Practice & Experience in using Parallel & Scalable Machine Learning in Remote Sensing from High Performance Computing over Cloud to Quantum Computing

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

15TH JULY, IEEE IGARSS 2021 CONFERENCE, DATA-INTENSIVE COMPUTING FOR REMOTE SENSING SESSION, ONLINE

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

IHPC National Competence Center for HPC & AI in Iceland

EuroHPC Joint Undertaking

EOSC NORDIC

RAISE Center of Excellence

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

EURO

HELMHOLTZAI | ARTIFICIAL INTELLIGENCE COOPERATION UNIT

DEEP Projects

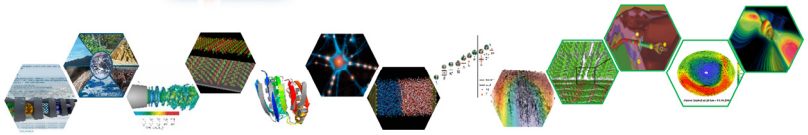
JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Outline

- Understanding Computing Technologies
  - High Performance Computing & Supercomputing
  - Critical Societal & Economic Application Examples
  - AI through Parallel & Scalable Machine & Deep Learning
- Practice & Experience in Remote Sensing
  - Co-Design and Use of High-Performance Computing Systems
  - Leverage Clouds & Apache Spark for Image Compression Tasks
  - Challenges & First steps in Quantum Annealing
- Summary & Future Work
- Selected References
- Acknowledgements

[1] PRACE – What is HPC, YouTube Video

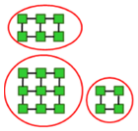
IHPC National Competence Center for HPC & AI in Iceland

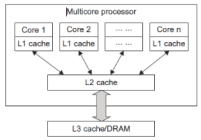


[10] Icelandic HPC Community Web page


Understanding Computing Technologies

High Performance Computing (HPC) & Supercomputing



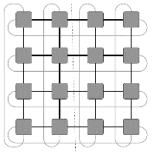


Multi-Core CPUs as Cluster

Large number of processors with high single thread performance and cache hierarchies

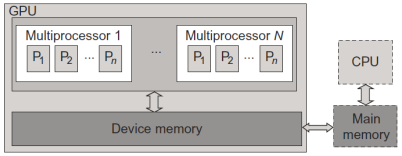
Fast Interconnects

Cluster nodes interconnected with a low-latency high-bandwidth network (e.g. Infiniband)



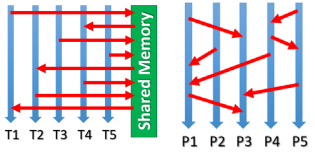
Additional Many-Core GPUs

Accelerators attached to host CPUs with moderate speed, but 100 – 1000 processors



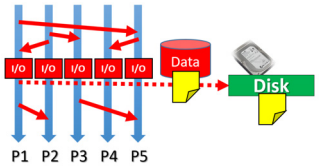
Parallel Programming Environment

Schedulers, monitoring systems, parallel libraries



Parallel File Systems & Storage

Using binary parallel file formats & large storage capacities on different levels (NVRAM, Disk, Tapes)

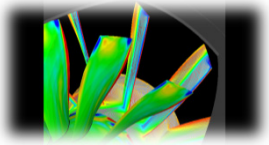


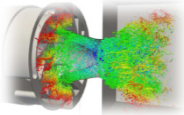
Building Infrastructure

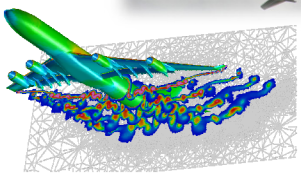
Cooling, cables, fire safety, etc.

[2] JUWELS – Zeitraffer, YouTube Video

Critical Societal & Economic Applications that require HPC Resources





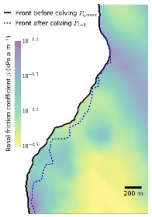


Aerospace Engineering

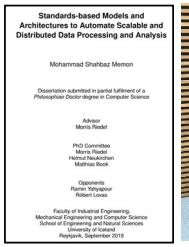
e.g. computational fluid dynamics

Ice Modeling

e.g. glacier calving



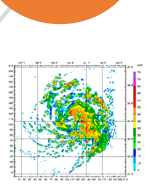
[29] Memon, M.S. & Riedel, M. et al.: Scientific workflows applied to the coupling of a continuum (Elmer v8.3) & a discrete element (HiDEM v1.0) ice dynamic model, GMD Vol 12 (7), 2019

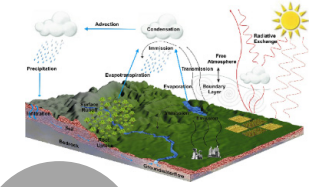


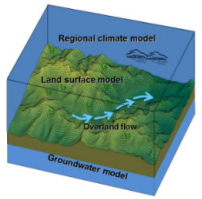
Dr. Shahbaz Memon (2019)
PhD Student Graduate, University of Iceland

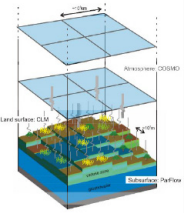
Terrestrial Systems & Climate

e.g. groundwater modeling





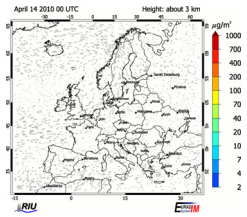




[5] SimLab Terrestrial Systems

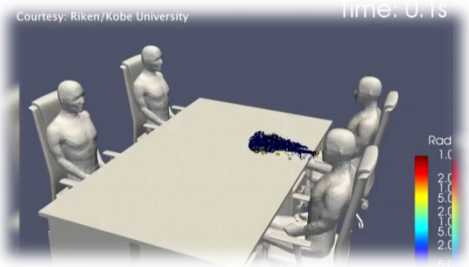
Volcanic Eruptions Modeling

e.g. spreading of ash clouds



COVID-19 Models

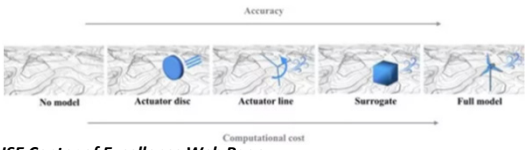
e.g. understanding spread of virus in detail



[3] Humidity in Covid-19, YouTube Video

Green Energy Research

e.g. understanding turbulence in windfarms



NEW

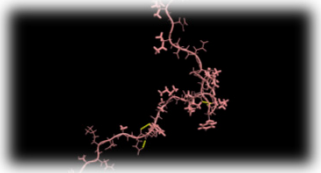
RAISE Center of Excellence

[4] RAISE Center of Excellence Web Page

Systems Biology & Medicine

e.g. protein folding

[6] SimLab Biology



NEW

Seyedreza Hassanianmoaref
Callsign "Reza"
PhD Student, University of Iceland
IHPC Simulation and Data Lab
Computational Fluid Dynamics (CFD)

[8] IHPC SimDataLab CFD Web Page

Focus Talk: Artificial Intelligence through Machine & Deep Learning

Artificial Intelligence (AI)

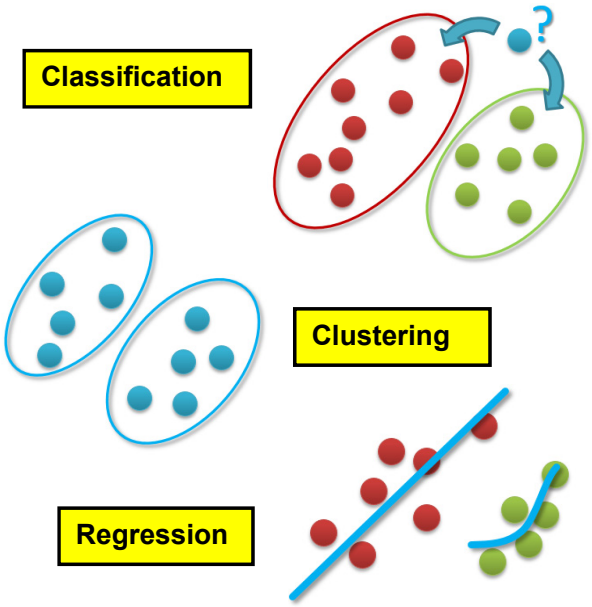
A wide area of techniques and tools that enable computers to mimic human behaviour (+ robotics)

