





## **Towards Simulation and Data Labs in the context of the LUMI Supercomputer**

PROF. DR. – ING. MORRIS RIEDEL, UNIVERSITY OF ICELAND / JUELICH SUPERCOMPUTING CENTRE (JSC)  $21^{TH}$  APRIL, LUMI STEERING COMMITTEE, ONLINE







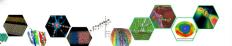




https://www.youtube.com/channel/UCWC4VKHmL4NZgFfKoHtANKg



IHPC National Competence Center for HPC & AI in Iceland















UNIVERSITY OF ICELAND SCHOOL OF ENGINEERING AND NATURAL SCIENCES

FACULTY OF INDUSTRIAL ENGINEERING, MECHANICAL ENGINEERING AND COMPUTER SCIEN











# Executive Summary - Major Icelandic HPC Activities - LUMI & People!



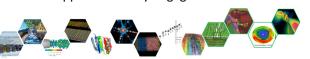
- ❖ HPC hardware funds by RANNIS; now via roadmap IReiP
- Proposals yearly required to obtain funds still
- Joint proposal from IHPC community

# **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

Veðurstofa

Islands





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





Co-Funds by EC and Iceland participation funds from: UoIceland,
 UoReykjavik, and Hannes Jonsson & Egill Skulason



- University of Reykjavik
- University of Iceland
- Arctic Webinar Series (with US partners)



❖ Digital/Horizon Europe MSc in HPC



- ❖ 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: Building an Icelandic National Lab with international cooperation together with Industry (e.g. Kaiser Global, other investors)





**HPC** 









**EuroHPC** 

# 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

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)

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



setting up NCCs

roadmap definition 1<sup>st</sup> phase of realisation & implementation

2<sup>nd</sup> phase of realisation & implementation

continuation funding planed

timeline

1<sup>st</sup> NCC meetings arranged <M01>

 $\Diamond$ 

roadmap <M04>

 $\Diamond$ 

periodic report <M12>

 $\Diamond$ 

final report <M24>

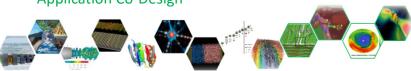
# **International Collaboration Partners: Juelich Supercomputing Centre**



in Iceland for education & research (!)

