



THANKS FOR JOINING

RAISE CoE Seminar: Graph Neural Networks

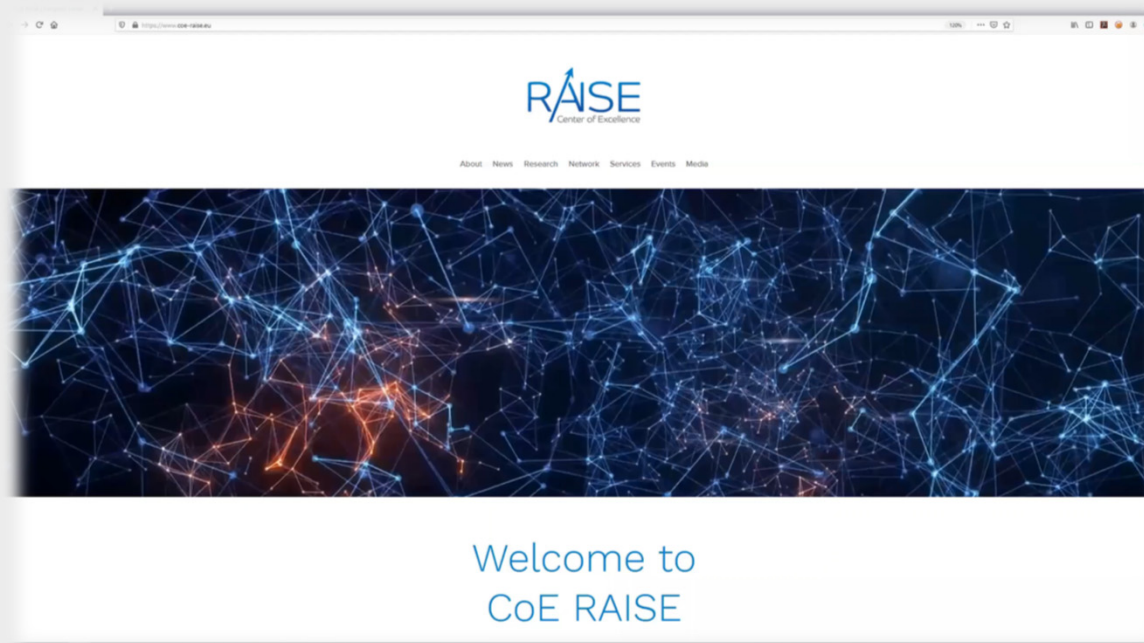
Prof. Dr. – Ing. Morris Riedel et al.

School of Engineering & Natural Sciences, University of Iceland, Iceland
National Competence Center (NCC) for HPC & AI in Iceland – IHPC
2022-03-31, RAISE CoE Seminar Graph Neural Networks, Online