Machine Learning (ML)

Learning from data without explicitly being programmed with common programming languages

Deep Learning (DL)

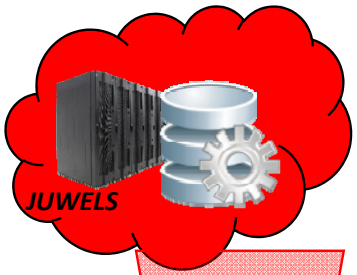
Systems with the ability to learn underlying features in data using large neural networks



[9] Neural Network 3D Simulation

Parallel & Scalable Machine & Deep Learning – AI & Big Data needs HPC/Clouds

@MorrisRiedel



High Performance Computing & Cloud Computing

Large Deep Learning Networks

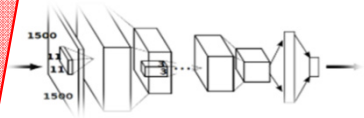
Training Time

Model Performance / Accuracy

'small datasets'

manual feature engineering' changes the ordering

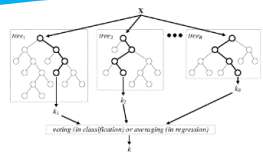
Medium Deep Learning Networks



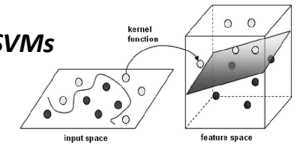
Small Neural Networks

Traditional Learning Models

Random Forests



SVMs



Statistical Computing with R

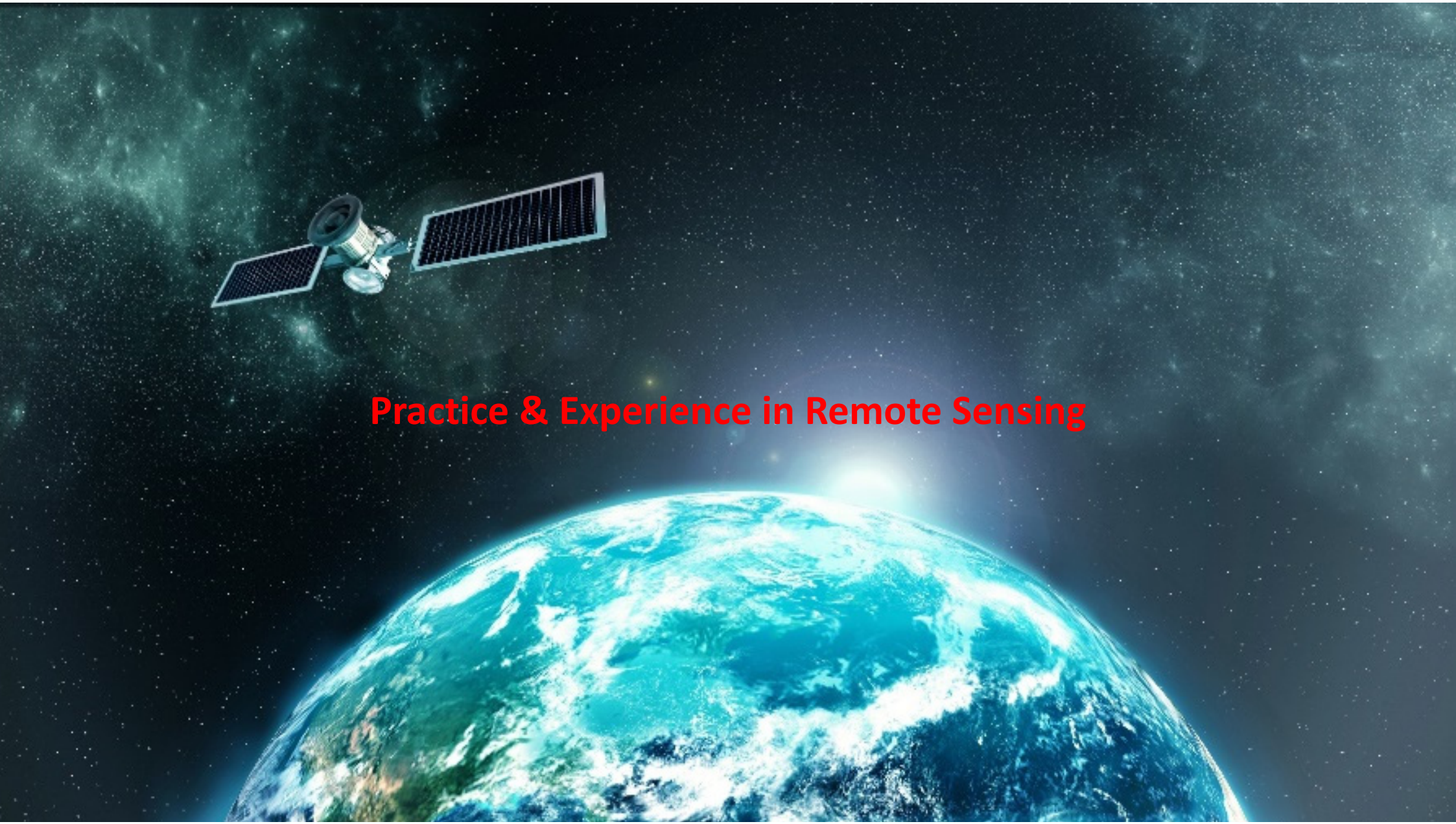
MatLab

scikit-learn *Weka* *Octave*

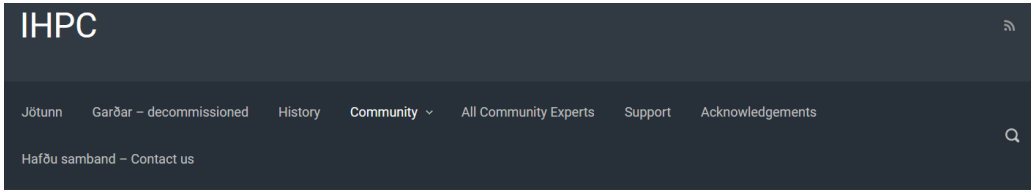
→ 'Big Data'

[7] www.big-data.tips

Dataset Volume


Practice & Experience in Remote Sensing

Icelandic HPC Community – Simulation & Data Lab Remote Sensing



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

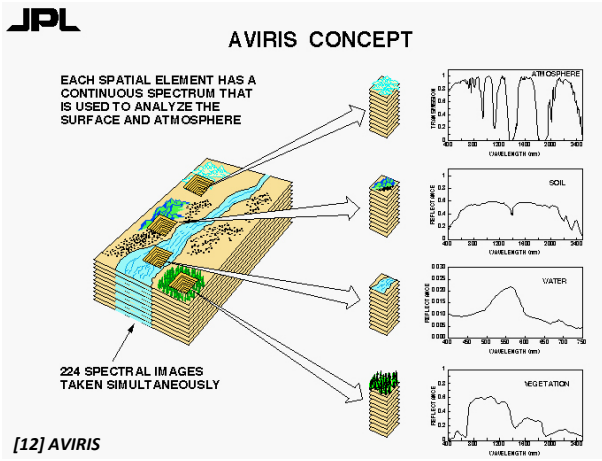
Dr. -Ing. Gabriele Cavallaro

Ing. Rocco Sedona

Surbhi Sharma

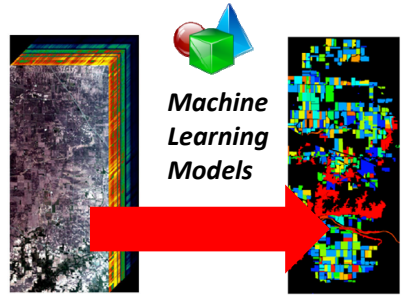
Ernir Erlingsson

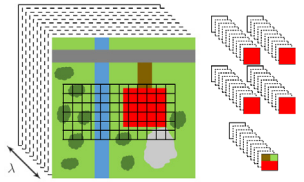
[11] IHPC SimDataLab Remote Sensing Web Page