**JUWELS** Cluster

**Application Co-Design** 

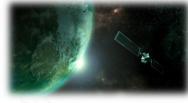


85 PF

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

# **DEEP Series of HPC Projects – Modular Supercomputing Architecture Research**







Strong collaboration with our industry partners Intel, Extoll & Megware

3 EU Exascale projects
 DEEP, DEEP-ER, DEEP-EST

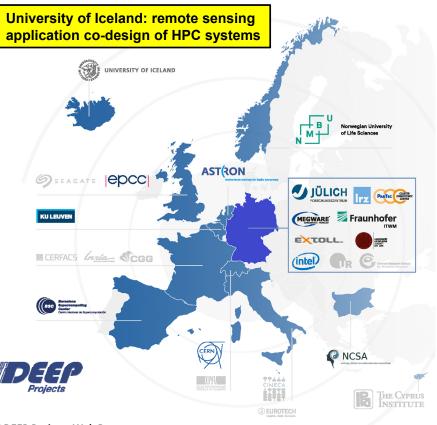
27 partners Coordinated by JSC

■ EU-funding: 30 M€ JSC-part > 5,3 M€

Nov 2011 – Mar 2021

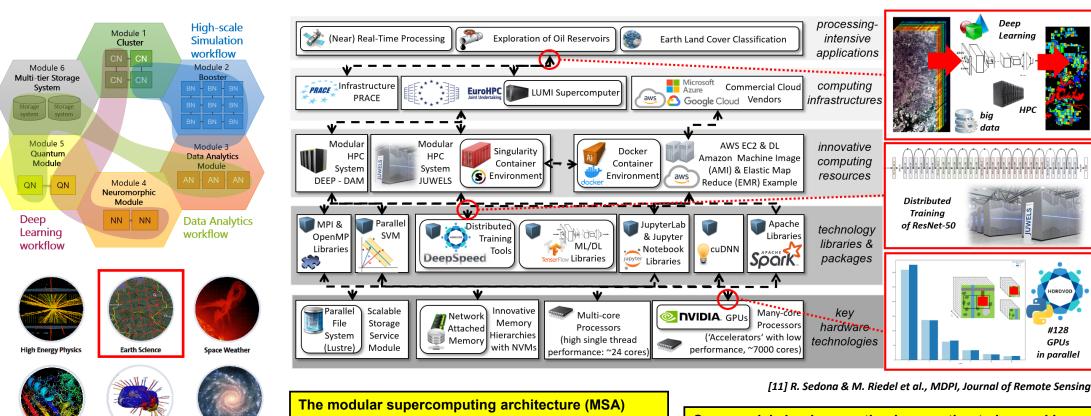
Strong collaboration with industry partners Intel, Extoll & Megware

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**



enables a flexible HPC system design co-designed by the need of diverse research application workloads

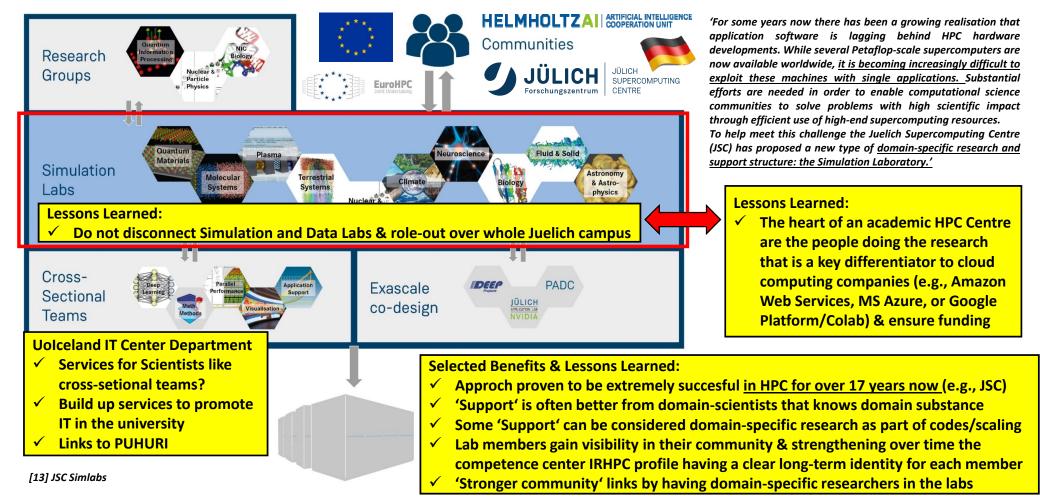
Commercial cloud computing is no option to be used here instead (e.g., Amazon Web Services charge 24\$/hour GPU

