

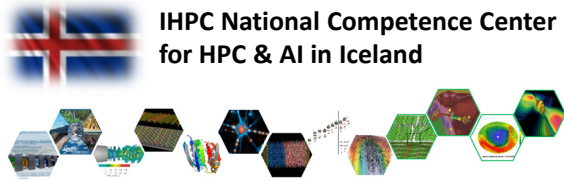


Overview IHPC National Competence Center for AI and HPC in Iceland @ EuroHPC Summit Week 2021

PROF. DR. – ING. MORRIS RIEDEL, UNIVERSITY OF ICELAND / JUELICH SUPERCOMPUTING CENTRE (JSC)

22TH MARCH, EUROHPC SUMMIT WEEK 2021 – ADDITIONAL INFORMATION, ONLINE

 @ProfDrMorrisRiedel
  @Morris Riedel
  @MorrisRiedel
  @MorrisRiedel
  <https://www.youtube.com/channel/UCWC4VKHmL4NZgFfKoHtANKg>



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



JÜLICH
 Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Prof. Dr. – Ing. Morris Riedel (from ~2004 in HPC) – Since 2013 @ UoIceland

- Holds **PhD in Computer Science** (from Karlsruhe Institute of Tech.)
 - MSc in data visualization and steering of data-intensive HPC & Grid applications
- Over the time many Positions at **Juelich Supercomputing Centre, Germany**
 - 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 Iceland Courses: HPC A / B, now High-Performance Computing**
 - **Statistical Data Mining, Cloud Computing & Big Data – Parallel & Scalable Machine & Deep Learning**



[15] Morris Riedel Web page

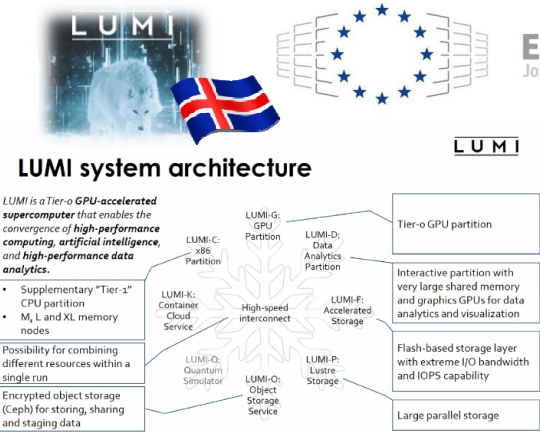
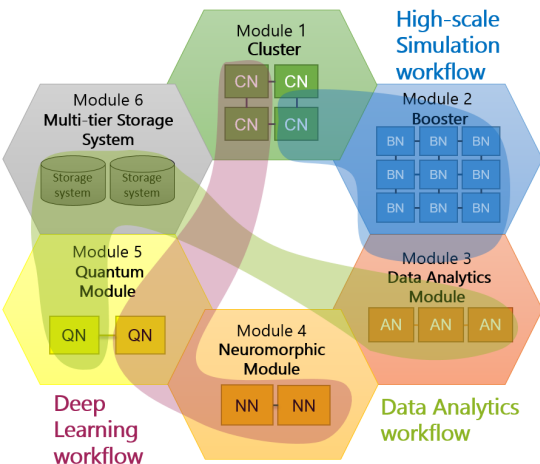
[5] EuroHPC Joint Undertaking



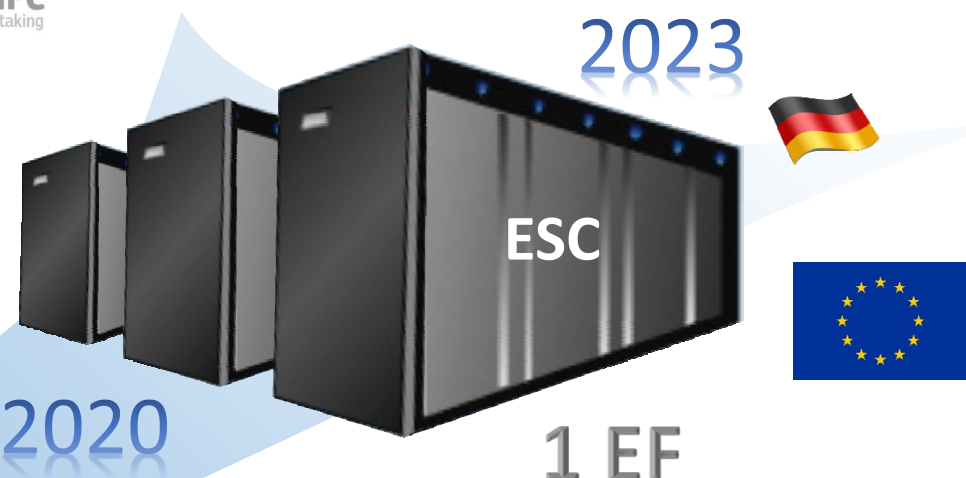
[16] High Performance Computing Course Fall 2019

[17] Cloud Computing & Big Data Course Fall 2020

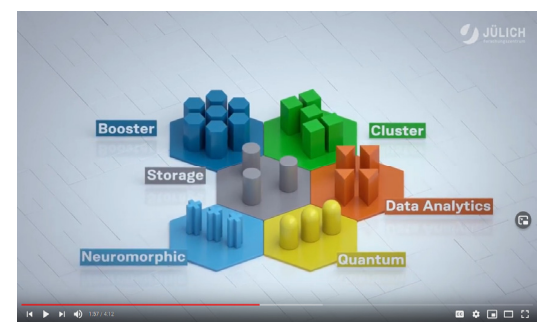
International Collaboration Partners: Juelich Supercomputing Centre & LUMI



[5] EuroHPC Joint Undertaking



[6] LUMI Supercomputer



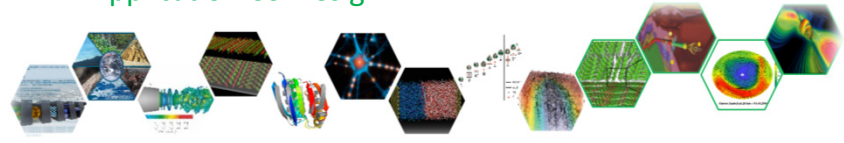
[2] YouTube, 'flexible and energy-efficient supercomputer: JUWELS is faster than 300 000 modern PCs'

[1] DEEP Series of Projects Web Page

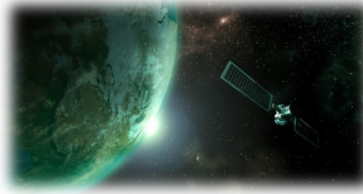
Despite the strong collaborations, it is important to have local HPC resources in Iceland for education & research (!)