[12] AVIRIS

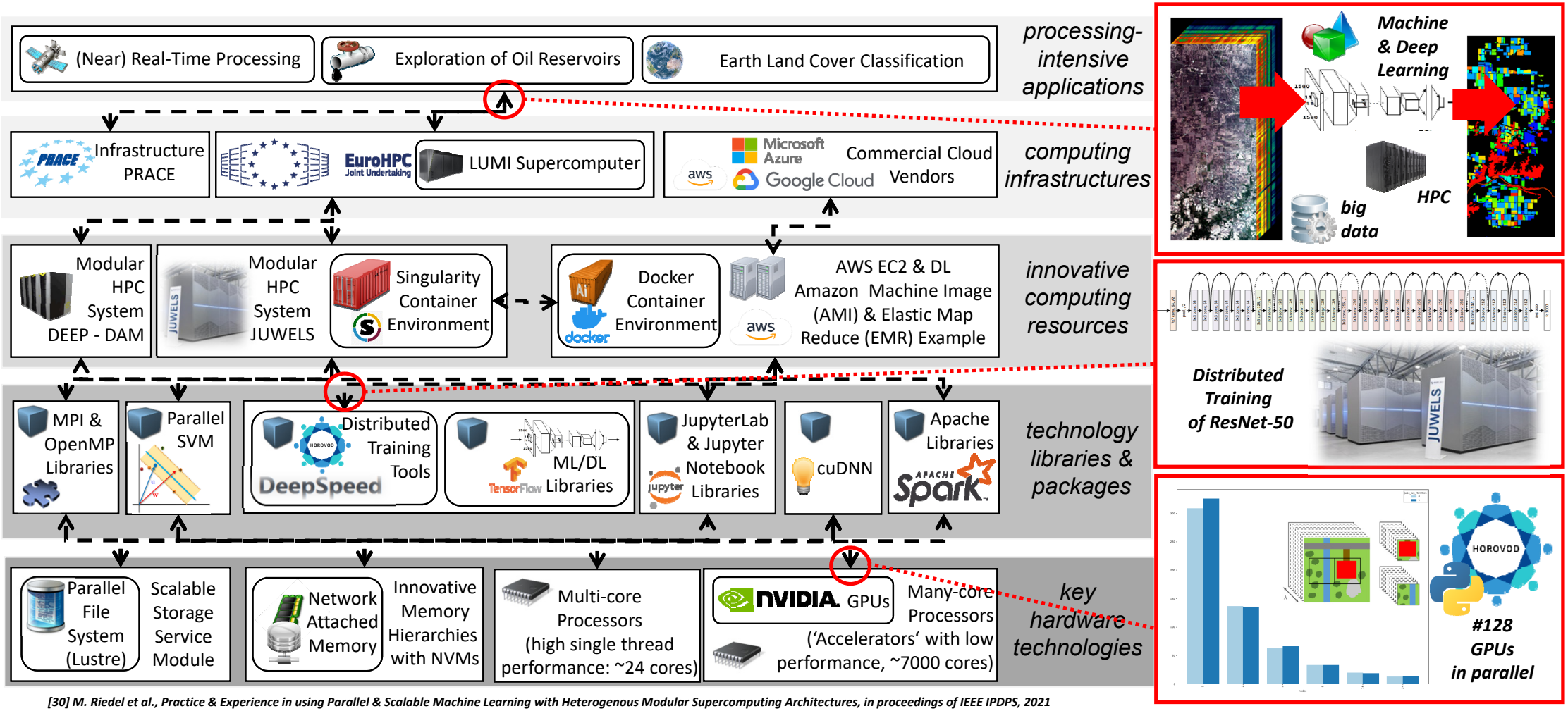
Example: Land cover classification





Challenges: mixed pixels & unbalanced land cover classes

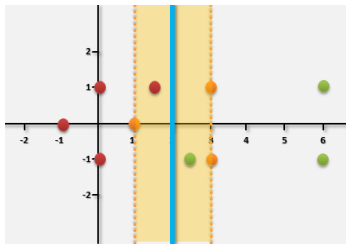
Research Examples – AI Applications in Remote Sensing using HPC



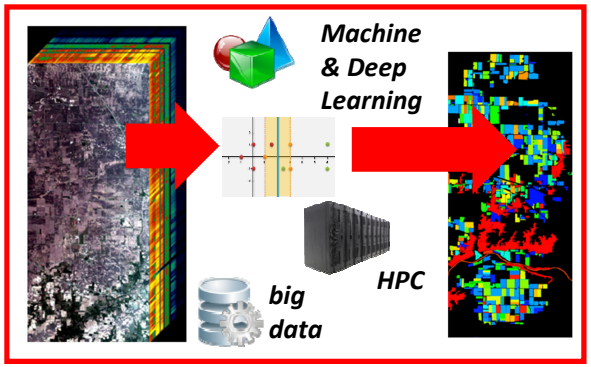
[30] M. Riedel et al., Practice & Experience in using Parallel & Scalable Machine Learning with Heterogenous Modular Supercomputing Architectures, in proceedings of IEEE IPDPS, 2021

Research on Parallel & Scalable Machine Learning Algorithms – SVM

- Parallel Support Vector Machine (SVM) piSVM
  - Being most scalable SVM (open source) still today
  - Significantly improved from original piSVM authors
  - Maintained by Simulation & Data Lab Remote Sensing

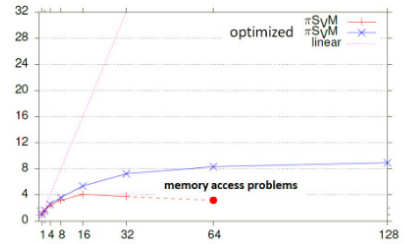


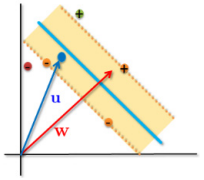
[14] C. Cortes & V. Vapnik, 'Support Vector Networks', Machine Learning, 1995

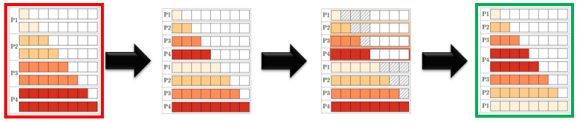


Scenario 'pre-processed data', 10xCV **serial**: accuracy (min)

γ/C	1	10	100	1000	10 000
2	48.90 (18.81)	65.01 (19.57)	73.21 (20.11)	75.55 (22.53)	74.42 (21.21)
4	57.53 (16.82)	70.74 (13.94)	75.94 (13.53)	76.04 (14.04)	74.06 (15.55)
8	64.18 (18.30)	74.45 (15.04)	**77.00** (14.41)	75.78 (14.65)	74.58 (14.92)
16	68.37 (23.21)	76.20 (21.88)	76.51 (20.69)	75.32 (19.60)	74.72 (19.66)
32	70.17 (34.45)	75.48 (34.76)	74.88 (34.05)	74.08 (34.03)	73.84 (38.78)



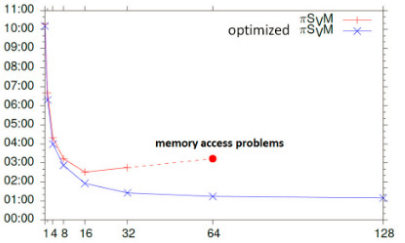




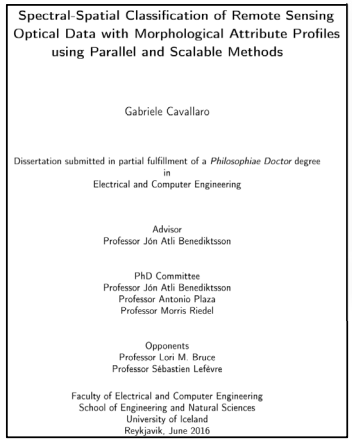
research challenges:
smart load balancing schemes for scaling up

Scenario 'pre-processed data', 10xCV **parallel**: accuracy (min)

