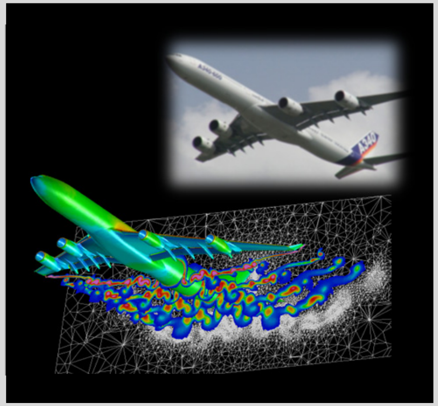


# High Performance Computing

ADVANCED SCIENTIFIC COMPUTING


**Prof. Dr. – Ing. Morris Riedel / Seyedreza Hassanianmoaref**

Full Professor / Senior PhD Student

School of Engineering and Natural Sciences, University of Iceland, Reykjavik, Iceland

Research Group Leader, Juelich Supercomputing Centre, Forschungszentrum Juelich, Germany


LECTURE 0

IHPC National Competence Center for HPC & AI in Iceland


@ProfDrMorrisRiedel @Morris Riedel @MorrisRiedel @MorrisRiedel

https://www.youtube.com/channel/UCWC4VKHmL4NZgFfKoHtANKg

morris@hi.is

@Reza Hassanian @RezaHassanian @RezaHassanian

seh@hi.is


# Prologue

January 8th, 2024

VR-2, Room 152

EUROPEAN OPEN SCIENCE CLOUD · TrustLLM · EUPEX European Pilot for Exascale · EuroHPC Joint Undertaking · ADMIRE malleable data solutions for HPC · EURO² · EUROPEAN DIGITAL INNOVATION HUB EDIH ICELAND

UNIVERSITY OF ICELAND · JÜLICH Forschungszentrum · JÜLICH SUPERCOMPUTING CENTRE · RAISE Center of Excellence · DEEP Projects · HELMHOLTZAI ARTIFICIAL INTELLIGENCE COOPERATION UNIT

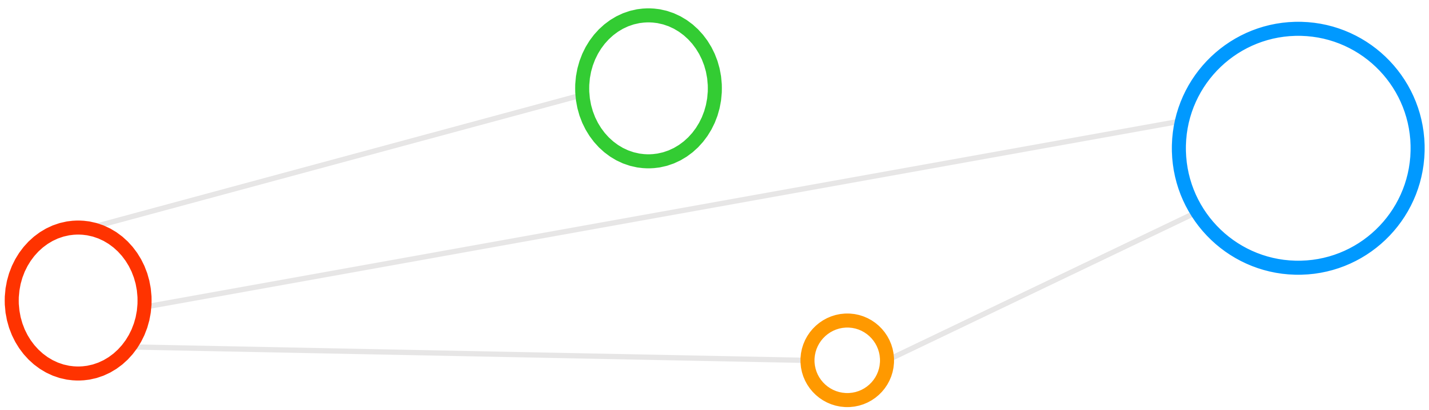
# Outline of the Course – CFD Special

1. High Performance Computing
2. Parallel Programming with MPI
3. Parallelization Fundamentals
4. Advanced MPI Techniques
5. Parallel Programming with OpenMP
6. Accelerators & Graphical Processing Units
7. Introduction to Deep Learning
8. Computational Fluid Dynamics (CFD)
9. CFD & Parallel Computing
10. OpenFoam Software & CFD Applications
11. Deep Sequence Models & CFD Applications
12. Lattice Boltzmann & CFD Applications
13. Transformer Models & CFD Applications
14. Solid Objects & Finite Elements Method
15. Green Energy & HPC Applications
16. Epilogue

+ additional invited lectures by experts & practical lectures for our hands-on assignments in context

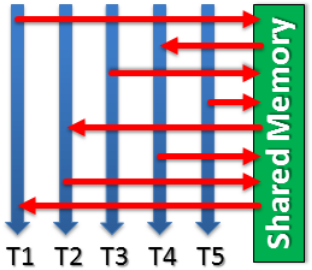
- Practical Topics
- Theoretical / Conceptual Topics

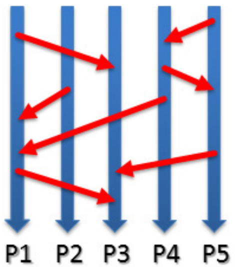
# Course Motivation & Information

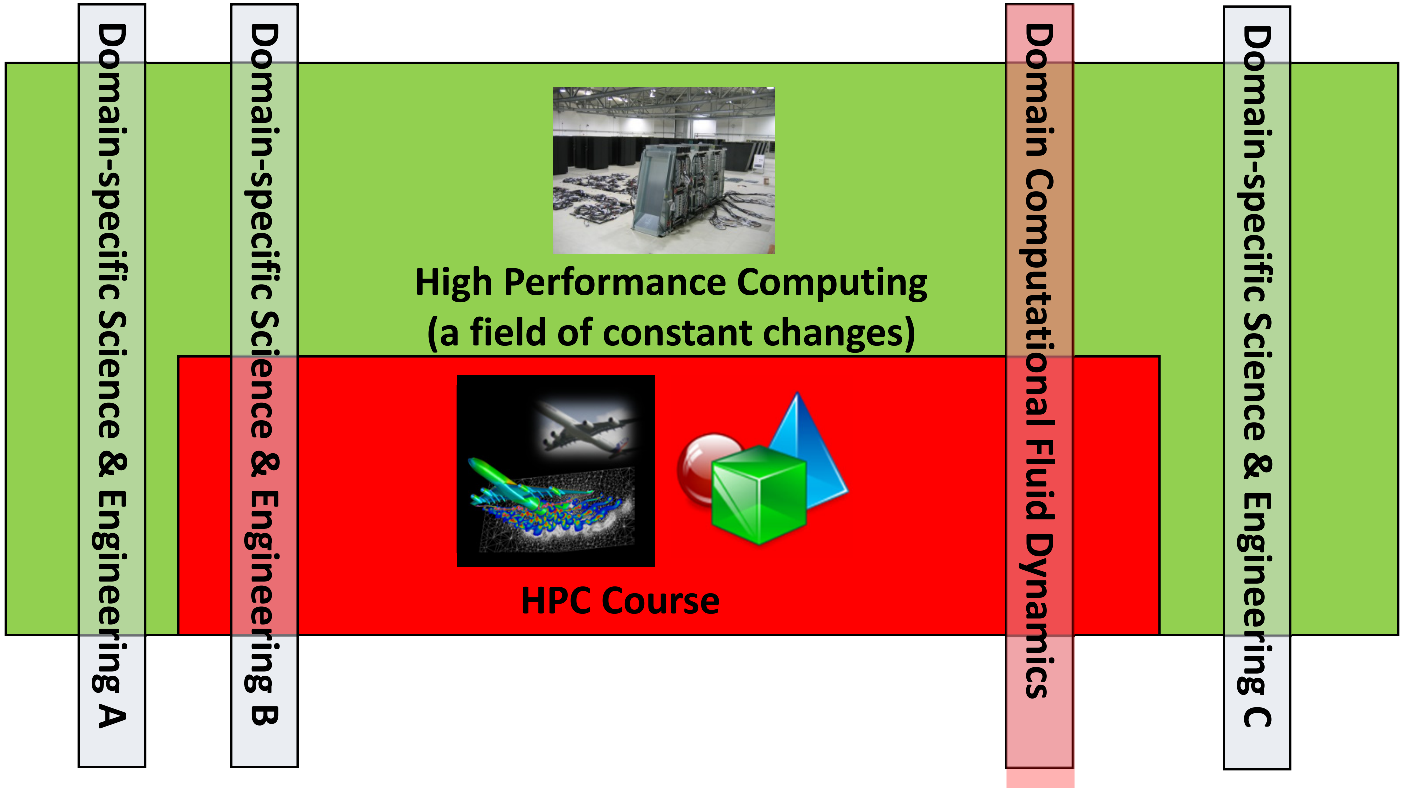


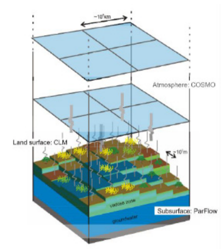
# Positioning in the Field of High Performance Computing (HPC)

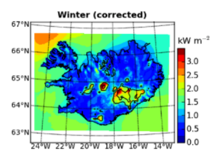
- Consists of techniques for programming & using large-scale HPC Systems
  - Approach: Get a broad understanding what HPC is and what can be done & CFD Special (new in 2023)
  - Goal: Train general HPC techniques and systems and selected details of domain-specific applications

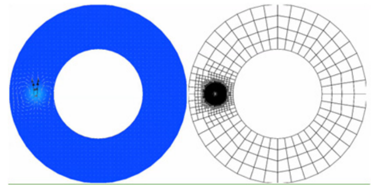


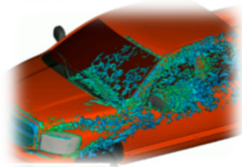



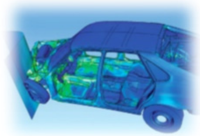



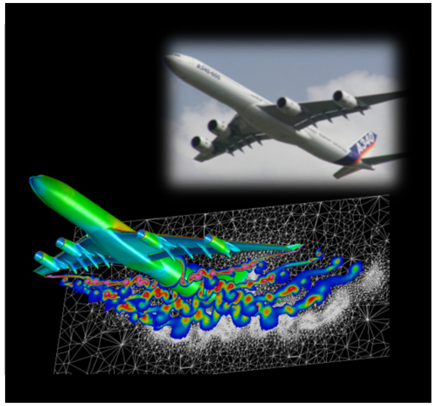






# Course Motivation

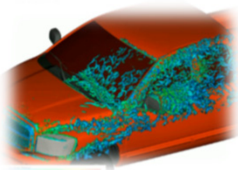


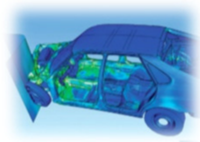
- Parallel processing and distributed computing
  - Matured over the past three decades
  - Both emerged as a well developed field in computer science
  - Still a lot of innovation, e.g. from hardware / software
- 'Scientific computing' with Maple, Matlab, etc.
  - Performed on small ('serial') computing 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
  - Computational Fluid Dynamics (CFD) Special as there are broadly known HPC Applications

# 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: Special Emphasis on Computational Fluid Dynamics (CFD) approaches (this year)

- 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

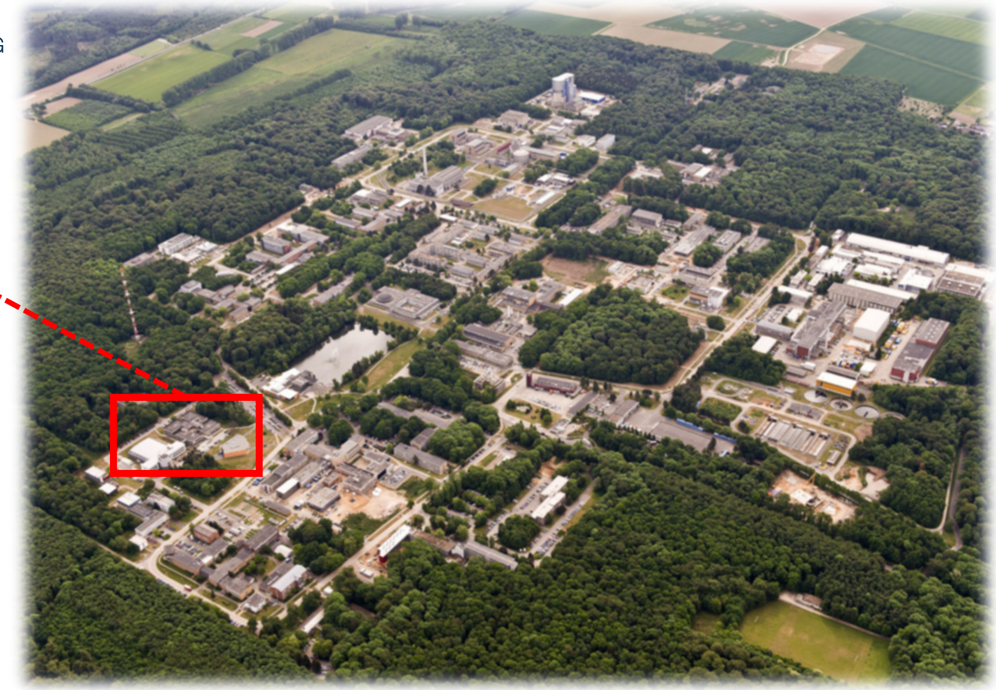


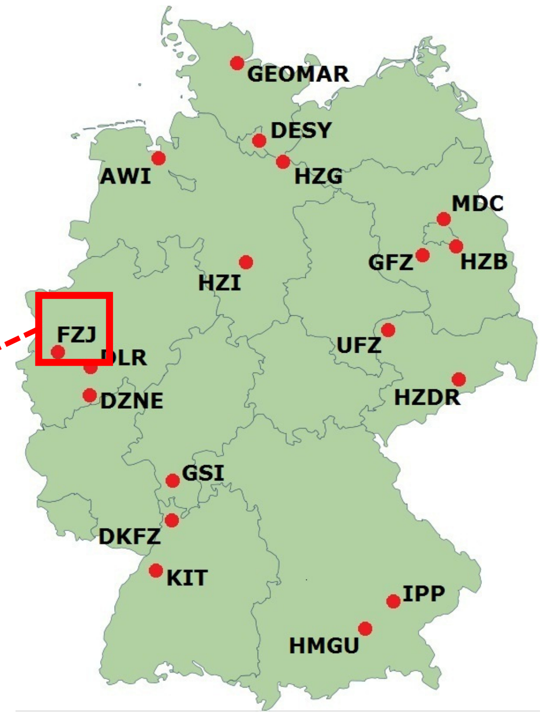


# Juelich Supercomputing Centre of Forschungszentrum Juelich – Germany

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

*[3] Forschungszentrum Juelich Web page*






HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES

*[2] Holmholtz Association 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, Clouds & Big Data)