Application Co-Design



DEEP Series of HPC Projects – Modular Supercomputing Architecture Research



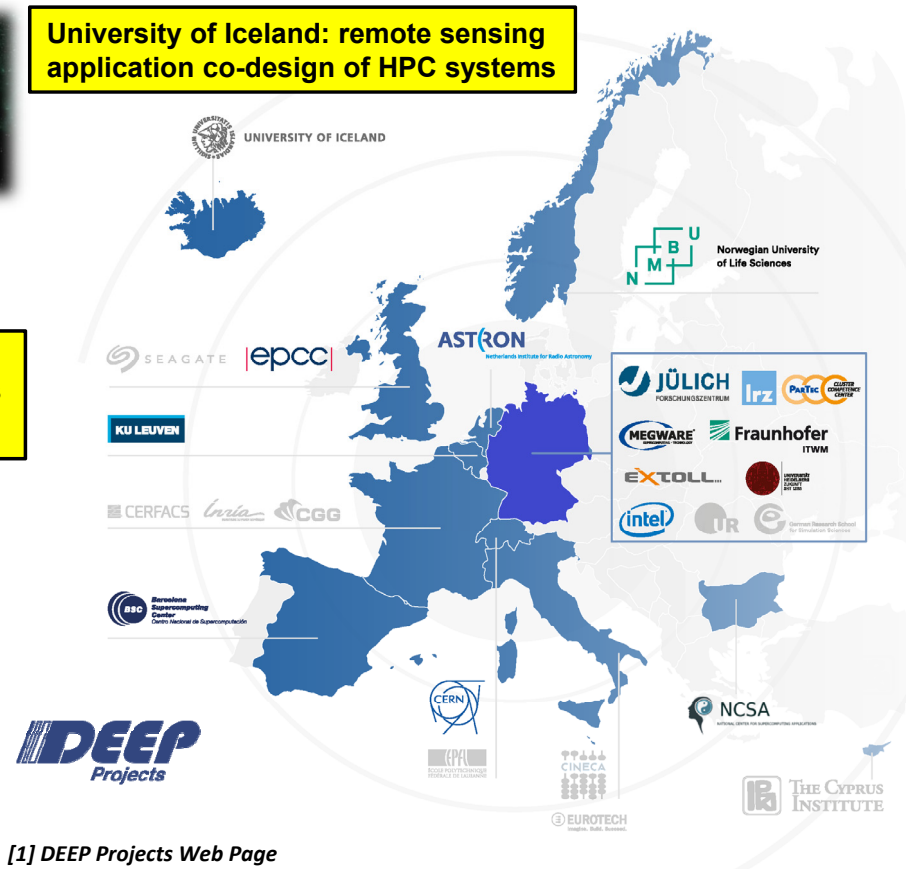
University of Iceland: remote sensing application co-design of HPC systems

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 – Mar 2021

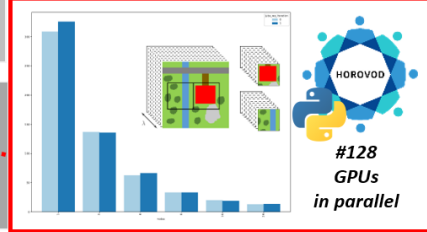
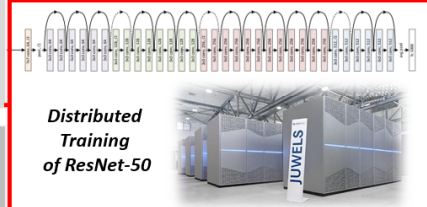
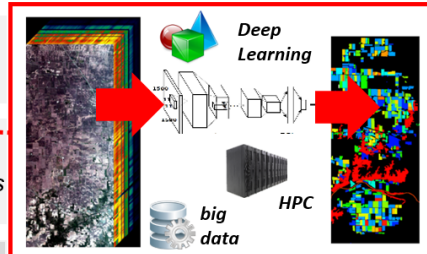
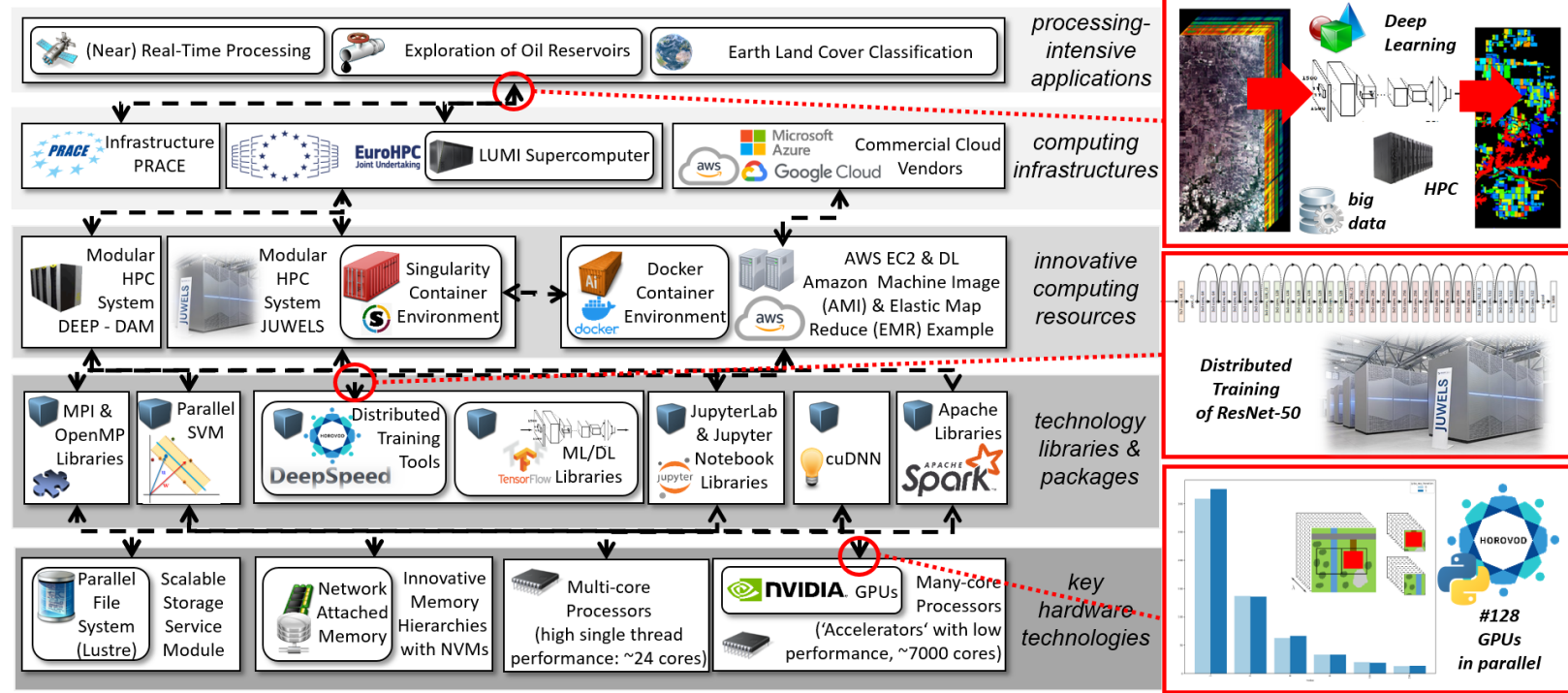
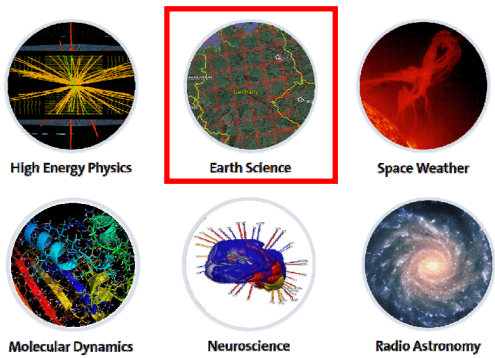
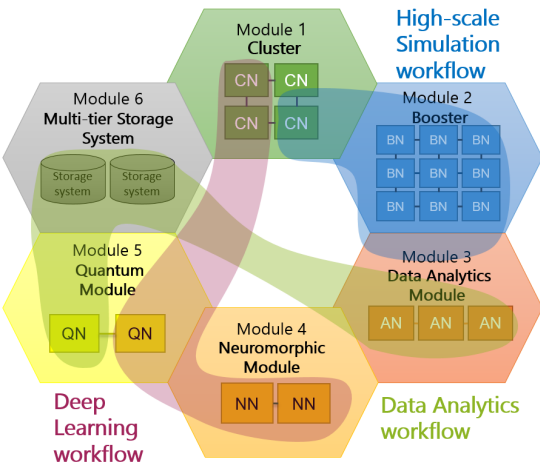
Strong collaboration with industry partners Intel, Extoll & Megware