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



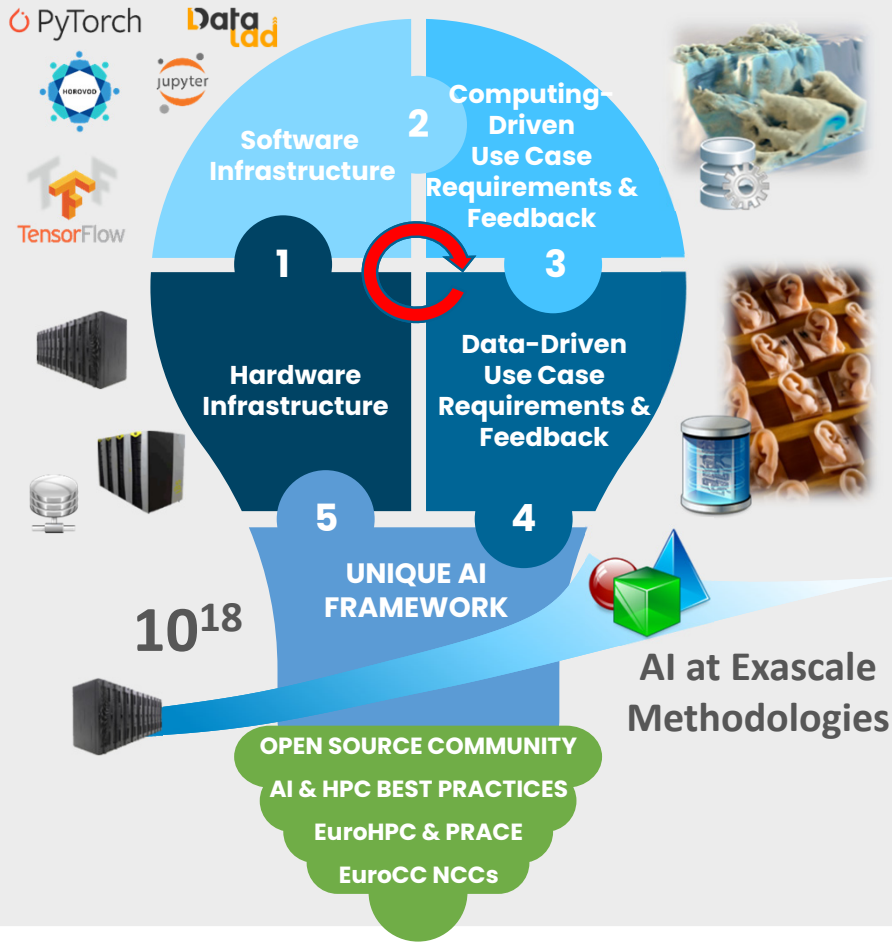
CoE RAISE Web Page & More Information



<https://www.coe-raise.eu>



Towards AI & HPC at Exascale with CoE RAISE Results



Hardware Infrastructure

Prepare & Document available production systems at partners' HPC centers

Examples: JUWELS (JUELICH), LUMI (UoICELAND), DEEP Modular Prototypes, JUNIQ (JUELICH), etc.

Software Infrastructure

Prepare & Document available open source tools & libraries for HPC & AI useful for implementing use cases

Examples: DeepSpeed and/or Horovod for interconnecting N GPUs for a scalable deep learning jobs

Computing-driven Use Cases Requirements & Feedback

Use cases with emphasize on computing bring in co-design information about AI framework & hardware

Examples: Use feedback that TensorFlow does not work nicely, so WP2 works with use cases on

Data-driven Use Cases Requirements & Feedback

Use cases with emphasize on data bring in co-design information about AI framework & hardware

Examples: Deployment blueprint by using AI training on cluster module & inference/testing on booster

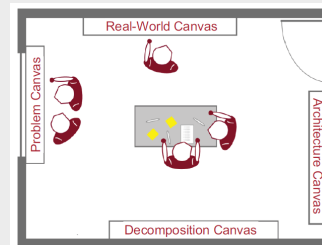
→ UNIQUE AI FRAMEWORK

Living design document & software framework blueprint for using HPC & AI offering also pretrained AI models

CoE RAISE YouTube Channel: Check our Trainings & Subscribe!

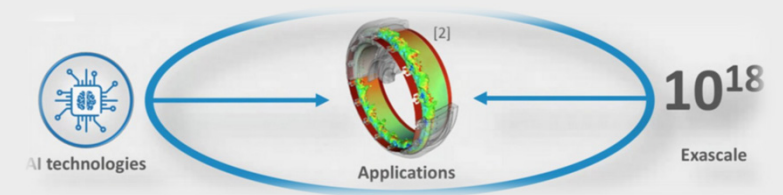
➤ Example: CoE RAISE Interaction Room Process

- Supports the proper software engineering design of the unique AI framework blueprint
- Expecting to work with WP3 & WP4 experts in an open minded way
- Process will be guided by Prof. Dr. Matthias Book (University of Iceland)
- Supported by Software Engineering & testing expert Prof. Dr. Helmut Neukirchen (University of Iceland)



HPC Systems Engineering in the Interaction Room

Matthias Book
with Morris Riedel, Jülich Supercomputing Centre / UoI and Helmut Neukirchen, University of Iceland

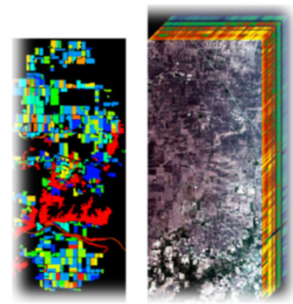
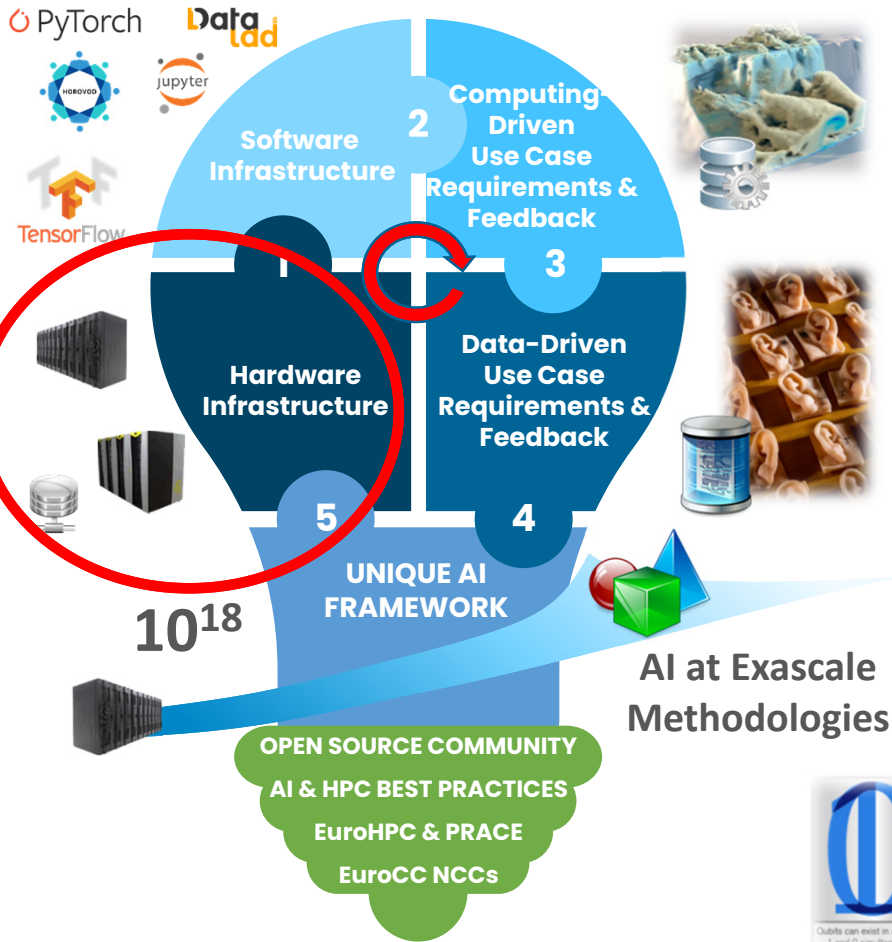


