszentrum Juelich Web page



## Selected Facts

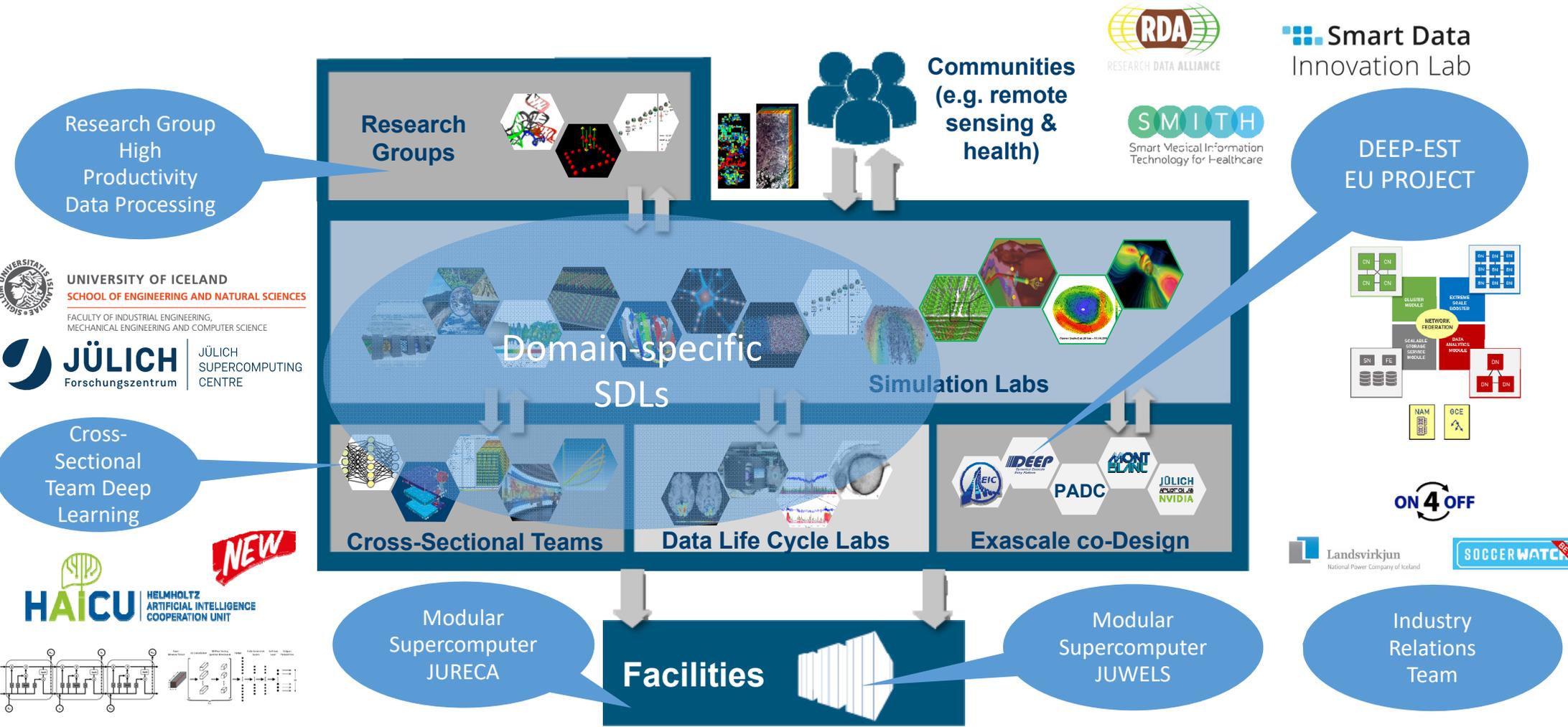
- One of EU largest inter-disciplinary research centres (~5000 employees)
- Special expertise in physics, materials science, nanotechnology, neuroscience and medicine & **information technology (HPC & Data)**



**HELMHOLTZ**  
RESEARCH FOR GRAND CHALLENGES

[4] Helmholtz Association Web Page

# Jülich Supercomputing Centre High Productivity Data Processing Research Group



# University of Iceland – School of Natural Sciences & Engineering (SENS)

## Selected Facts

- Ranked *among the top 300 universities in the world* (by Times Higher Education)
- Ranked *#6 in the field of remote sensing* (by Shanghai list)
- ~2900 students at the SENS school
- Long collaboration with Forschungszentrum Juelich
- ~350 MS students & ~150 PhD students
- Many foreign & Erasmus students
- English courses

[6] University of Iceland SENS Web Page



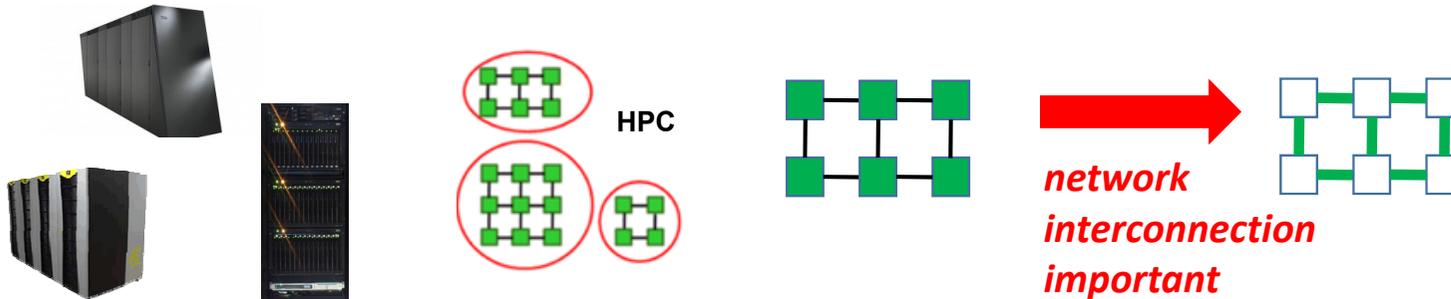
UNIVERSITY OF ICELAND  
SCHOOL OF ENGINEERING AND NATURAL SCIENCES

FACULTY OF INDUSTRIAL ENGINEERING,  
MECHANICAL ENGINEERING AND COMPUTER SCIENCE



# Understanding High Performance Computing (HPC)

- High Performance Computing (HPC) is based on computing resources that enable the efficient use of parallel computing techniques through specific support with dedicated hardware such as high performance cpu/core interconnections.



- High Throughput Computing (HTC) is based on commonly available computing resources such as commodity PCs and small clusters that enable the execution of 'farming jobs' without providing a high performance interconnection between the cpu/cores.



➤ The complementary Cloud Computing & Big Data – Parallel Machine & Deep Learning Course focusses on High Throughput Computing

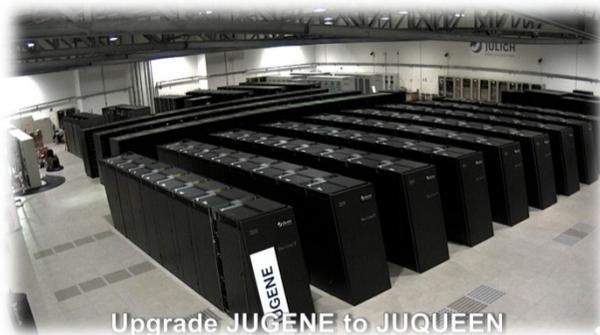
# HPC & Data-intensive Sciences – A Field of Constant Evolution

1.000.000 FLOP/s  
~1984



- Floating Point Operations per one second (FLOPS or FLOP/s)
- 1 GigaFlop/s =  $10^9$  FLOPS
- 1 TeraFlop/s =  $10^{12}$  FLOPS
- 1 PetaFlop/s =  $10^{15}$  FLOPS
- 1 ExaFlop/s =  $10^{18}$  FLOPS

1.000.000.000.000.000 FLOP/s  
~295.000 cores ~2009 (JUGENE)



>5.900.000.000.000.000 FLOP/s  
~ 500.000 cores  
~2013 → end of service in 2018

# German GAUSS Centre for Supercomputing



**GCS**  
Gauss Centre for Supercomputing

[7] GCS Web page

## ■ Supercomputer JUWELS @ JSC

- Juelich Wizard for European Leadership Science (JUWELS)
- Cluster architecture based on commodity multi-core CPUs
- 2,550 compute nodes: two Intel Xeon 24-core Skylake CPUs & 48 accelerated compute nodes (4 NVIDIA Volta GPUs)

## ■ Supercomputer SuperMUC @ LRZ

- 155,000 cores

## ■ Supercomputer Hazel Hen @HLRS

- 185,088 compute cores

- GCS represents Germany in the Partnership for Advanced Computing in Europe (PRACE) HPC infrastructure