Radio Astronomy

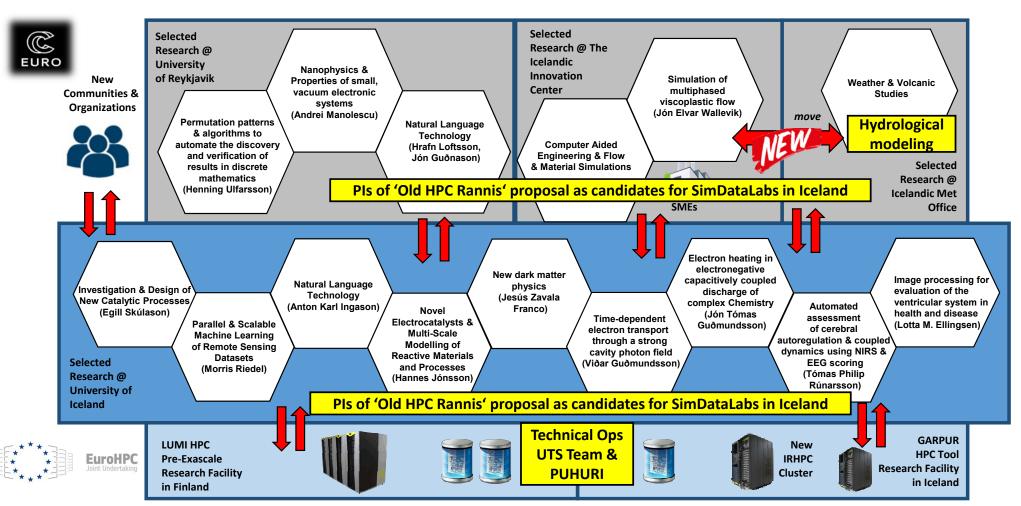
Neuroscience

Molecular Dynamics

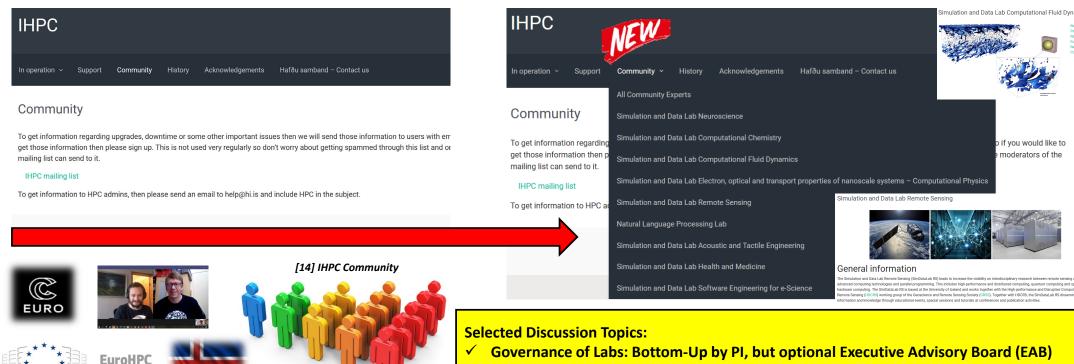
# Community-building with Simulation & Data Labs (SDLs) – Lessons Learned



# First Steps towards Potential Simulation and Data Labs in Iceland



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

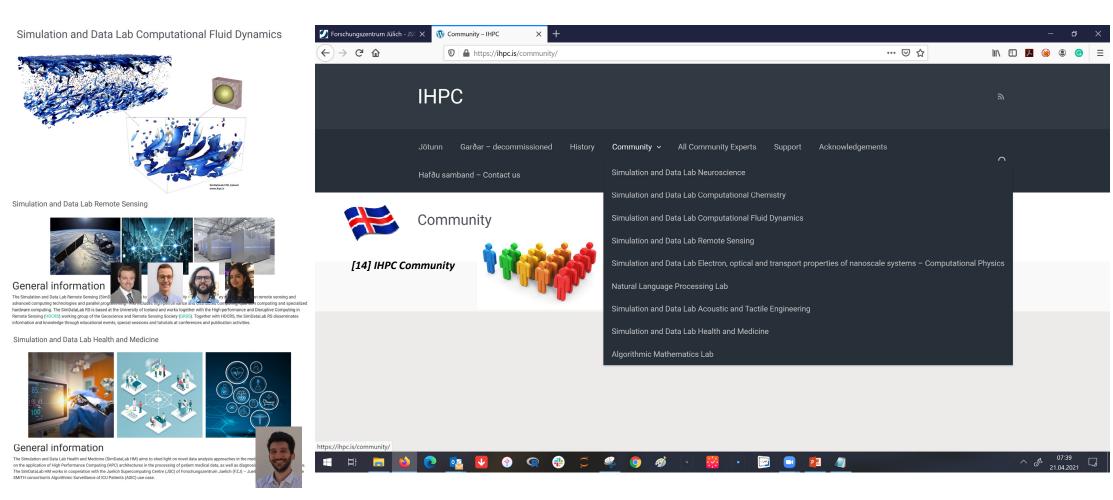


Jointly engage in future funding together, e.g. EuroHPC Master of Science in HPC program and many other activities planed in Horizon Europe



- 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 (Accoustic, done), others?
- ✓ Teaching better topics of relevance in HPC Course for Iceland, other activities?

