



Prof. – Dr. Ing. Morris Riedel (Iceland NCC / EuroCC WP33)

2021-06-07

NCC Iceland at a Glance & Collaboration



 Iceland, NCC 33



Icelandic National Infrastructure for HPC

- ❖ HPC hardware funds by RANNIS; now via roadmap IReiP
- ❖ Proposals yearly required to obtain funds still
- ❖ Joint proposal from IHPC community



EuroHPC LUMI Supercomputer in Finland

- ❖ Supercomputer funded by Finland, Belgium, Czech Republic, Denmark, Estonia, Iceland, Norway, Poland, Sweden, Switzerland
- ❖ Co-Funds by EC and Iceland participation funds from: UoIceland, UoReykjavik, and Hannes Jonsson & Egill Skulason



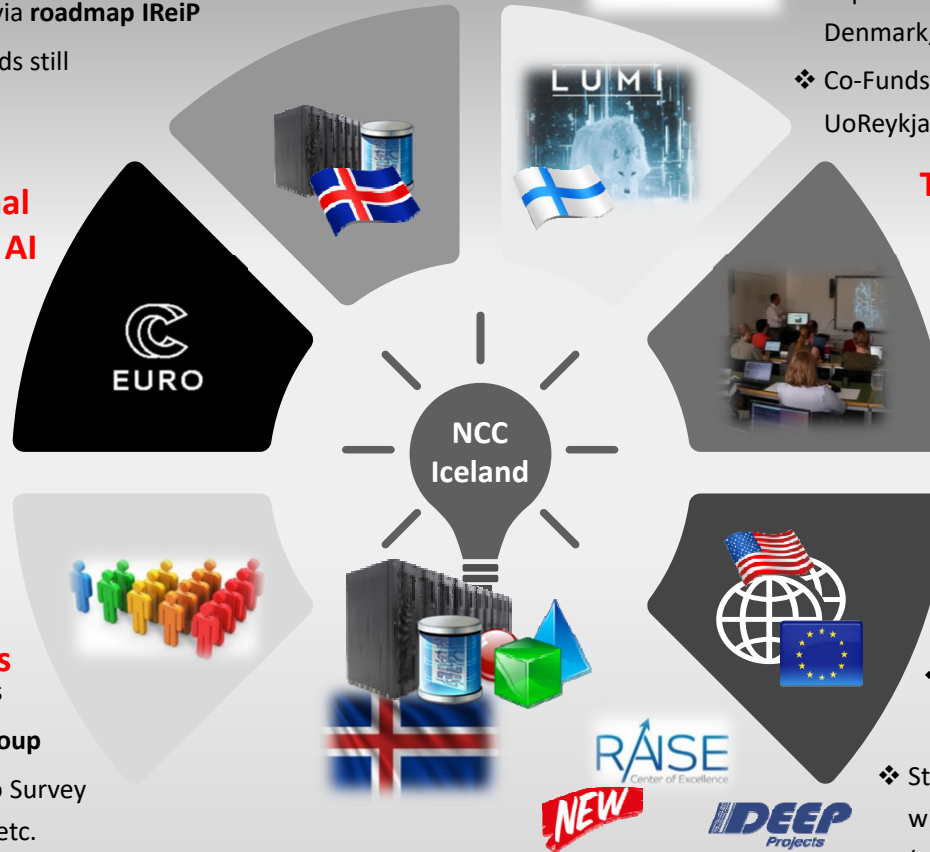
EuroHPC EuroCC National Competence Center for HPC & AI

- ❖ EU Project (09/2019-08/2021), 2 years
- ❖ Building **Simulation and Data Labs (SDLs)** of the IHPC Community of Users
- ❖ Supports industry engagement in HPC



IHPC Community of Users

- ❖ Organized around RANNIS proposals
- ❖ ~53 scientific experts & research group
- ❖ UoIceland/UoReykjavik, Iceland Geo Survey ÍSOR, Met Office & industry: Matis, etc.



Teaching & Education in HPC & AI

- ❖ University of Reykjavik
- ❖ University of Iceland
- ❖ Arctic Webinar Series (with US partners)
- ❖ Digital/Horizon Europe MSc in HPC



HÁSKÓLI ÍSLANDS



International Cooperations

- ❖ Tactical: ~4 Joint PhDs with **Juelich Supercomputing Centre** in Germany (#1 HPC System in Europe)
- ❖ Tactical: **EC Projects** like DEEP-EST, EOSC-Nordic, RAISE Center of Excellence (CoE)
- ❖ Strategic: Plans of building an **Icelandic National Lab** with international cooperation together with Industry (e.g. Kaiser Global, other investors)



The Competences of the NCC at a Glance



Iceland, NCC 33

Competence category	Level of HPC readiness of users				
	Digitalization needed	Digitally ready	HPC ready	HPC users	HPC champions
Awareness creation					
Expert technical consultancy			Experience in teaching technical topics like HPC & HPDA systems ¹	Experience in Modular Supercomputing Architecture Technologies ²	Experience in parallel & distributed training of HPDA / AI models ³
Services and products				Application Experience in HPDA & Remote Sensing (#6 in the world) ⁴	
Business & project consultancy					
Technological assessment and PoCs					Experience in Quantum Computing (i.e., quantum annealing) ⁵
Mastering the EU HPC ecosystem				Experience in forming Simulation & Data Labs (science & industry partners) ⁶	

Example Competence 1



Experience in Teaching Technical Topics like HPC & HPDA Systems



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



HÁSKÓLINN Í REYKJAVÍK
REYKJAVÍK UNIVERSITY

- Expert Technical Consultancy
→ HPC ready users
 - E.g. **High-Performance Computing Course**
(Advanced Scientific Computing)
 - E.g. **Cloud Computing & Big Data Course**
(Parallel & Scalable Machine & Deep Learning)
 - E.g. **Natural Language Processing (NLP)**
 - Selected domain-specific courses with HPC relevance

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. Hybrid Programming & Patterns
8. Debugging & Profiling & Performance Analysis
9. Accelerators & Graphical Processing Units
10. Parallel & Scalable Machine & Deep Learning
11. HPC in Health & Neurosciences
12. Computational Fluid Dynamics & Finite Elements
13. Systems Biology & Bioinformatics
14. Molecular Systems & Material Sciences
15. Terrestrial Systems & Climate
16. Epilogue