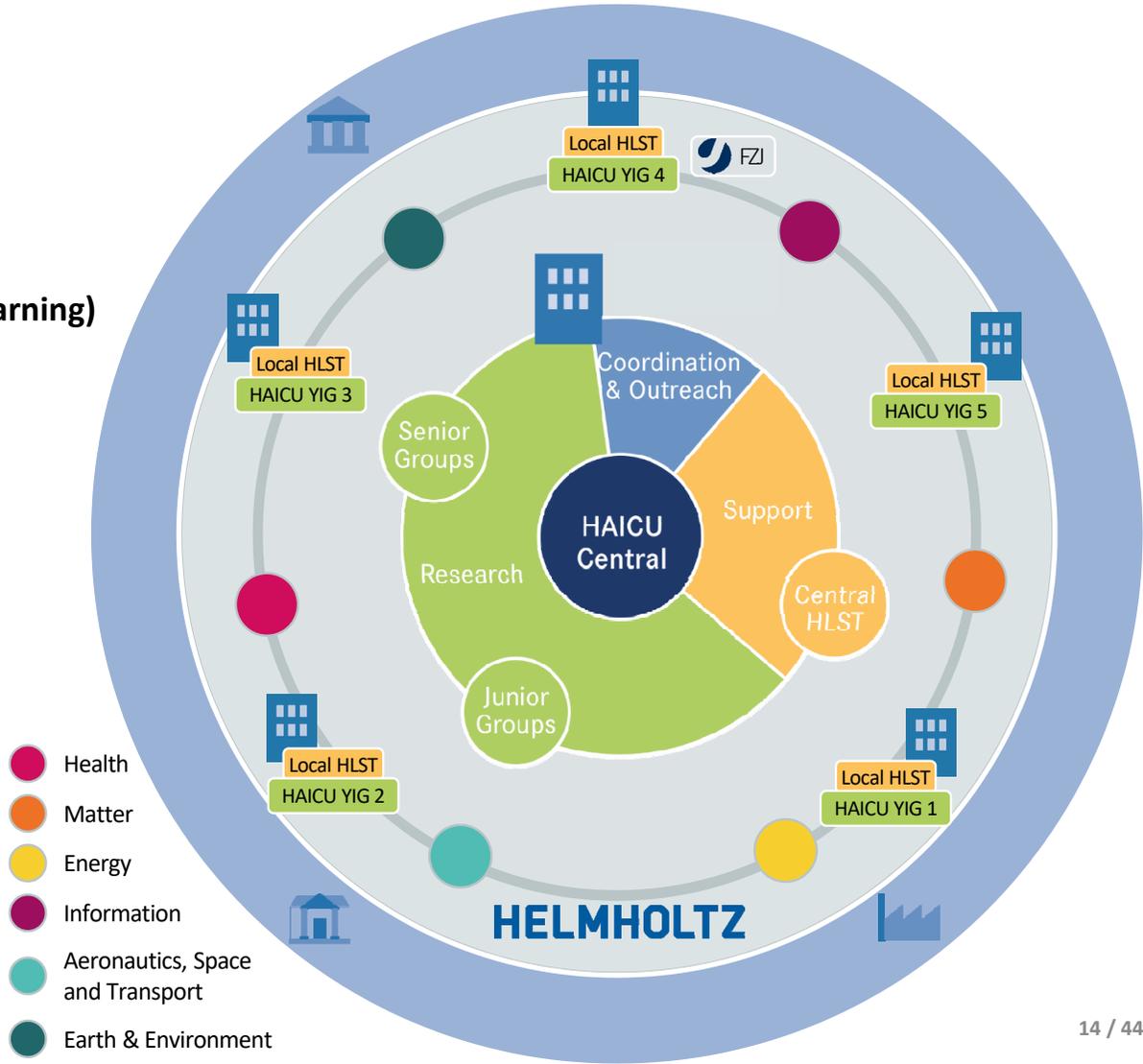
[8] PRACE Web page

# Artificial Intelligence & HPC

- **Forschungszentrum Jülich (HAICU Local ‘Information’)**
  - **Young Investigator Group at INM-1 (~3 FTEs)**
  - **High Level Support Team (HLST) at JSC (~ 5 FTEs)**  
(specific expertise in parallel & scalable machine learning)
- Helmholtz Zentrum München (HMGU)  
(HAICU Central ‘Health’)
- Karlsruhe Institute of Technology (KIT)  
(HAICU Local ‘Energy’)
- Helmholtz-Zentrum Geesthacht (HZG)  
(HAICU Local ‘Earth & Environment’)
- Helmholtz-Zentrum Dresden Rossendorf (HZDR)  
(HAICU Local ‘Matter’)
- German Aerospace Center (DLR)  
(HAICU Local ‘Aeronautic/Space & Transport’)