# Simulation and Data Labs – Iceland NCC – Examples



# Simulation and Data Labs – Juelich Supercomputing Centre – Examples

### Simulation Laboratory Neuroscience



The SimLab Neuroscience is an interdisciplinary team of scientists and engineers with complementary backgrounds and skills, dedicated to supporting neuroscientists in using high-performance computing and data resources for their research. Expertise in both neuroscience and HPC is based on in-house research and development, as well as collaborative joint projects with the Institute of Neuroscience and Medicine (INM), Forschungszentrum Jülich, and other national and international partners.

[13] JSC Simlabs

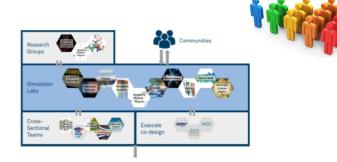


### Simulation and Data Laboratories

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 Jülich Supercomputing Centre (JSC) has proposed a new type of domain-specific research and support structure: the Simulation and Data Laboratory. Four such units have now been established at JSC in the fields of Computational Biology, Molecular Systems, Plasma Physics, and Climate Modelling, which have already been actively engaged with user groups from their respective communities over the past year. In October 2012 the SimLab Terrestrial Systems was started. Another SimLab in Neuroscience came on stream early 2013.

In collaboration with JARA-HPC at RWTH Aachen, the JARA Simulation and Data Laboratories "Highly Scalable Fluids and Solids Engineering" and "Ab-Initio Methods in Chemistry and Physics" have been established.



# Supercomputers JUNIQ User Support 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

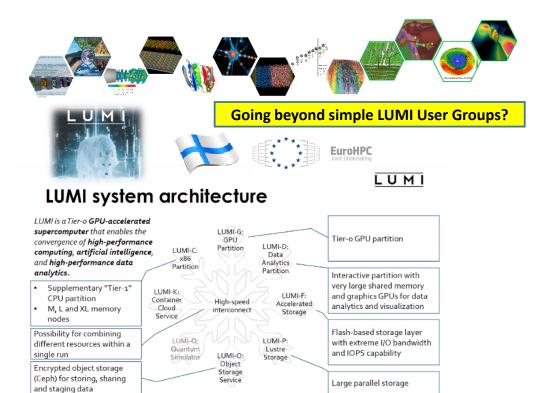
Data Management

Services

Scientific Cloud Services

Test projects on JSC Resources

# **EuroHPC – LUMI – What Strategy for People(!) in Research & Support?**





LUMI's computing power will be over 550 petaflops.



LUMI's computing power is equivalent to the combined performance of 1.5 million of the latest laptop computers. These would form over 23-kilometer high tower.



In total, LUMI will have astounding storage of 117 petabytes and an impressive aggregated I/O bandwidth of 2 terabytes per second.



LUMI is using 100% hydropowered energy. Up to 200MWs are available. The waste heat of LUMI will produce 20 percent of the district heat of the area.

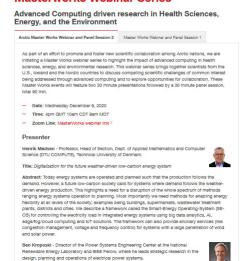
- The strategy of people around LUMI will be key to success of the LUMI consortium, not simple hardware
- Possibilities. Jointly engage in CoE or other Calls for creating Simulation and Data Labs around LUMI over time, e.g. also Digital Twins might contribute Digital/Horizon Europe, etc. Bottom-up; E.g. approach like EOSC-Nordic was one idea
  - Some approach also for cross-sectional teams that could be the SIGs in a way, but will they provide support & answers?