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

▪ Practical Topics
▪ Theoretical / Conceptual Topics

2021 High Performance Computing Lecture 0 Prologue Part1

395 views • Jan 13, 2021

Prof Dr. Ing Morris Sledel
538 subscribers

ANALYTICS EDIT VIDEO

Outline of the Course

1. Cloud Computing & Big Data Introduction
2. Machine Learning Models in Clouds
3. Apache Spark for Cloud Applications
4. Virtualization & Data Center Design
5. Map-Reduce Computing Paradigm
6. Deep Learning driven by Big Data
7. Deep Learning Applications in Clouds
8. Infrastructure-As-A-Service (IAAS)
9. Platform-As-A-Service (PAAS)
10. Software-As-A-Service (SAAS)
11. Big Data Analytics & Cloud Data Mining
12. Docker & Container Management
13. OpenStack Cloud Operating System
14. Online Social Networking & Graph Databases
15. Big Data Streaming Tools & Applications
16. Epilogue

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

▪ Practical Topics
▪ Theoretical / Conceptual Topics

2020 Cloud Computing and Big Data Lecture 0 Prologue Part1

10,082 views • Aug 26, 2020

Prof Dr. Ing Morris Sledel
538 subscribers

ANALYTICS EDIT VIDEO



[1] YouTube Channel: <https://www.youtube.com/channel/UCWC4VKHmL4NZgFfKoHtANKg>

Example Competence 1 – PhD Students

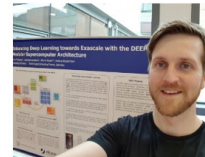


Experience in Teaching Technical Topics like HPC & HPDA Systems



Pétur Helgi Einarsson

PhD Student in Computational Neuroscience & HPC



Ernir Erlingsson

PhD Student in HPC Application Co-Design



Reza

PhD Student in Computational Fluid Dynamics (CFD) & HPC



Rocco Sedona

PhD Student in **Remote Sensing & HPC**



Marcel Aach

PhD Student in Computational Fluid Dynamics (CFD) & HPC



Surbhi Sharma

PhD Student in **Remote Sensing & HPC**



Dirk Helmrich

PhD Student in Preserving Environments with Plants & HPC



Eric Michael Sumner

PhD Student in Accoustic & Tactile Engineering & HPC



Chadi Barakat

PhD Student in computational healthcare & HPC

Guiding & Recruiting MSc Students



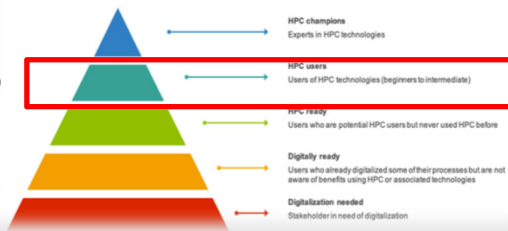
Great joint students to start PhDs like Gísli Ingolfsson & Liang Tian



Example Competence 2



Experience in Modular Supercomputing Architecture Technologies



Potentially first
Exascale system
in Europe



[3] DEEP Series of Projects Web Page

- Expert Technical Consultancy
→ HPC users



[2] YouTube, 'flexible and energy-efficient supercomputer:
JUWELS is faster than 300 000 modern PCs



2018

12 PF



2020
85 PF

NEW

JUWELS Booster – A Supercomputer for
Large-Scale AI Research

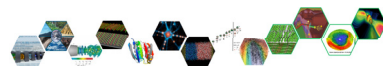
Stefan Kesselheim¹*, Andreas Horten¹*, Kai Krajsek¹*, Jan Ebert¹*,
Jens Jites¹*, Mehdi Chertil¹*, Michael Langguth¹*, Bing Gong¹*,
Scarlet Stadler¹*, Amirpasha Mozaffari¹*, Gabriele Cavallaro¹*,
Rocco Sedona^{1,2}*, Alexander Schug^{1,3}*, Alexandre Strübel¹, Roshni Kamathi¹,
Martin G. Schulz¹, Morris Riedel^{1,2}, Thomas Lippert¹

¹ Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH, Germany,
contact: <cc>:cc@fz-juelich.de

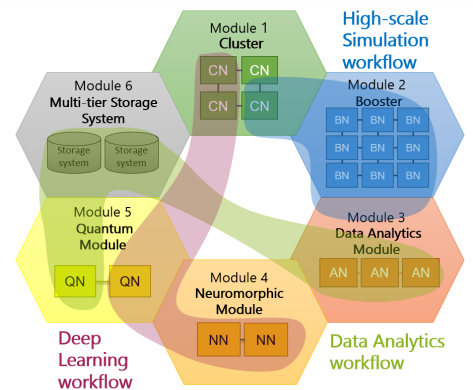
² School of Engineering and Natural Sciences,
University of Iceland, Reykjavik, Iceland

