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

RAISE Center of Excellence

EURO

WP2 AI- & HPC-Cross Methods at Exascale

Prof. Dr. – Ing. Morris Riedel

School of Engineering & Natural Sciences, University of Iceland

2021-01-22, RAISE Kick-Off Meeting, Online

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https://www.youtube.com/channel/UCWC4VKHmL4NZgFfKoHtANKg morris@hi.is

WP2 Vision – Intertwined HPC Simulations & AI – 'full loop' ?

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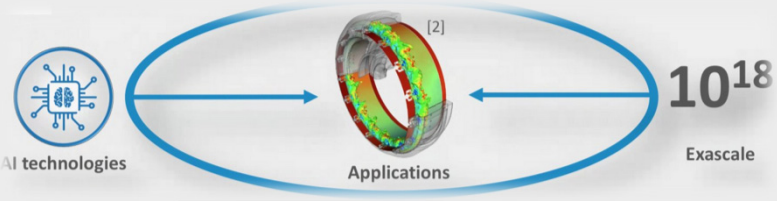
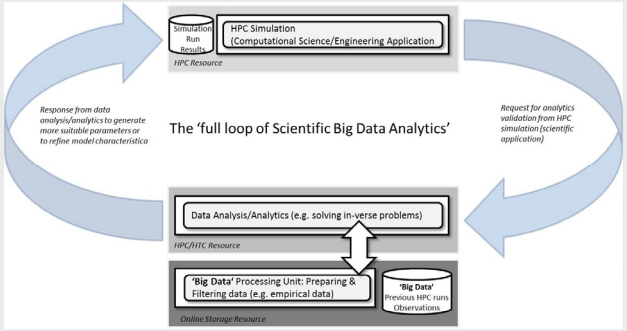
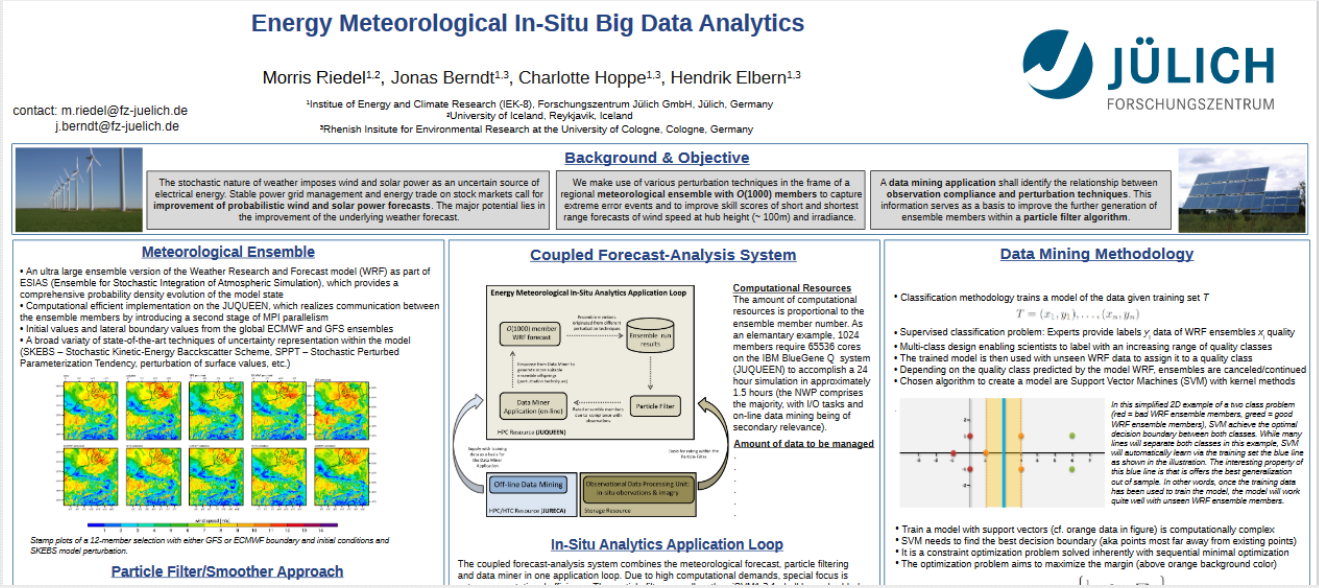
- What means AI & HPC Cross Methods at Exascale?