γ/C	1	10	100	1000	10 000
2	75.26 (1.02)	65.12 (1.03)	73.18 (1.33)	75.76 (2.35)	74.53 (4.40)
4	57.60 (1.03)	70.88 (1.02)	75.87 (1.03)	76.01 (1.33)	74.06 (2.35)
8	64.17 (1.02)	74.52 (1.03)	**77.02 (1.02)**	75.79 (1.04)	74.42 (1.34)
16	68.57 (1.33)	76.07 (1.33)	76.40 (1.34)	75.26 (1.05)	74.53 (1.34)
32	70.21 (1.33)	75.38 (1.34)	74.69 (1.34)	73.91 (1.47)	73.73 (1.33)



First Result: best parameter set from 14.41 min to 1.02 min
Second Result: all parameter sets from ~9 hours to ~35 min


Spectral-Spatial Classification of Remote Sensing Optical Data with Morphological Attribute Profiles using Parallel and Scalable Methods

Gabriele Cavallaro

Dissertation submitted in partial fulfillment of a *Philosophiae Doctor* degree in Electrical and Computer Engineering

Advisor
Professor Jón Atli Benediktsson

PhD Committee
Professor Jón Atli Benediktsson
Professor Antonio Plaza
Professor Morris Riedel

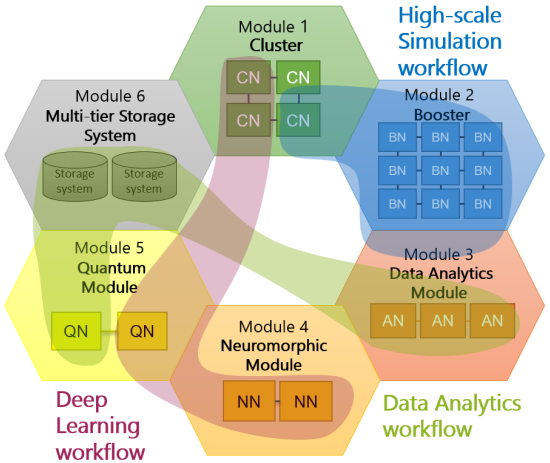
Opponents
Professor Lori M. Bruce
Professor Sébastien Lefèvre

Faculty of Electrical and Computer Engineering
School of Engineering and Natural Sciences
University of Iceland
Reykjavik, June 2016

Dr. – Ing. Gabriele Cavallaro (2016)
PhD Student Graduate, University of Iceland
IHPC Simulation and Data Lab
Remote Sensing

[13] G. Cavallaro & M. Riedel & J.A. Benediktsson et al., 'On Understanding Big Data Impacts in Remotely Sensed Image Classification Using Support Vector Machine Methods', Journal of Applied Earth Observations and Remote Sensing, 2015

Moving towards Exascale HPC Systems – Juelich Supercomputing Centre



[17] DEEP Series of Projects Web Page

Simulation and Data Laboratories
SDL Biology
SDL Plasma Physics
SDL Molecular Systems
SDL Climate Science
SDL Fluid & Solid Engineering
SDL Quantum Materials
SDL Terrestrial Systems
SDL Numerical Quantum Field Theory
SL Neuroscience
SDL Astrophysics

[18] JSC Simlabs

Potentially first Exascale system in Europe

2023

1 EF

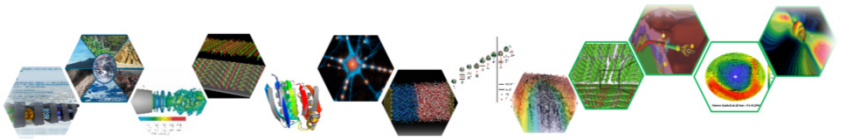
2020

85 PF

2018

12 PF

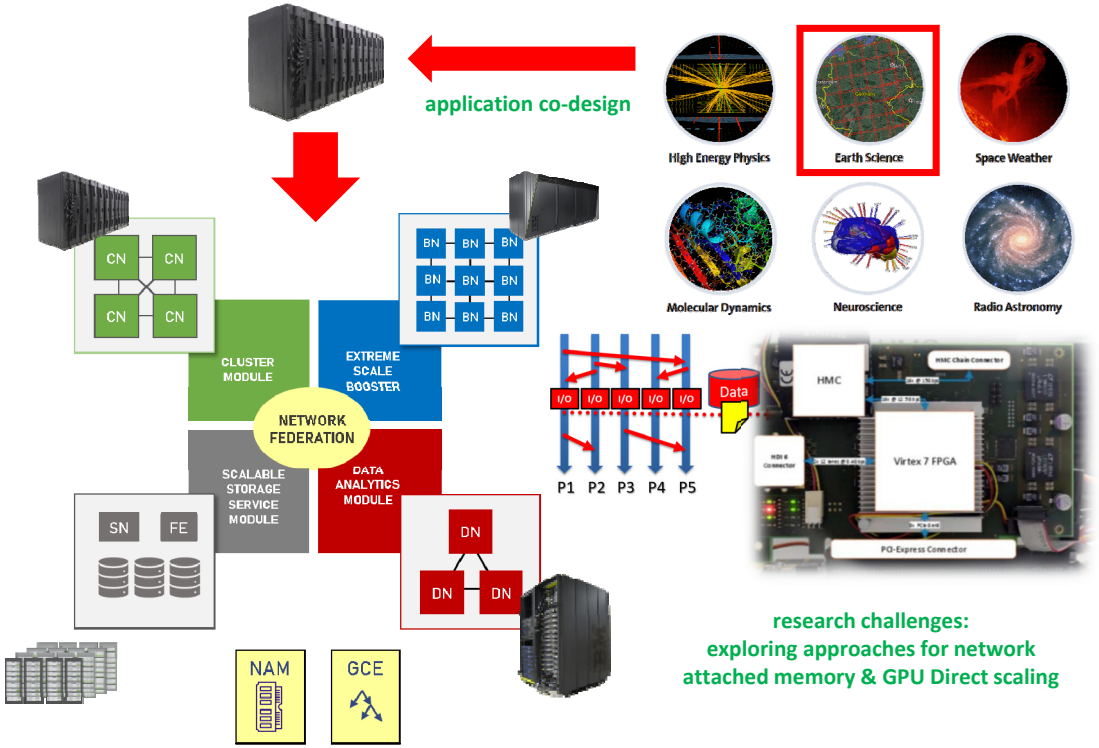
Application Co-Design



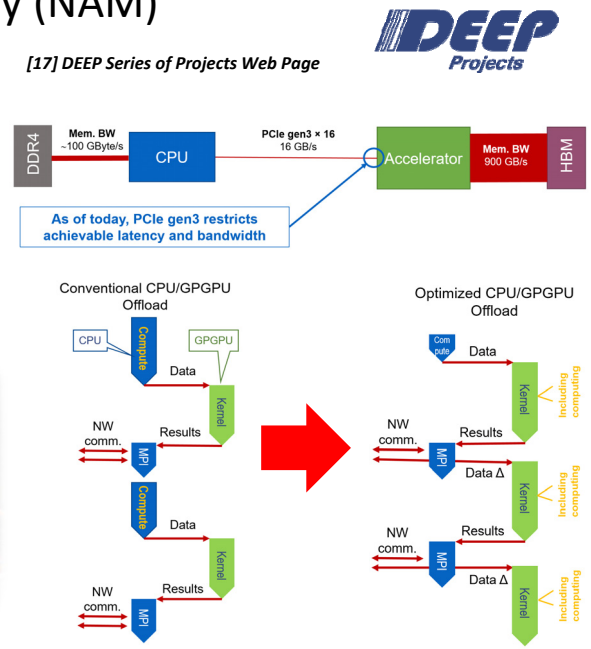
[20] YouTube, 'flexible and energy-efficient supercomputer: JUWELS is faster than 300 000 modern PCs

Research on Parallel & Scalable Machine Learning using Innovative Hardware

- Co-designing EU Modular Supercomputing Architecture (MSA)
  - Improved design on SVM & DBSCAN algorithms (NextDBSCAN/NextSVM)
  - E.g. also research on Network Attached Memory (NAM)



research challenges:
exploring approaches for network attached memory & GPU Direct scaling