# Lecturer Prof. Dr. – Ing. Morris Riedel (since ~2004 in HPC)

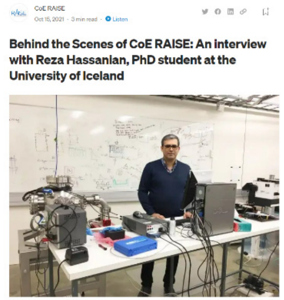
- Holds PhD in Computer Science (from Karlsruhe Institute of Tech.)
  - MSc in data visualization and steering of HPC & Grid applications
- Over the time several Positions at Juelich Supercomputing Centre
  - OS, Grid divisions; later deputy division leader federated systems and data
  - Currently: Research 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 design, steering group of Helmholtz Artificial Intelligence Initiative
  - European EuroHPC Joint Undertaking Governing Board member for Iceland
- University courses
  - University of IcelandCourses: HPC A / B, Statistical Data Mining, Cloud Computing & Big Data
  - Slides from previous years available under teaching of instructors personal Web page

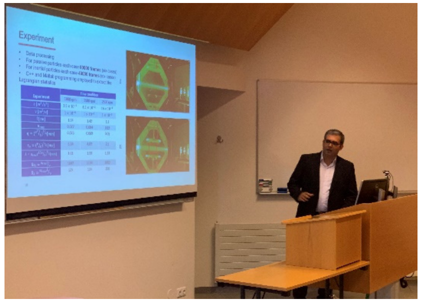
*[1] Morris Riedel Web page*

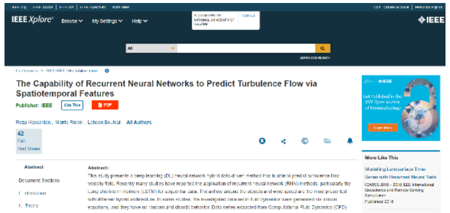
EuroHPC
Joint Undertaking

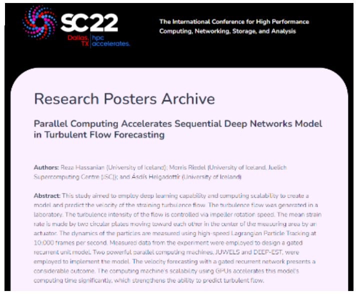
# Lecturer “Reza” (Seyedreza Hassanian)

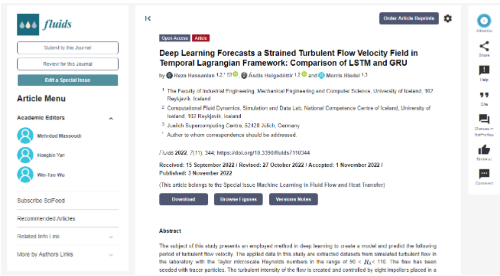
- BSc and MSc degree in Mechanical Engineering/ MSc Degree in Sustainable Energy Engineering
- PhD Student, Computational Engineering, University of Iceland
  - Computational Fluid Dynamics/ High Performance Computing/ Artificial intelligence/ Scalability
- European Union Commission project participation
  - Center of Excellence (**COE-RAISE**)/ **EuroCC-1 / EuroCC-2**
- Member of National Competence Center of Iceland (**NCC**)
  - Simulation and Data Lab Computational Fluid Dynamics
- Member of :
  - American Physical Society (APS),
  - American Society of Mechanical Engineers (ASME),
  - Institute of Electrical and Electronics Engineers (IEEE)
- Recent Publication Area: Turbulent flow, Deep Learning, HPC, Energy
- Selected other recent activities
  - Working with Julich Supercomputer center (JSC), Modeling prediction for turbulent Flow
  - Work Package 3 use-cases of CoE-Raise, CERN, JSC, Technical University of Achen, Barcelona Supercomputer Center
  - Laboratory of Fundamental of Turbulent Flow , Reykjavik University, Experiment of Turbulent Flow
  - Reviewer of Physics of Fluids, AIP Publishing LLC (Melville, New York, US)
- University courses
  - University of Iceland Courses: HPC/ Fluid Mechanics / Computational Fluid Dynamics
  - Reykjavik University, etc: Wind Power Lab/ Heat Transfer/ Finite Element

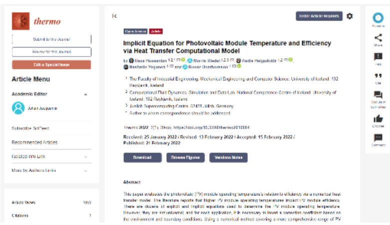


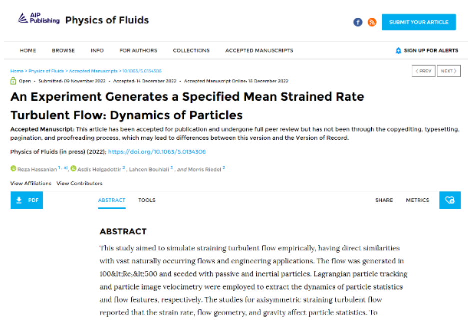





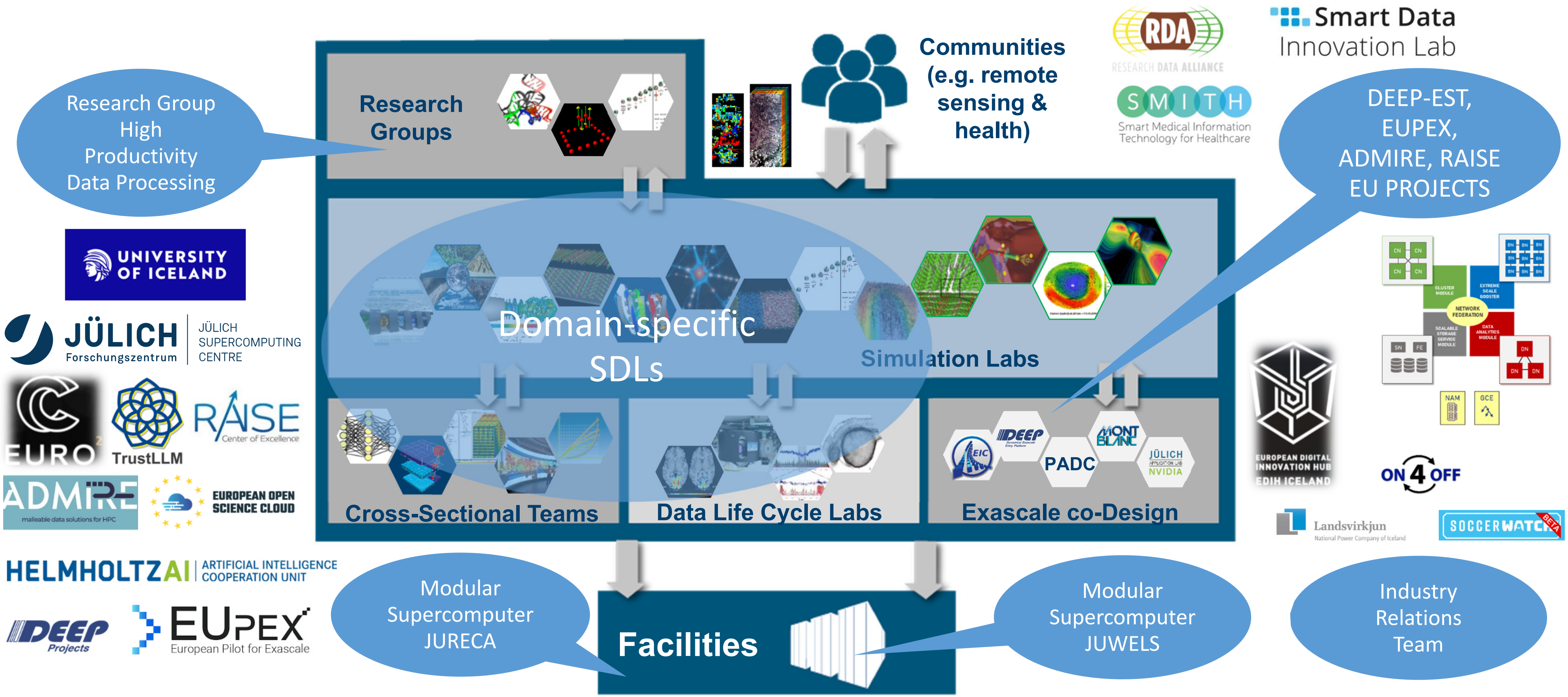
# University of Iceland – School of Natural Sciences & Engineering (SENS)

- 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*




UNIVERSITY OF ICELAND

# Jülich Supercomputing Centre High Productivity Data Processing Research Group



# Intertwined: High Performance Computing & Cloud Computing & Big Data

- European EuroHPC Joint Undertaking
  - EU EuroCC project in Iceland: user support & structuring of High Performance Computing (HPC) communities & roadmaps
  - EU ADMIRE Project: Remote Sensing application co-design of HPC systems
  - EU EUPEX Project: EU Exascale Prototype Project
- European Open Science Cloud (EOSC)
  - Provides services and tools for large-scale datasets (aka ‘big data‘) for EU researchers
  - Offers computing capacity for scientists in EU
  - EU EOSC-Nordic project in Iceland: provisioning of a couple of data services for selected application communities in Iceland

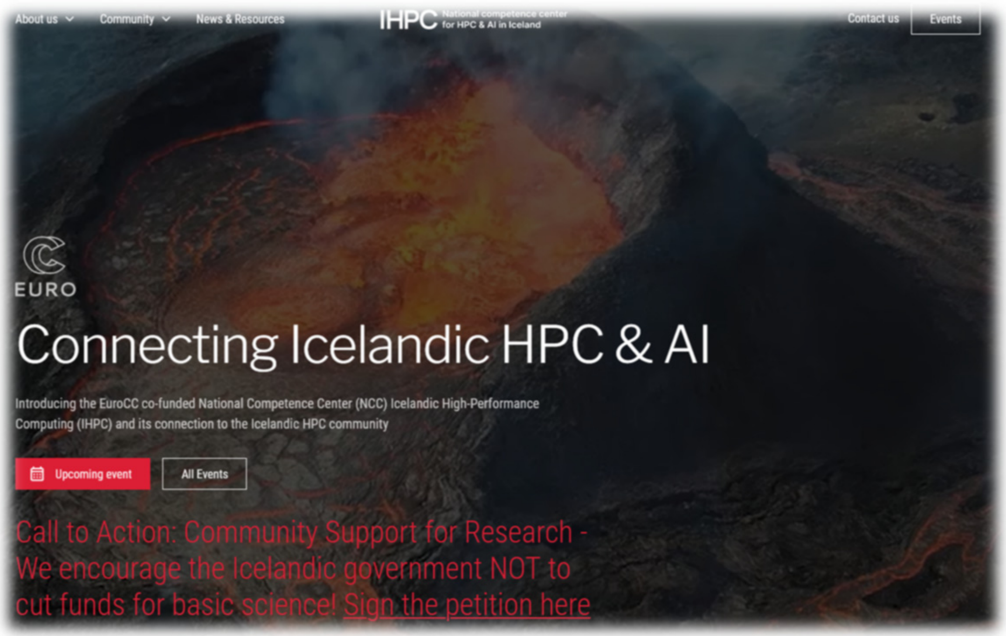
[36] EUPEX Web Page

[4] EuroHPC Joint Undertaking

[30] EuroCC EuroHPC Project

[29] ADMIRE EuroHPC Project

[31] Icelandic HPC Community

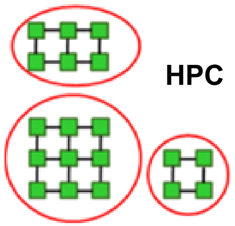



[5] EOSC Web page

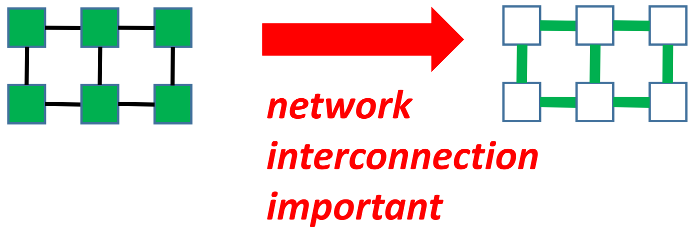
[6] EOSC-Nordic Web page

# Understanding High Performance Computing (HPC)

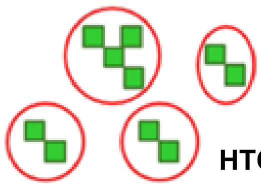
- **High Performance Computing (HPC) is based on computing resources that enable the efficient use of parallel computing techniques through specific support with dedicated hardware such as high performance cpu/core interconnections.**



HPC

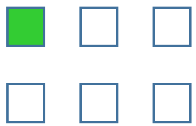



- **High Throughput Computing (HTC) is based on commonly available computing resources such as commodity PCs and small clusters that enable the execution of 'farming jobs' without providing a high performance interconnection between the cpu/cores.**