[6] LUMI Supercomputer

# Simulation and Data Labs - Recruiting links to Teaching & Education in HPC & Al



### **Masterworks Webinar Series**



### **Webinar Series Organizing Committee**

Electric Power Systems

- Morris Riedel, Associate Professor, University of Iceland
- David Martin, Industry Partnerships and Outreach Manager, Argonne National Laboratory
- Henning Úlfarsson, Assistant Professor, Reykjavík University
- Steve Hammond, Senior Research Advisor, National Renewable Energy Laboratory







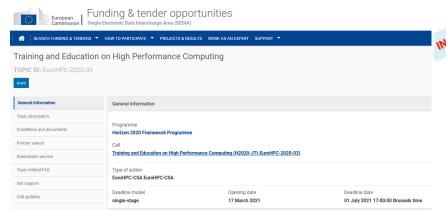


emerging education activities



### Teaching HPC & Al university courses at two universities

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

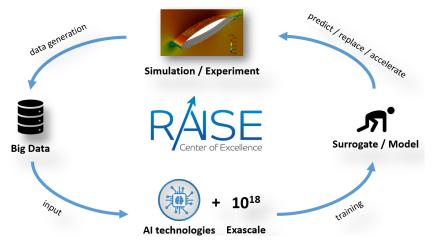




PILLAR	ACTION	Total EU (21 - 27)
Usage & Skill	Supporting Networking National Centres of Competence (CoC) on HPC (Actions to strengthen the wide application of HPC and increasing the innovation potential of SMEs using advanced HPC services)	€100M
Usage & Skill	Education (Curricula development) - Short Term trainings/Traineeships	€30M
Usage & Skill	M.Sc. HPC	€20M



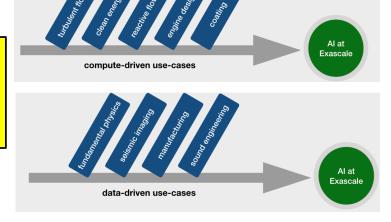
# RAISE Center of Excellence (CoE) EU Project – CFD SDLs Join Forces