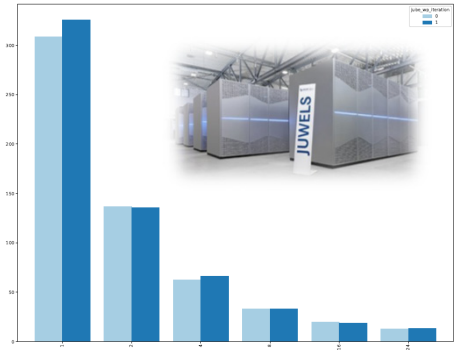
[19] E. Erlingsson, M. Riedel et al., IEEE MIPRO Conference, 2018

Ernir Erlingsson (mid-term 2019)
PhD Student, University of Iceland
IHPC Simulation and Data Lab
Remote Sensing

Research on Deep Learning Architectures using Distributed Training Approaches

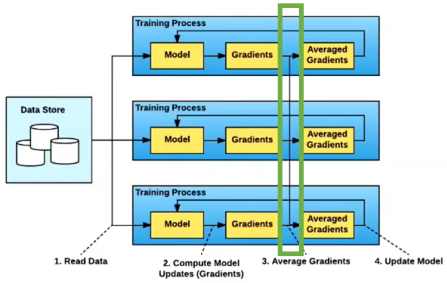
- RESNET-50 Architecture: Case for interconnecting GPUs
  - RESNET-50 is a known neural network architecture that has established a strong baseline in terms of accuracy
  - Computational complexity of training the RESNET-50 architecture relies in the fact that is has ~ 25.6 millions of trainable parameters
  - RESNET-50 still represents a good trade-off between accuracy, depth and number of parameters
  - Distributed training challenges (i.e. large batch size)

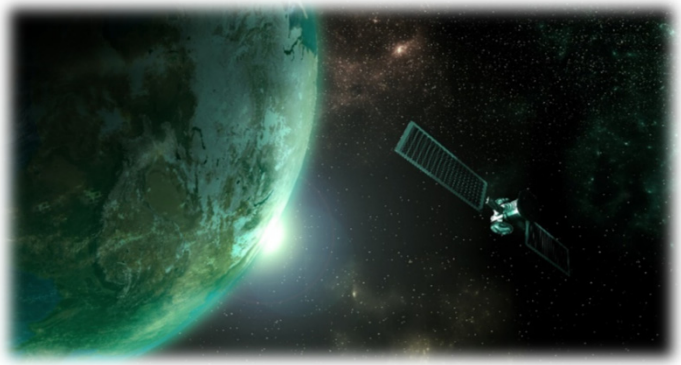
Partition of the JUWELS system has 56 compute nodes, each with 4 NVIDIA V100 GPUs (equipped with 16 GB of memory)



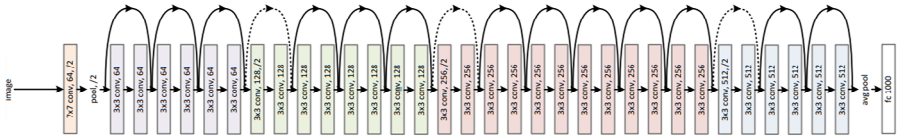
24 nodes x 4 GPUs = 96 GPUs

Horovod distributed training via MPI_Allreduce()





[23] Horovod



[24] 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

Rocco Sedona
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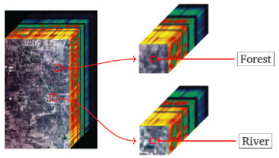
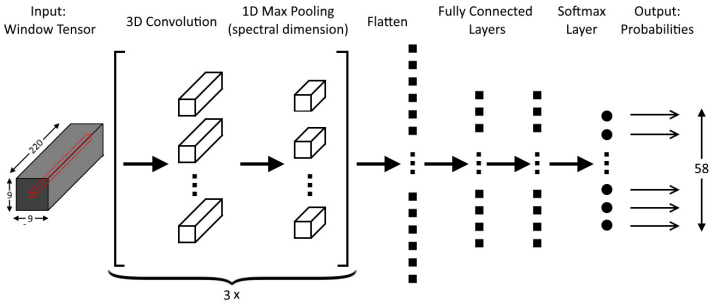
Remote Sensing

Research on Deep Learning Architectures for Remote Sensing – CNNs

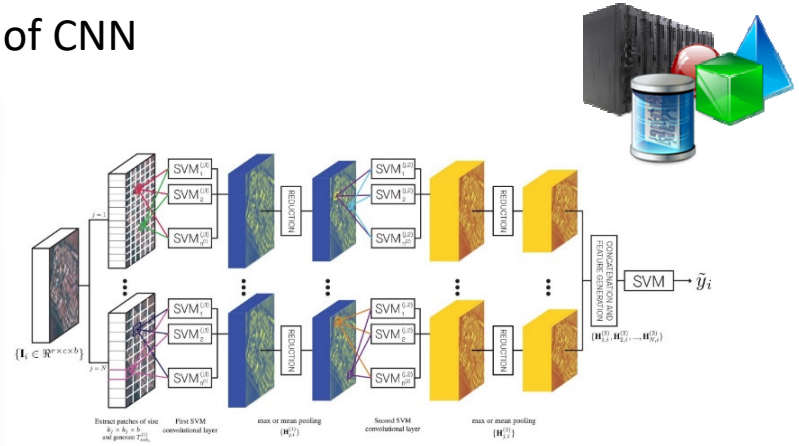
- Convolutional Neural Networks (CNNs)
  - Used with hyperspectral remote sensing data
  - Rare labeled/annotated data in science
    (e.g. 36,000 vs. 14,197,122 images ImageNet)
  - Scene vs. pixel-wise classification challenges
- Combining Machine Learning Models
  - Using CNNs basic principle
  - Apply SVMs in different layers of CNN





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

research challenges:
rare groundtruth and surrounding labels bias in training, but key challenge remain: hyper-parameter tuning

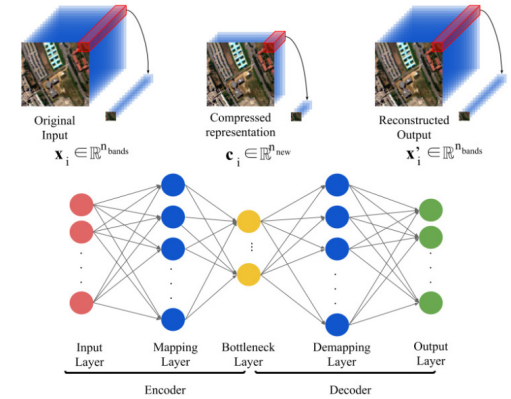


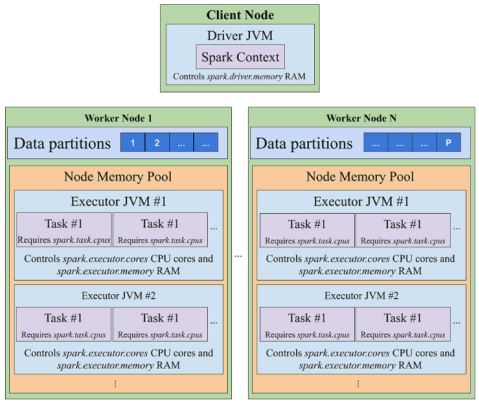
[22] G. Cavallaro, M. Riedel et al., IGARSS 2019