HTC

*network interconnection less important!*



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

# HPC & Data-intensive Sciences – Constant Evolution & Technology Changes

**1.000.000 FLOP/s**

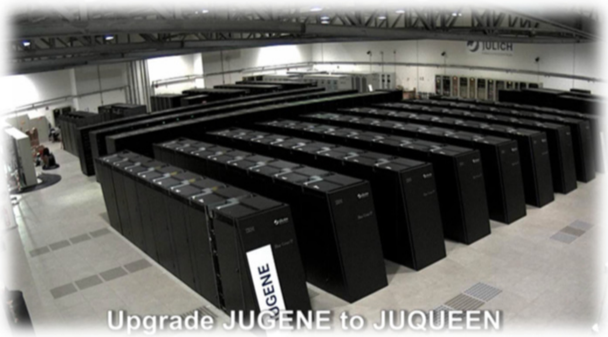
**~1984**

© Photograph by Rama, Wikimedia Commons

- **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**

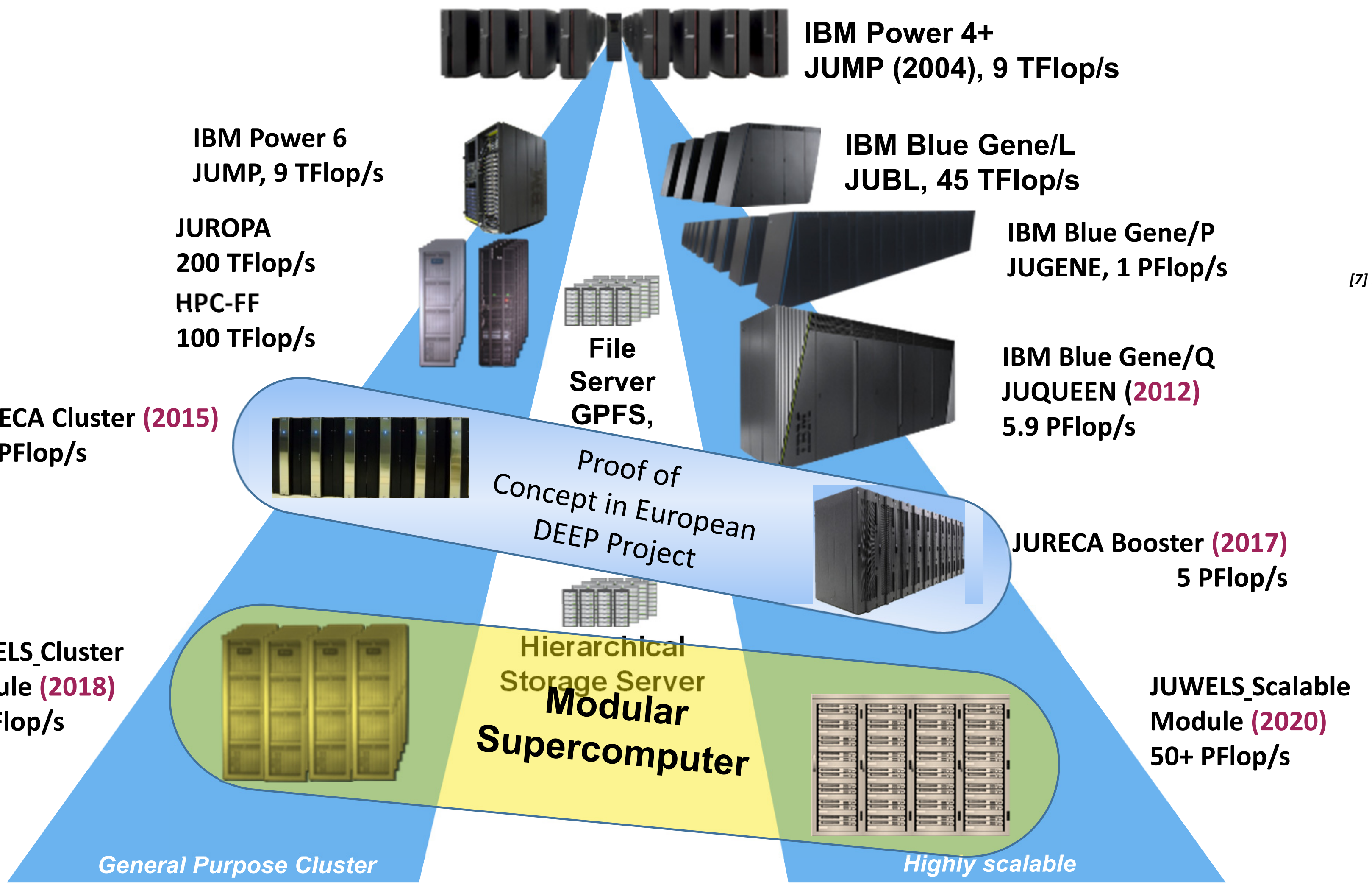
**1.000.000.000.000.000 FLOP/s**

**~295.000 cores~2009 (JUGENE)**





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

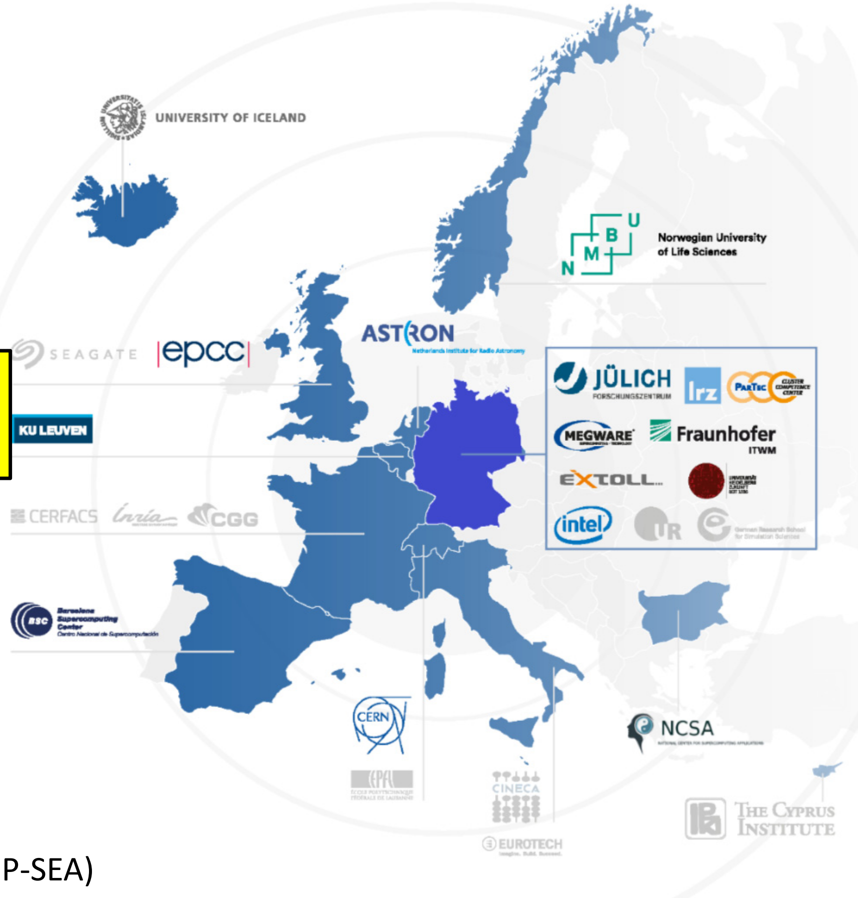



[7] DEEP Projects Web Page

# DEEP Series of Projects – Modular Supercomputing Architecture Research

*[7] DEEP Projects Web Page*

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

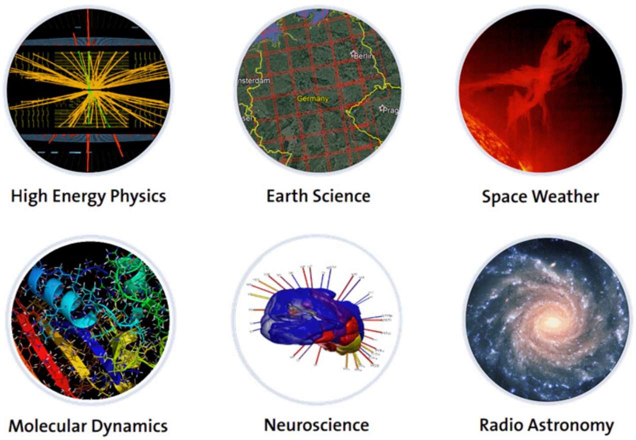


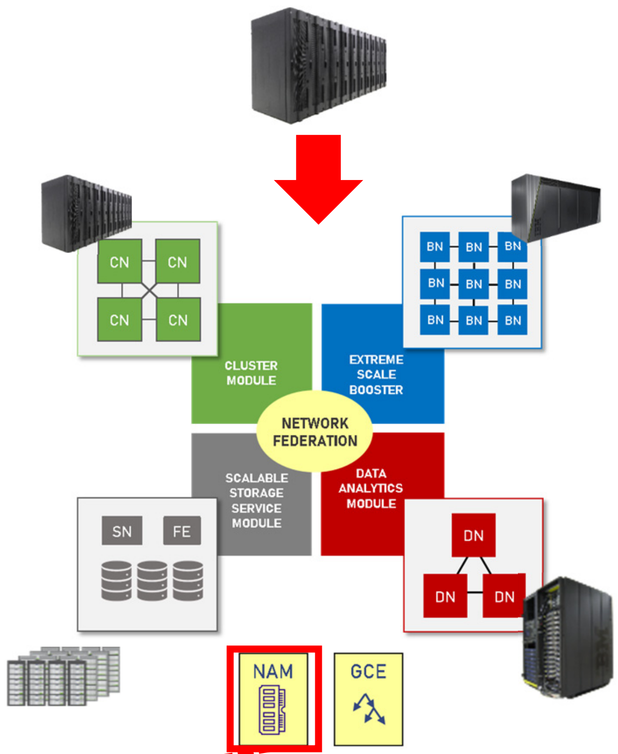

- 3 EU Exascale projects
  DEEP, DEEP-ER, DEEP-EST
- 27 partners
  Coordinated by JSC
- EU-funding: 30 M€
  JSC-part > 5,3 M€
- Nov 2011 – Dec 2020
- New DEEP Project launched, e.g., DEEP-Software for Exascale Architectures (DEEP-SEA)

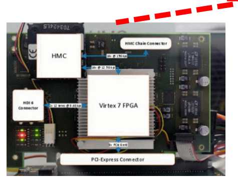
- **Strong collaboration with industry partners Intel, Extoll & Megware**

- **Juelich Supercomputing Centre implements the DEEP projects designs in its HPC infrastructure**

# Application Co-Design for Machine & Deep Learning in HPC

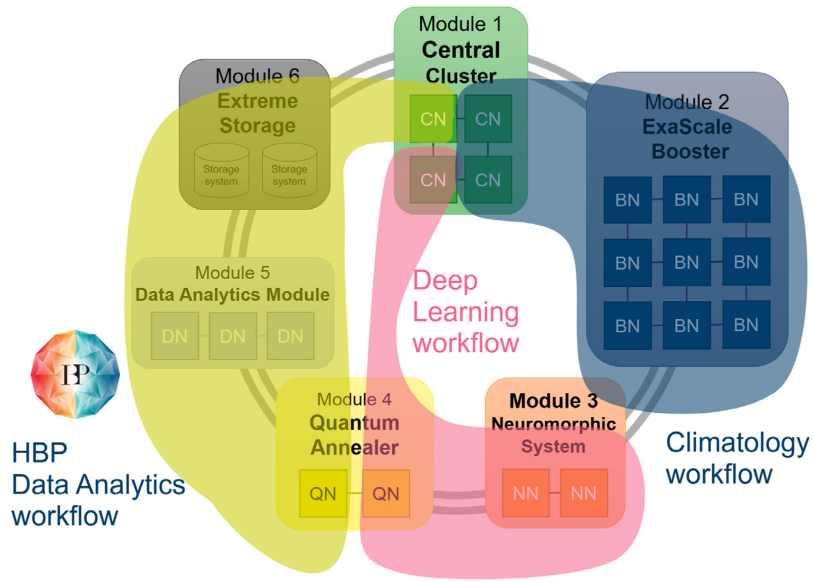


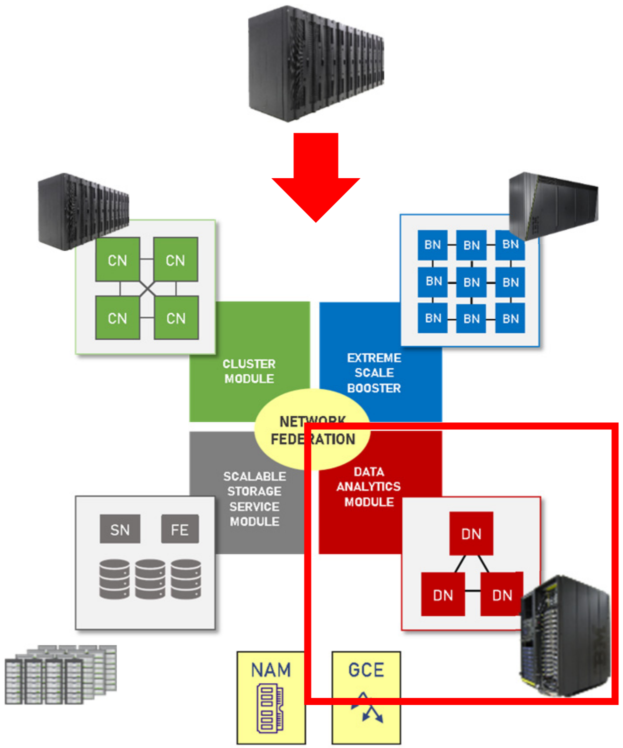
*[28] E. Erlingsson & M. Riedel et al., Modular Supercomputing Design Supporting Machine Learning Applications*