³ University of Duisburg-Essen, Germany

Application Co-Design



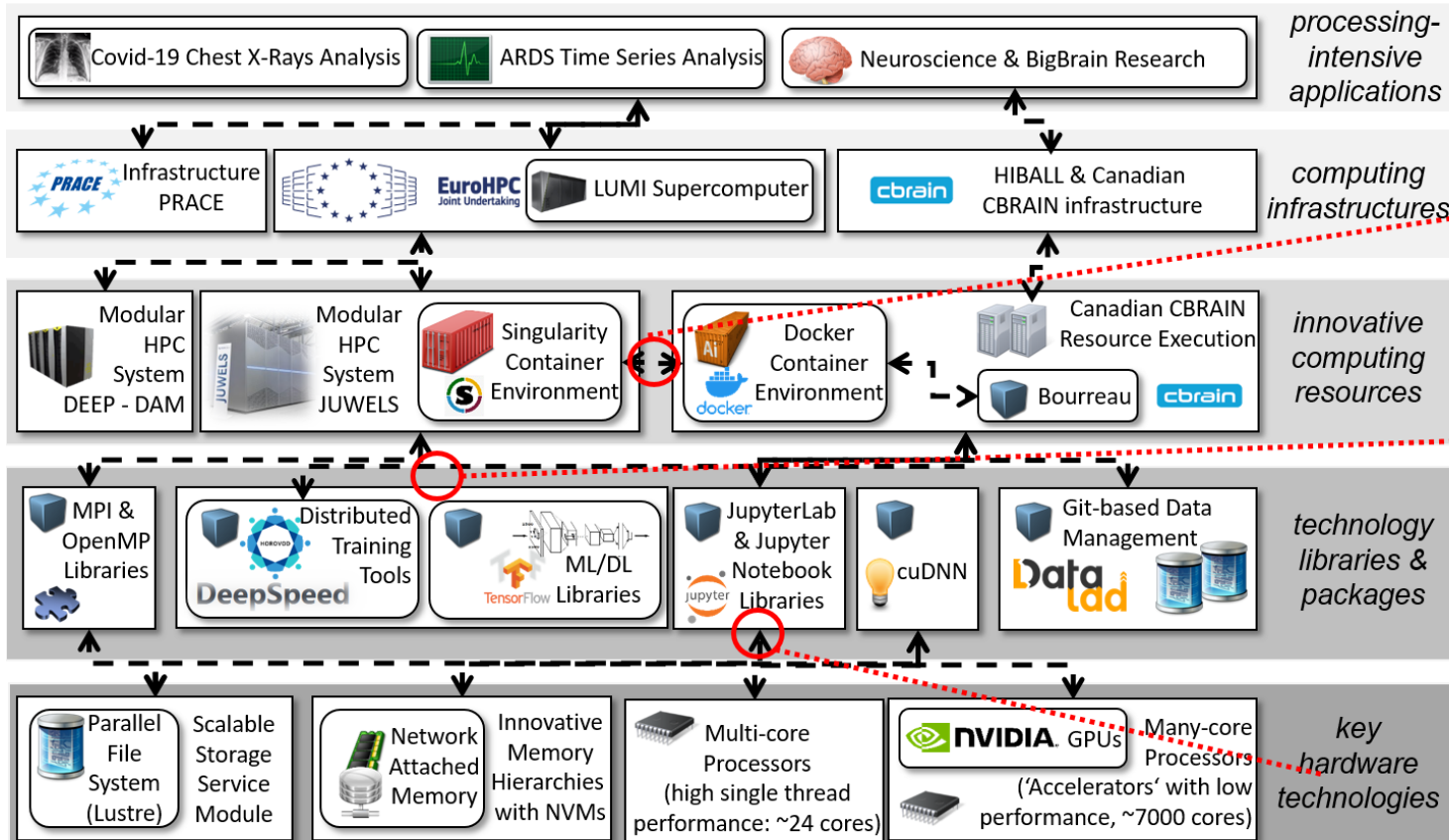
1 EF



[6] S. Kesselheim et al., 'JUWELS Booster - A Supercomputer
for Large-Scale AI Research', ICS 2021, to appear

Example Competence 2 – Summary

Experience in Modular Supercomputing Architecture Technologies



Some preparation

```
$ mkdir winterschool winterschool_cache winterschool_tmp
$ chmod -w winterschool_cache
$ export SINGULARITY_CACHEDIR=$(mktemp -d -p "$(pwd)/winterschool_cache")
$ export SINGULARITY_TMPDIR=$(mktemp -d -p "$(pwd)/winterschool_tmp")
```

Pull the docker image:

```
$ cd winterschool
$ singularity pull hws.sif docker://glatard/hws
```

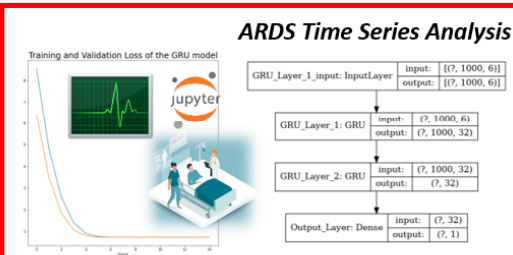
Step into the container

```
$ singularity shell ./hws.sif
(the prompt changes to `>Singularity`)
```

download a dataset:

```
$ git config --global user.name "Your name"
$ git config --global user.email "peturhelgi@gmail.com"
```

Singularity> datalad install https://github.com/COMP-PCNO/comp-dataset.git



Covid-19 Chest X-Ray Analysis

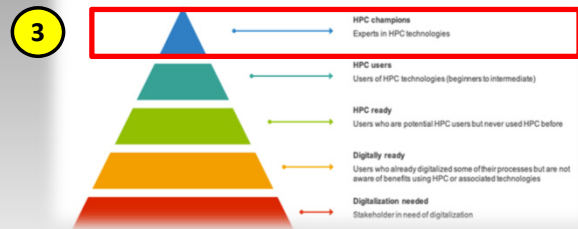
Covid-Net jupyter Covid-X Dataset

```
#!/bin/bash
# Load required modules
module purge
module use $OTHERSTAGES
module load Stages/2020
module load GCCcore/9.3.0
module load Python/3.8.5
module load TensorFlow/2.3.1-Python-3.8.5
module load OpenCV/4.5.0-Python-3.8.5
# Activate Python virtual environment
source /p/project/training2104/ingolfsson1/jupyter/kernels/ingolfsson1_kernel/bin/activate
# Ensure python packages installed in the virtual environment are always preferred
export PYTHONPATH=/p/project/training2104/ingolfsson1/jupyter/kernels/ingolfsson1_kernel/11b
exec python -m ipynbkernel $@
```

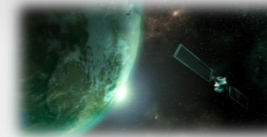
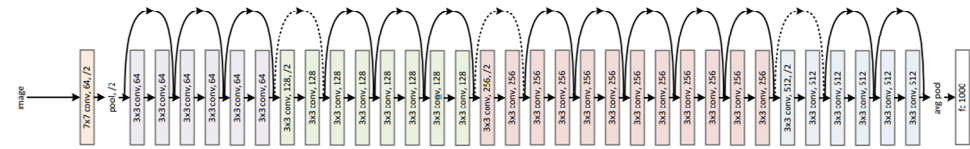
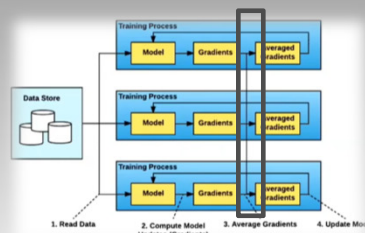