~11.4 million € / year  
[9] HAICU Web Page



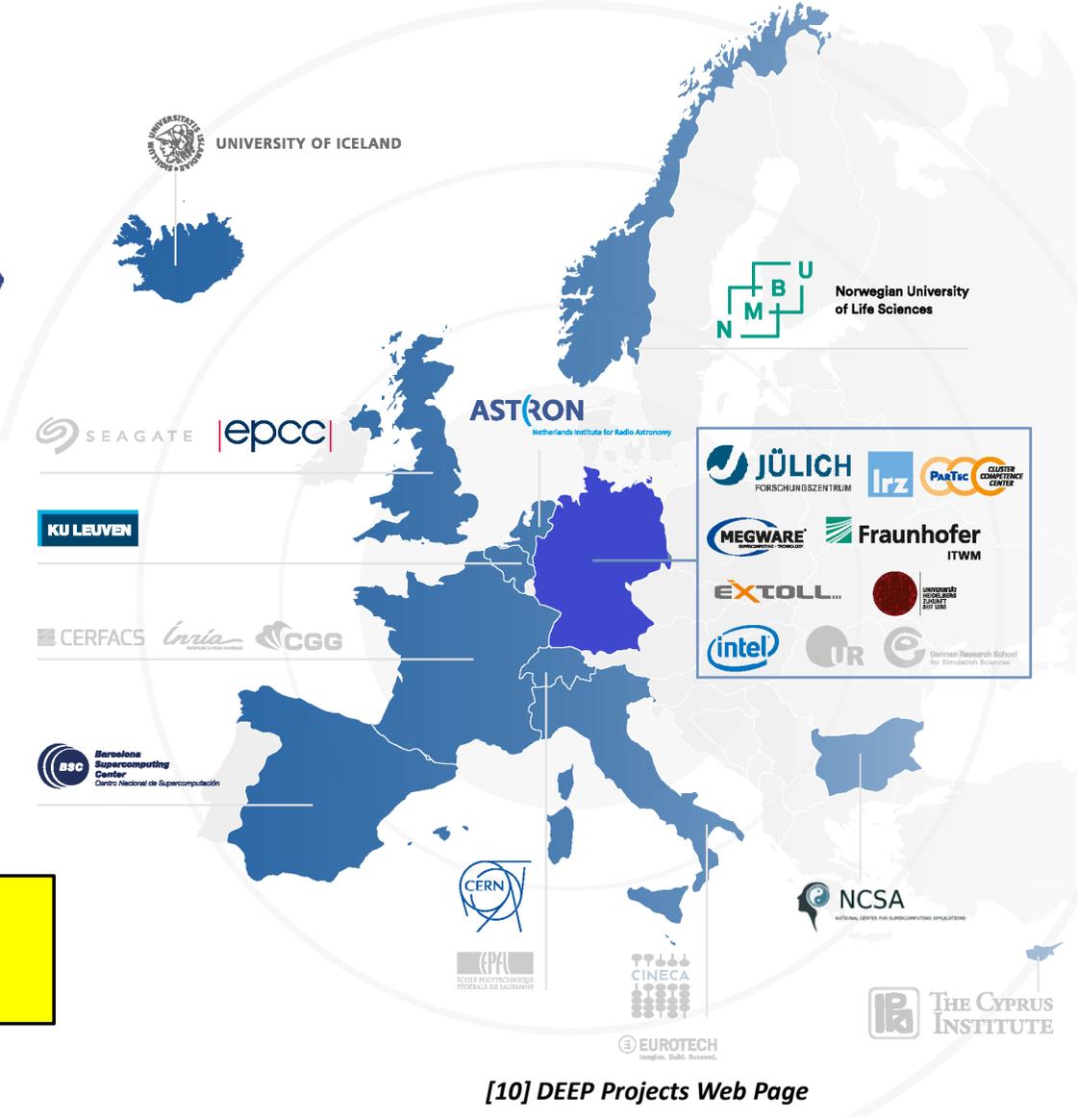
# DEEP series of PROJECTS & HPC



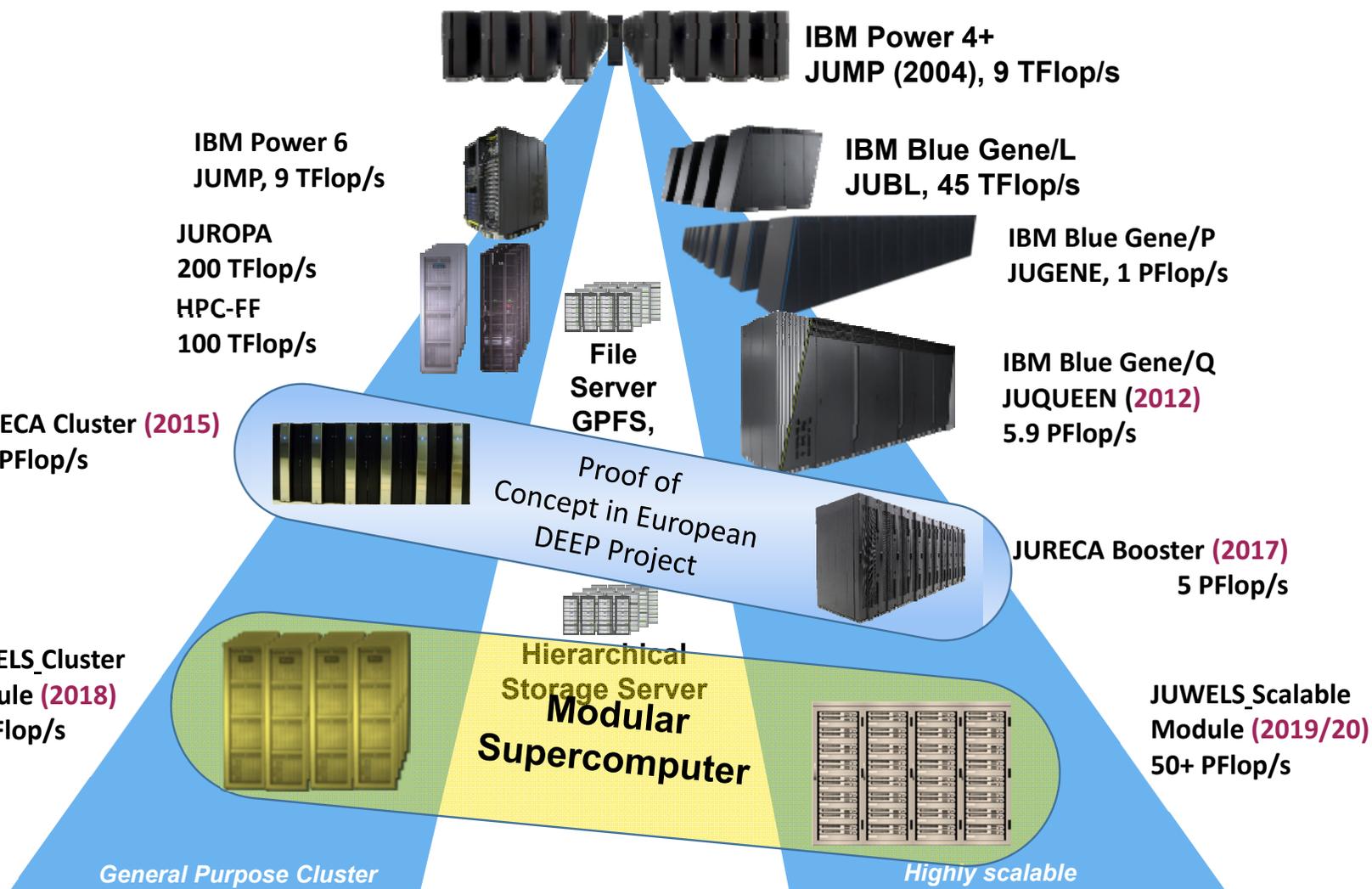
- 3 EU Exascale projects  
DEEP, DEEP-ER, DEEP-EST
- 27 partners  
Coordinated by JSC
- EU-funding: 30 M€  
JSC-part > 5,3 M€
- Nov 2011 – Dec 2020

▪ Strong collaboration with our industry partners Intel, Extoll & Megware

▪ Juelich Supercomputing Centre implements the DEEP projects designs in its HPC production infrastructure



[10] DEEP Projects Web Page



# UGLA Tool & Office Hours (!)

- Reference course information

- [High Performance Computing](#)
- [REI105M, Fall 2019](#)



- Use it for course communication

- Every course member requires account
- Contact other students & discuss topics
- Contact lecturer

- Find course materials

- Slides of Lectures and Practical Lectures
- Handouts and Recordings
- Further reading topics (e.g. papers, etc.)

- **Questions, major difficulties, etc.? → Don't wait long!**

- [Use my office hours](#), send meeting request email to [morris@hi.is](mailto:morris@hi.is)



*[13] High Performance Computing  
UGLA Course Page Online*

# Overall Course Organization

- 3 Assignments (40% of grade)
  - Guided by **practical lectures in context** with hands-on elements for all
  - Cloud configuration & cloud programming projects
  - Influence in the overall grade
  - **TBD(all): Create Groups of 2-3 and send the group to [morris@hi.is](mailto:morris@hi.is)**
- Quizzes (10% of grade)
  - Small quiz from time to time (pre-announced) to check understanding
  - Minor influence in the overall grade – good preparation for exam
- Exam (50% of grade)
  - End of the lecture series (~December) – major part of the overall grade
  - **'Not knowing everything is key – but understand the important elements'**
- Invited Lectures
  - A couple of presentations (e.g. companies, interesting projects, etc.)

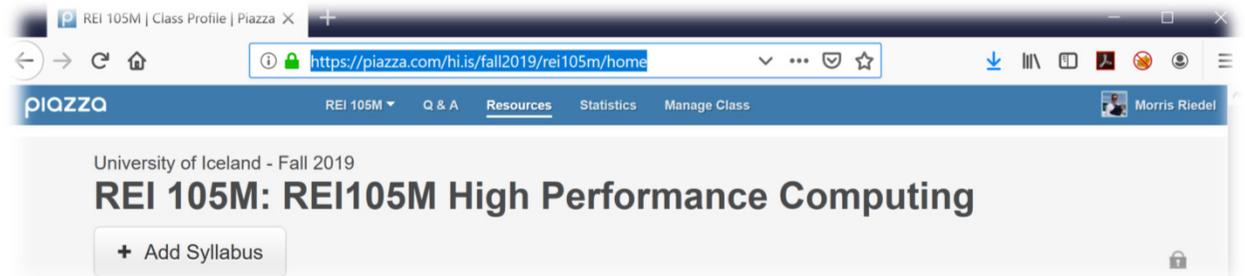
# Course @ Q&A Platform Piazza

## ■ Q&A Platform

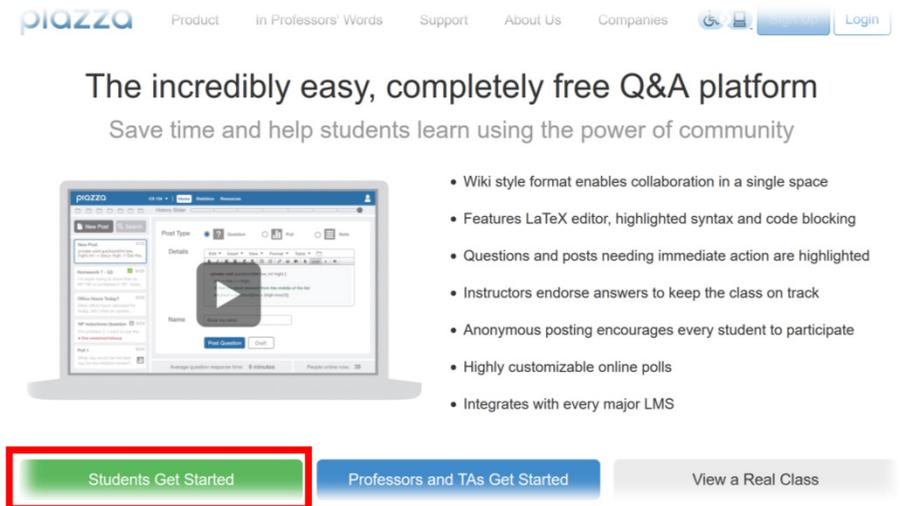
- Mixture between a wiki and a forum for students
- Can be used by academic institutions for free
- Idea: come together to share ideas and knowledge
- E.g. ask questions about course assignments/ content

## ■ Course information

- Name: REI105M High Performance Computing
- Semester: Fall 2019
- URI: <https://piazza.com/hi.is/fall2019/rei105m/home>
- TBD (all students): Please check whether you have been registered for the course
- TBD (all students): Get familiar with Piazza