*[7] DEEP Projects Web Page*

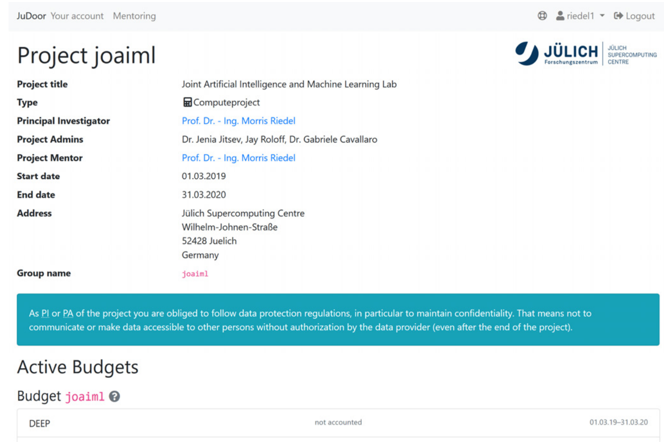



- **The modular supercomputing architecture (MSA) enables a flexible HPC system design co-designed by the need of different application workloads**

# Hands-On Training System – Data Analytics Module (DAM)




- Data Analytics Module (DAM)
  - Specific requirements for data science & analytics frameworks
  - 16 nodes with 2x Intel Xeon Cascade Lake; 24 cores
  - 1x NVIDIA V100 GPU / node
  - 1x Intel STRATIX10 FPGA PCIe3 / node
  - 384 GB DDR4 memory / node
  - 2 TB non-volatile memore / node
- DAM Prototype
  - 3 x 4 GPUs Tesla Volta V100
  - Slurm scheduling system


JuDoor Your account Mentoring riedel1 Logout

Project joaiml

| | |
|---|---|
| Project title | Joint Artificial Intelligence and Machine Learning Lab |
| Type | Computeproject |
| Principal Investigator | Prof. Dr. - Ing. Morris Riedel |
| Project Admins | Dr. Jenia Jitsev, Jay Roloff, Dr. Gabriele Cavallaro |
| Project Mentor | Prof. Dr. - Ing. Morris Riedel |
| Start date | 01.03.2019 |
| End date | 31.03.2020 |
| Address | Jülich Supercomputing Centre<br>Wilhelm-Johnen-Straße<br>52428 Juelich<br>Germany |
| Group name | joaiml |

As PI or PA of the project you are obliged to follow data protection regulations, in particular to maintain confidentiality. That means not to communicate or make data accessible to other persons without authorization by the data provider (even after the end of the project).

Active Budgets

Budget joaiml

| | | |
|---|---|---|
| DEEP | not accounted | 01.03.19–31.03.20 |

(easy join via JOAIML ab with JuDoor)

DEEP Projects

*[7] DEEP Projects Web Page*

> ➢ **The DEEP modular HPC system will be used for a couple of different machine & deep learning exercises in the context of our lectures**

# Canvas Tool & Office Hours (!)

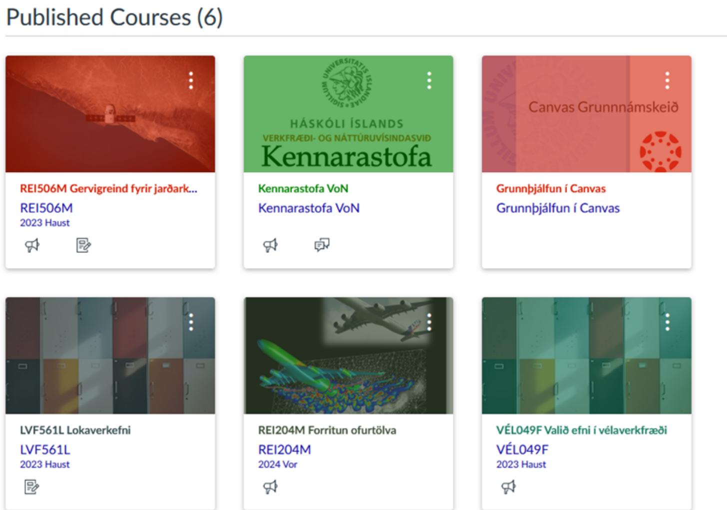
- Reference course information
  - High Performance Computing
  - REI204M, Spring 2024
- Use it for course communication
  - Every course member requires account
  - Contact other students & discuss topics
  - Contact lecturer & access to all materials
- Find course materials
  - Slides of Lectures and Practical Lectures
  - Handouts and Recordings
  - Further reading topics (e.g. papers, etc.)
- Questions, major difficulties, etc.? → Don't wait long!
  - Use our online office hours, send request: morris@hi.is & katrine@hi.is or she@hi.is (Reza)

UNIVERSITY OF ICELAND
UGLA - intraweb

*changes to*

CANVAS

*[8] High Performance Computing Course Catalogue Web page*



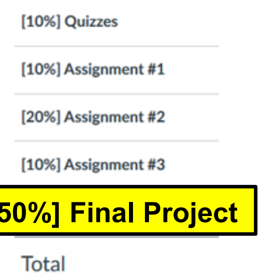
# Overall Course Organization – Course Activities

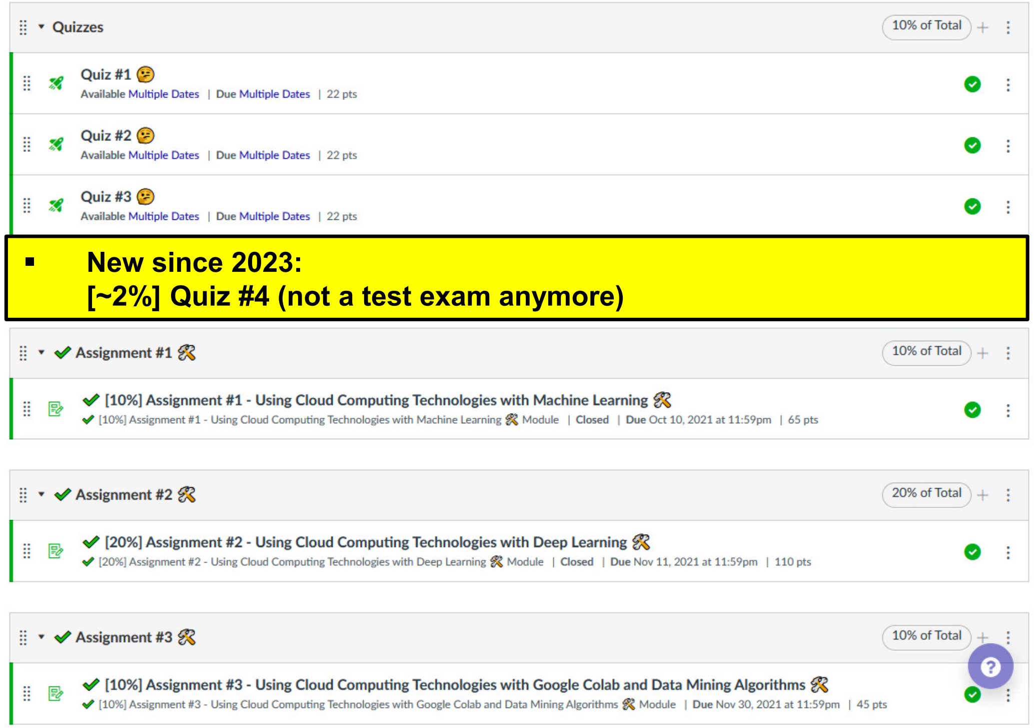
- 3 Assignments (40% of grade)
  - Guided by practical lectures in context with hands-on elements for all
  - Scheduling scripts configuration & parallel programming projects
  - Important influence in the overall grade
  - TBD(all): Create Groups of 2-3 & send group to morris@hi.is & katrine@hi.is
- Quizzes (10% of grade)
  - Small quiz from time to time (pre-announced) to check understanding
  - Minor influence in the overall grade
- Final Project (50% of grade)
  - End of the lecture series (~April) – major part of the overall grade
  - ‘Specific topics will be discussed with each assignment team‘
- Selected Invited Lectures
  - A couple of presentations (e.g. companies, interesting projects, PhD students, etc.)

> - **Each lecture will have these type of yellow blocks**
> - **The most important course material and information is usually summarized in these yellow blocks**
> - **It is essential to know these elements of the course, so pay attention on learning and understanding those**
> - **Knowing the substance of these yellow blocks in context of some associated figures and illustrations fundamentally helps to have good quiz outcomes**

# Overall Course Organization – Q&A & Grading via Canvas

- Questions (Q) & Answers (A)
  - E.g., for Lectures & overall course aspects in Ed Tool reachable from Canvas
  - Quizzes to be in Canvas
  - E.g. overall course discussion section via Ed Tool
  - Once per week Q&A session via Zoom (online, might not work every week due to conferences)
- Submissions & Grading via Canvas
  - Submission of Assignments, Quizzes & Project
  - Note: Final grades in UGLA might not always in sync with Canvas (delay in administration)
  - Examples here from Cloud Computing & Big Data Course in Fall 2021



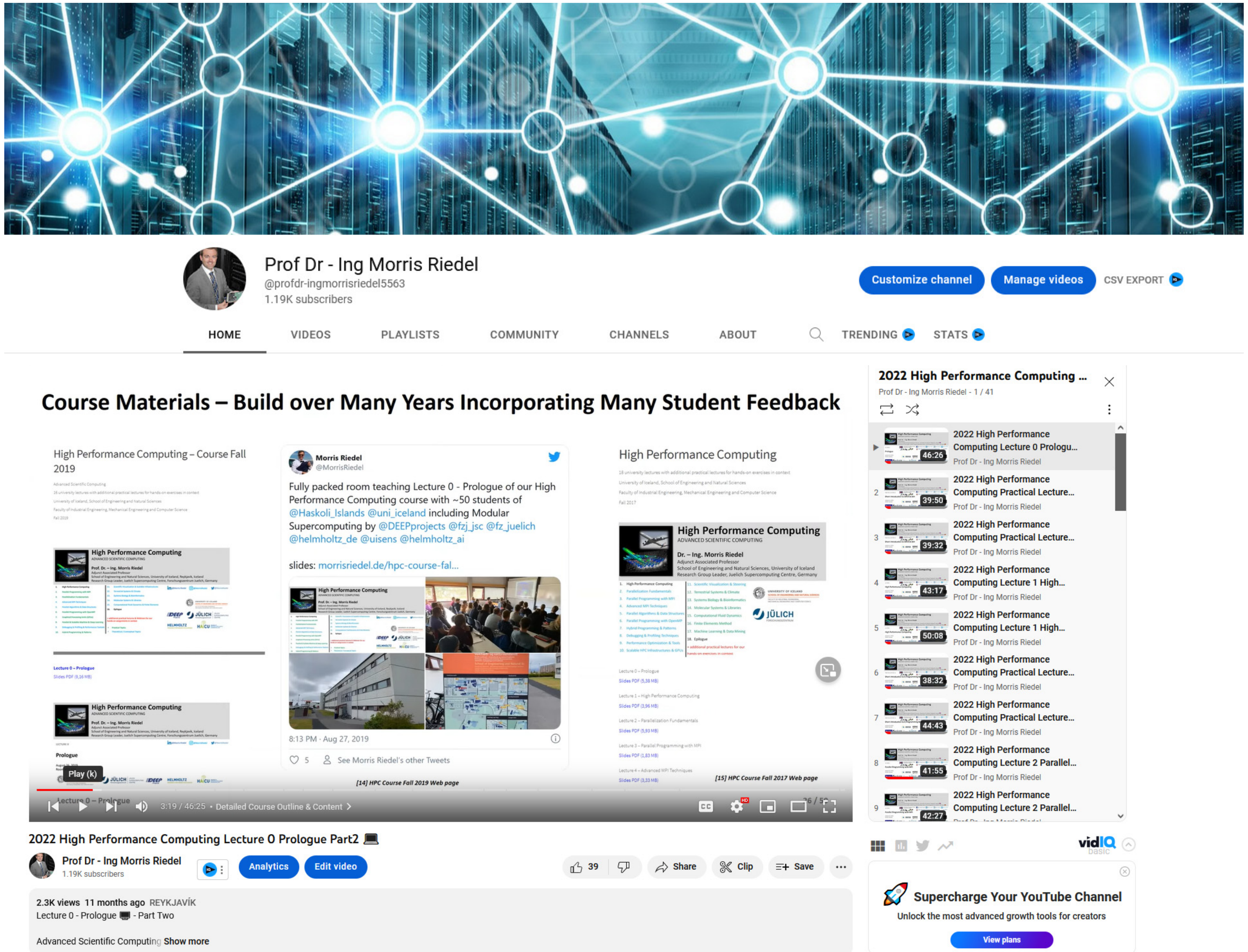

- **New since 2023:** **[~2%] Quiz #4 (not a test exam anymore)**

- **New since 2023:** **[50%] Final Project instead of Exam** **(student surveys indicated that students prefer final project)**

# Overall Course Organization – Recordings of Each Lecture

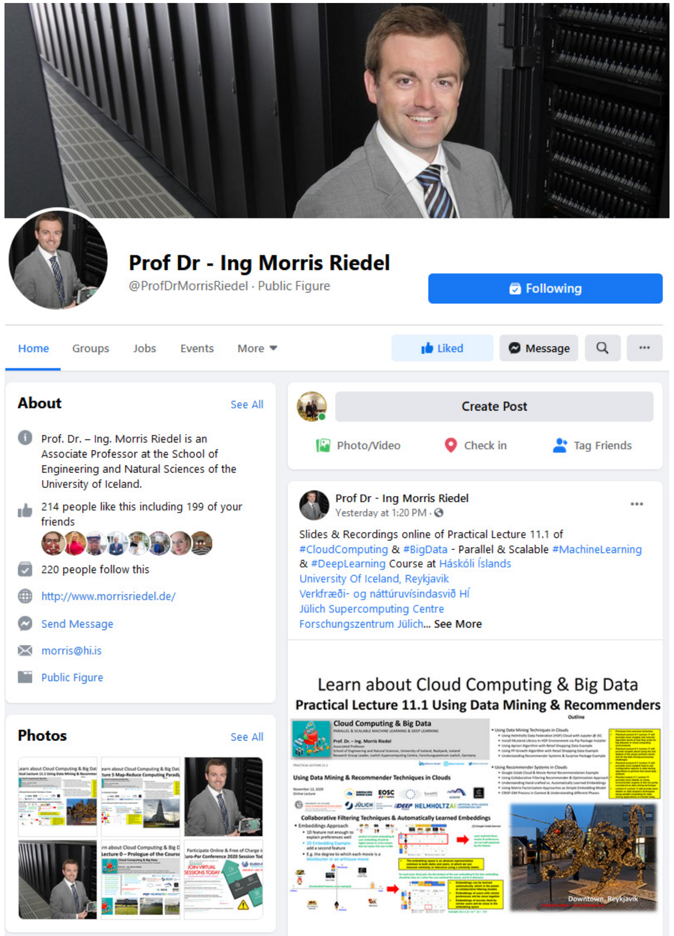
*[20] Morris Riedel YouTube Channel*

- Recordings at YouTube Channel
  - Public Lectures and Practical Lectures on YouTube Channel
  - Usually each lecture will be recorded in two parts
  - Practial lectures will include demonstrations of technology and/or processes (e.g. compiling)
  - E.g. like from HPC Course in Spring 2021/2022 – Playlist
- Recordings in Panopto in Canvas
  - Course recordings of Quizzes & Assignment Debriefs, etc.