Example Competence 3



Experience in Parallel & Distributed Training of HPDA / AI Models



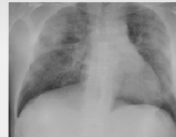
[4] Horovod



using satellite images in remote sensing

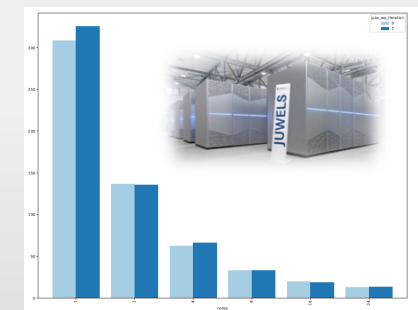
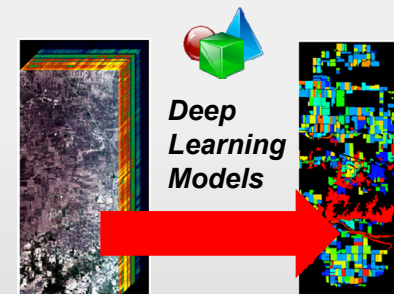


Healthy Patient



Covid-19 Patient

- Expert Technical Consultancy
 - HPC Champions
 - E.g. **using Horovod to scale-up TensorFlow & Keras for Deep Learning**
 - E.g. with remote sensing applications (land cover analysis)
 - E.g. with health sciences applications (Covid-19 Xray analysis)

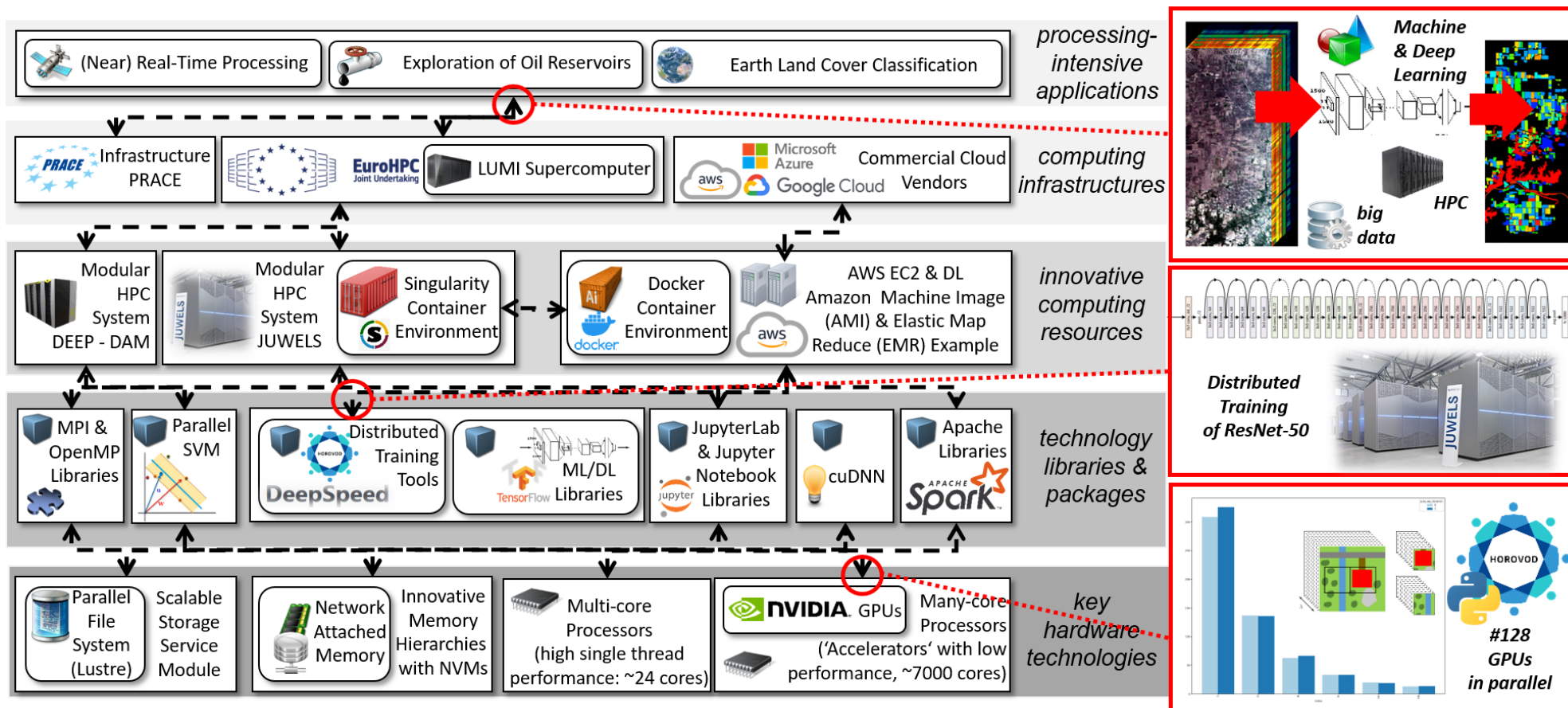


24 nodes x 4 GPUs = 96 GPUs

[5] R. Sedona, G. Cavallaro, M. Riedel, J.A. Benediktsson et al.: Remote Sensing Big Data Classification with High Performance Distributed Deep Learning, *Journal of Remote Sensing*, Multidisciplinary Digital Publishing Institute (MDPI), Special Issue on Analysis of Big Data in Remote Sensing, 2019

Example Competence 3 – Summary

Experience in Parallel & Distributed Training of HPDA / AI Models



[7] M. Riedel et al., Practice & Experience in using Parallel & Scalable Machine Learning with Heterogenous Modular Supercomputing Architectures, in proceedings of IEEE IPDPS, 2021

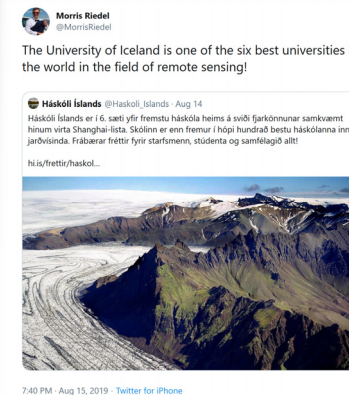
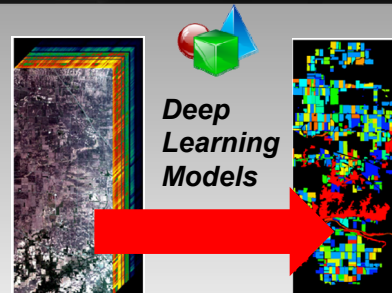
Example Competence 4



Application Experience in HPDA & Remote Sensing (#6 in the world)