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



[1] DEEP Projects Web Page

DEEP Series of Projects – Research Examples & Need for Academic HPC Centres

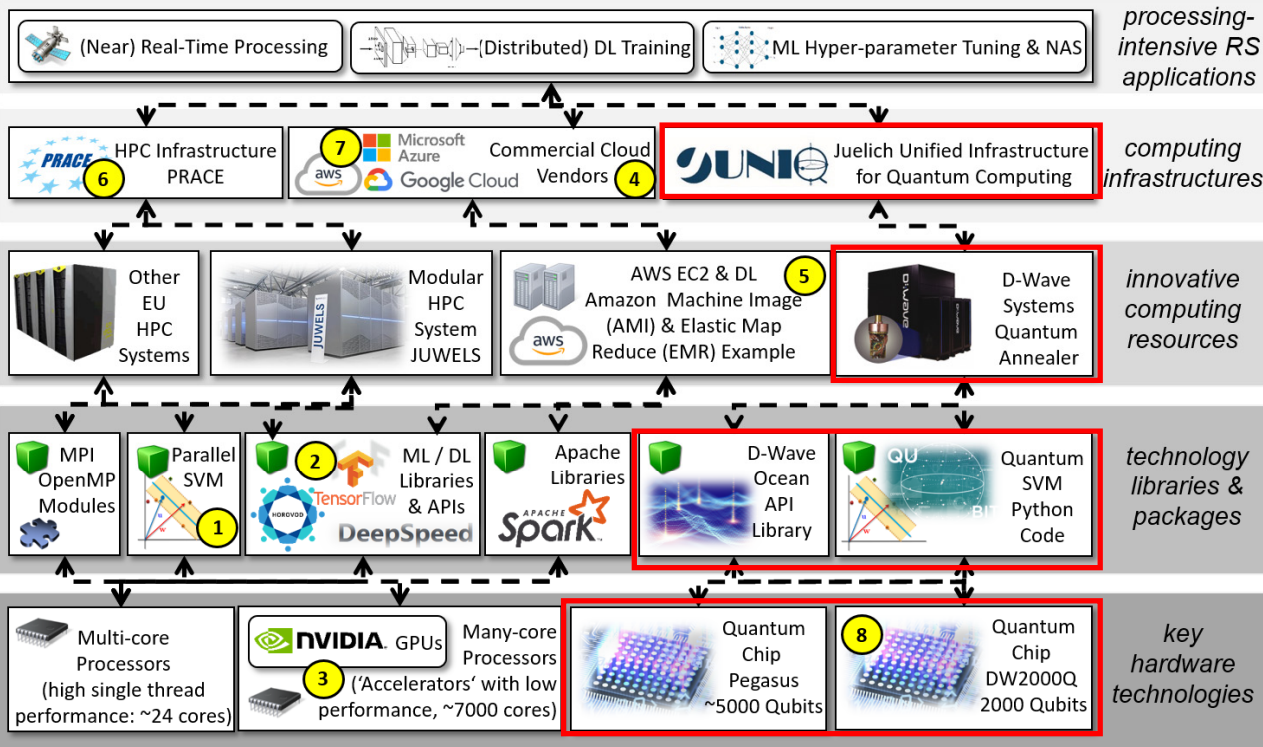


The modular supercomputing architecture (MSA) enables a flexible HPC system design co-designed by the need of diverse research application workloads

Commercial cloud computing is no option to be used here instead (e.g., Amazon Web Services charge 24\$/hour GPU)

[11] R. Sedona & M. Riedel et al., MDPI, Journal of Remote Sensing

Research Examples – Quantum Module with D-Wave Systems Quantum Annealer



- 1 Parallel ML implementations still rare (MPI/OpenMP)
- 2 Open source tools good, but all need to fit in versions
- 3 Using very many GPUs beyond NVlink could be tricky
- 4 Look & feel of CC vendor ML services differ significantly
- 5 Costs of GPUs of CC vendors (e.g., EC2) tough, 24\$/hour
- 6 GPU hours are free, but requires time grant proposal
- 7 Free GPUs in Google Colab vary in the available types
- 8 Works not yet with multi-class problems & large data

Legend:
N Highlighted Challenges & Experiences



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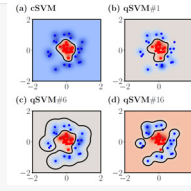
In [ ]: from quantum_svm import *
import numpy as np
from utils import *
from sklearn.model_selection import KFold
from sklearn import preprocessing

# Write the data
experiment=0
slices=0 # Number of samples to use for the training
fold=int(len(X_train)/40)

print(fold)

for i in range(0,experiment):
    cv = KFold(n_splits=fold, random_state=i, shuffle=True)
    count=0
    for test_index, train_index in cv.split(X_train):
        #print("Train Index: ", len(train_index), "\n")
        X_train_slice = X_train[train_index], Y_train[train_index]
        X_train_slice = preprocessing.scale(X_train_slice)

        X_test_slice = X_train[test_index], Y_train[test_index]
        X_test_slice = preprocessing.scale(X_test_slice)
    