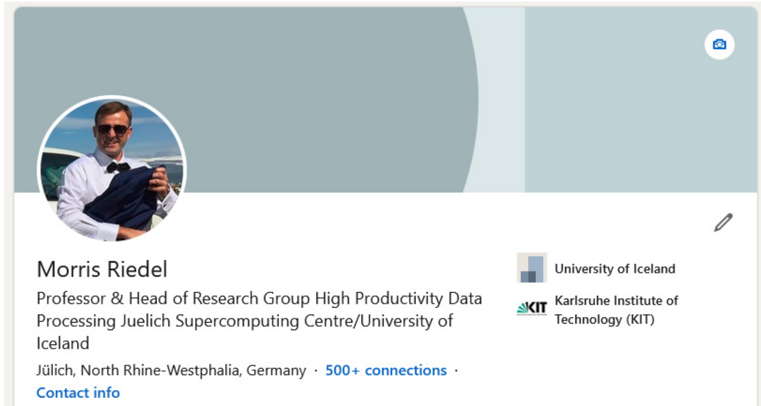


# Social Media – Spread the Word about HPC & our Course Contents – Thanks!

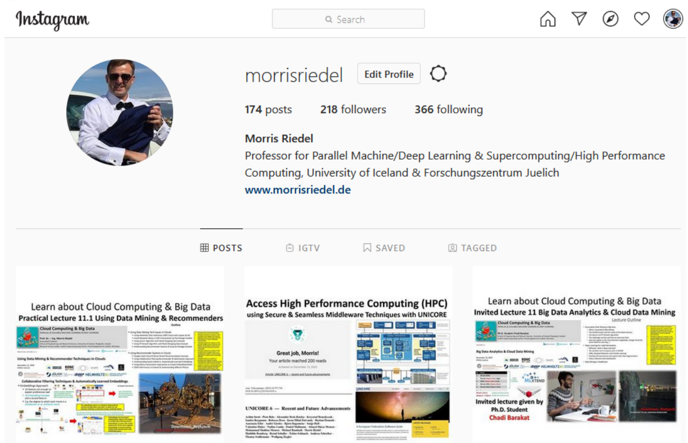

@MorrisRiedel [16] Morris Riedel Twitter Profile




@ProfDrMorrisRiedel [17] Morris Riedel Facebook Profile




@Morris Riedel [18] Morris Riedel LinkedIn Profile

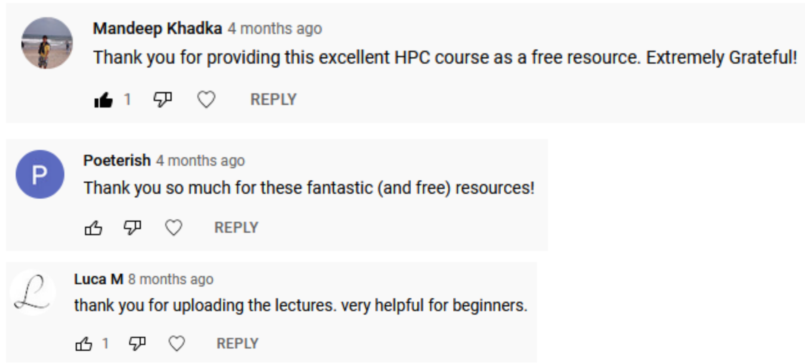



@MorrisRiedel [19] Morris Riedel Instagram Profile

# Associated Literature & Bibliography in Each Lecture & Community Feedback


**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*




- Much more further up-to-date bibliography & readings will be provided in context
  - E.g., HPC community Web pages, HPC community tutorials, courses, lessons-learned, infrastructure, policy links, etc.
  - E.g., YouTube links to videos in context of lectures that increase the overall understanding of the subject
  - E.g., papers, public Web pages, etc.

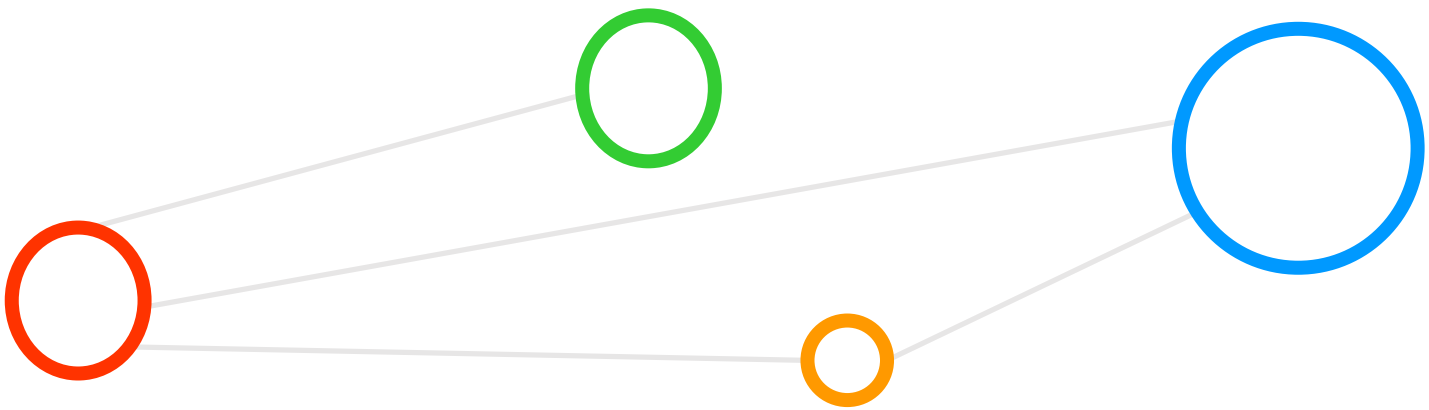
**Lecture Bibliography (1)**


- [1] Morris Riedel Web page, Online: http://www.morrisriedel.de
- [2] Helmholtz Association Web Page, Online: https://www.helmholtz.de/en/
- [3] Forschungszentrum Juelich Web page, Online: http://www.fz-juelich.de
- [4] European EuroHPC Joint Undertaking, Online: https://eurohpc-ju.europa.eu/
- [5] European Open Science Cloud (EOSC) Web page, Online: https://www.eosc-portal.eu/
- [6] EU EOSC-Nordic Project Web page, Online: https://www.eosc-nordic.eu/
- [7] DEEP Series Projects Web Page, Online: http://www.deep-projects.eu/
- [8] High Performance Computing Course Catalogue Web page, Online: https://ugla.hi.is/kennsluskra/index.php?tab=nam&chapter=namskeid&id=70067120210
- [9] PRACE – Dare to Think the Impossible, Online: https://www.youtube.com/watch?v=CbMCHs-Rv_w&feature=emb_logo
- [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, Dreamworks, High Performance Computing, Online: http://www.youtube.com/watch?v=TGSRvV9u32M
- [12] K. Hwang, G. C. Fox, J. J. Dongarra, 'Distributed and Cloud Computing', Book, Online: http://store.elsevier.com/product.jsp?locale=en_EU&isbn=9780128002049

# [Video] PRACE – What is High Performance Computing


*[9] YouTube, PRACE – Dare to Think the Impossible*

# Detailed Course Outline & Content



# Course Materials – Build over Many Years Incorporating Many Student Feedback

## High Performance Computing – Course Fall 2019

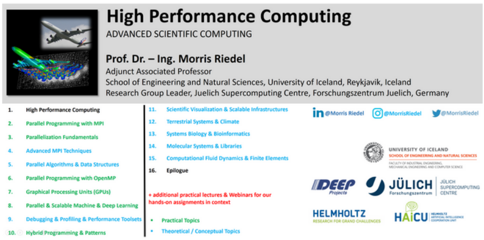
Advanced Scientific Computing

16 university lectures with additional practical lectures for hands-on exercises in context

University of Iceland, School of Engineering and Natural Sciences

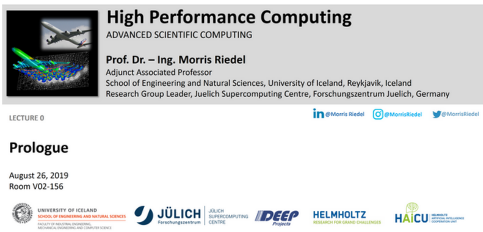
Faculty of Industrial Engineering, Mechanical Engineering and Computer Science

Fall 2019




**Lecture 0 – Prologue**

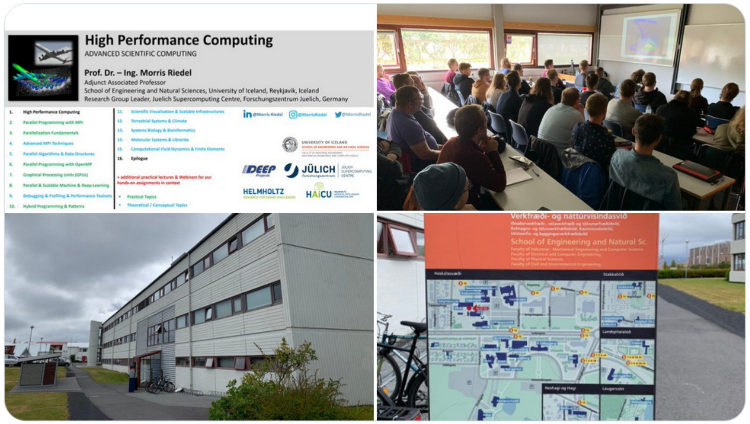
Slides PDF (9,16 MB)




**Morris Riedel**
@MorrisRiedel

Fully packed room teaching Lecture 0 - Prologue of our High Performance Computing course with ~50 students of @Haskoli_Islands @uni_iceland including Modular Supercomputing by @DEEPprojects @fzj_jsc @fz_juelich @helmholtz_de @uisens @helmholtz_ai

slides: morrisriedel.de/hpc-course-fal...




8:13 PM · Aug 27, 2019

5 See Morris Riedel's other Tweets

*[14] HPC Course Fall 2019 Web page*

## High Performance Computing

18 university lectures with additional practical lectures for hands-on exercises in context

University of Iceland, School of Engineering and Natural Sciences

Faculty of Industrial Engineering, Mechanical Engineering and Computer Science

Fall 2017


Lecture 0 – Prologue

Slides PDF (5,38 MB)

Lecture 1 – High Performance Computing

Slides PDF (3,96 MB)

Lecture 2 – Parallelization Fundamentals

Slides PDF (5,93 MB)

Lecture 3 – Parallel Programming with MPI

Slides PDF (1,83 MB)

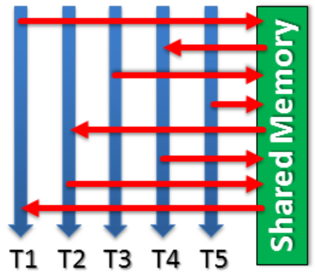
Lecture 4 – Advanced MPI Techniques

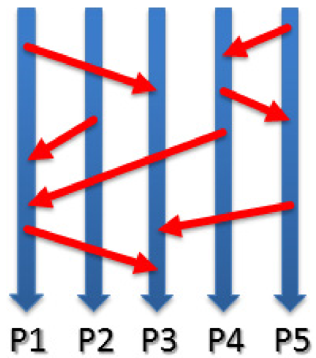
Slides PDF (3,33 MB)

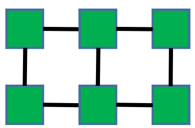
*[15] HPC Course Fall 2017 Web page*

# 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
  - EuroHPC Joint Undertaking & Resource Provisioning
  - Emerging Quantum Computing Systems