Today rather high performance data analytics (HPDA)





Lippert, T., Mallmann, D., **Riedel, M.**: Scientific Big Data Analytics by HPC, in Symposium proceedings of NIC Symposium 2016 – publication Series of the John von Neumann Institute for Computing (NIC), NIC Series 48 (417), ISBN 978-3-95806-109-5, February 11-12, 2016, Juelich, Germany

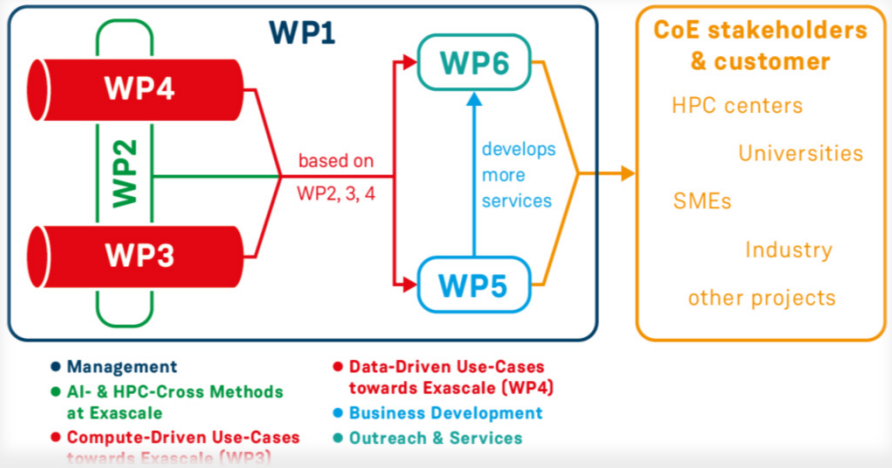
Riedel, M., Berndt, J., Hoppe, C., Elbern, H., Energy Meteorological In-Situ Big Data Analytics, Helmholtz Program Meeting, Karlsruhe Institute of Technology (KIT), July 1, 2016, Karlsruhe, Germany, [PDF (~ 4,08 MB)]