[1] Piazza Web page



# Course @ Gradescope

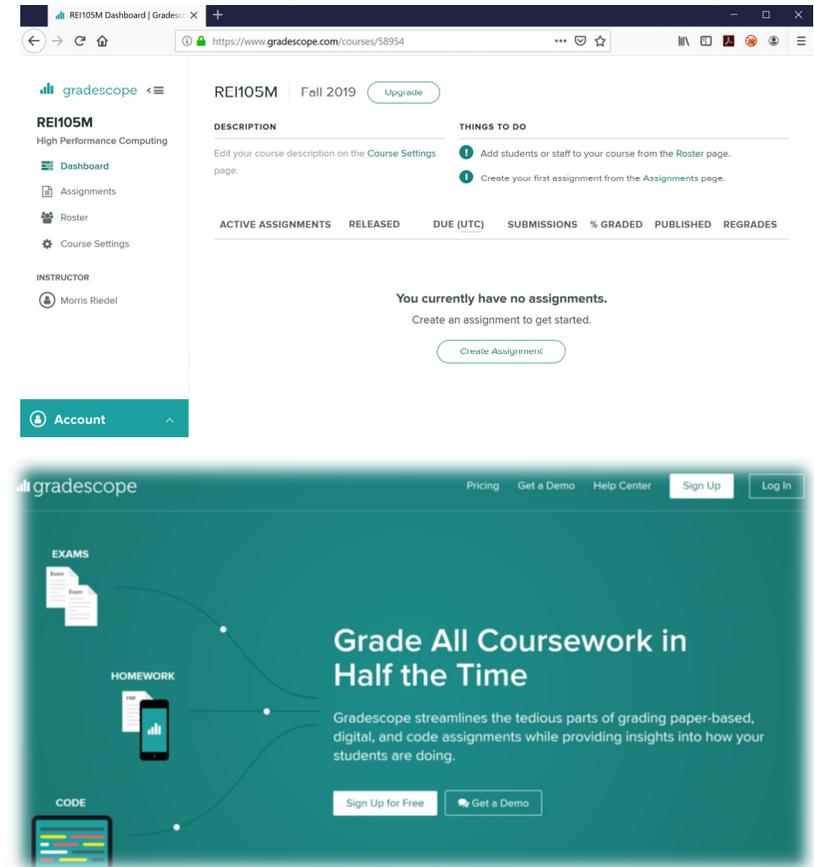
## ■ Student Grading Platform

- Grading for quizzes, assignments & exam will be performed
- Can be used by academic institutions for free
- Idea: get faster feedback for course content and a more fair grading process
- E.g. professor does not see the name of students per task

## ■ Course information

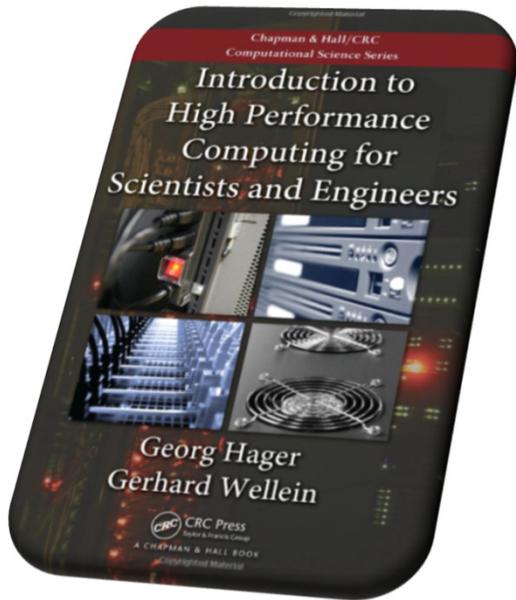
- Name: REI105M High Performance Computing
- Semester: Fall 2019
- URI: <https://www.gradescope.com/courses/58954>
- TBD (all students): Please check whether you have been registered for the course
- TBD (all students): Get familiar with Gradescope

[2] Gradescope Web page



## Associated Literature

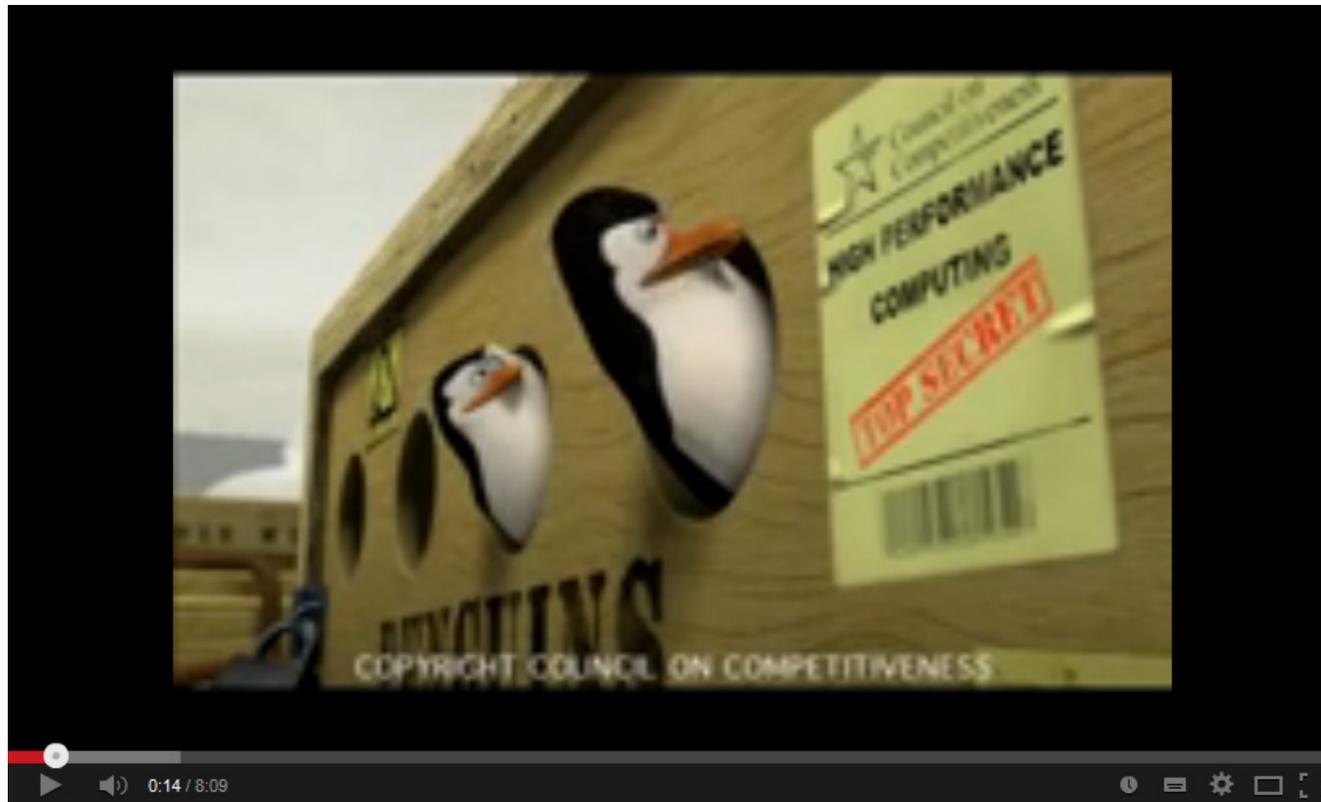
**Introduction to High Performance Computing for Scientists and Engineers,**  
Georg Hager & Gerhard Wellein,  
Chapman & Hall/CRC Computational Science,  
ISBN 143981192X, English, ~330 pages, 2010



*[14] Introduction to High Performance Computing, 2010*

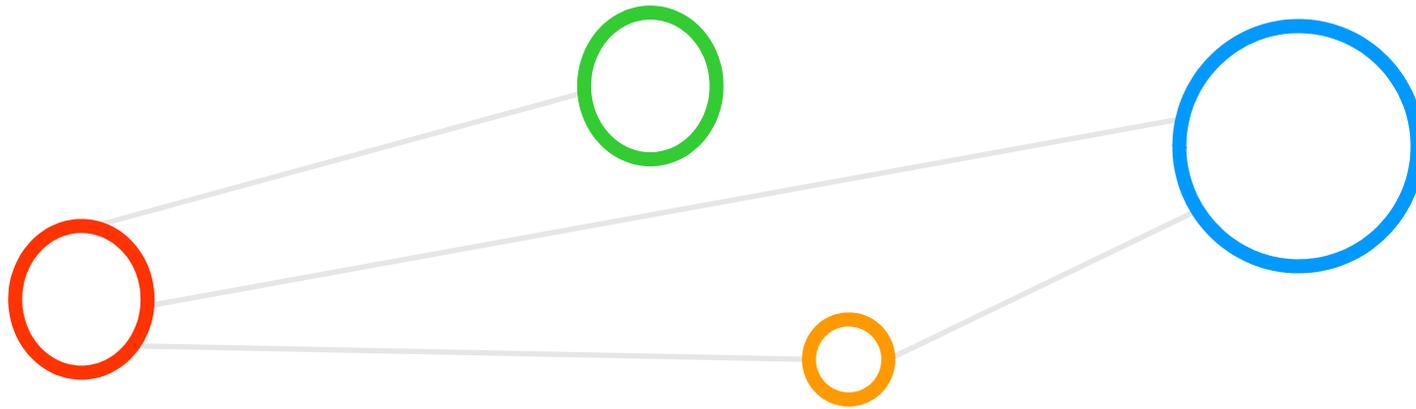
- Further bibliography and readings will be provided in context
  - E.g. Papers, Web pages, etc.