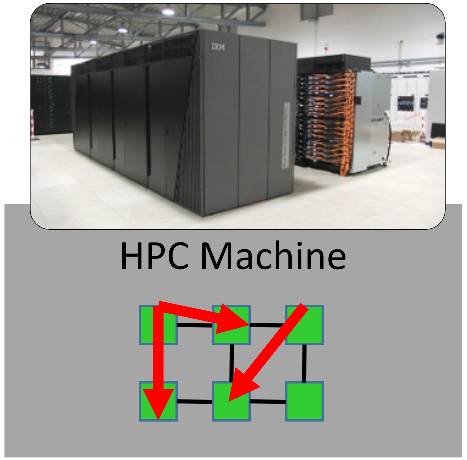



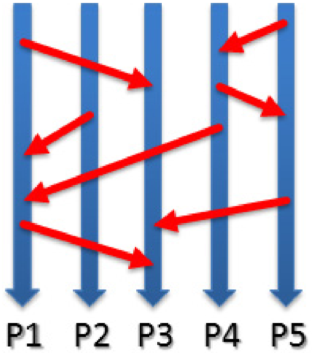



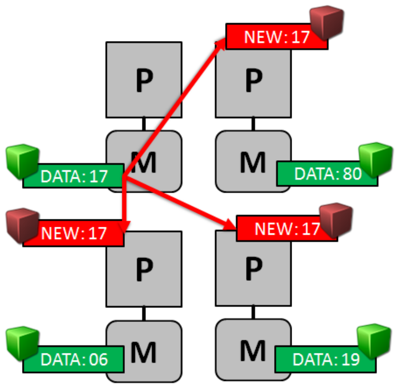
EuroHPC
Joint Undertaking

# 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

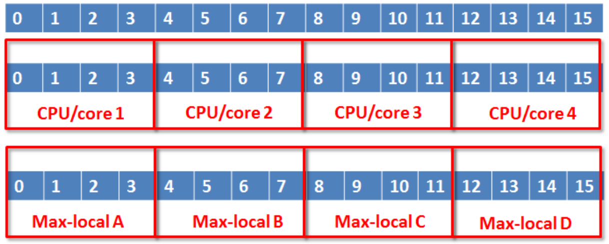


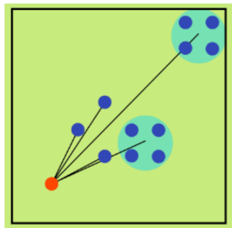



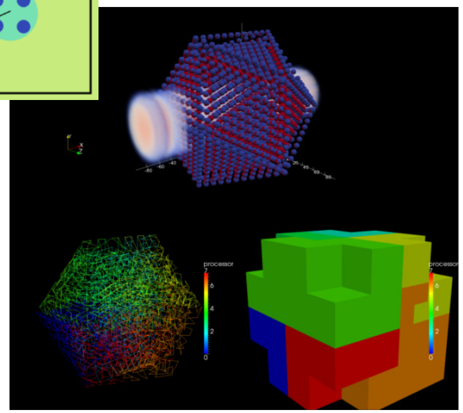



# Lecture 3 – Parallelization Fundamentals

- 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





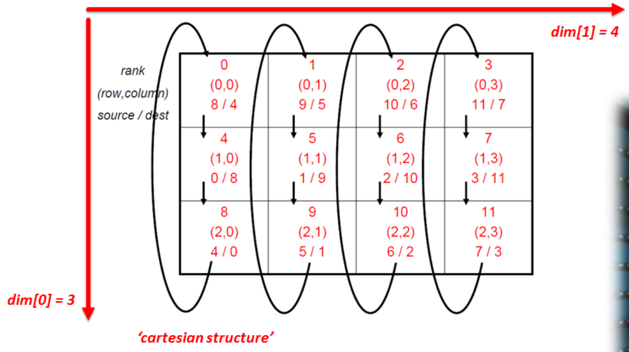
- Amount of work/overall problem size:

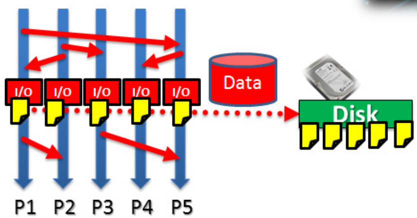
  **$s + p = 1$**
- s = serial (nonparallelizable part)
- p = parallelizable part

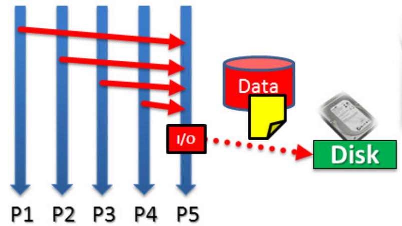
$T_f^P = s + p/N$

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



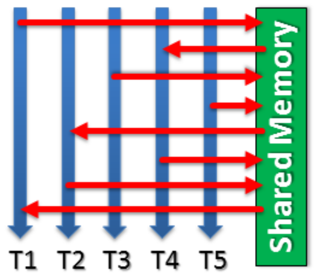



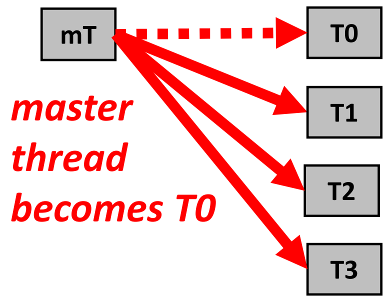




# Lecture 5 – Parallel Programming with OpenMP

- Shared-Memory Programming Concepts
  - Parallel and Serial Regions
  - Fork & Joins
  - Master and Worker Threads
  - Portability
  - Application Examples
  - Differences to distributed memory
- OpenMP Parallel Programming Basics
  - Basic building blocks
  - Local/shared variables & Loops
  - Synchronization & Critical Regions
  - Selected Comparisons with MPI
  - Simple Applications

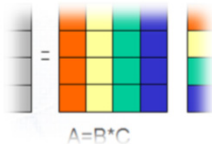
```
int main()
{
  #pragma omp parallel
  printf(„Hello World");
}
```



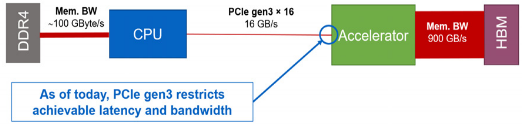



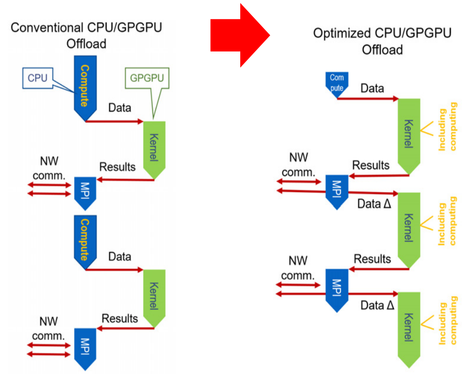
# Lecture 6 – Graphical Processing Units (GPUs)

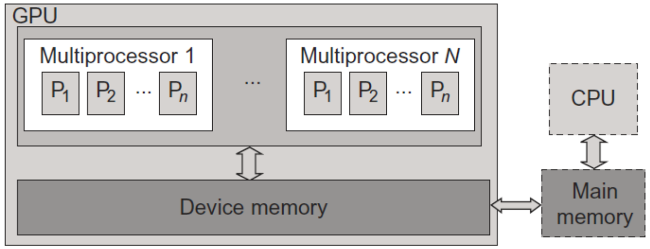
- General Purpose Graphical Processing Units (GPGPUs)
  - Often known as just 'GPU'
  - Many-core vs. Multi-core
  - Terminology & Architecture
  - Architecture differences from Kepler, Pascal, Volta
  - Programming Models
  - Usage Models & Applications
  - NVidia & CUDA Examples
  - Programming with OpenACC
  - Programming with HIP
  - GPU Toolsets & GPU Direct
  - Scalability with GPUs
- Selected GPU Applications
  - Scientific Computing Examples
  - Simulation Sciences
  - Machine & Deep Learning







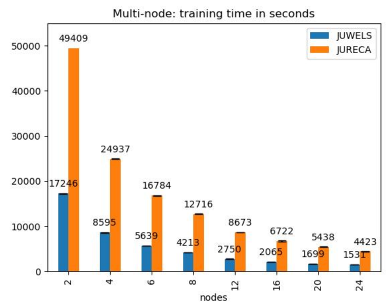



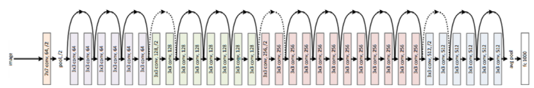




*[12] Distributed & Cloud Computing Book*

A partition of the JUWELS system
has 56 compute nodes,
each with 4 NVIDIA V100 GPUs
(equipped with 16 GB of memory)

24 nodes x 4 GPUs = 96 GPUs

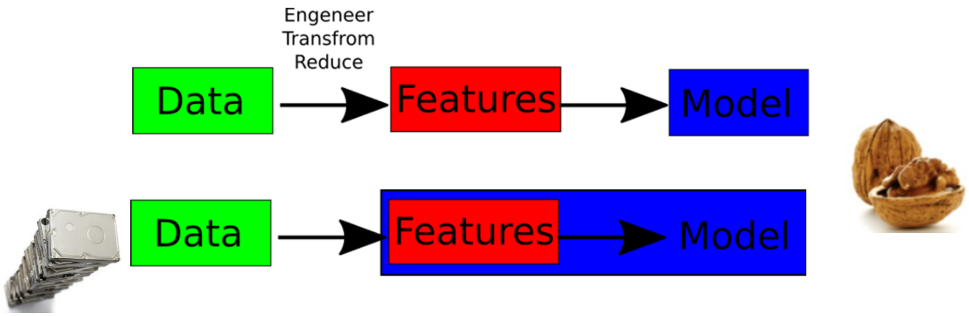


*[37] R. Sedona, G. Cavallaro, & M. Riedel et al.,
Remote Sensing Big Data Classification
with High Performance Distributed Deep Learning*

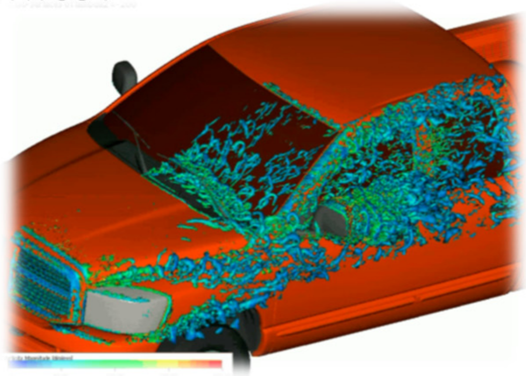
# Lecture 7 – Introduction to Deep Learning

- Deep Learning Fundamentals
  - Artificial Neural Networks (ANNs) foundations
  - Backpropagation Algorithm
  - Role of big data sets
  - Feature learning
  - Transfer learning
- Deep Learning Models
  - Using libraries as PyTorch, TensorFlow & Keras
  - E.g. Convolutional Neural Networks (CNNs) models for image data sets
  - E.g. Long Short Term Memory (LSTM) models for time series data sets
  - Advantage of HPC for deep learning models
  - Role of GPUs and scalable models
  - Hyperparameter Tuning benefits using HPC

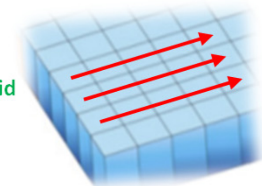


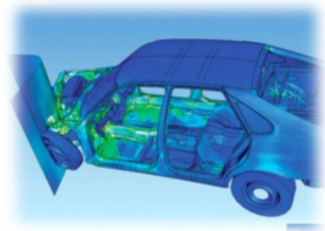
# Lecture 8 – Computational Fluid Dynamics (CFD)

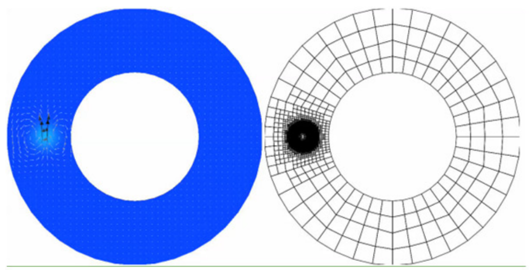
- What is Computational Fluids Dynamics?
  - Why CFD and the Background
  - Range of the applications
  - Navier-Stokes Equation
  - Numerical schemes
- Applying CFD techniques
  - Classification of flows
  - Solution methods
  - Meshing
  - Boundary conditions
  - RANS/LES/DNS

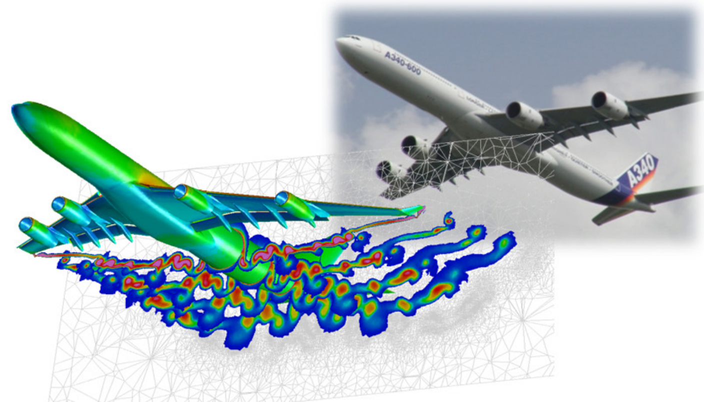


(classical mechanics solutions
are rather trajectories
of positions of a certain particle, here fluid
velocity is in focus)