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}

Leverage Clouds & Apache Spark for Image Compression Tasks

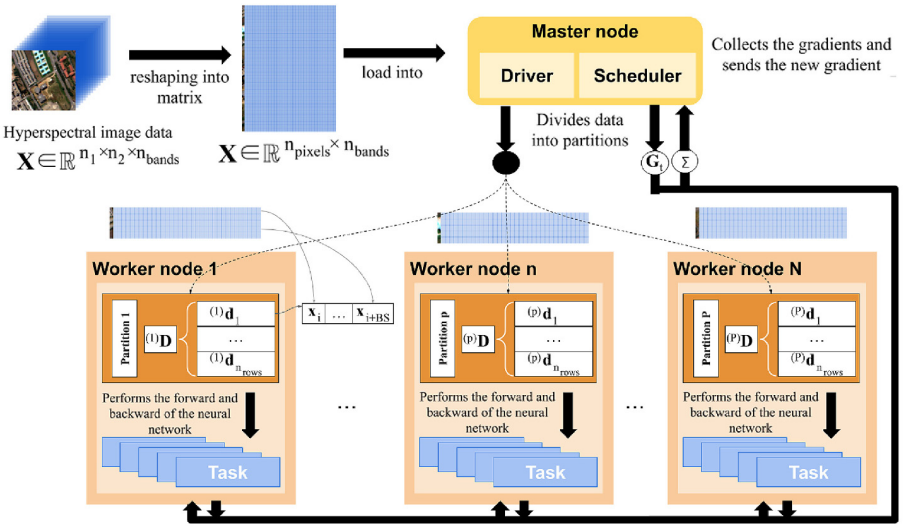
- Cloud Computing Vendors
  - Amazon Web Services (AWS)
  - Microsoft Azure
  - Google Cloud Platform
  - Many others
- Similar set of Tools
  - Jupyter Notebooks
  - Hadoop & Apache Spark
  - Generally quite good portability between clouds
  - Use of Containers (e.g., Docker)





Using Autoencoder deep neural networks with Cloud computing for image compression

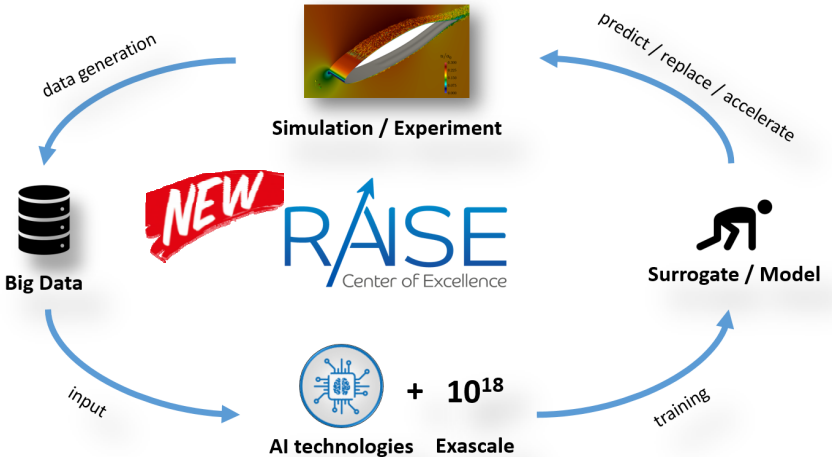
Performing parallel computing with Apache Spark across different worker nodes

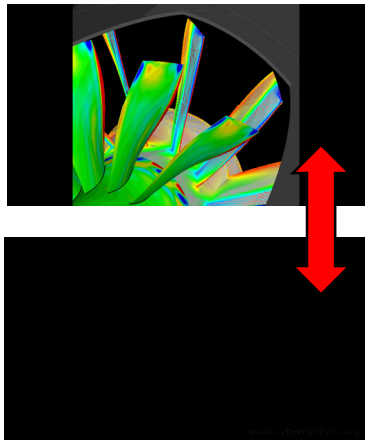


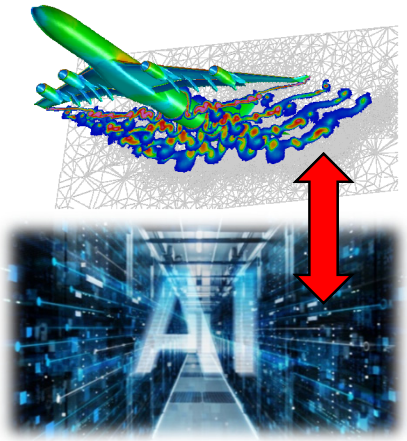
[32] Apache Spark Web page

[31] J. Haut, G. Cavallaro and M. Riedel et al., IEEE Transactions on Geoscience and Remote Sensing, 2019

RAISE Center of Excellence (CoE) EU Project – HPC Intertwined with AI



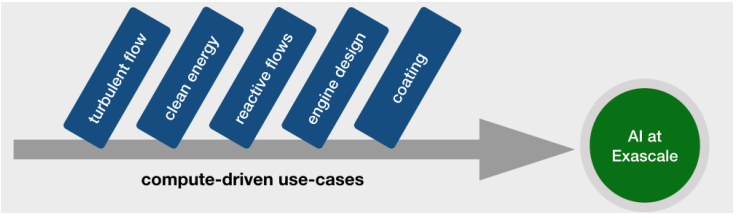




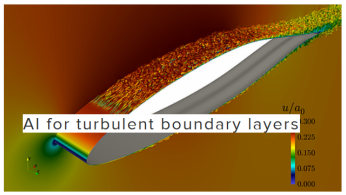
Computational expensive use cases

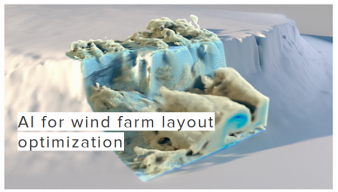
[4] RAISE Center of Excellence Web Page

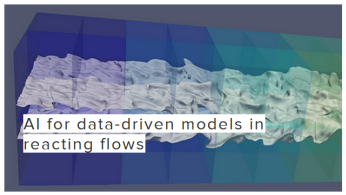
SAFRAN · JÜLICH Forschungszentrum · Atos · CERFACS · Delphi Consortium · 1862 RĪGAS TEHNISKĀ UNIVERSITĀTE · CERN · UNIVERSITY OF ICELAND · FLANDERS MAKE · ParTec Cluster Competence Center The Modular Supercomputing Company · RWTH AACHEN UNIVERSITY · BSC Barcelona Supercomputing Center Centro Nacional de Supercomputación · The Cyprus Institute Research·Technology·Innovation

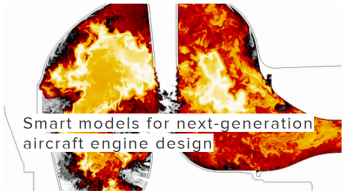


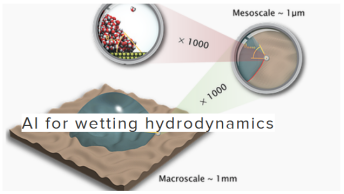
Starting Research with CoE RAISE to intertwine more AI with Simulations

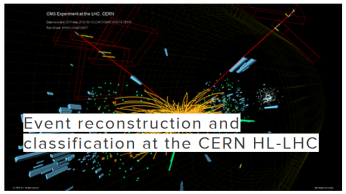


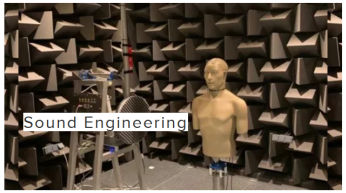












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[11] IHPC SimDataLab Remote Sensing Web Page

NEW RAISE Center of Excellence

[4] RAISE Center of Excellence Web Page

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Computational Fluid Dynamics (CFD)