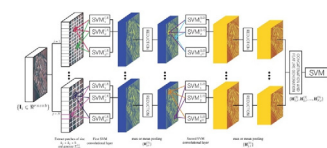
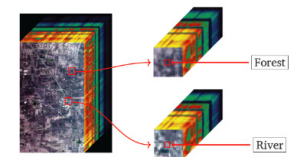


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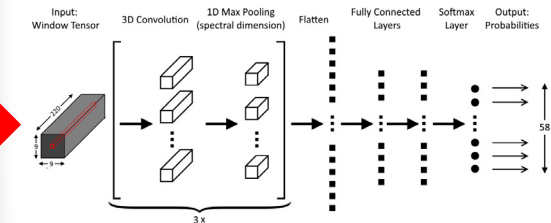


[10] J. Lange, G. Cavallaro, M. Riedel et al., IGARSS Conference, 2018

- Services and Products
→ HPC Users
- E.g. Feature Selection & Engineering Methods
- E.g. Transfer-Learning expertise with succesful deep learning networks
- E.g. Combination of traditional machine learning & new deep learning models



[11] G. Cavallaro, M. Riedel et al., IGARSS 2019

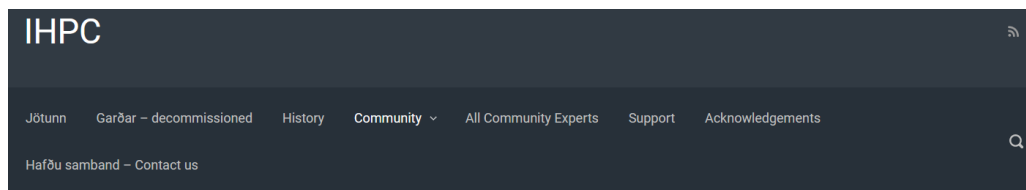


Feature	Representation / Value
Conv. Layer Filters	48, 32, 32
Conv. Layer Filter size	(3, 3, 5), (3, 3, 5), (3, 3, 5)
Dense Layer Neurons	128, 128
Optimizer	SGD
Loss Function	mean squared error
Activation Functions	ReLU
Training Epochs	600
Batch Size	50
Learning Rate	1
Learning Rate Decay	5×10^{-6}

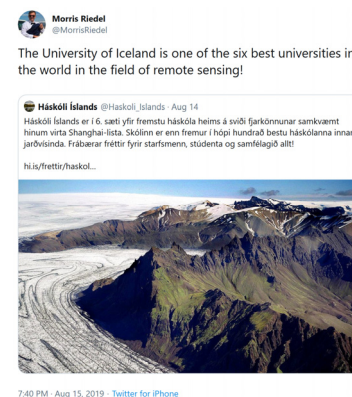
Example Competence 4 – Contacts



Application Experience in HPDA & Remote Sensing (#6 in the world)



Simulation and Data Lab Remote Sensing



General information

The Simulation and Data Lab Remote Sensing (SimDataLab RS) leads to increase the visibility on interdisciplinary research between remote sensing and advanced computing technologies and parallel programming. This includes high-performance and distributed computing, quantum computing and specialized hardware computing. The SimDataLab RS is based at the University of Iceland and works together with the High-performance and Disruptive Computing in Remote Sensing (HDCRS) working group of the Geoscience and Remote Sensing Society (GRSS). Together with HDCRS, the SimDataLab RS disseminates information and knowledge through educational events, special sessions and tutorials at conferences and publication activities.

Members

Prof. Dr. – Ing. Morris Riedel



Dr. -Ing. Gabriele Cavallaro



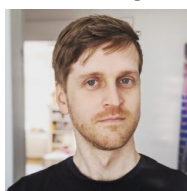
Ing. Rocco Sedona



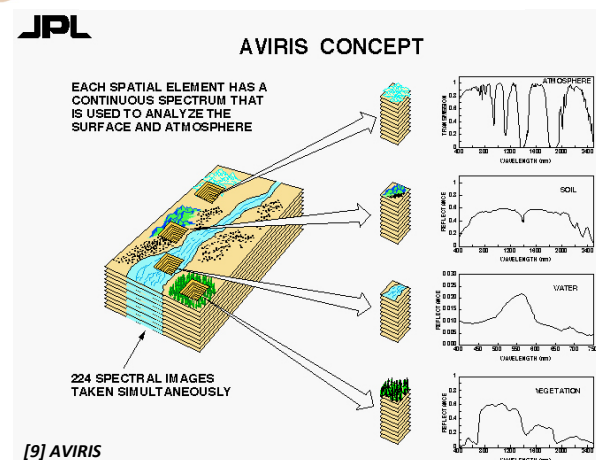
Surbhi Sharma



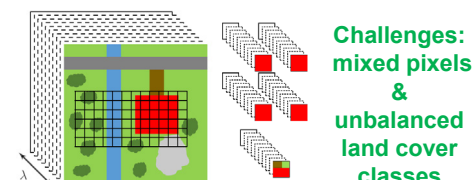
Ernir Erlingssson



[8] IHPC SimDataLab Remote Sensing Web Page



Example: Land cover classification



Challenges:
mixed pixels
&
unbalanced
land cover
classes

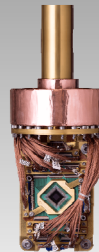
Example Competence 5



Experience in Quantum Computing (i.e., quantum annealing)



5

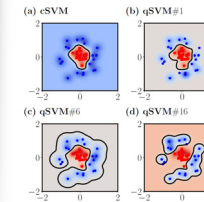


```
In [ ]: from quantum_SVM import *
import numpy as np
from sklearn import *
from sklearn.model_selection import KFold
from sklearn import preprocessing

# Write the data
# Load the data
# Number of samples to use for the training
fold = KFold(n_splits=10, random_state=1, shuffle=True)

print(fold)

for i in range(10):
    cv = KFold(n_splits=10, random_state=1, shuffle=True)
    for test_index, train_index in cv.split(X_train):
        X_train_allow = X_train[train_index]
        X_test_allow = X_train[test_index]
        X_test_allow = preprocessing.scale(X_test_allow)
```