## [Video] High Performance Computing by Dreamworks



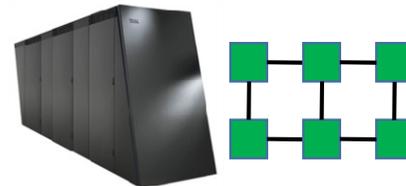
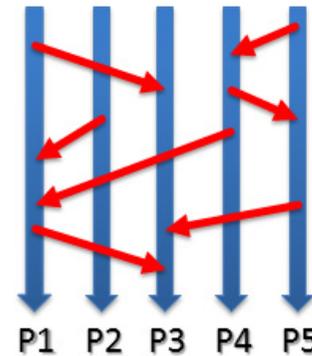
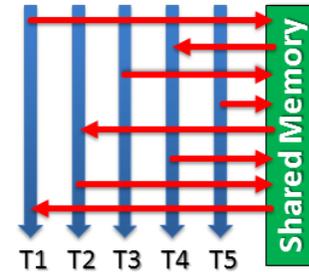
[11] YouTube, Dreamworks

# Course Organization & Content



# Lecture 1 – High Performance Computing

- What means ‘high performance’?
  - Four basic building blocks of HPC
  - TOP500 and Performance Benchmarks
  - Relationship to ‘Parallelization’
- HPC Architectures
  - Shared Memory & Distributed Memory Architectures
  - Hybrid and Emerging Architectures
  - Parallel Applications and Infrastructures
- HPC Ecosystem
  - Software Environments & Scheduling
  - System Architectures & Data Access
  - Multicore Processor Design
  - Network Topologies
  - Interesting international HPC Projects



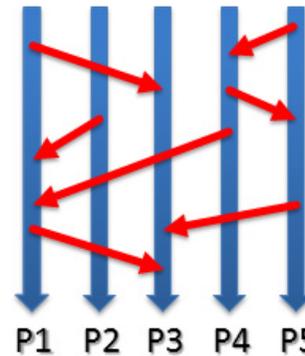
# Lecture 2 – Parallel Programming with MPI

## ■ Message Passing Interface (MPI) Concepts

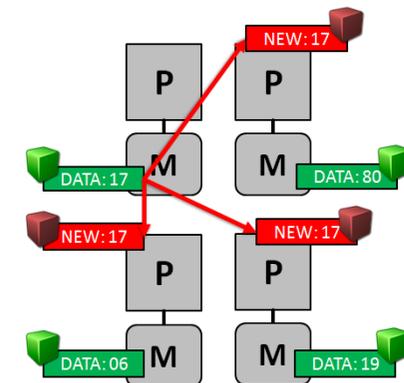
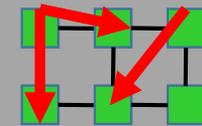
- Distributed memory systems
- Message passing functions
- Understanding the functionality of MPI collectives
- Standardization & portability
- Using MPI rank and communicators
- MPI collective communications

## ■ MPI Parallel Programming Basics

- Environment with libraries & modules
- Thinking parallel
- Basic building blocks of a program
- Compilations of codes
- Parallel executions and MPI runtime
- ‘Bad’ code examples vs. good code examples



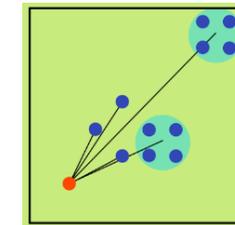
HPC Machine



# Lecture 3 – Parallelization Fundamentals

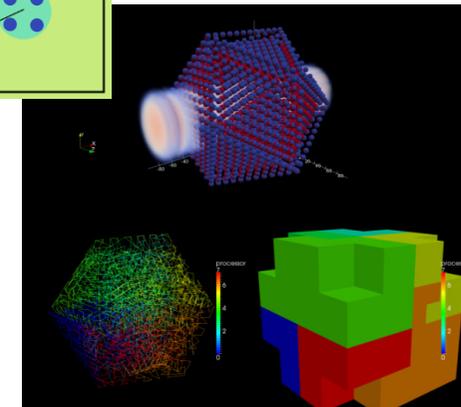
- Parallel Applications
  - Simple first parallel application examples
  - Gradually more complex applications
- Common Strategies for Parallelization
  - Moore's law
  - Parallelization reasons and approaches
  - Various domain decompositions
  - Data parallelism methods
  - Functional parallelism methods
- Parallelization Terms & Theory
  - Speedup & Load Imbalance
  - Role of Serial Elements
  - Scalability Metrics & Performance
  - Amdahl's Law & Performance Analysis

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
CPU/core 1				CPU/core 2				CPU/core 3				CPU/core 4			
0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Max-local A				Max-local B				Max-local C				Max-local D			



Amount of work/overall problem size:  
 $s + p = 1$   
 ▪  $s$  = serial (nonparallelizable part)  
 ▪  $p$  = parallelizable part

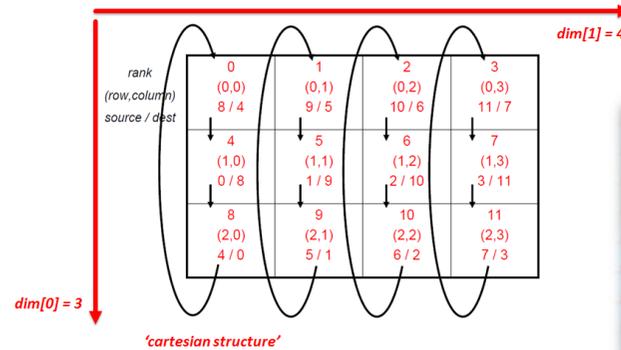
$$T_i^p = s + p/N$$



# Lecture 4 – Advanced MPI Techniques

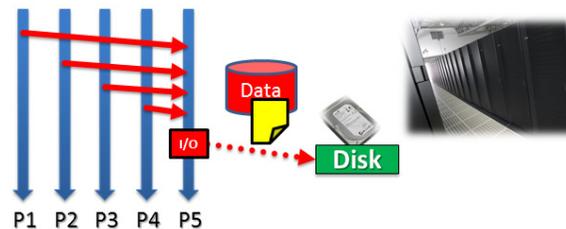
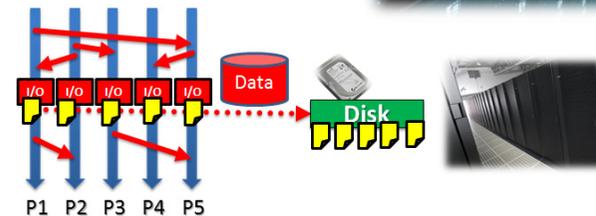
## ■ MPI Communication Techniques

- MPI Communicators
- Cartesian Communicator
- Hardware & Communication Issues
- Network Interconnects
- Task-Core Mappings
- Application examples



## ■ MPI Parallel I/O Techniques

- I/O Terminologies & Challenges
- Parallel Filesystems
- MPI I/O Techniques
- Higher-Level I/O Libraries
- Portable File Formats
- Application examples