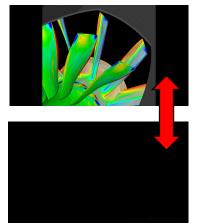


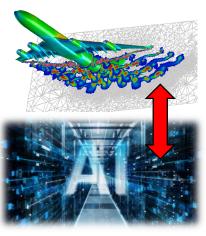
[4] CoE RAISE Web Page

[3] Simulation Figure

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





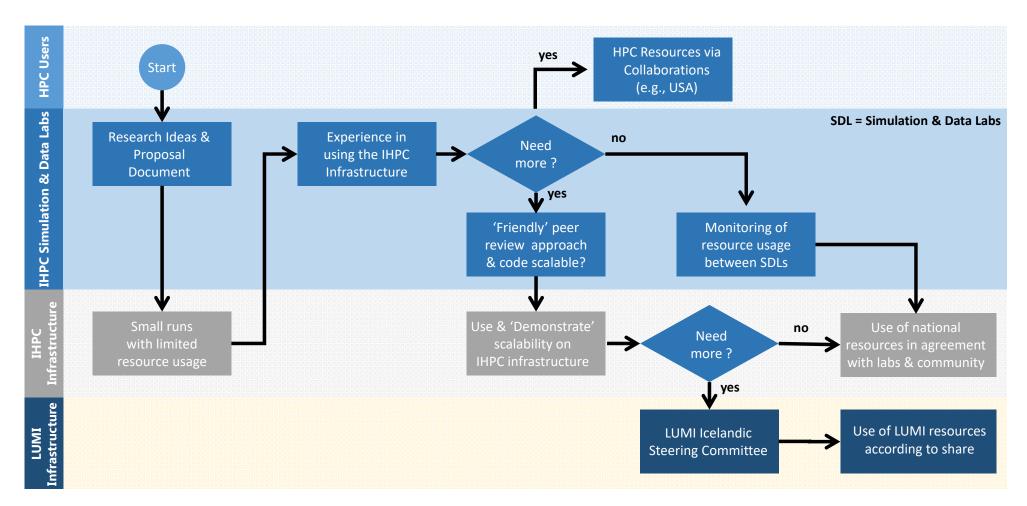




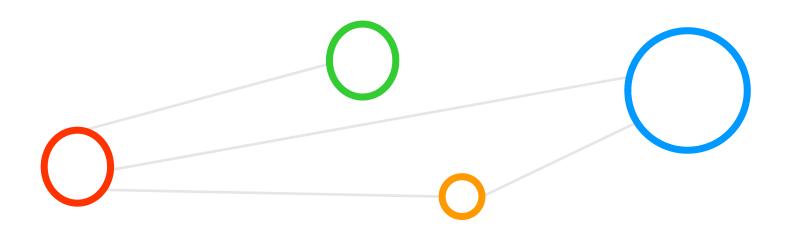


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# **Icelandic National Resource Allocation Principle & LUMI – Work-in-Progress**



# **Lecture Bibliography**



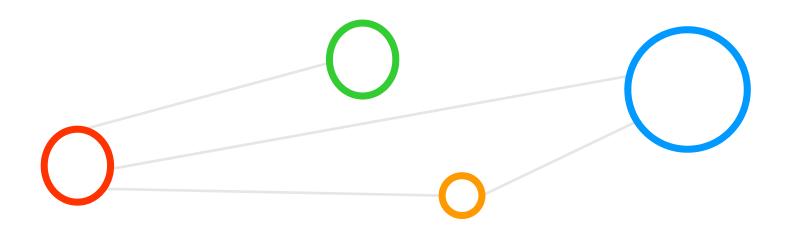
# **Selected References (1)**

- [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: <a href="https://www.sciencedirect.com/science/article/pii/S001046551930342X951733">https://www.sciencedirect.com/science/article/pii/S001046551930342X951733</a>
- [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, Hawai, USA, to appear, Online: <a href="https://igarss2020.org/Papers/ViewPapers.asp?PaperNum=1416">https://igarss2020.org/Papers/ViewPapers.asp?PaperNum=1416</a>
- [10] Open PhD Position for the RAISE EU project @ Iceland, Online: https://www.gabriele-cavallaro.com/news/fully-funded-phd-position

# **Selected References (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/

# **ACKNOWLEDGEMENTS**



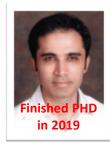
# **Acknowledgements – High Productivity Data Processing Research Group**



PD Dr. G. Cavallaro



Senior PhD Student A.S. Memon



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PhD Student R. Sedona



PhD Student P. H. Einarsson





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(now other division)



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MSc C. Bodenstein (now Soccerwatch.tv)



MSc G.S. Guðmundsson (Landsverkjun)