```



(ensembles due to small datasets compared to full datasets on CPUs/GPUs)

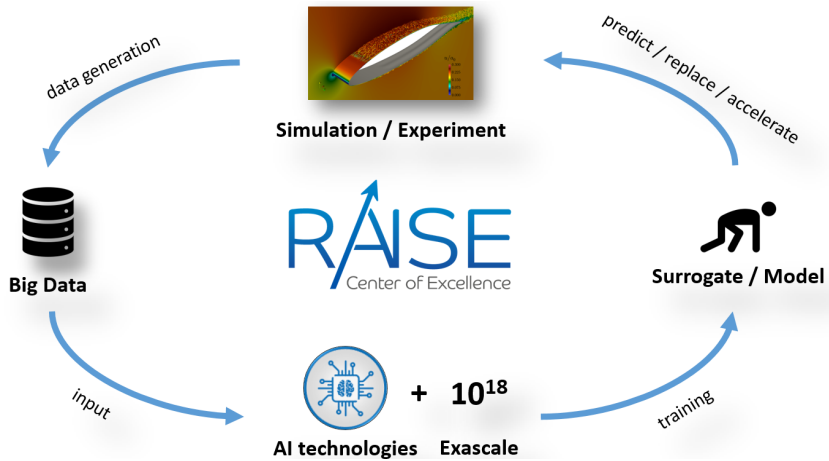
[9] Approaching Remote Sensing Image Classification with Ensembles of SVMs on the D-Wave Quantum Annealer, G. Cavallaro & M. Riedel et al.



[8] Quantum SVM, D. Willsch et al. [7] M. Riedel, UTMessan 2020 YouTube Video

NEW

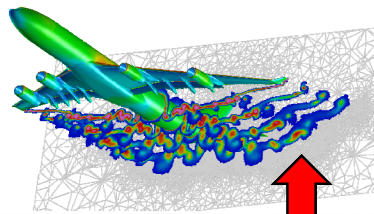
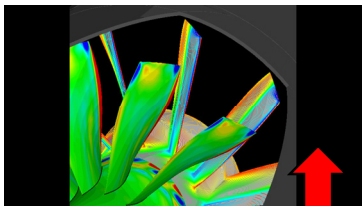
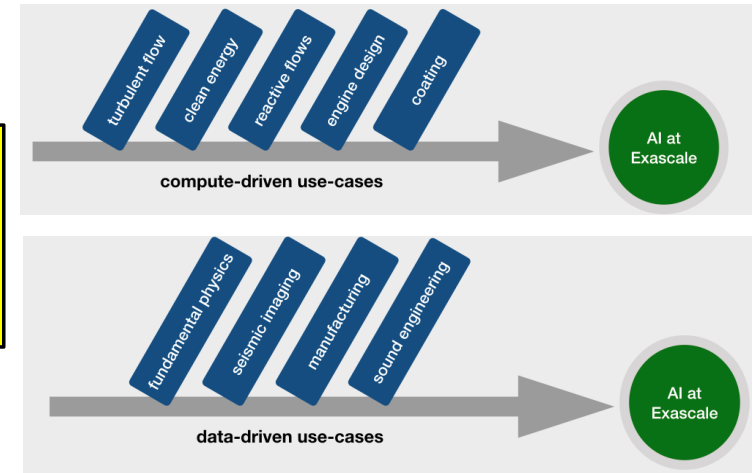
RAISE EU Project: Intertwined HPC Simulations & AI



[4] CoE RAISE Web Page

[3] Simulation Figure

RAISE funds three use cases for the University of Iceland in the area of AI-enabled remote sensing, sound engineering, and links with our computational fluid dynamics activities

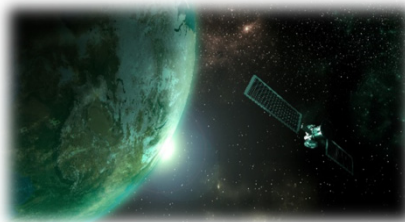


[8] Neural Network 3D Simulation

IHPC Icelandic National Competence Center for High Performance Computing and Artificial Intelligence



Open PhD Position Available in EU Project RAISE @ Iceland



Information

The PhD position is funded by the EU project Center of Excellence "Research on AI- and Simulation-Based Engineering at Exascale" (CoE RAISE). This project will be the excellent enabler for the advancement of European multi-physics and/or multi-scale applications on industrial and academic level and a driver for novel intertwined AI and HPC technologies.

👤 **Supervisor:** Prof. Morris Riedel (University of Iceland)

👥 **Co-Supervisors:** Dr. Gabriele Cavallaro (Jülich Supercomputing Centre) and Prof. Magnús Örn Úlfarsson (University of Iceland)

📅 **Starting date:** January 2021

⚠️ (Due to the current corona pandemic, the first work period can be conducted remotely)

📍 **Location:** Reykjavík (Iceland). You will be employed at the University of Iceland. A research stay at the Jülich Supercomputing Centre (Forschungszentrum Jülich, Germany) is envisaged for a minimum period of time of 6 months. To obtain your PhD degree at the University of Iceland you will have to acquire 30 ECTS from courses and seminars. Your working hours will be not monitored and working from home will be largely permitted.

🎯 **Goal:** pioneer the research of advanced deep transfer learning methods in the context of complex learning scenarios in applications from remote sensing. The priority will be put on the investigation of the transferability capacity of Deep Learning (DL) models with meta-learning and Neural Architecture Search methods.

👥 **Research Group:** be part of our joint research group "High Productivity Data Processing" at University of Iceland and Jülich Supercomputing Centre. The group is highly active in developing parallel and scalable machine (deep) learning algorithms for remote sensing data processing and many other types of applications (i.e., medical research and retail sectors).