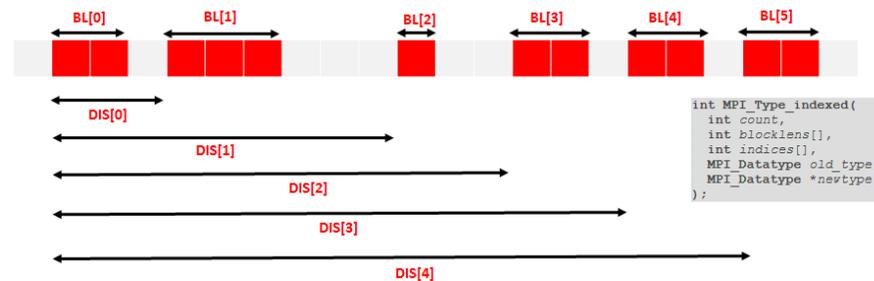
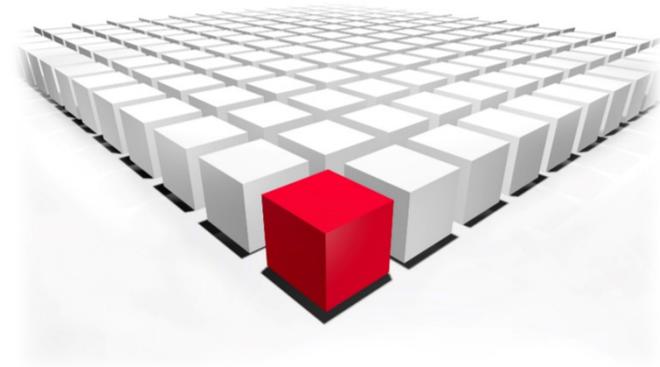
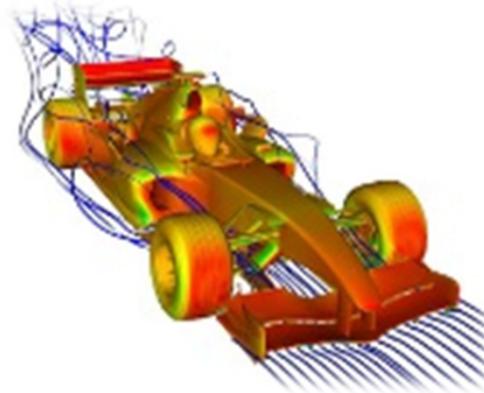
# Lecture 5 – Parallel Algorithms & Data Structures

## Selected Parallel Algorithms

- Vector Addition in MPI & OpenMP
- Matrix – Vector Multiplication in MPI
- Fast Fourier Transform with MPI
- Advanced Algorithm Examples
- Use of MPI collectives in applications

## Selected Data Structures

- Basic MPI Datatypes
- Arrays & Multi-dimensional datasets
- Derived MPI Datatypes
- Relationships to Parallel IO & Filesystems

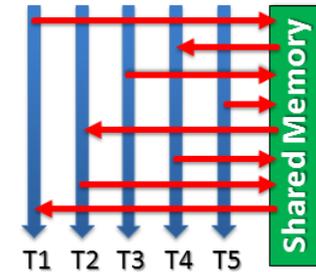


# Lecture 6 – Parallel Programming with OpenMP

## ■ Shared-Memory Programming Concepts

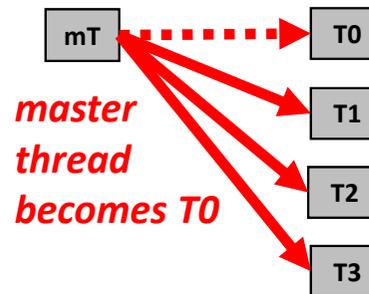
- Parallel and Serial Regions
- Fork & Joins
- Master and Worker Threads
- Portability
- Application Examples
- Differences to distributed memory

```
int main()
{
    #pragma omp parallel
    printf(„Hello World“);
}
```



## ■ OpenMP Parallel Programming Basics

- Basic building blocks
- Local/shared variables & Loops
- Synchronization & Critical Regions
- Selected Comparisons with MPI
- Simple Applications



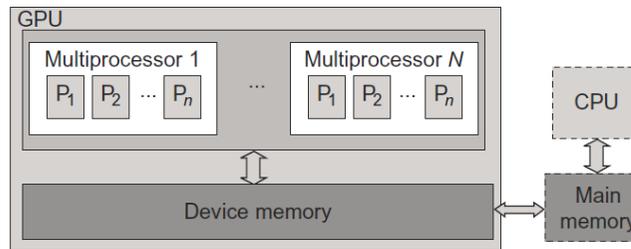
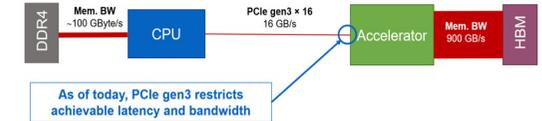
# Lecture 7 – Graphical Processing Units (GPUs)

- General Purpose Graphical Processing Units (GPGPUs)

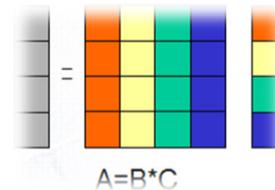
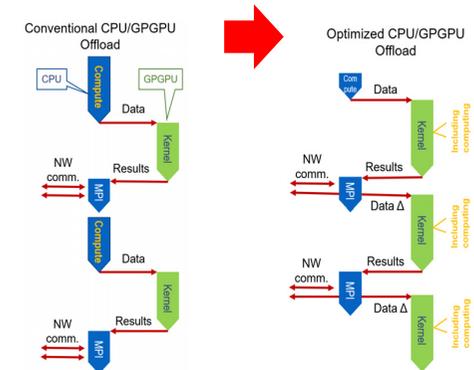
- Often known as just ‘GPU’
- Many-core vs. Multi-core
- Terminology & Architecture
- Architecture differences from Kepler, Pascal, Volta
- Programming Models
- Usage Models & Applications
- NVidia & CUDA Examples
- Programming with OpenACC
- Programming with HIP
- GPU Toolsets
- GPU Direct

- Selected GPU Applications

- Simple Examples
- Simulation Sciences
- Machine & Deep Learning



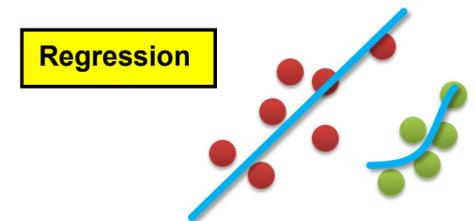
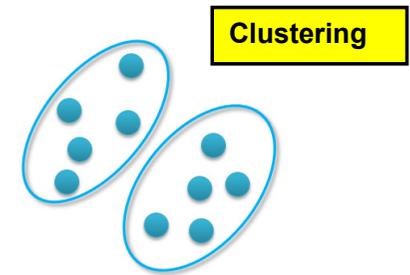
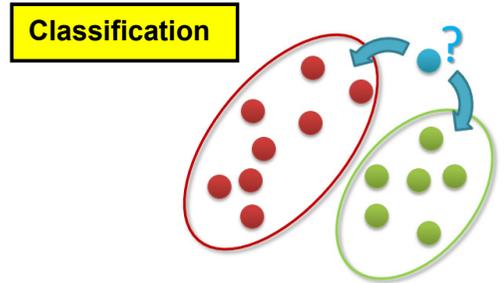
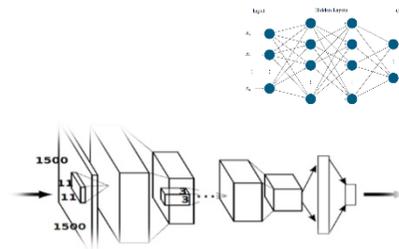
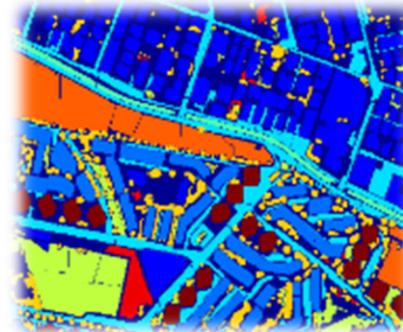
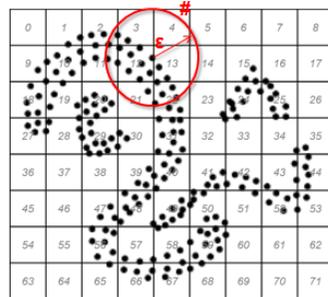
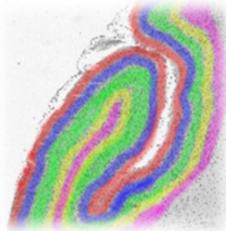
[15] Distributed & Cloud Computing Book



# Lecture 8 – Parallel & Scalable Machine & Deep Learning

## Machine Learning & Deep Learning

- Terminology & Motivation
- Contrast to High Throughput Computing
- HPC for Classification, Clustering & Regression
- Selected Remote Sensing Use Case
- Parallel Support Vector Machines
- HBDBSCAN for Clustering
- Deep Learning with Keras & TensorFlow
- Inverse Problems
- Relationship to Parallel I/O
- Application Examples