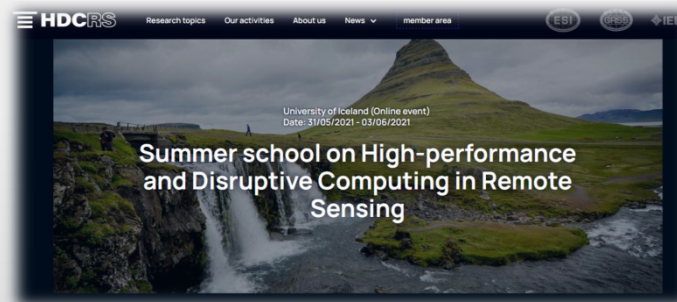
ID	Sensor	Data points	Train Samples	Classes
Im16	Landsat	200×200×7	500	2
Im40	Landsat	200×200×7	500	2

[16] G. Cavallaro & M. Riedel et al., *Approaching Remote Sensing Image Classification with Ensembles of SVMs on the D-Wave Quantum Annealer*, *Proceedings of the IEEE IGARSS 2020 Conference*

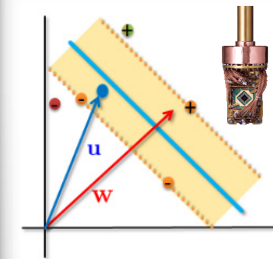
[15] A. Delilbasic, G. Cavallaro, F. Melgani, M. Riedel, K. Michielsen: *QUANTUM SUPPORT VECTOR MACHINE ALGORITHMS FOR REMOTE SENSING DATA CLASSIFICATION*, *Proceedings of the IEEE IGARSS 2021 Conference, to appear*

• Technological assessment & PoCs → HPC Champions

- Experience with D-Wave Quantum Annealer System
- Cutting-edge IEEE Training Events



[17] Summerschool Web Page



[13] Quantum SVM, D. Willsch et al.

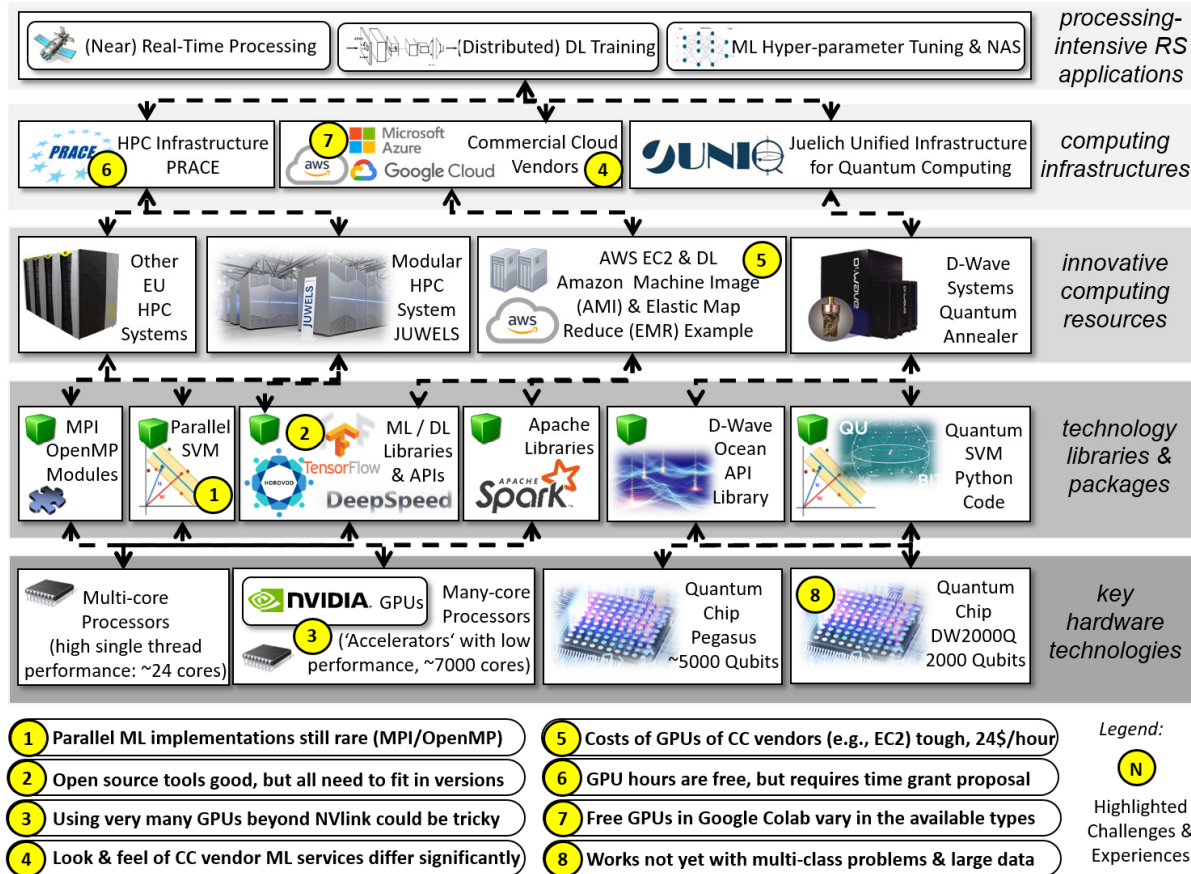


[14] M. Riedel, UTMessan 2020 YouTube Video

Example Competence 5 – Challenges



Experience in Quantum Computing (i.e., quantum annealing)



[12] M. Riedel, G. Cavallaro, J.A. Benediktsson, 'PRACTICE AND EXPERIENCE IN USING PARALLEL AND SCALABLE MACHINE LEARNING IN REMOTE SENSING FROM HPC OVER CLOUD TO QUANTUM COMPUTING', in *Proceedings of the IGARSS 2021 Conference, to appear*