⚙️ **Working Environment:** Direct access to high performance multi-GPU systems equipped with the state-of-the-art of DL frameworks (TensorFlow, pyTorch, Chainer, Horovod, DeepSpeed). There is also the possibility to access innovative quantum computing systems.

📖 **Other information:** You will have the possibility to participate in international top conferences in the field of machine learning, HPC and remote sensing. You will be put in contact with several international partners for initiating research collaborations that match the topic of the PhD.

🎓 **Background education:** MSc degree in computer science or computer engineering. Level of English >= B2.

🧠 **Required knowledge and experience:** deep learning (Convolutional Neural Networks and/or Transformers) and Python programming (TensorFlow and/or pyTorch). Experience with parallel programming (OpenMP and MPI), High Performance Computing (HPC) and remote sensing data processing are a substantial plus.

✉️ **Apply:** Send your CV, a cover letter and the transcripts of records of your bachelor and master to Gabriele Cavallaro: g.cavallaro@fz-juelich.de.

Apply now

A screenshot of a Facebook post. At the top, it shows the profile of Morris Riedel, Professor & Head of Research Group High Productivity Data Processing Juelich. Below that, it shows a post by Dr. Ing. Gabriele Cavallaro, 1st Deputy Head of a research group at Jülich. The main text of the post reads: "Fully-funded PhD position in our 'High Productivity Data Processing' research group at the University of Iceland - Háskóli Íslands". Below the text is a large, scenic photograph of a mountain peak with a waterfall in the foreground. At the bottom of the image, the text "PHD POSITION IN ICELAND" is overlaid in large, bold, white letters.

[10] Open PhD Position, RAISE EC Project @ Iceland

NEW EuroCC EU Project: Building National Competence Centers for HPC & AI



- EuroHPC Joint Undertaking Project
- 33 Countries as Partners
- 50% funding only for University of Iceland (in-kind funding by person Prof. Dr. – Ing. Morris Riedel & Prof. Dr. Ebba Hvanberg)
- Goal: Establish National Competence Centers (NCCs) in the area of HPC & AI to bring national activities together



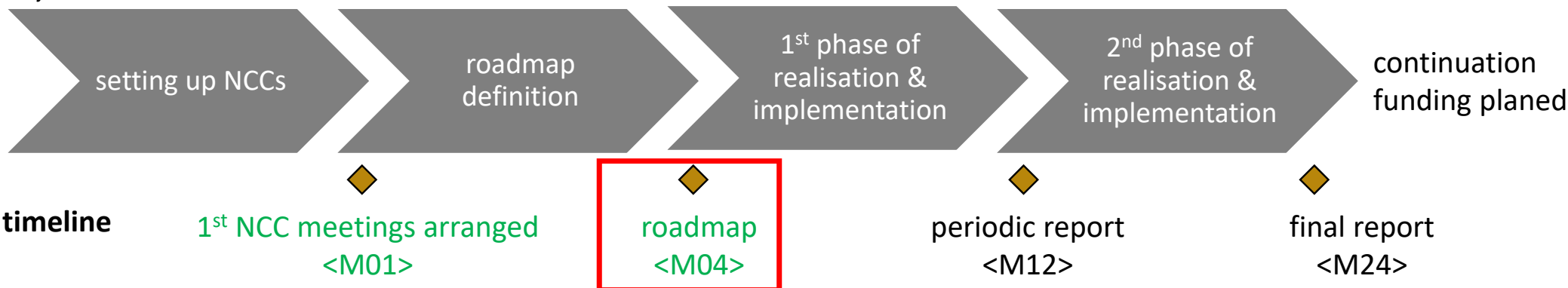
EuroCC funds two research activities for the University of Iceland in the area of neuroscience & computational fluid dynamics