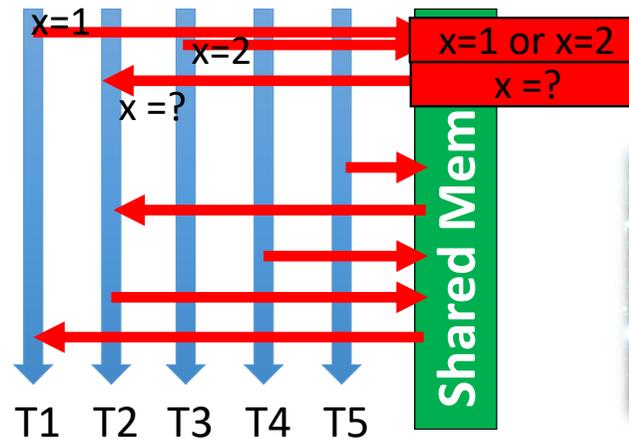
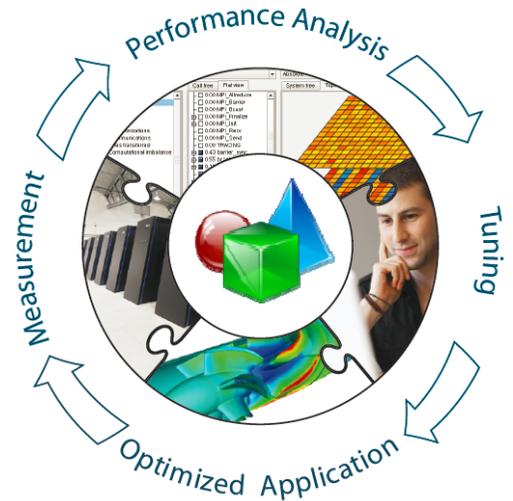
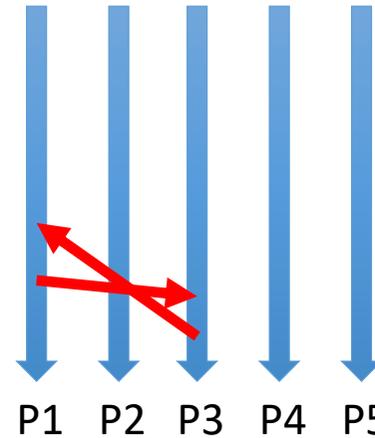
# Lecture 9 – Debugging & Profiling & Performance Toolsets

## ■ Debugging & Profiling Techniques

- Origin and Terminologies
- Bug Prevention Approaches
- Review Printf Debugging
- Advanced Debugging Techniques
- Selected Debugging Tools
- Understanding Wall-clock time
- Simple MPI Timing Approaches
- MPI Profiling Interface & Tools

## ■ Selected Profiling Tools

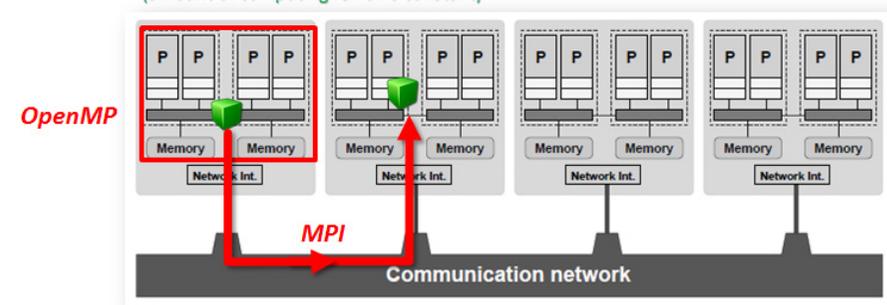
- Performance Optimization
- Tracing Technique & Open Trace Format
- MPI & OpenMP Problem Patterns
- Tensorflow & Deep Learning Tool Support



# Lecture 10 – Hybrid Programming and Patterns

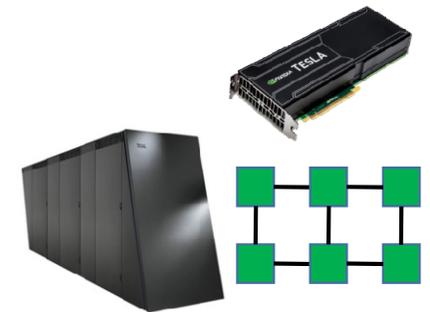
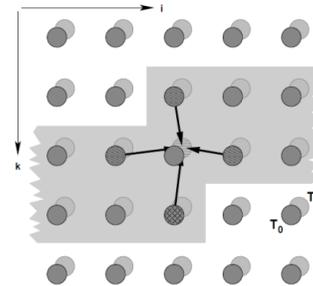
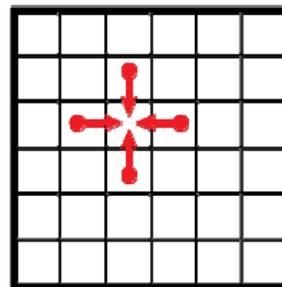
## ■ Hybrid Programming

- Motivation and Memory Benefits
- Programming Hybrid Systems
- Vector Mode and Task Mode
- Lessons Learned & Performance
- Another type of Hybrid Programming
- Application Examples in OpenMP, MPI & GPUs



## ■ Programming Patterns

- Nearest Neighbour Communication
- Cartesian Communicator Shifts
- Stencil-based Iterative Methods
- Jacobi 2D Application Example
- Working with Halo Regions
- Application Examples



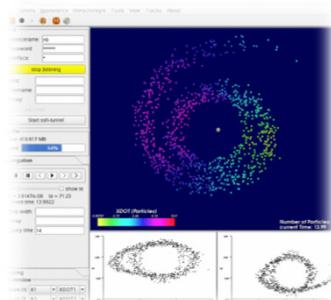
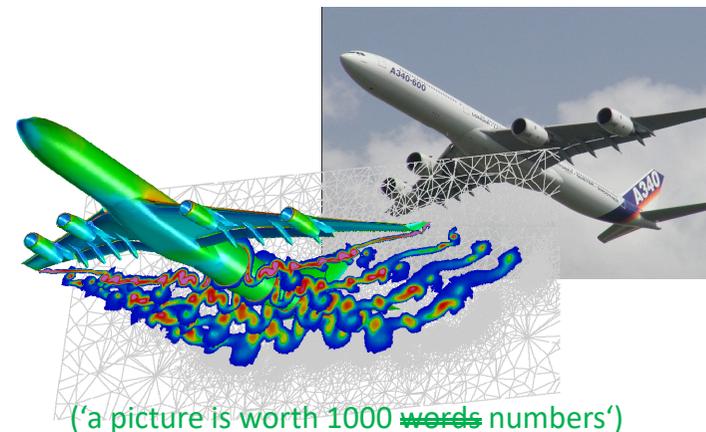
# Lecture 11 – Scientific Visualization & Scalable Infrastructures

## ■ Scientific Visualization

- Motivation & Objectives
- Understanding HPC Simulation Data
- Selected Visualization & Computational Steering Techniques
- Selected Tools and Technologies
- Multi-scale Visualization Example
- Application Examples

## ■ Scalable Infrastructures

- Large Scale HPC Infrastructures
- e-Science and Grid Computing
- Cloud Computing Infrastructures
- Collaborative Data Infrastructures
- Scientific Workflows
- Applications

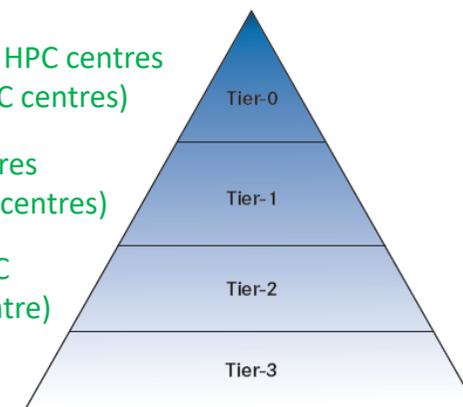


Large-scale HPC centres  
(e.g. EU HPC centres)

National HPC centres  
(e.g. German HPC centres)

Topical and Regional HPC  
Centres (e.g. climate centre)

Servers and small clusters  
(e.g. universities, institutes)



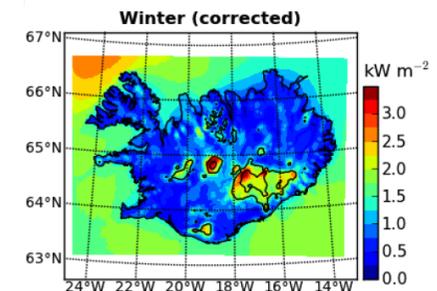
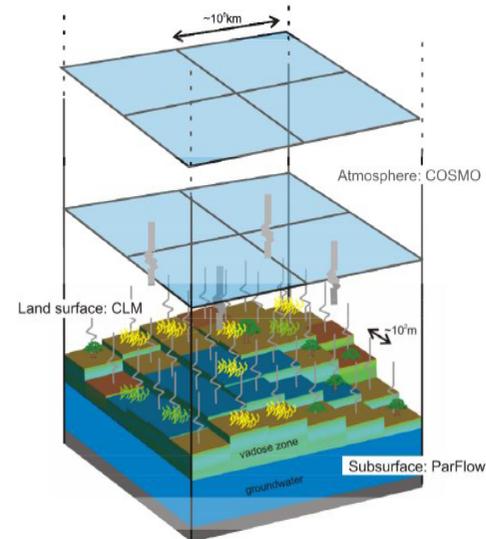
# Lecture 12 – Terrestrial Systems & Climate