WP2 Partners & Funding Levels

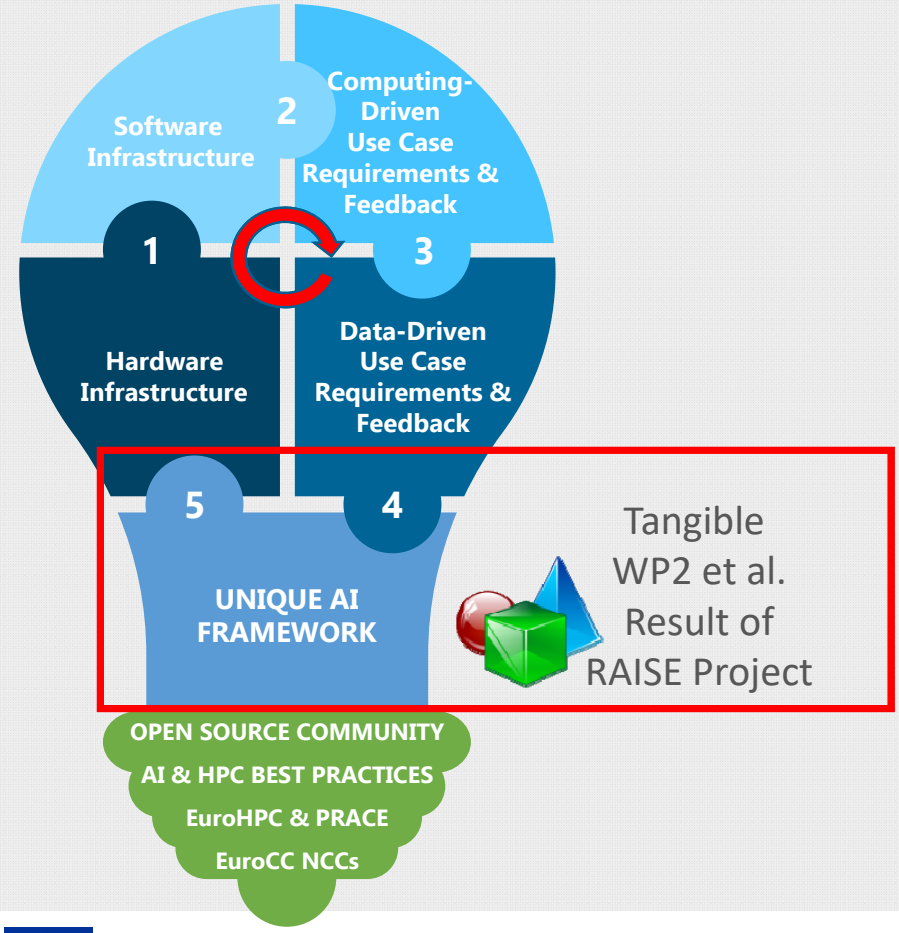
Work package title	AI- and HPC-Cross Methods at Exascale											
Participant No.	1	**2**	3	4	5	6	7	8	9	10	11	
Short name of participant	FZJ	**UOI**	CYI	RWTH	BSC	CERN	CERFACS	BULL	RTU	FM	SAFRAN	**TOT**
PM per partner	43	**24**	0	10	8	8	0	8	22	12	0	**135**
Start month	**1**			**End month**								**36**

WP2 & Connections to other WPs – 'WP2 in a nutshell'

- WP3 (Compute-Driven Use-Cases towards Exascale)
- WP4 (Data-Driven Use-Cases towards Exascale
- Developments in these WPs will be supported by the cross-linking activities of WP2
  - E.g. scaling machine & deep learning codes with frameworks like Horovod/Deepspeed
  - E.g. introduction to new AI methods such as Long-Short Term Memory (Time series)
  - E.g. data augmentation approaches
  - E.g. benchmarking HPC machines and offer also pre-trained AI algorithms (i.e., transfer learning)
  - E.g. offer neural architecture search methods for hyperparameter – tuning in semi-automatic way



WP2 Objectives – 'AI & HPC at Exascale backbone'



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 (→ WP3)

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 pyTorch

Data-driven Use Cases Requirements & Feedback (→ WP4)

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

WP2 Objectives – Can AI do Exascale & use Disruptive Technologies?