The National Competence Center (NCC) for Iceland of the EuroCC project represents our already established IHPC & IRHPC activities is fully complementary to those activities

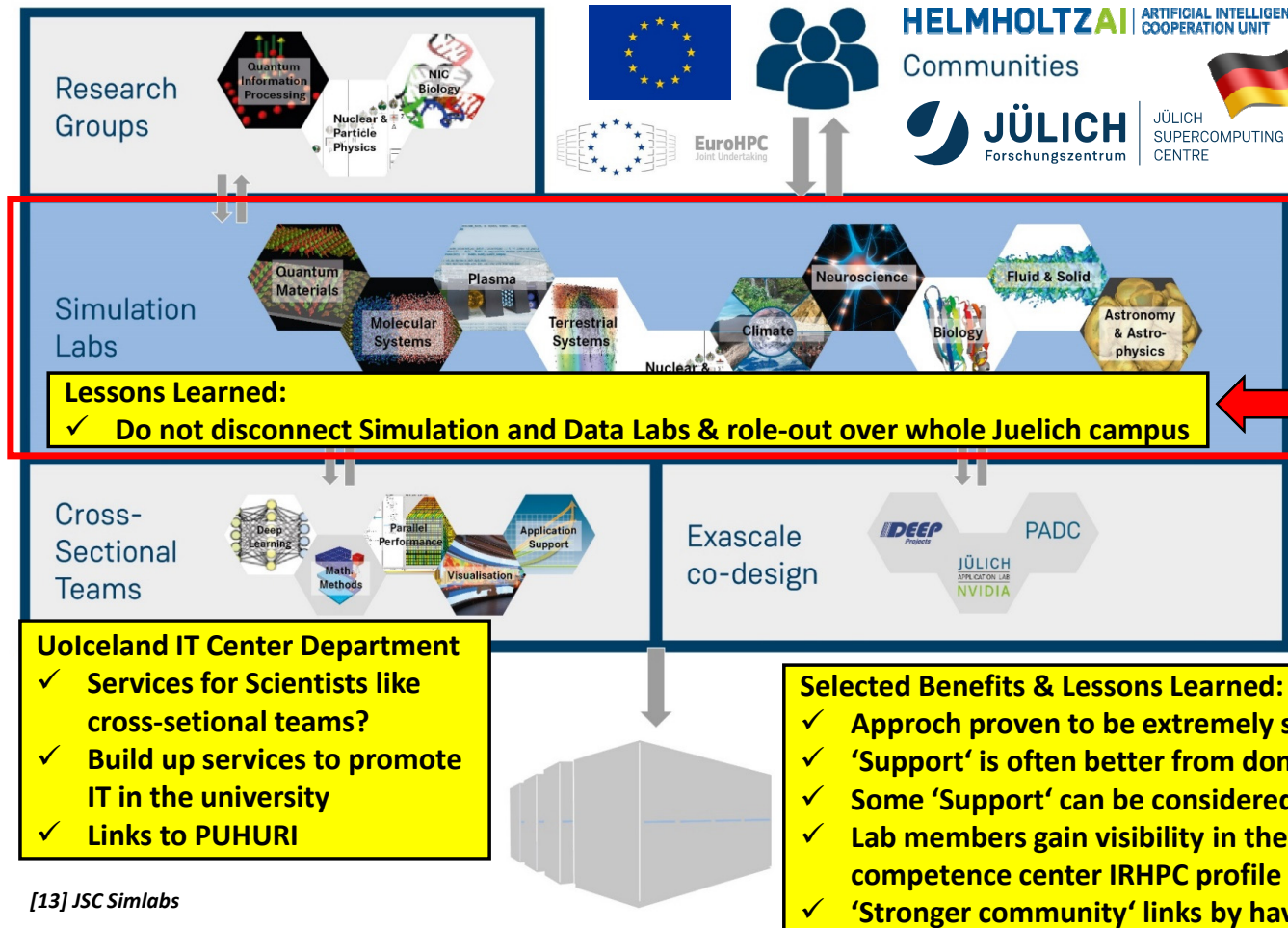


- Major activities: Community building (including industry)

[12] EuroCC Project



Community-building with Simulation & Data Labs – Lessons Learned



'For some years now there has been a growing realisation that application software is lagging behind HPC hardware developments. While several Petaflop-scale supercomputers are now available worldwide, it is becoming increasingly difficult to exploit these machines with single applications. Substantial efforts are needed in order to enable computational science communities to solve problems with high scientific impact through efficient use of high-end supercomputing resources. To help meet this challenge the Juelich Supercomputing Centre (JSC) has proposed a new type of domain-specific research and support structure: the Simulation Laboratory.'

Lessons Learned:

- ✓ The heart of an academic HPC Centre are the people doing the research that is a key differentiator to cloud computing companies (e.g., Amazon Web Services, MS Azure, or Google Platform/Colab) & ensure funding

Uolceland IT Center Department

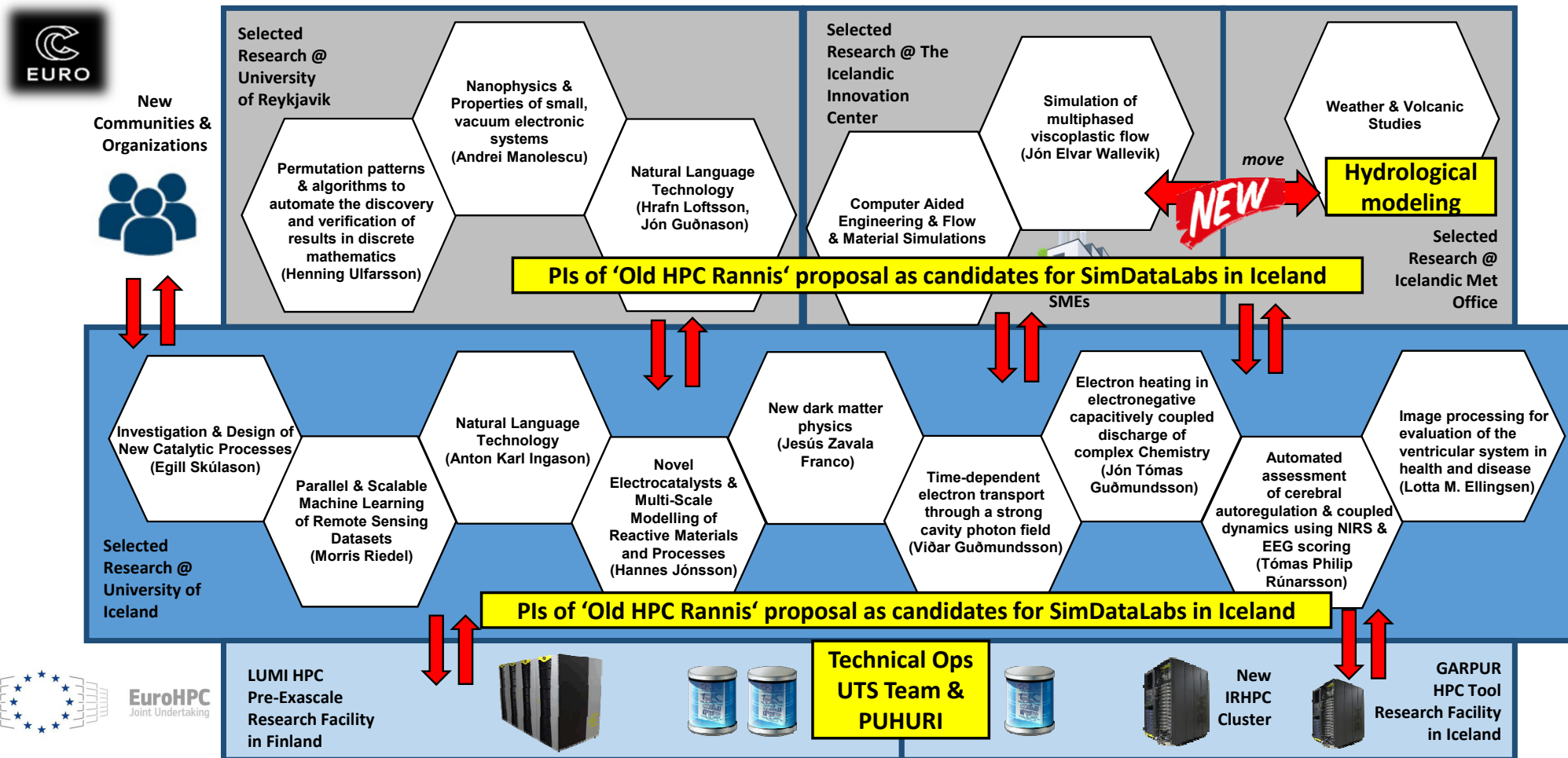
- ✓ Services for Scientists like cross-sectional teams?
- ✓ Build up services to promote IT in the university
- ✓ Links to PUHURI

Selected Benefits & Lessons Learned:

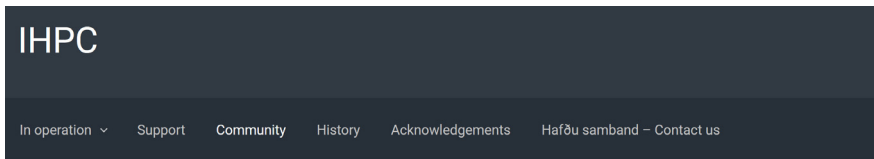
- ✓ Approach proven to be extremely successful in HPC for over 15 years now (e.g., JSC)
- ✓ 'Support' is often better from domain-scientists that knows domain substance
- ✓ Some 'Support' can be considered domain-specific research as part of codes/scaling
- ✓ Lab members gain visibility in their community & strengthening over time the competence center IRHPC profile having a clear long-term identity for each member
- ✓ 'Stronger community' links by having domain-specific researchers in the labs

[13] JSC Simlabs

EuroCC Proposal – First Steps towards Potential SimDataLabs in Iceland



SimDataLabs in Iceland – Confirmed Participation (Work-in-Progress)

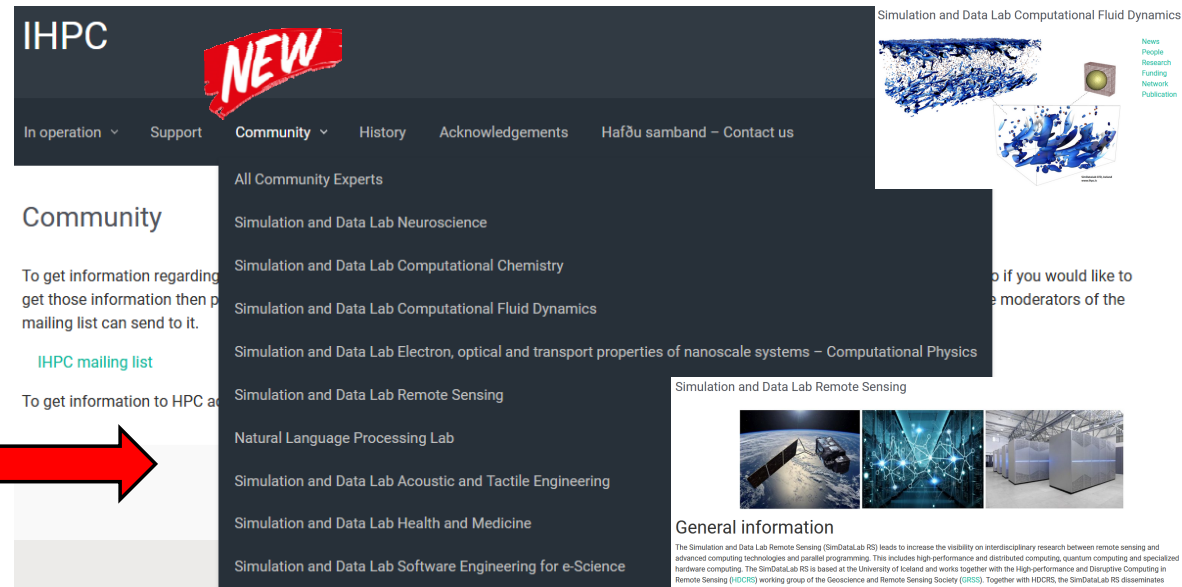


Community

To get information regarding upgrades, downtime or some other important issues then we will send those information to users with email. If you get those information then please sign up. This is not used very regularly so don't worry about getting spammed through this list and our mailing list can send to it.

[IHPC mailing list](#)

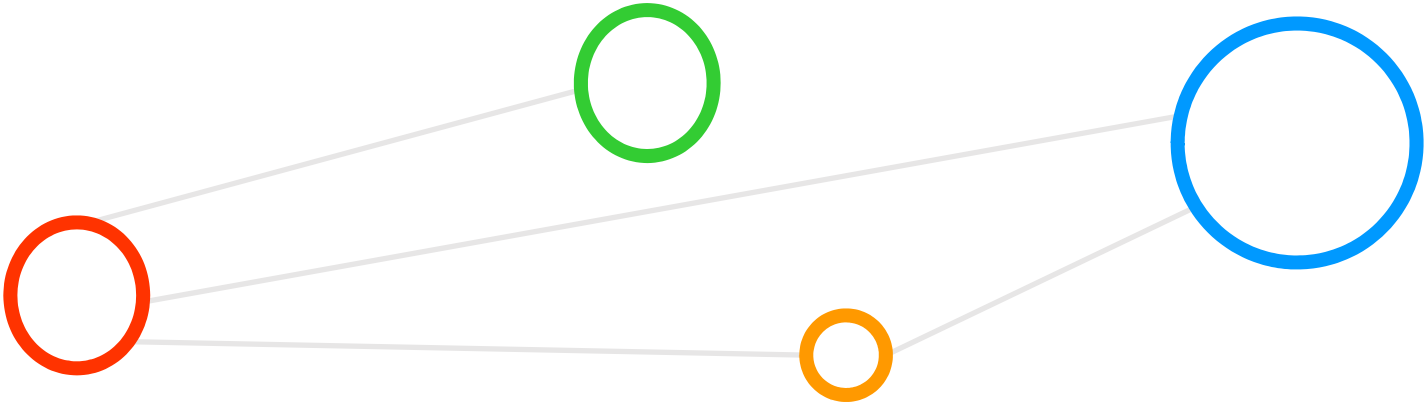
To get information to HPC admins, then please send an email to help@hi.is and include HPC in the subject.