## ■ Terrestrial Systems

- Numerical Terrestrial Simulations & Models
- ParFlow Hydrology Parallel Application
- CLM Land-Surface Model Parallel Application
- COSMO Weather Model Parallel Application
- Coupled Models & Other Models & Libraries
- Application Examples

## ■ Climate

- Numerical Weather Prediction & Forecast
- Role of Partial Differential Equations (PDEs)
- WRF Model Parallel Application
- SAR Weather Project & Business Case
- Other Models & Libraries
- Application Examples



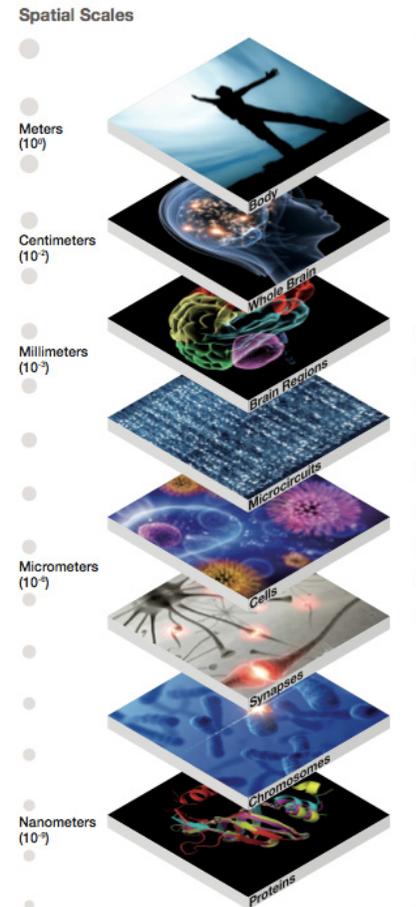
# Lecture 13 – Systems Biology & Bioinformatics

## ■ Systems Biology

- Motivation & Basic Terminology
- Selected Scientific Case Protein Folding
- Role of Monte Carlo Methods
- SMMP & Neuroscience Parallel Applications
- Other Models & Libraries
- Application Examples

## ■ Bioinformatics

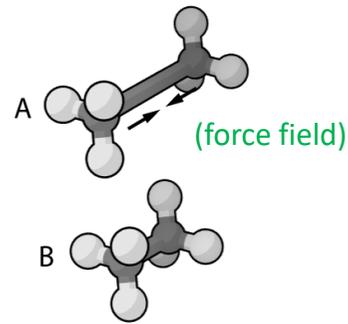
- Motivation & Basic Terminology
- Selected Scientific Case Gene Sequencing
- Role of Databases and Web-based Portals
- BLAST Parallel Application
- Other Tools & Techniques
- Application Examples



# Lecture 14 – Molecular Systems & Libraries

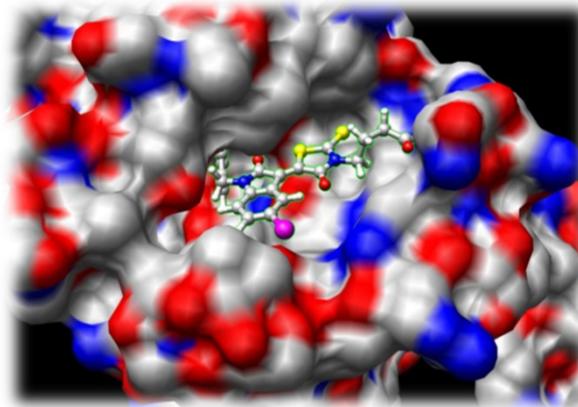
## ■ Molecular Systems

- Terminology & Motivation
- Ab Initio Calculations
- Molecular Docking & Dynamics
- Application Examples



## ■ Selected Methods & Libraries

- NAMD
- CPMD
- MP2C
- AMBER
- Parallel Interoperability Application



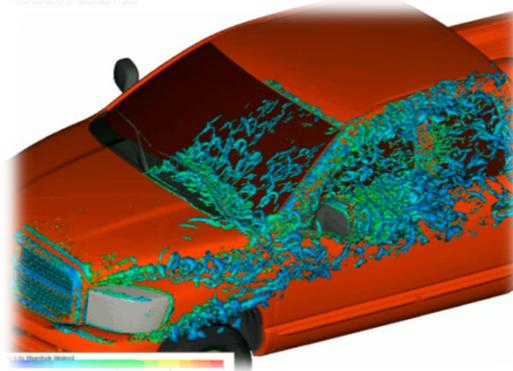
# Lecture 15 – Computational Fluid Dynamics & Finite Elements

## ■ Computational Fluid Dynamics

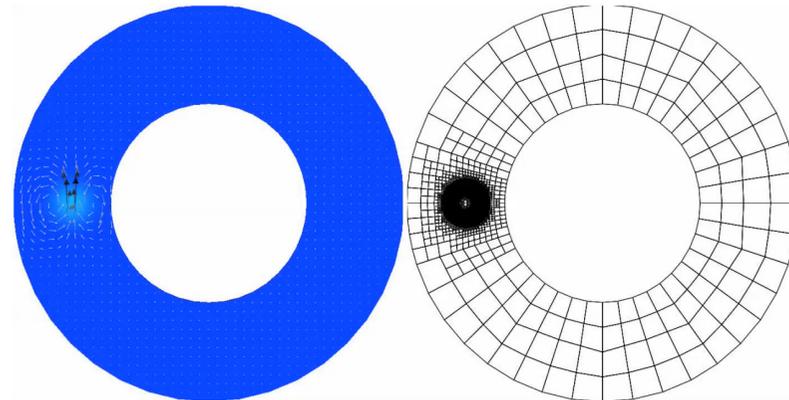
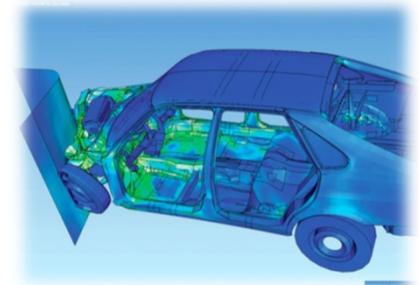
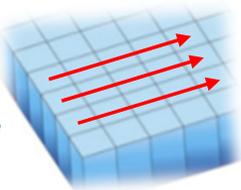
- Terminology & Motivation
- Navier-Stokes Method
- Lattice-Boltzmann Method
- Large Eddy Turbulence Model
- Modelling Methodology Revisited
- Application Examples & Libraries

## ■ Finite Elements

- Terminology & Motivation
- Boundary Value Problems
- Mesh Generation Technique
- Adaptive Mesh Refinement
- Application Examples & Libraries



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



# 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.

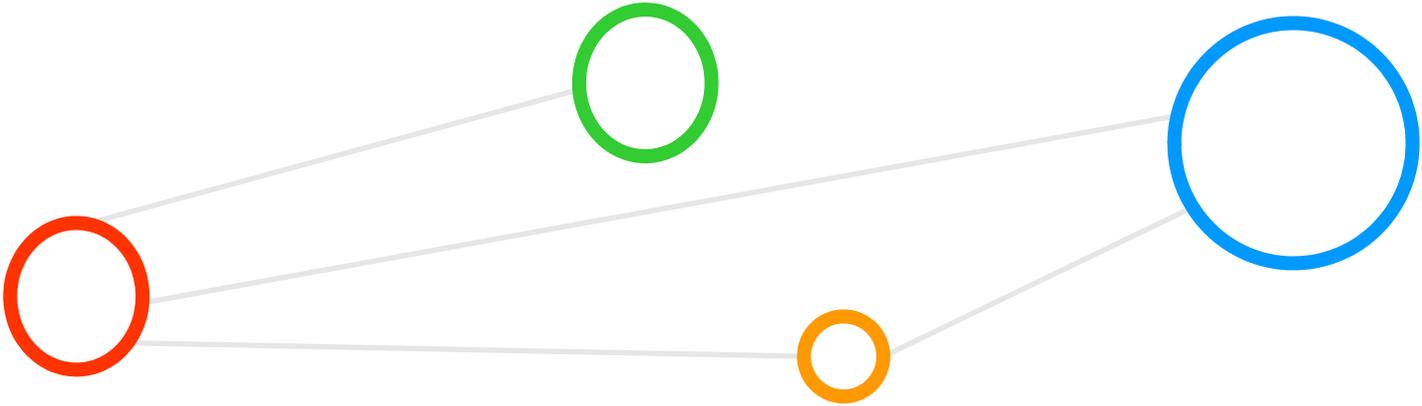


## [Video] PRACE – What is High Performance Computing



[12] YouTube, PRACE – Dare to Think the Impossible

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