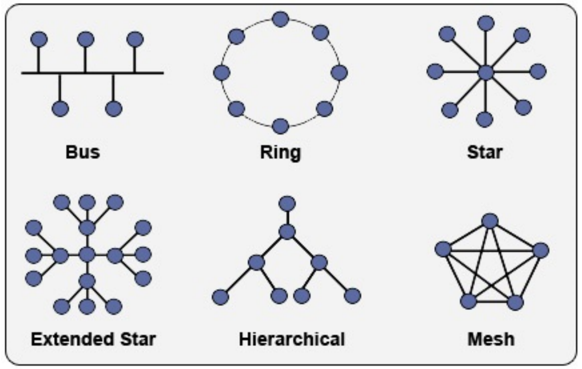




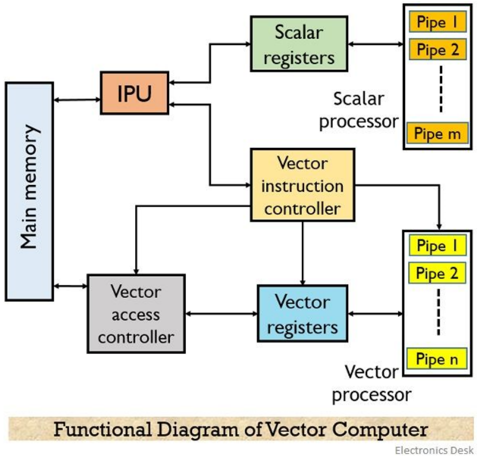


# Lecture 9 – CFD & Parallel Computing

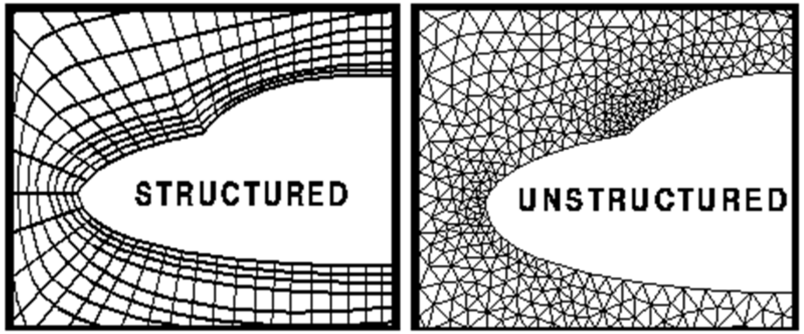
- Parallel computing in CFD
  - Vector computers
  - Superscaler computers
  - Parallel architecture
  - Topology
  - Parallel programming
- Explicit and Implicit methods
  - Grid techniques
  - Strucured explicit
  - Unstructured explicit
  - Parallel iterative schemes
  - Gradient methods
  - Particle methods




[21] CompTIA® Network+ Exam Notes



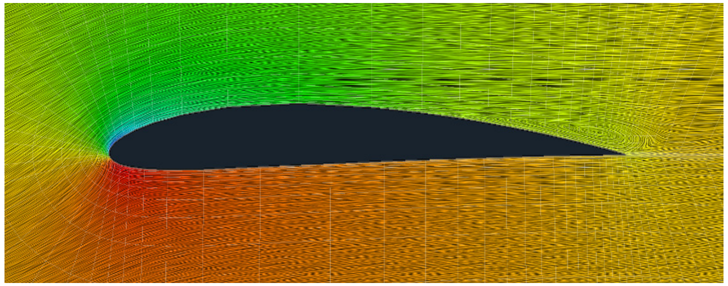

[22] Vector Processor



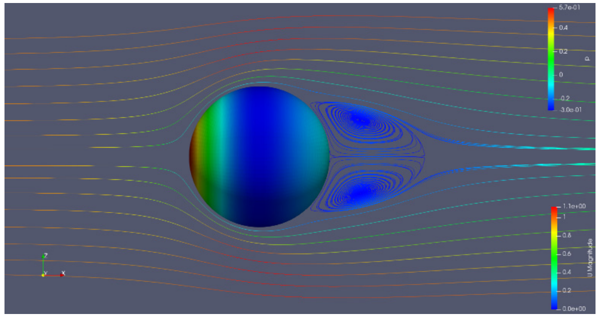

[23] FAST :Computational Fluid Dynamics ,Robert Neely, NASA Langley

# Lecture 10 – OpenFoam Software & CFD Applications

- Openfoam
  - Open source
  - Geometry
  - Meshing
  - Boundary
  - Solver
  - Laminar and turbulent
  - Example in openfoam
- Running parallel
  - Decoposition of domain
  - Input/output
  - Running decopoosed
  - Distributing data

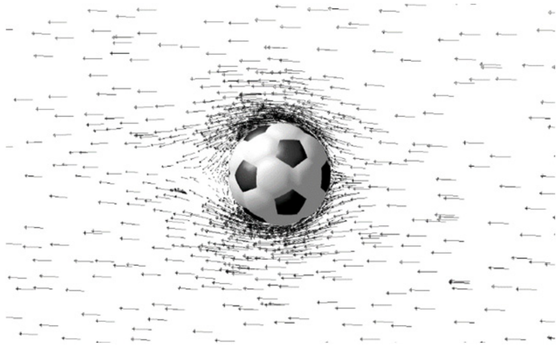


[25] NACA4412 Airfoil Tutorial

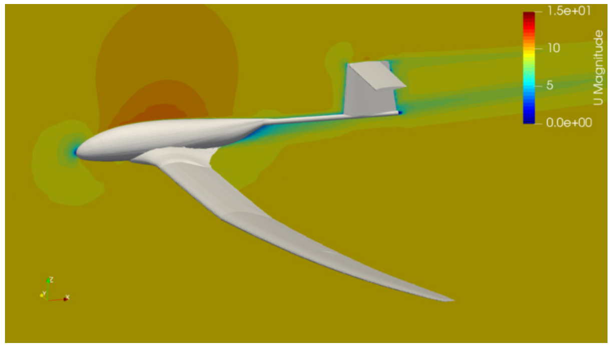


[26] CD error simulating laminar steady-state flow over a sphere (OpenFOAM)

OpenFOAM®



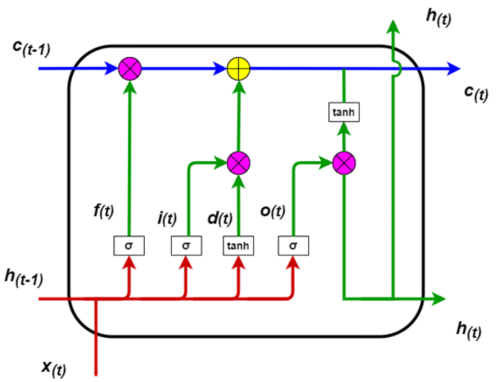
[27] Lecture of Applied Computational Fluids Dynamics, André Bakker, 2008

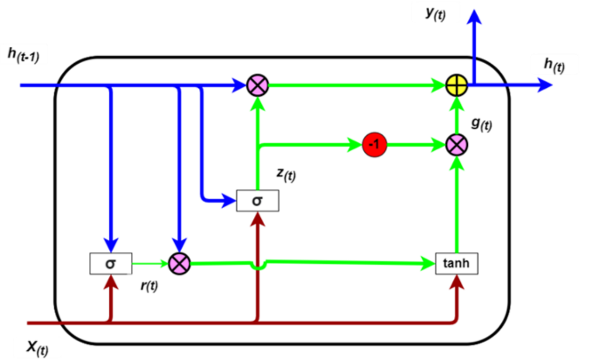


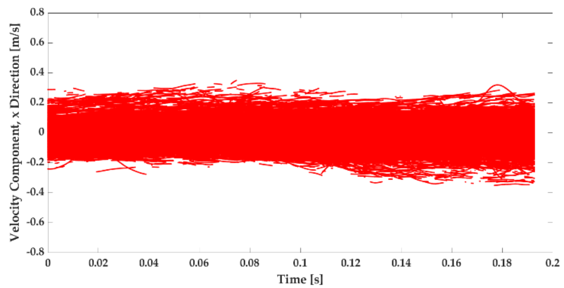

[33] 3D Analysis of Aircraft

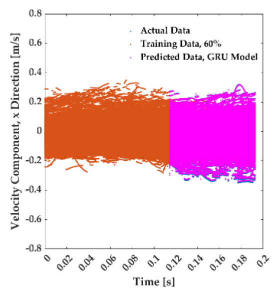
# Lecture 11 – Deep Sequence Models & CFD Applications

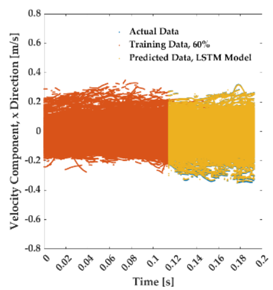
- Fluids flow prediction
  - Turbuent flow
  - Forcasting and its matter
  - Example of wind energy forecasting
  - Deep learning capability
  - Flow forcasting via deep learning
- LSTM/GRU forecasting model
  - Long short-term memory (LSTM)
  - Gated recurrent units (GRUs)
  - Define turbulent flow in framework
  - LSTM and GRU model
  - Considerable prediction
  - Larger data and more computing



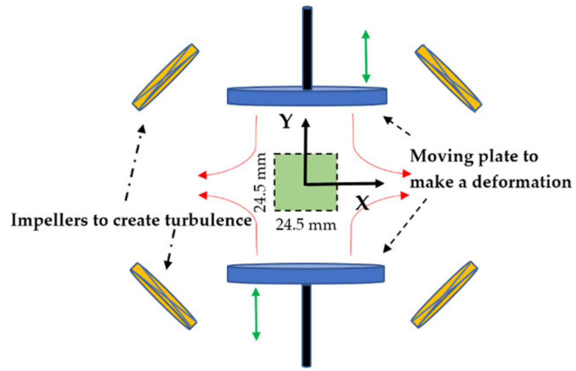



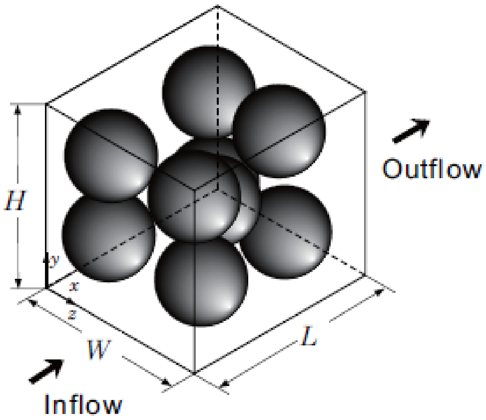




[24] Hassanian R, Riedel M et al. Deep Learning Forecasts a Strained Turbulent Flow Velocity Field in Temporal Lagrangian Framework: Comparison of LSTM and GRU. Fluids. 2022; 7(11):344

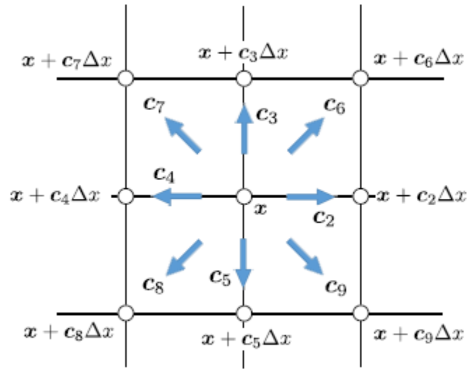


# Lecture 12 – Lattice Boltzmann & CFD Applications

- Lattice Boltzmann
  - History and concept
  - Boltmann equation
  - Boundary condition
  - Advantages and disadvantages
  - Applications
- Methodology
  - Modeling
  - Gas-particle flow
  - Particle tracking
  - LBM for turbulent flow
  - LBM base on LES

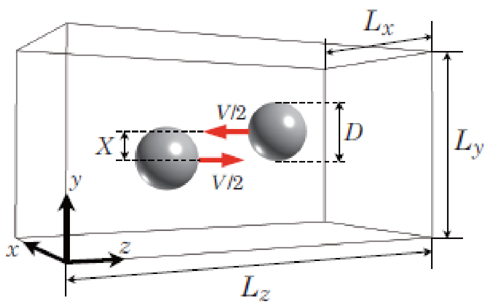



Three-dimensional porous structure.




Computational lattice and particle velocities in the D2Q9 model.

[34] Kosuke Suzuki et al., Introduction To The Lattice Boltzmann Method: A Numerical Method for Complex Boundary and Moving Boundary Flows, worldscientific publisher, November 2021




Computational domain of droplet collisions.

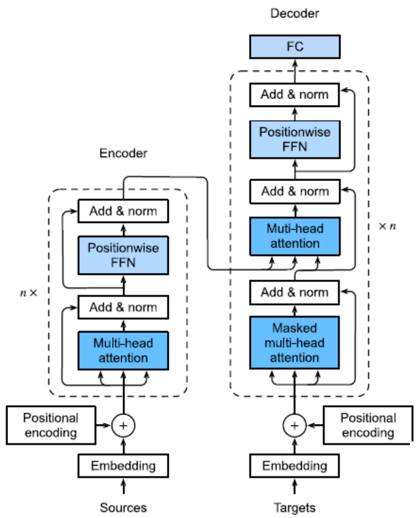
$$f\left(\vec{r} + \vec{c}dt, \vec{c} + \frac{\vec{P}}{m}dt, t + dt\right) - f(\vec{r}, c, t) = \left(\frac{\partial f}{\partial t}\right)dt$$

Streaming = Collision

$$\frac{\partial f}{\partial t} + \vec{c}.\nabla f = \Omega(f)$$ Boltzman Equation (1872)

# Lecture 13 – Transformer Models & CFD Applications

- Attention mechanisms
  - Attention and visual environment
  - Attention Cues
  - Self-Attention and Positional Encoding
  - Encoder-decoder architecture
  - Transformer Architecture
- Transformers application
  - Fluid framework
  - Dataset
  - Transformers model
  - Model architecture
  - Fluid prediction
  - Validation