[8] IHPC SimDataLab CFD Web Page

Eric Michael Sumner
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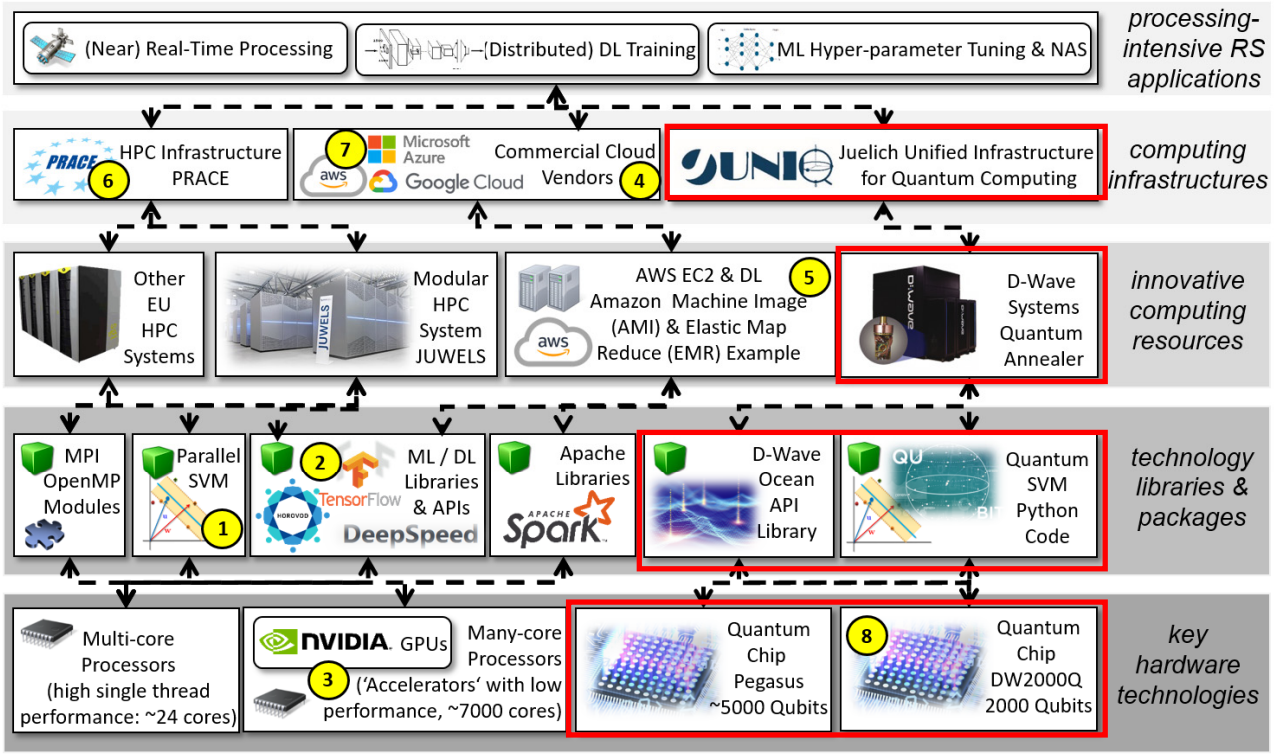
IHPC Simulation and Data Lab
Accoustic & Tactile Engineering

[15] IHPC SimDataLab Accoustic & Tactile Engineering Web Page

Research on Quantum Machine Learning using D-Wave Quantum Annealer

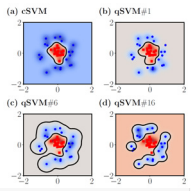


1. Parallel ML implementations still rare (MPI/OpenMP)
2. Open source tools good, but all need to fit in versions
3. Using very many GPUs beyond NVlink could be tricky
4. Look & feel of CC vendor ML services differ significantly
5. Costs of GPUs of CC vendors (e.g., EC2) tough, 24$/hour
6. GPU hours 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