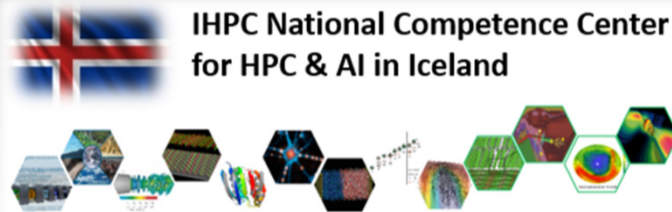
Example Competence 6



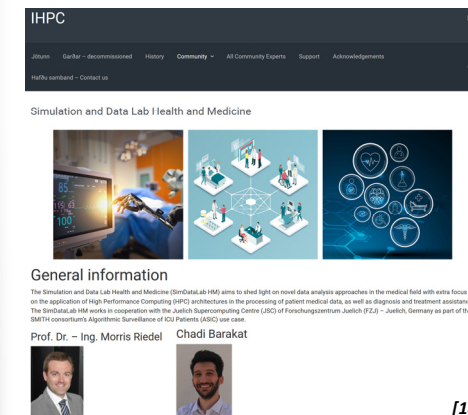
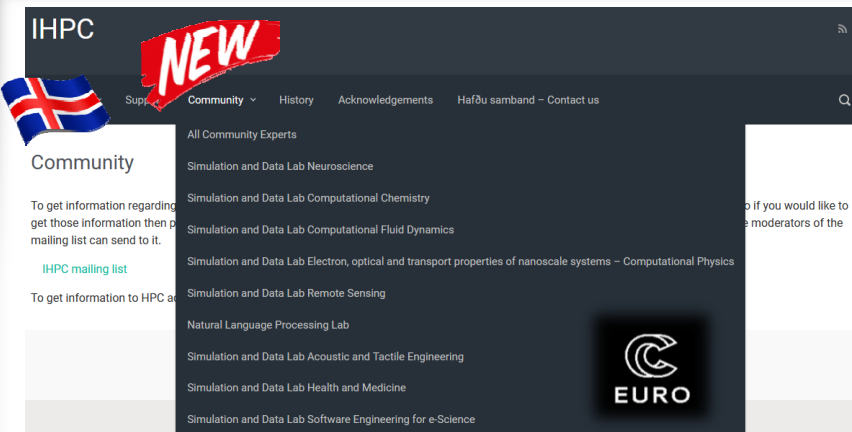
Experience in forming Simulation & Data Labs (science & industry)



6



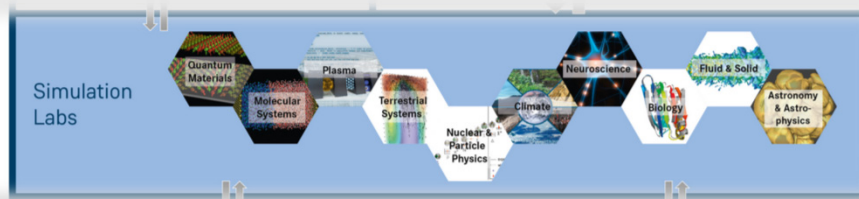
[10] Icelandic HPC Community Web page



[18] IHPC SimDataLab Health & Medicine Web Page

- Mastering the EU HPC ecosystem
→ HPC Users
 - Experience in **establishing Simulation & Data Labs (SimDataLabs)** for Community Building
 - Based on experience over 15 years

[20] JSC Simulation Labs Web Page



Deep Learning Models for ARDS

Example Competence 6 – SMEs



Experience in forming Simulation & Data Labs (science & industry)



Simulation and Data Lab Acoustic and Tactile Engineering

Acoustic and Tactile Engineering

General information

The focus of the Acoustic and Tactile Engineering (ACUTE) lab is both on research and product development. For the last few years, our main focus has been on the development of wearable assistive devices for visually impaired persons and cochlear implant recipients. We are also working on other projects, such as solutions for delivering virtual acoustics (i.e., sounds generated by computers) as realistically as possible and on multi-channel recording/playback.

Some of our current collaborations include: Oticon Medical, DTU (Technical University of Denmark), University of Southampton and Treble technologies.

Members

[22] IHPC SimDataLab Acoustic & Tactile Engineering Web Page



Prof. Dr. Ing Rúnar Úrnþórsson

Dr. Rúnar Úrnþórsson is a Professor (100%) at the faculty of Industrial engineering, Mechanical engineering, and Computer Science at the University of Iceland. Rúnar's main research interests are in performance engineering and the engineering application of acoustics / vibrations for sensory substitution, non-destructive evaluations, tactile/acoustic displays and product design.

Prof. Rúnar Úrnþórsson, coordinated the AME H2020 RIA project Sound of Vision (no. 643636) which was carried out in the years 2015-2017. The project received the EC's 2018 Innovation Radar Prize in the category Tech for Society for the development of an assistive device for the visually impaired. In 2017, the lab was awarded the 2nd prize for its tactile display at the University of Iceland's Science and Innovation Awards. The ACUTE lab is currently working on the development of the tactile display – with support from the Technology Development Fund (tdfa.is)



Dr. Ing. Finnur Pind

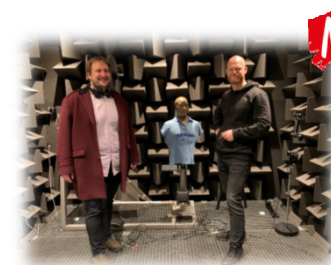
Dr. Finnur Pind received his MSc in acoustical engineering in 2013 from the Technical University of Denmark (DTU), and his PhD from the same institution in 2020. His PhD research was centered on virtual acoustics and was done in collaboration with the architectural studio Henning Larsen. Between his MSc and PhD studies, Finnur was an acoustic consultant in the building industry for some three years, and before entering the world of acoustics he was a software engineer in the telecom industry. His research interests include wave-based (numerical) acoustic simulations, acoustic virtual reality, room surface modeling, high-performance computing and spatial audio. He is currently a postdoctoral researcher at the ACUTE (Acoustics and Tactile Engineering) group at the University of Iceland and co-founder / CEO of Treble Technologies, which develops state-of-the-art virtual acoustics software.



Elvar Aili Áriðsson worked as an electronics technician for many years, specializing in professional sound system installation. He completed his MSc degree in electrical and computer engineering at the University of Iceland in 2020, having spent time as an exchange student at the Technical University of Denmark (DTU) taking acoustical engineering courses. He is currently a PhD student in industrial engineering at the University of Iceland working with the ACUTE group and focusing on audio-tactile integration.



[10] Icelandic HPC Community Web page



NEW

RAISE
Center of Excellence

[21] RAISE Center of Excellence Web Page



[23] EuroCC Project



Natural Language Processing Lab

General information

The Natural Language Processing Lab (NLP Lab) connects a community of researchers in NLP. The main focus is on large language models that require high-performance distributed computing environments to train efficiently.

The NLP Lab is based at the University of Iceland and works together with startups and companies on research projects and innovation. Currently, the lab is working with Nordverse and Miðind. The NLP Lab disseminates information and knowledge through educational events, special sessions, and tutorials at conferences and publication activities.

Members

Prof. Dr. Hafsteinn Einarsson

Hafsteinn is an assistant professor at the School of Engineering and Natural Sciences of the University of Iceland. He received his Ph.D. in Computer Science from ETH in 2018. He has worked on applied ML solutions for startups and in the Icelandic banking sector. He is currently focused on natural language processing, interpretable ML methods and optimization problems.