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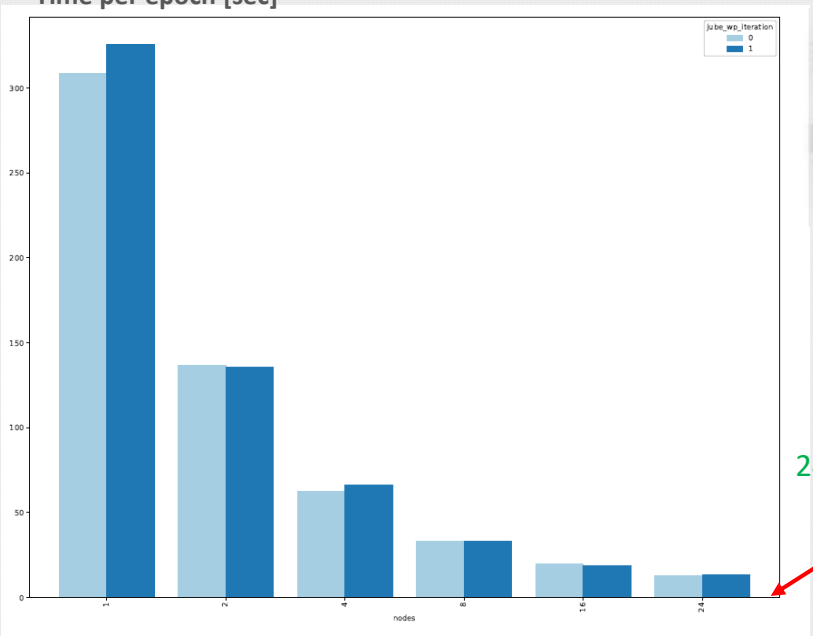
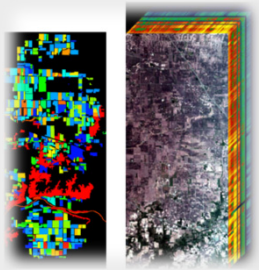
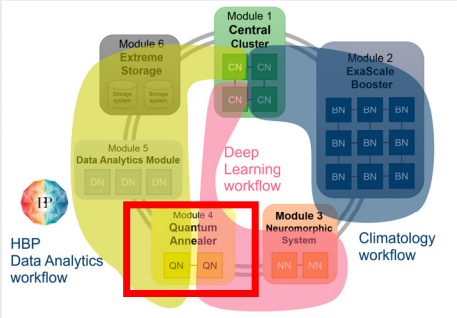
Time per epoch [sec]



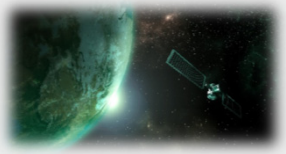
Example from 2019:
Using partition of the JUWELS system has 56 compute nodes, each with 4 NVIDIA V100 GPUs (equipped with 16 GB of memory)

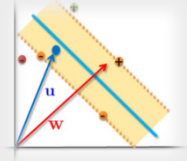
24 nodes x 4 GPUs = 96 GPUs






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





Sedona, R., Cavallaro, G., Jitsev, J., Strube, A., **Riedel, M.**, Book, M.: SCALING UP A MULTISPECTRAL RESNET-50 TO 128 GPUS, 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

Sedona, R., Cavallaro, G., Jitsev, J., Strube, A., **Riedel, M.,** Benediktsson, J.A.: 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

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

WP2 Tasks

Task 2.4 Software design of a unique AI framework plan (M1-M36)

UNIQUE AI FRAMEWORK

Preparing AI Design Plan 1

Preparing AI Design Plan 2

Preparing AI Design Plan 3

Revising the project plan

Revising the AI design plan 1

Revising the AI design plan 2

Revising the AI design plan 3

SOFTWARE INFRASTRUCTURE

Task 2.5 Cross-Sectional AI Methods (M3-M36)

WP3 & WP4 INTERACTIONS

Task 2.2 Hardware prototypes (M1-M18)

Task 2.3 Benchmarking on disruptive technologies (M19-M36)

Task 2.1 Modular and heterogeneous supercomputing architectures (M1-M36)