[16] 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

```
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
experiments=1
slice=40 # Number of samples to use for the training
fold=int(len(X_train)/40)

print(fold)

for i in range(0,experiments):
    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, y_train_slice = X_train[train_index], Y_train[train_index]
        X_train_slice = preprocessing.scale(X_train_slice)

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

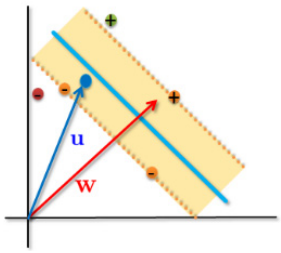


[25] G. Cavallaro & M. Riedel et al., Approaching Remote Sensing Image Classification with Ensembles of SVMs on the D-Wave Quantum Annealer, Proceedings of the IEEE IGARSS 2020 Conference

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

(research challenges: ensembles due to small datasets compared to full datasets on CPUs/GPUs & disruptive technology)

[28] 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



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

[27] M. Riedel, UTMessan 2020 YouTube Video


Summary & Outlook

Summary & Outlook

- HPC needed for science & engineering, including Remote Sensing Applications
- Remote Sensing can benefit from HPC, Clouds & Quantum Computing

- Landscape of HPC, Clouds & Quantum Computing gets increasingly complex
- Inter-disciplinary teams strive: Technologists, remote sensing experts, programmers

- Wide variety of great tools exist for HPC, Clouds, and Quantum Computing
- Mastering the many toolsets is not trivial for remote sensing scientists

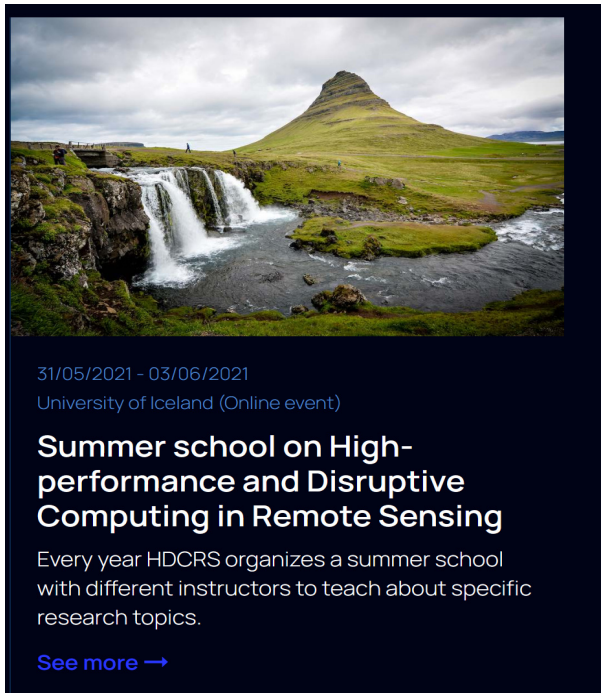
Urgent need of more remote sensing experts on the intersection of AI, HPC and specific scientific & engineering domains: 'finding good talent in HPC is a world-wide problem we all face in academia (PhD recruiting problem)'

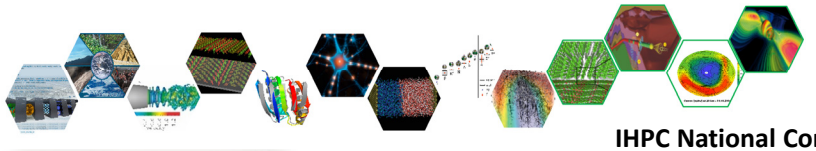
RAISE Center of Excellence

[4] RAISE Center of Excellence Web Page

Working towards Pan-European MSc in HPC – Strengthening Teaching in HPC & AI

[33] IEEE GRSS Working Group HDCRS Web poage





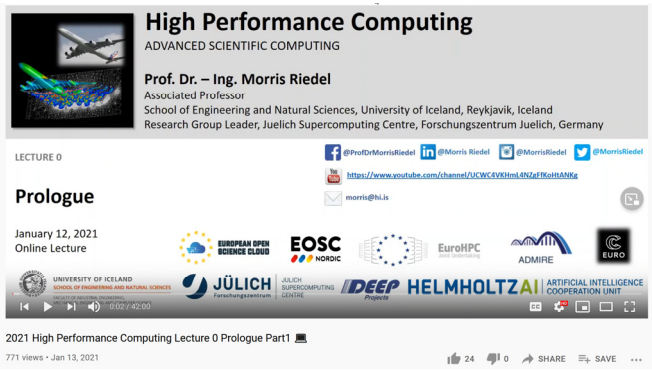
[10] Icelandic HPC Community Web page

IHPC National Competence Center for HPC & AI in Iceland

HÁSKÓLI ÍSLANDS

HÁSKÓLINN Í REYKJAVÍK
REYKJAVIK UNIVERSITY

Teaching HPC & AI university courses at two universities



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

EuroHPC Joint Undertaking

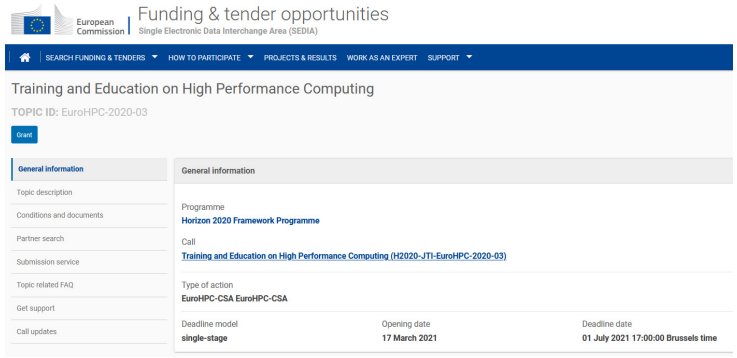
emerging education activities

RAISE Center of Excellence

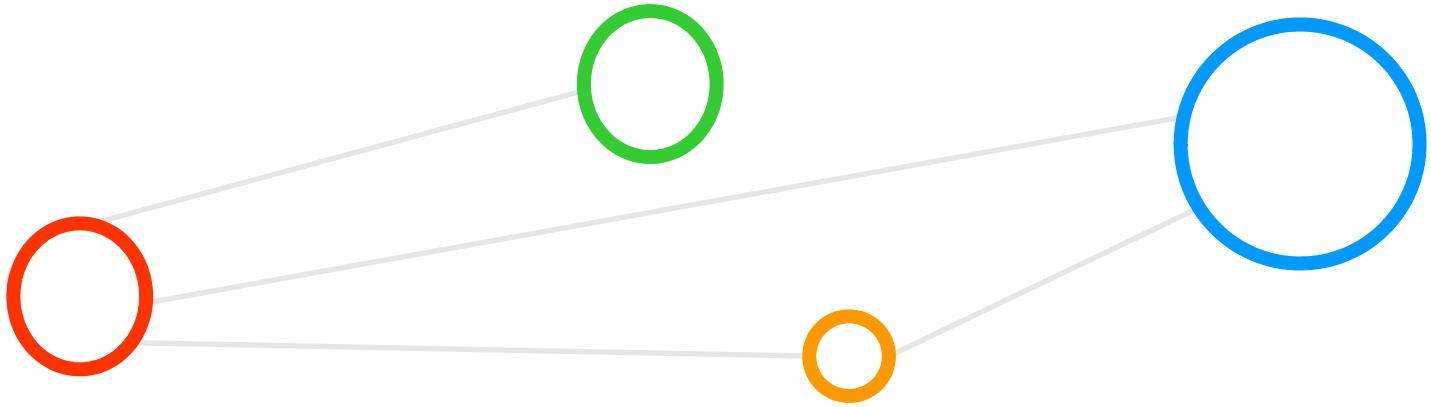
[4] RAISE Center of Excellence Web Page

long-term center of excellence in HPC, e.g. RAISE

Future Ideas of MSc of HPC with Remote Sensing Specialization



Selected References



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- [2] Zeitraffervideo des Aufbaus unseres Supercomputers JUWELS, YouTube Video, Online: https://www.youtube.com/watch?v=8Y8zTG2a-UE
- [3] Supercomputer shows humidity effect on COVID-19, YouTube Video, Online: https://www.youtube.com/watch?v=4TUrsRvKZOc
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- [5] JSC Terrestrial Systems Simulation Lab, Online: http://www.hpsc-terrsys.de/simlab
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- [7] www.big-data.tips, Online: http://www.big-data.tips
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- [9] Neural Network 3D Simulation, YouTube Video, Online: https://www.youtube.com/watch?v=3JQ3hYko51Y
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- [13] G. Cavallaro, M. Riedel, M. Richerzhagen, J. A. Benediktsson and A. Plaza, "On Understanding Big Data Impacts in Remotely Sensed Image Classification Using Support Vector Machine Methods," *in the IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, vol. 8, no. 10, pp. 4634-4646, Oct. 2015, Online: https://www.researchgate.net/publication/282524415_On_Understanding_Big_Data_Impacts_in_Remotely_Sensed_Image_Classification_Using_Support_Vector_Machine_Methods
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- [15] Icelandic HPC Simulation and Data Lab Accoustic & Tactile Engineering, Online: https://ihpc.is/simulation-and-data-lab-acoustic-and-tactile-engineering/
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- [18] Juelich Supercomputing Centre – SimLabs Blueprint, Online: https://www.fz-juelich.de/ias/jsc/EN/Expertise/SimLab/simlab_node.html
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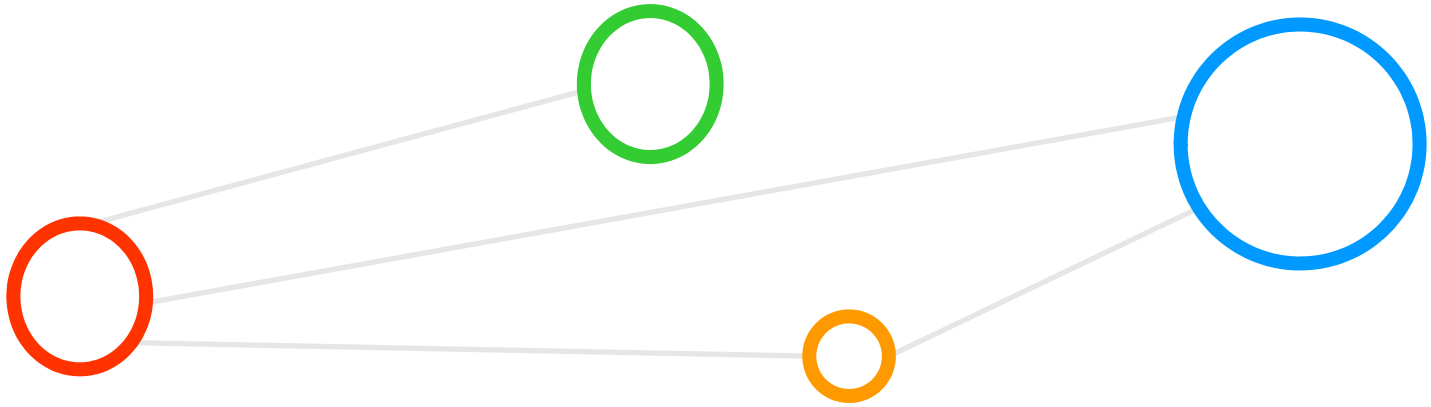

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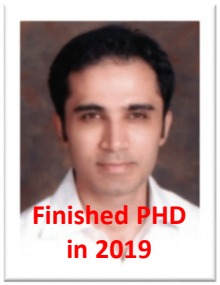

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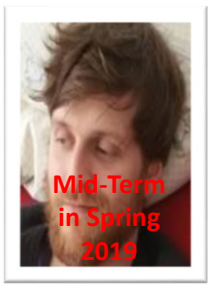

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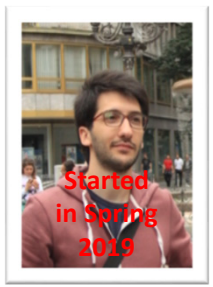

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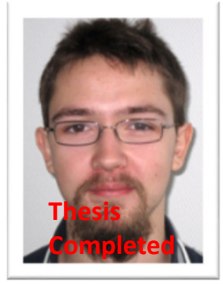

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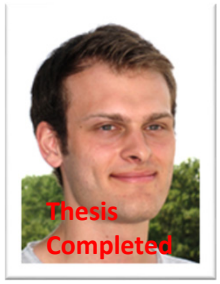

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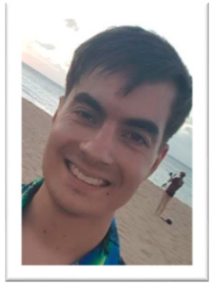

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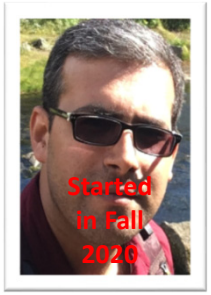

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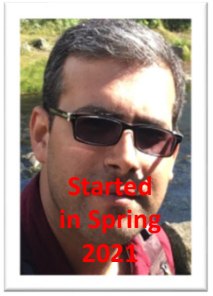

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