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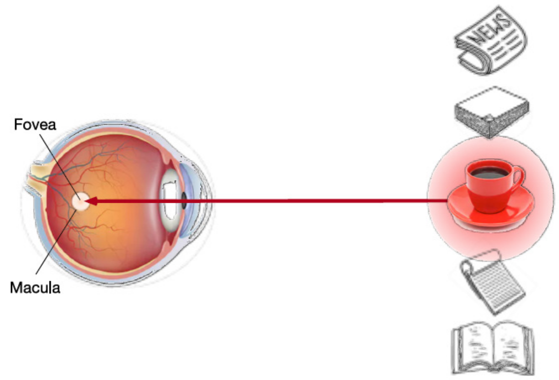
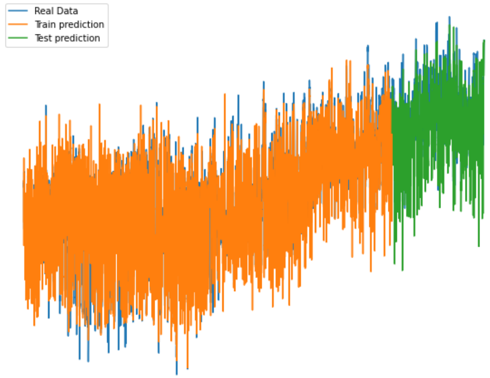
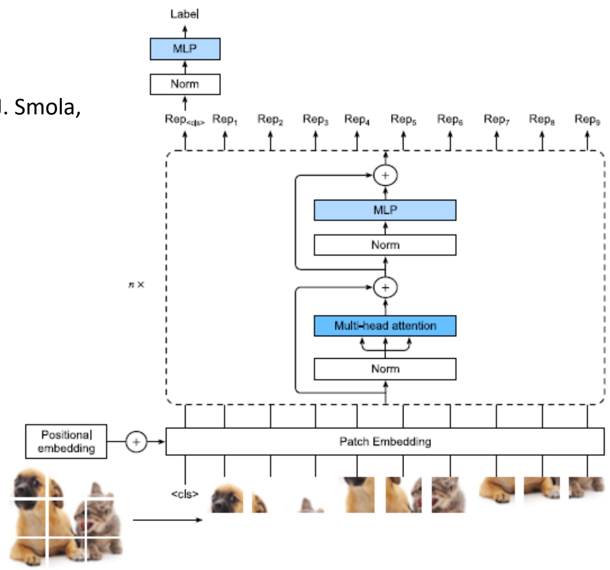
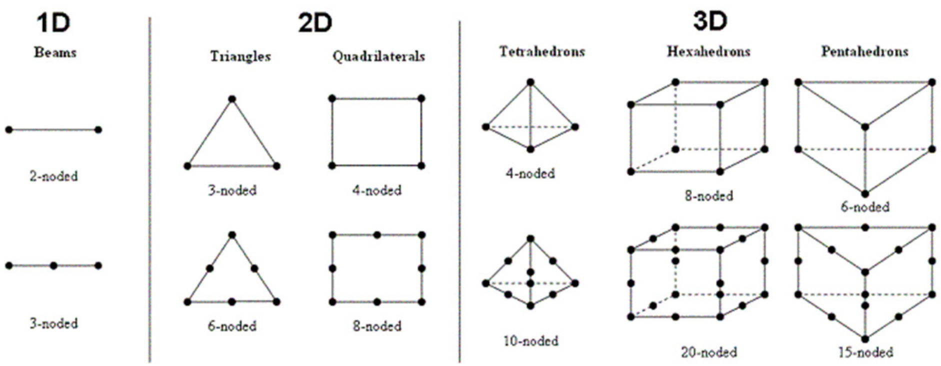


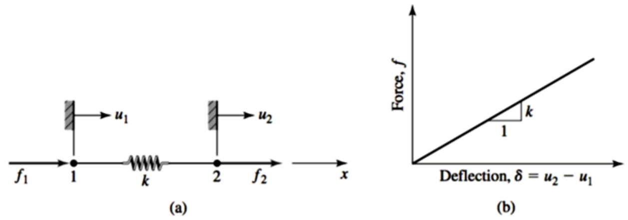



# Lecture 14 – Solid Objects & Finite Elements Method

- Numerical method in Solid objects
  - Finite element
  - Direct method
  - Variational method
  - Weighted residual method
  - applications
- Finite element meshes
  - Element types
  - Interpolation functions
  - Features and procedures
  - Stifness matrix



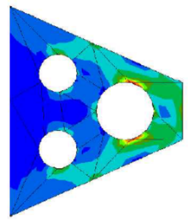




$$\begin{bmatrix} k & -k \\ -k & k \end{bmatrix} \begin{Bmatrix} u_1 \\ u_2 \end{Bmatrix} = \begin{Bmatrix} f_1 \\ f_2 \end{Bmatrix} \quad \text{or} \quad [k_e]\{u\} = \{f\}$$

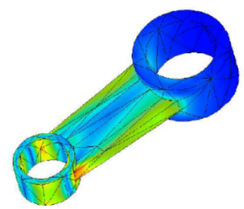
where

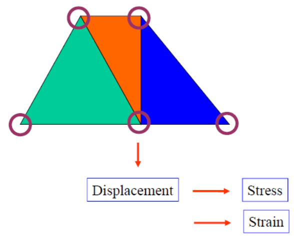
$$[k_e] = \begin{bmatrix} k & -k \\ -k & k \end{bmatrix}$$ Stiffness matrix for one spring element

Examples of FEA - 2D



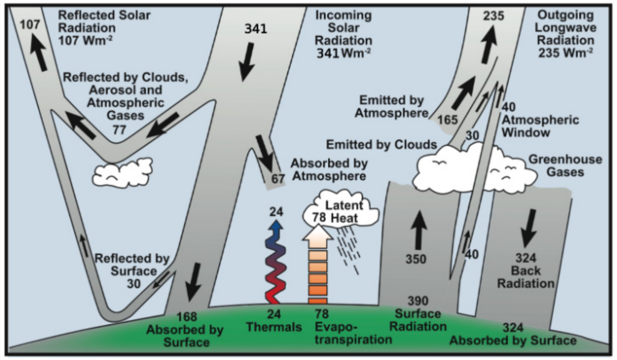
Examples of FEA – 3D





# Lecture 15 – Green Energy & HPC Applications

- Green Energy
  - Smart cities
  - Smart power grid
  - HPC needed for smart system
  - Large data
  - Extensive computing
- HPC energy supply
  - HPC system and its demand
  - Energy supply
  - Green energy tranistion
  - Renewable energy options





[13] J. T. Kiehl and Kevin E. Trenberth, Bulletin of the American Meteorological Society, Vol. 78, No. 2, February 1997, Planet Energy bala


| | Size ID | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | A | B | C | D | E | F | G | H | I | J | K | L |
| X | 128 | 256 | 256 | 256 | 256 | 256 | 512 | 512 | 768 | 768 | 1024 | 512 |
| Y | 128 | 256 | 256 | 512 | 256 | 256 | 512 | 512 | 768 | 768 | 1024 | 512 |
| Z | 128 | 256 | 512 | 512 | 1024 | 2048 | 512 | 1024 | 768 | 1024 | 704 | 2832 |
| MB | 32 | 256 | 512 | 1024 | 1024 | 2048 | 2048 | 4096 | 6912 | 9216 | 11266 | 11328 |

Input sizes used in experiments with 3D Wave Propagation.

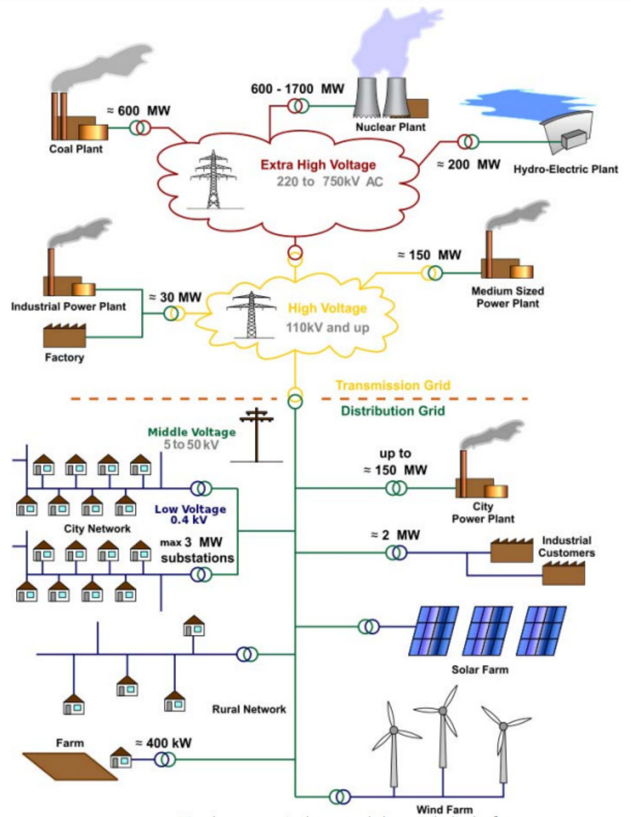
| | | CPU | | | GPU | | |
|---|---|---|---|---|---|---|---|
| | | System | Monitor | App | System | Monitor | App |
| Energy (J) | Serial Region | 13,770 | 972 | 2,916 | 17,989 | 811 | 1,758 |
| | Parallel region | 15,470 | 1,092 | 10,556 | 5,721 | 258 | 4,990 |
| Power (W) | Serial region | 170 | 12 | 36 | 266 | 12 | 26 |
| | Parallel region | 170 | 12 | 116 | 266 | 12 | 232 |

Results for the ComCiDis's CPU and GPU.

| Size | Cluster | Time to solution | Energy to solution |
|---|---|---|---|
| A | SDumont | 9,5 sec | 1,092 J |
| A | ComCiDis | 7,9 sec | 2,291 J |
| G | SDumont | 4 min 12 sec | 36,802 J |
| G | ComCiDis | 6 min 32 sec | 101,703 J |
| L | SDumont | 22 min 50 sec | 200,740 J |

Time and Energy to Solution on GPUs.


[39] M. Ferro et al."Analysis of GPU Power Consumption Using Internal Sensors", in Anais do XVI Workshop em Desempenho de Sistemas Computacionais e de Comunicação, São Paulo, 2017, doi: https://doi.org/10.5753/wperformance.2017.3360.


Electric power production, transmission and distribution


[38] Marcin. P, , Jean. P. N, Ladina. G, Francois. R., Norbert M, Radoslaw j. Electricity in HPC Centres, Whitepaper, Partnership for Advanced Computing in Europe.

# Final Lecture 16 – 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 & parallel computing & programming skills
  - PhD positions & Master Thesis topics in HPC applications & techniques


- Toolset
  - Knowledge of HPC system tools & scientific computing libraries
  - Future Topics to study: Quantum computing, neural networks on the chip, neuromorphic computing, modular supercomputing

# [Video] High Performance Computing by Dreamworks


*[11] YouTube, Dreamworks HPC*

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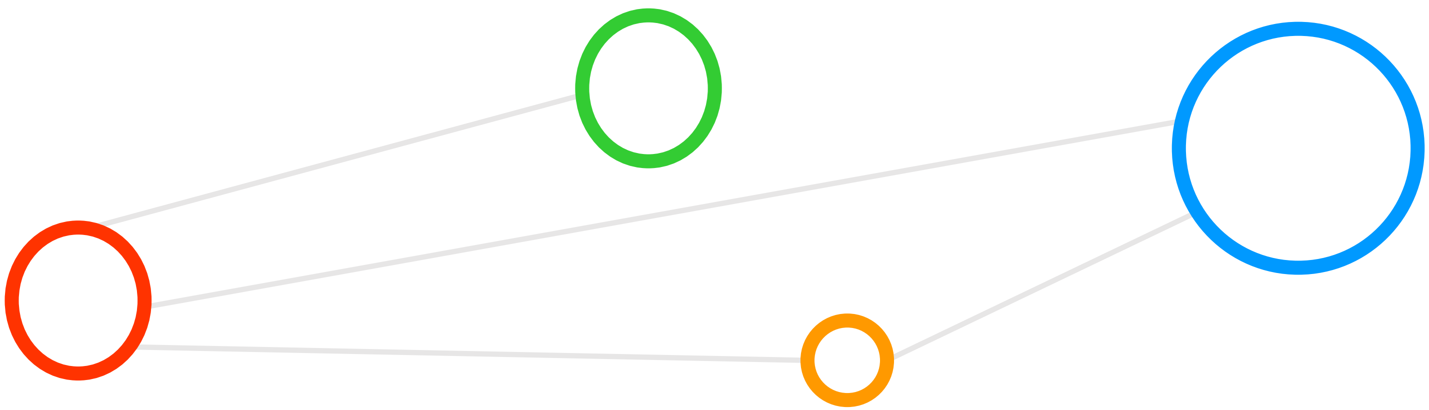

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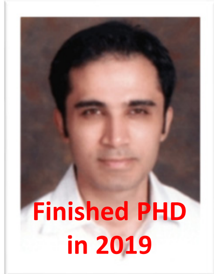


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PD Dr.
A.S. Memon


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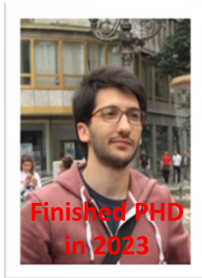
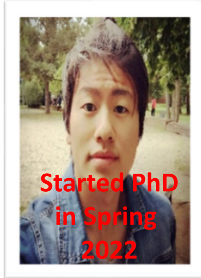



PD Dr.
S. Bakarat

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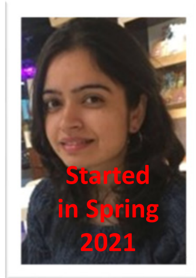


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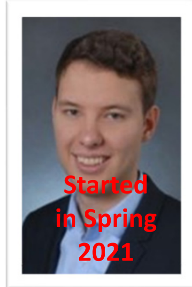


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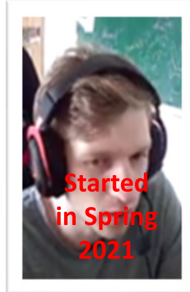


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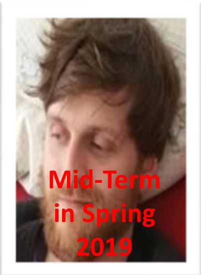


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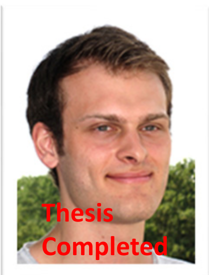


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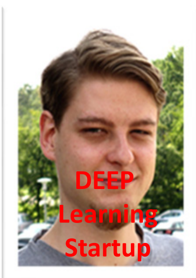


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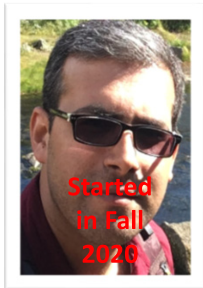


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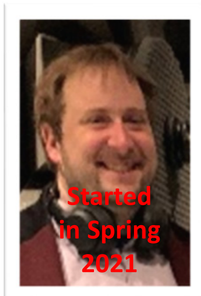


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