Vésteinn Snæbjarnarson

Vésteinn is a researcher at language technology company and an MSc student at the School of Engineering and Natural Sciences of the University of Iceland. He works in machine translation, language modeling and question answering.

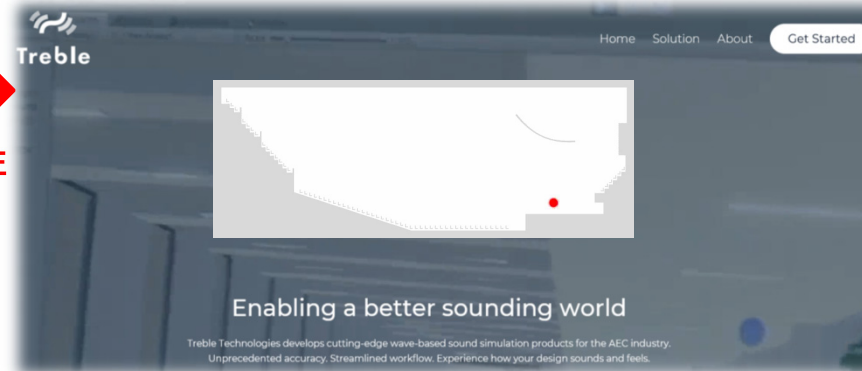


We create software that simplifies complex health information to empower valuable human care.

Nordverse is a Nordic based health tech startup created in 2019 by two medical doctors and a PhD computer scientist. Nordverse has received numerous grants and awards as well as having built a strong team to deliver high-quality software originating from clinical experience and aimed to deliver real clinical value.



Our Partners

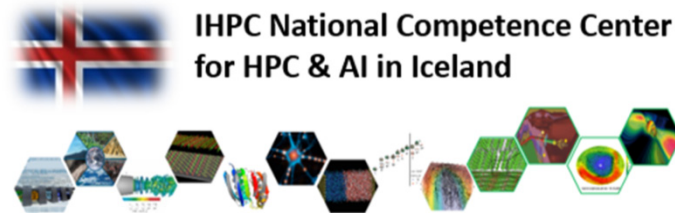


[24] Treble Technologies

[25] Nordverse

Topics of interest for networking

To share with other NCCs



[10] Icelandic HPC Community Web page

- Simulation & Data Lab Communities
 - Get in contact w.r.t. **domain-specific topics**
- Technology Topics
 - Interest to work together w.r.t. **Modular Supercomputing & Quantum Computing**



Simulation and Data Lab Computational Chemistry

General Information

Advancement of theory and methodology for atomic scale simulations, with broad ranging applications for chemistry and physical chemistry, reaction rate theory, adsorption spectroscopy, and magnetism, to name a few.

Prof. Hannes Jonsson

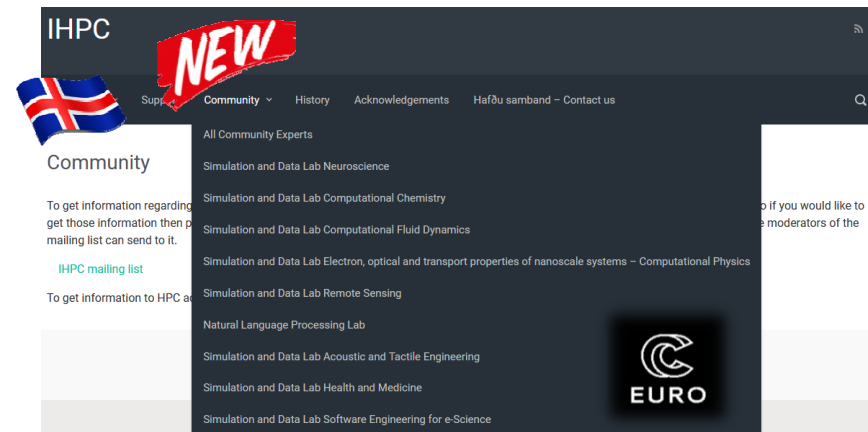
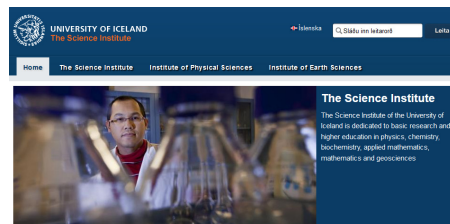
Dr. Elvar Örn Jónsson

Development of explicit polarizable classical solvent models and methodology for hybrid simulations coupling classical and quantum mechanics for the simulation of solvated molecules and the solid / liquid interface.

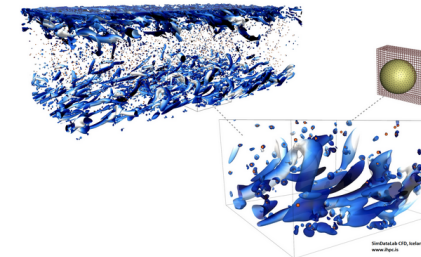
Dr. Pavel Bessarab

[27] IHPC SimDataLab Computational Chemistry Web Page

[28] Science Institute



Simulation and Data Lab Computational Fluid Dynamics



Dr. Pedro Costa



Dr. Ásdís Helgadóttir



Ph.D. Student S. Reza Hassanian, M



Prologue

[26] IHPC SimDataLab CFD Web Page

The Simulation and Data Lab computational fluid dynamics (SimDataLab CFD) is leading parallel computing in Computational fluid dynamics in Iceland at the University of Iceland. The SimDataLab is Iceland's representative in the international projects in CFD and parallel computing. SimDataLab CFD aims to develop parallel code applications in CFD and support users who have already developed parallel application codes. SimDataLab CFD participates in the European project network in parallel computing and has an infrastructure and access to powerful parallel systems in-memory optimization, processing system architecture, high scalability, and have performance optimization computer nodes.

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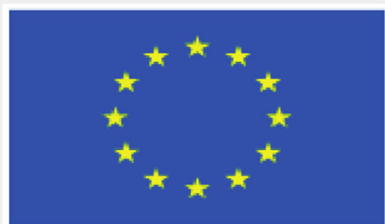
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Thanks!



Iceland, NCC 33
Prof. Dr. – Ing. Morris Riedel
University of Iceland
e-mail address: morris@hi.is



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