HARDWARE INFRASTRUCTURE

TIME

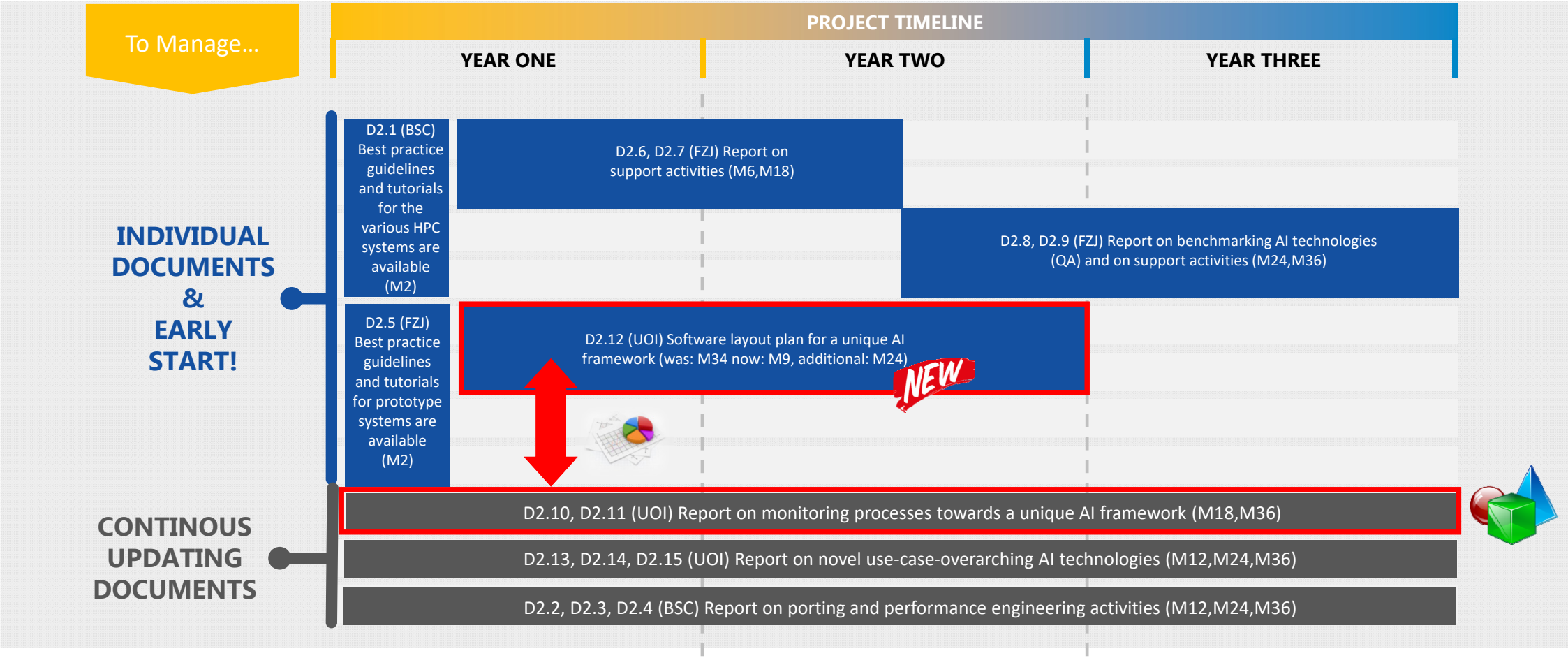
PRE KICK-OFF STAGE

YEAR 1

YEAR 2

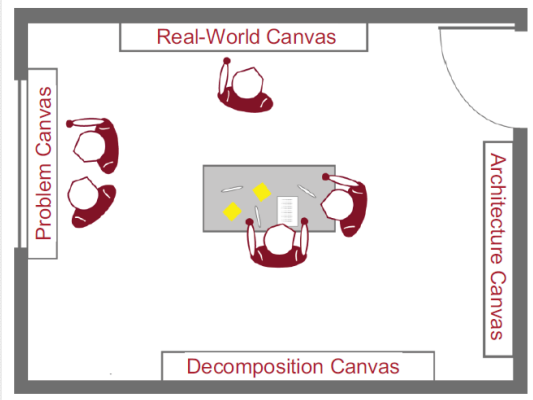
YEAR 3

WP2 Work on Deliverables & Milestones



WP2 Expectations & Requirements

- Start: 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** (Software Engineering, University of Iceland)
  - Supported by Software Engineering & testing expert **Prof. Dr. Helmut Neukirchen** (University of Iceland)



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drive. enable. innovate.

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