PhD Student Reza



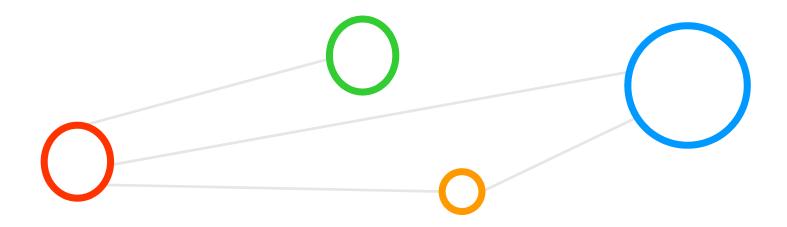




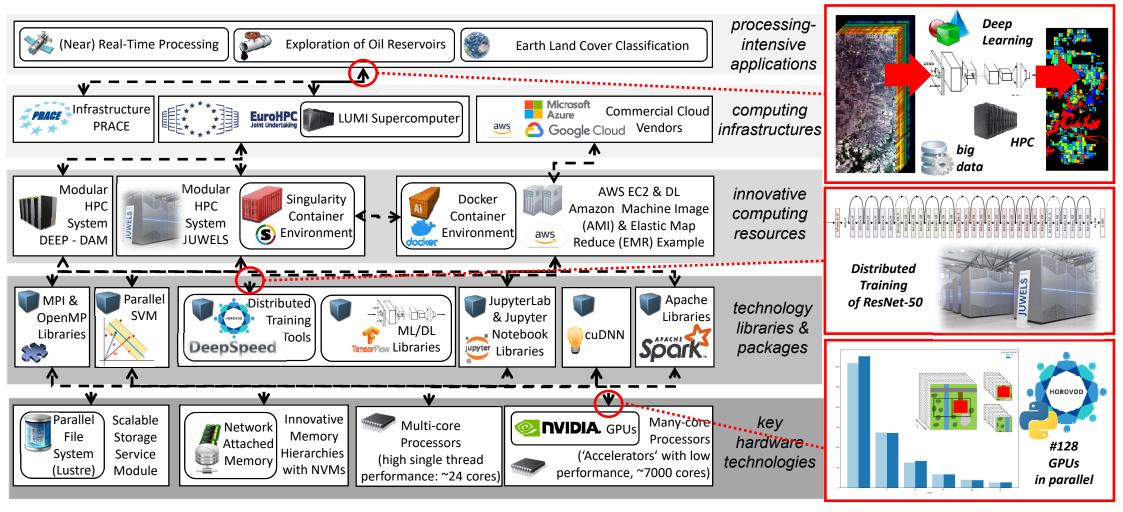
This research group has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 763558 (DEEP-EST EU Project) and grant agreement No 951740 (EuroCC EU Project) & 951733 (RAISE EU Project)