Jointly engage in future funding together, e.g. EuroHPC Master of Science in HPC program and many other activities planned in Horizon Europe

- Selected Discussion Topics:**
- ✓ **Governance of Labs: Bottom-Up by PI, but optional Executive Advisory Board (EAB) members could be used to guide & 'review' labs on a yearly basis (could be useful): labs of Juelich are 'friendly' reviewed on a 1-2 years basis as part of funding program**
 - ✓ **Engagement with Industry: ISOR, MATIS, MAREL, DECODE (work-in-progress), etc.**
 - ✓ **Including Start-Ups: Nordverse (medical NLP, done), Treble (Acoustic, done), others?**
 - ✓ **Relationship to our new IRHPC & steering board activities → Logo for IRHPC/NCC?!**
 - ✓ **Teaching better topics of relevance in HPC Course for Iceland, other activities?**

Lecture Bibliography



Lecture Bibliography (1)

- [1] DEEP Series of Projects Web page, Online:
<http://www.deep-projects.eu/>
- [2] YouTube Video, 'flexible and energy-efficient supercomputer: JUWELS is faster than 300 000 modern PCs' Online:
<https://www.youtube.com/watch?v=t5kNxPT5rSY&list=PLCer2BlxxQ2zToC6SRVlfwj0MO1-xli6I>
- [3] Copyright Institute of Aerodynamics and Chair of Fluid Mechanics, RWTH Aachen University, Online:
<https://www.aia.rwth-aachen.de>
- [4] CoE RAISE Web page, Online:
<http://www.coe-raise.eu>
- [5] EuroHPC Joint Undertaking Web page, Online:
<https://eurohpc-ju.europa.eu/>
- [6] LUMI EuroHPC Supercomputer hosted at CSC Finland, Online:
<https://www.lumi-supercomputer.eu/>
- [7] YouTube, Morris Riedel, UTMessan 2020 - Demystifying Quantum Computing, Online:
<https://www.youtube.com/watch?v=EQGshhspn9A>
- [8] D. Willsch, M. Willsch, H. De Raedt, K. Michielsen, 'Support Vector Machines on the D-Wave Quantum Annealer', Online:
<https://www.sciencedirect.com/science/article/pii/S001046551930342X951733>
- [9] Cavallaro, G., Willsch, D., Willsch, M., Michielsen, K., Riedel, M.: APPROACHING REMOTE SENSING IMAGE CLASSIFICATION WITH ENSEMBLES OF SUPPORT VECTOR MACHINES ON THE D-WAVE QUANTUM ANNEALER, in conference proceedings of the IEEE International Geoscience and Remote Sensing Symposium (IGARSS 2020), September 26 – October 2nd, 2020, Virtual Conference, Hawaii, USA, to appear, Online:
<https://igarss2020.org/Papers/ViewPapers.asp?PaperNum=1416>
- [10] Open PhD Position for the RAISE EU project @ Iceland, Online:
<https://www.gabriele-cavallaro.com/news/fully-funded-phd-position>

Lecture Bibliography (2)

- [11] R. Sedona, G. Cavallaro, J. Jitsev, A. Strube, M. Riedel, J.A. Benediktsson, 'Remote Sensing Big Data Classification with High Performance Distributed Deep Learning', MDPI Journal of Remote Sensing, Online:
https://www.researchgate.net/publication/338077024_Remote_Sensing_Big_Data_Classification_with_High_Performance_Distributed_Deep_Learning
- [12] EuroCC Project, Online:
<http://www.eurocc-project.eu>
- [13] Juelich Supercomputing Centre – SimLabs Blueprint, Online:
https://www.fz-juelich.de/ias/jsc/EN/Expertise/SimLab/simlab_node.html
- [14] Icelandic HPC Community Page, Online:
<https://ihpc.is/>
- [15] Morris Riedel Web page, Online:
<http://www.morrisriedel.de/>
- [16] High Performance Computing Course Fall 2019, Online:
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- [17] Cloud Computing and Big Data – Parallel and Scalable Machine & Deep Learning Course Fall 2020, Online:
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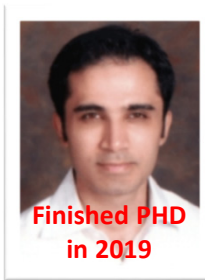
Acknowledgements – High Productivity Data Processing Research Group



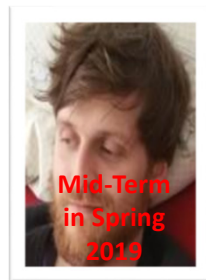
PD Dr.
G. Cavallaro



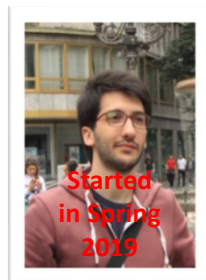
Senior PhD Student
A.S. Memon



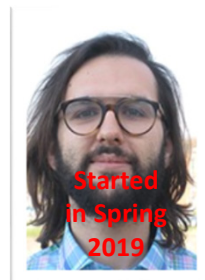
PD Dr.
M.S. Memon



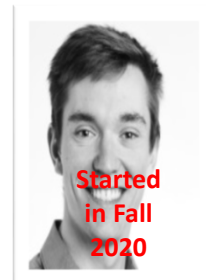
PhD Student
E. Erlingsson



PhD Student
S. Bakarar



PhD Student
R. Sedona



PhD Student
P. H. Einarsson



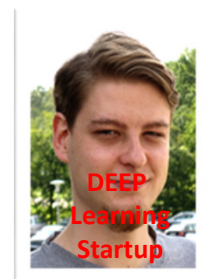
Dr. M. Goetz
(now KIT)



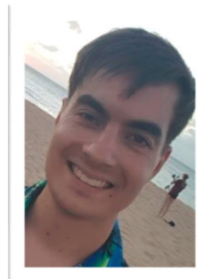
MSc M.
Richerzhagen
(now other division)



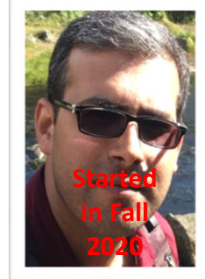
MSc
P. Glock
(now INM-1)



MSc
C. Bodenstein
(now Soccerwatch.tv)



MSc G.S.
Guðmundsson
(Landsverkjun)

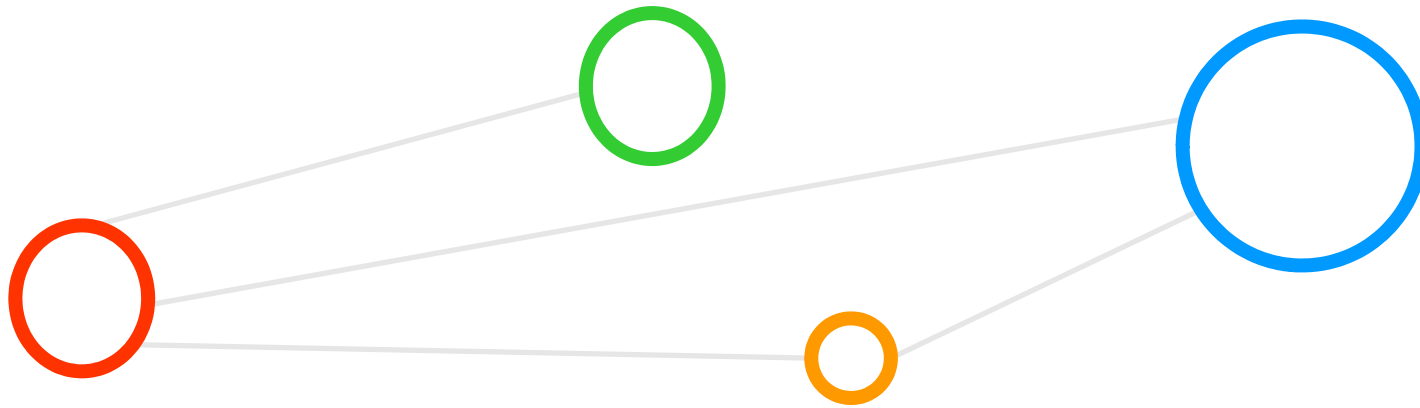


PhD Student
Reza

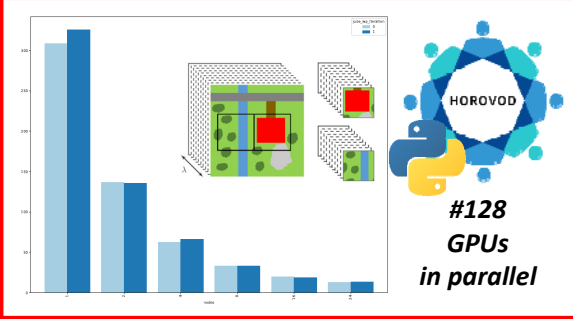
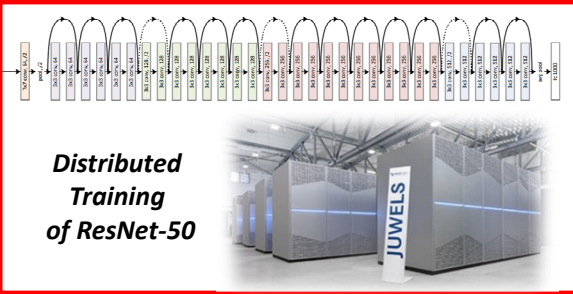
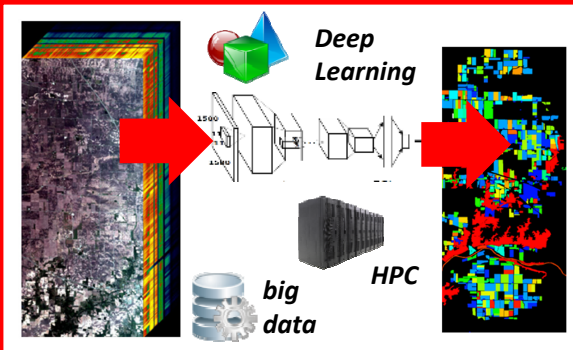
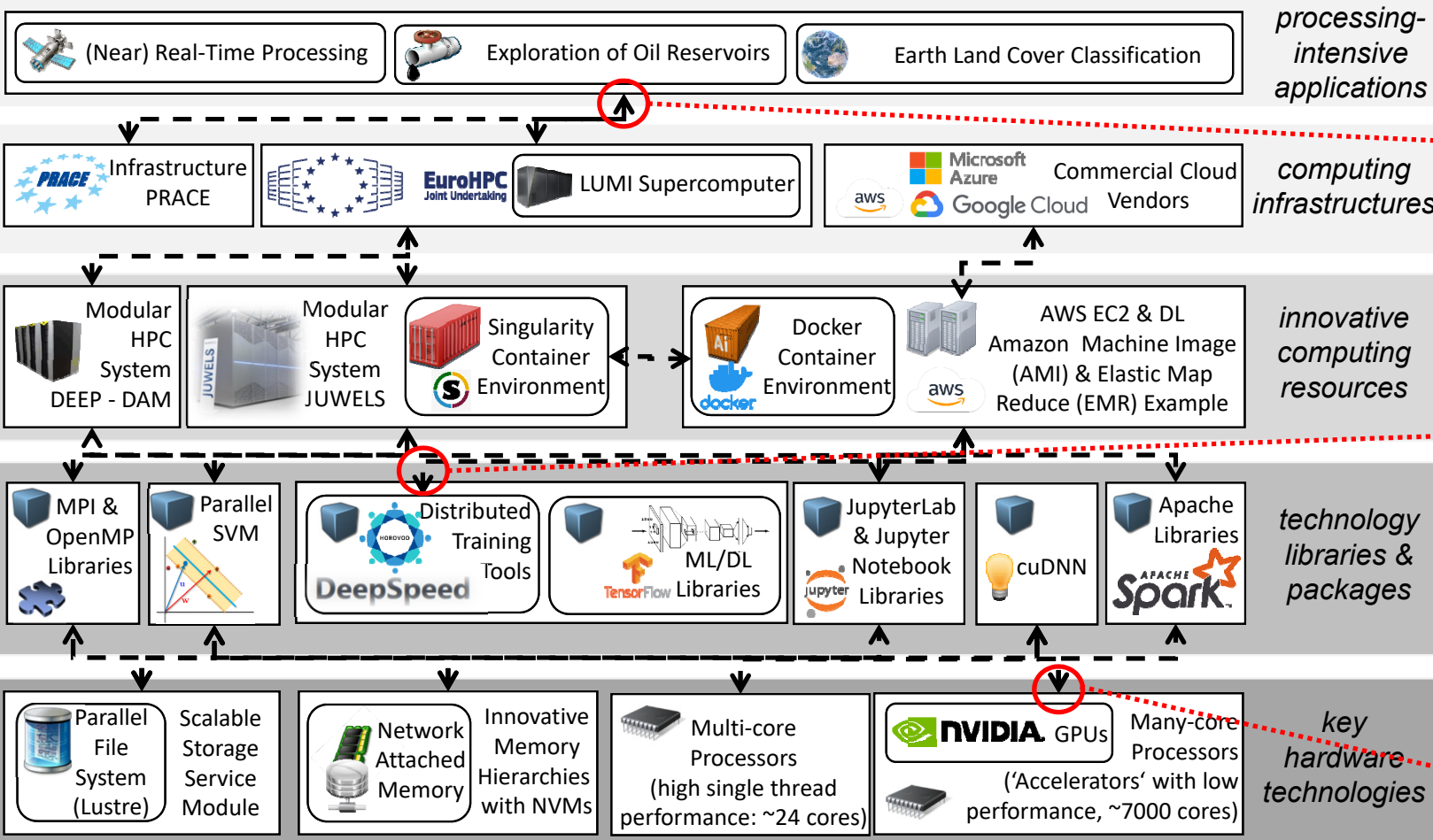


This research group has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 763558 (DEEP-EST EU Project) and grant agreement No 951740 (EuroCC EU Project) & 951733 (RAISE EU Project)

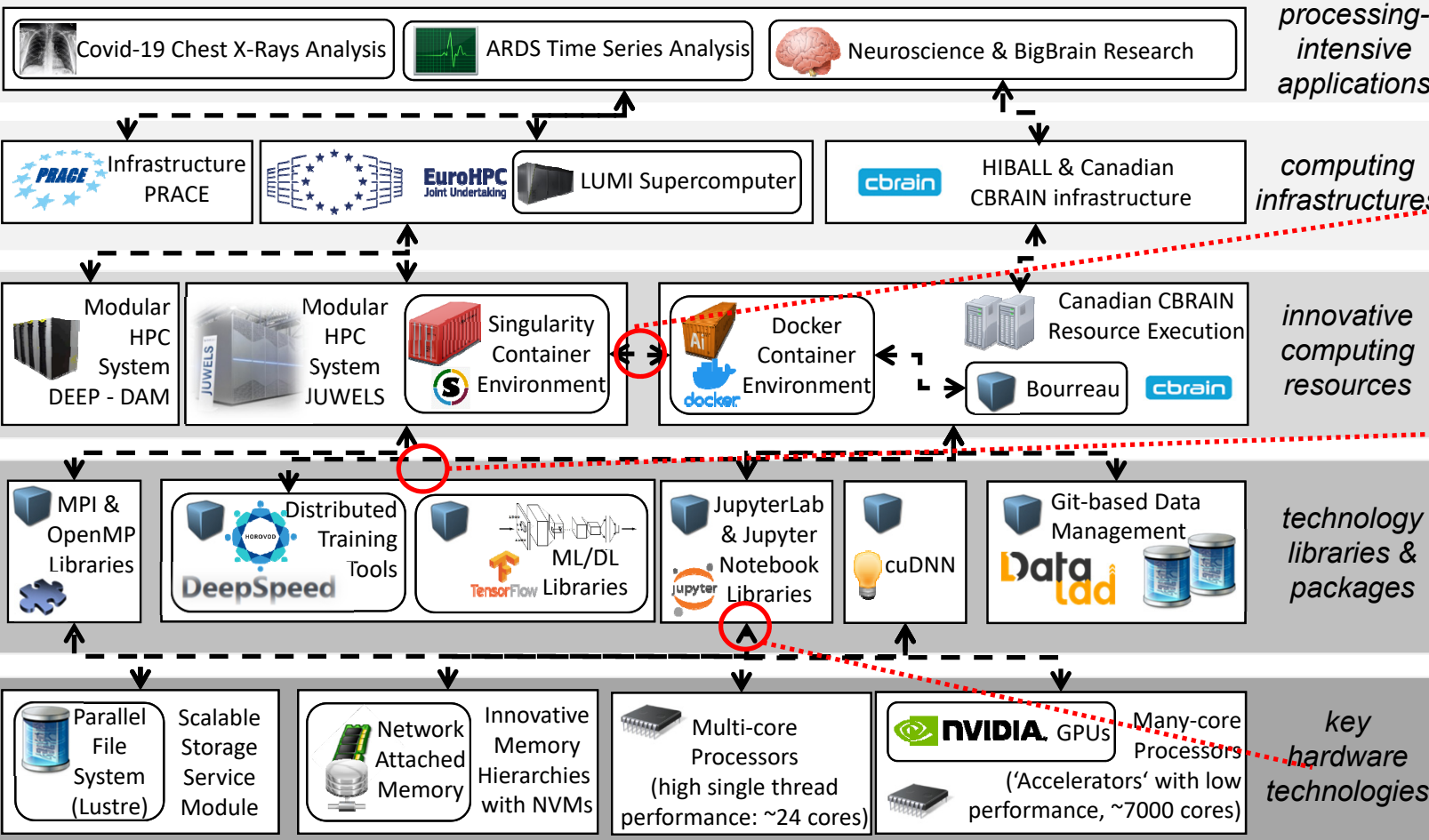
Appendix



Research Examples – Remote Sensing AI & HPC Applications



Research Examples – Health & Medical AI & HPC Applications



```

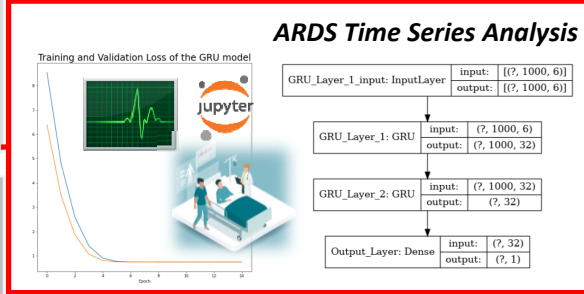
Some preparation
$ mkdir winterschool winterschool_cache winterschool_tmp
$ chmod +w winterschool_cache
$ export SINGULARITY_CACHEDIR=$(mktemp -d -p "$(pwd)/winterschool_cache")
$ export SINGULARITY_TMPDIR=$(mktemp -d -p "$(pwd)/winterschool_tmp")

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/CONP-PCNO/conp-dataset.git
    
```



Covid-19 Chest X-Ray Analysis

```

#!/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 $@
    
```