- CoE RAISE @ YouTube: <https://www.youtube.com/channel/UCAdIZ-v6cWwGdapwYxdN7dg>
- **Methology as one CoE RAISE outcome**

Book, M., Riedel, M., Neukirchen, H., Goetz, M.: **Facilitating Collaboration in High-Performance Computing Projects with an Interaction Room**, in conference proceedings of the 4th ACM SIGPLAN International Workshop on Software Engineering for Parallel Systems (SEPS 2017), October 22-27, 2017, Vancouver, Canada

JOIN US IN APRIL – DATE & TIME WILL BE ANNOUNCED

RAISE Quantum Computing Use Case



```
In [ ]: from quantum_SVM import *

# Hyperparameters
B=[2,3,5,10]
K=[2,3]
xi=[0,1,5]
gamma=[-1,0.125,0.25,0.5,1,2,4,8]
n_experiments=len(B)*len(K)*len(xi)*len(gamma)

hyperparameters=np.zeros([n_experiments,4], dtype=float)

path_data_key='input_datasets/calibration/'+id_dataset+'/'
data_key = id_dataset+'calibtrain'
path_out='outputs/calibration/'+id_dataset+'/'

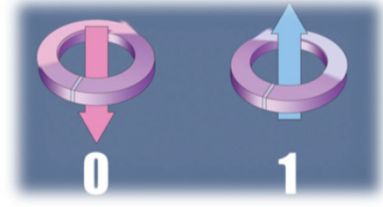
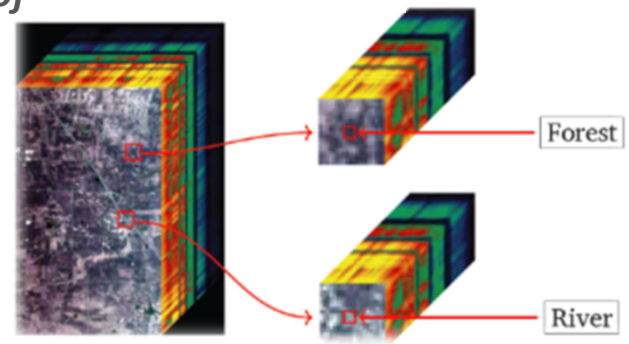
trainacc=np.zeros([fold], dtype=float)
trainauc=np.zeros([fold], dtype=float)
trainauprc=np.zeros([fold], dtype=float)
```



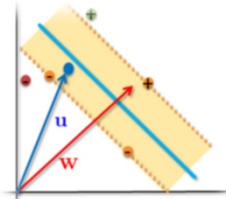
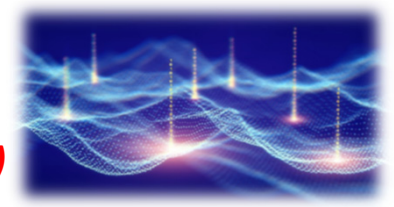
Training based on labeled data of land cover

$$E = \sum_{i \leq j} a_i Q_{ij} a_j$$

Testing based on unseen data



Using Support Vector Machines Machine Learning Models with Quantum Computing (Annealing)



drive. enable. innovate.



The CoE RAISE project receives funding from the European Union's Horizon 2020 – Research and Innovation Framework Programme H2020-INFRAEDI-2019-1 under grant agreement no. 951733