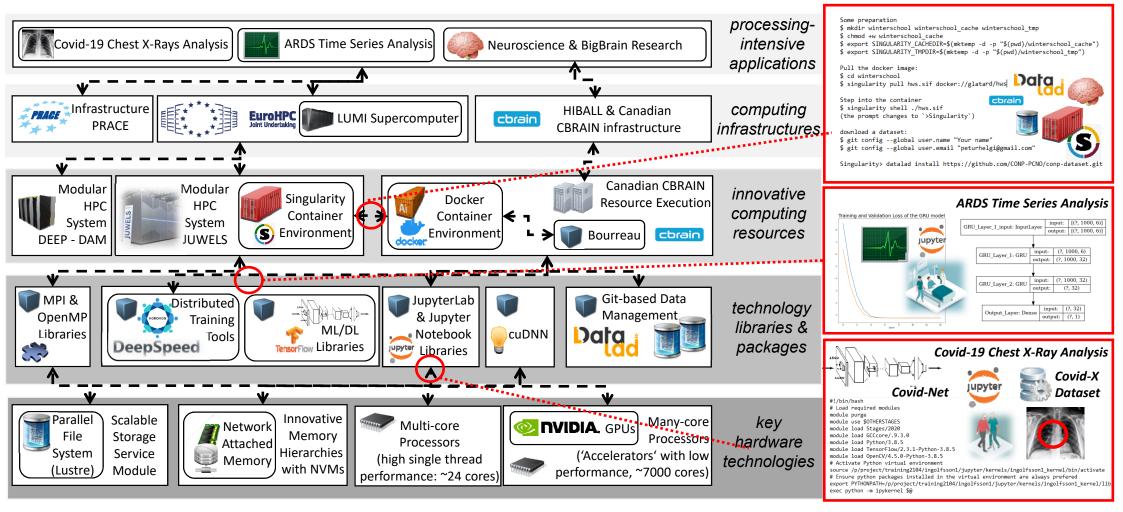
# **Appendix**



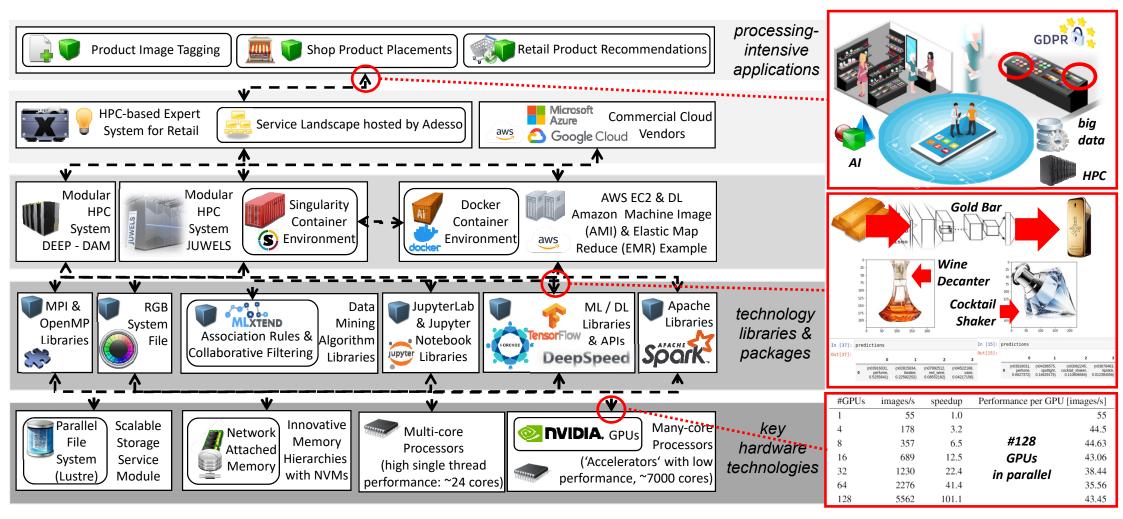
# **Research Examples – Remote Sensing AI & HPC Applications**



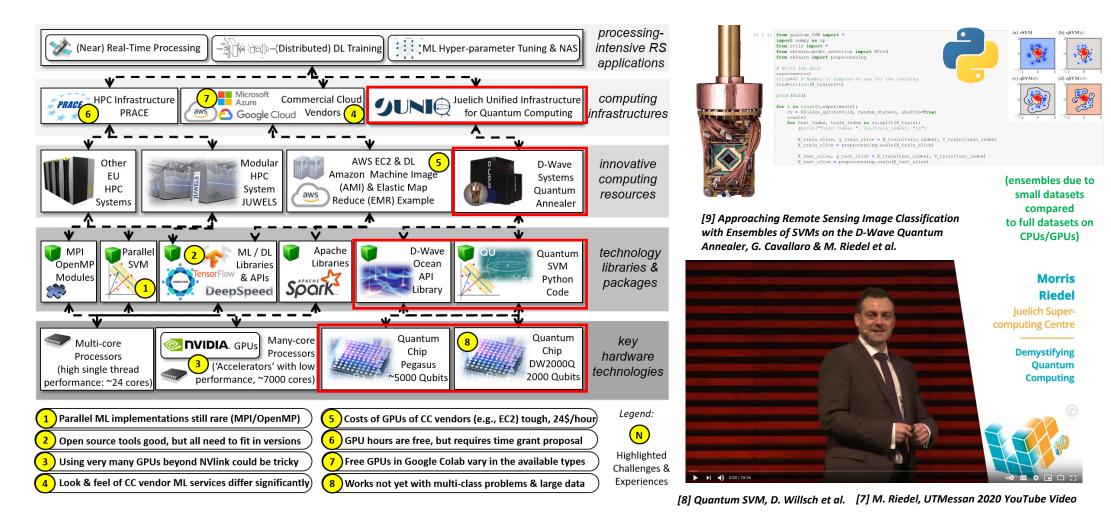
# Research Examples - Health & Medical AI & HPC Applications



# Research Examples – Retail AI & HPC Applications



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



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# Open PhD Position Available in EU Project RAISE @ Iceland











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

(A 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.

② ② ② ② ② Presearch 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).

**xWorking 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: q.cavallaro@fz-juelich.de.

Apply now

