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

RAISE Center of Excellence

EURO

CoE RAISE – Role of MLOps

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Juelich Supercomputing Centre, Forschungszentrum Juelich, Germany

2021-09-30, RAISE CoE Seminar MLOps with ClearML, Online

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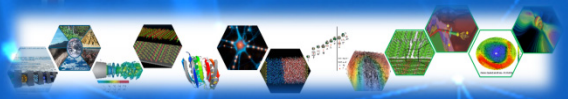
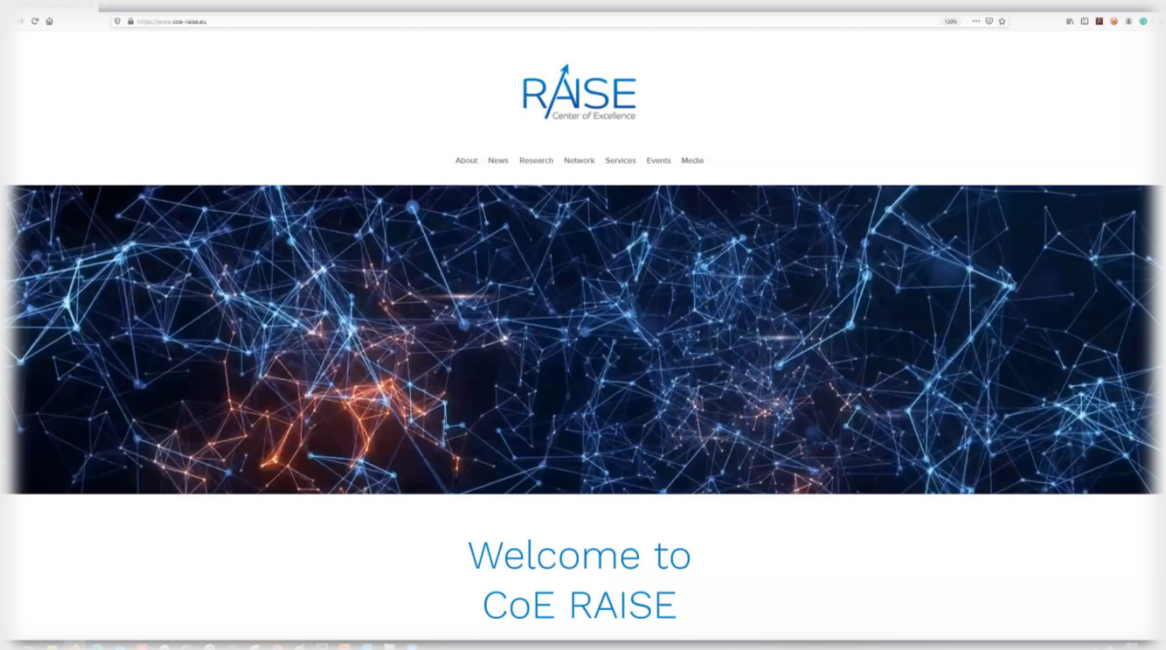
https://www.youtube.com/channel/UCWC4VKHmL4NZgFfKoHtANKg morris@hi.is

IHPC National Competence Center (NCC) for HPC & AI in Iceland

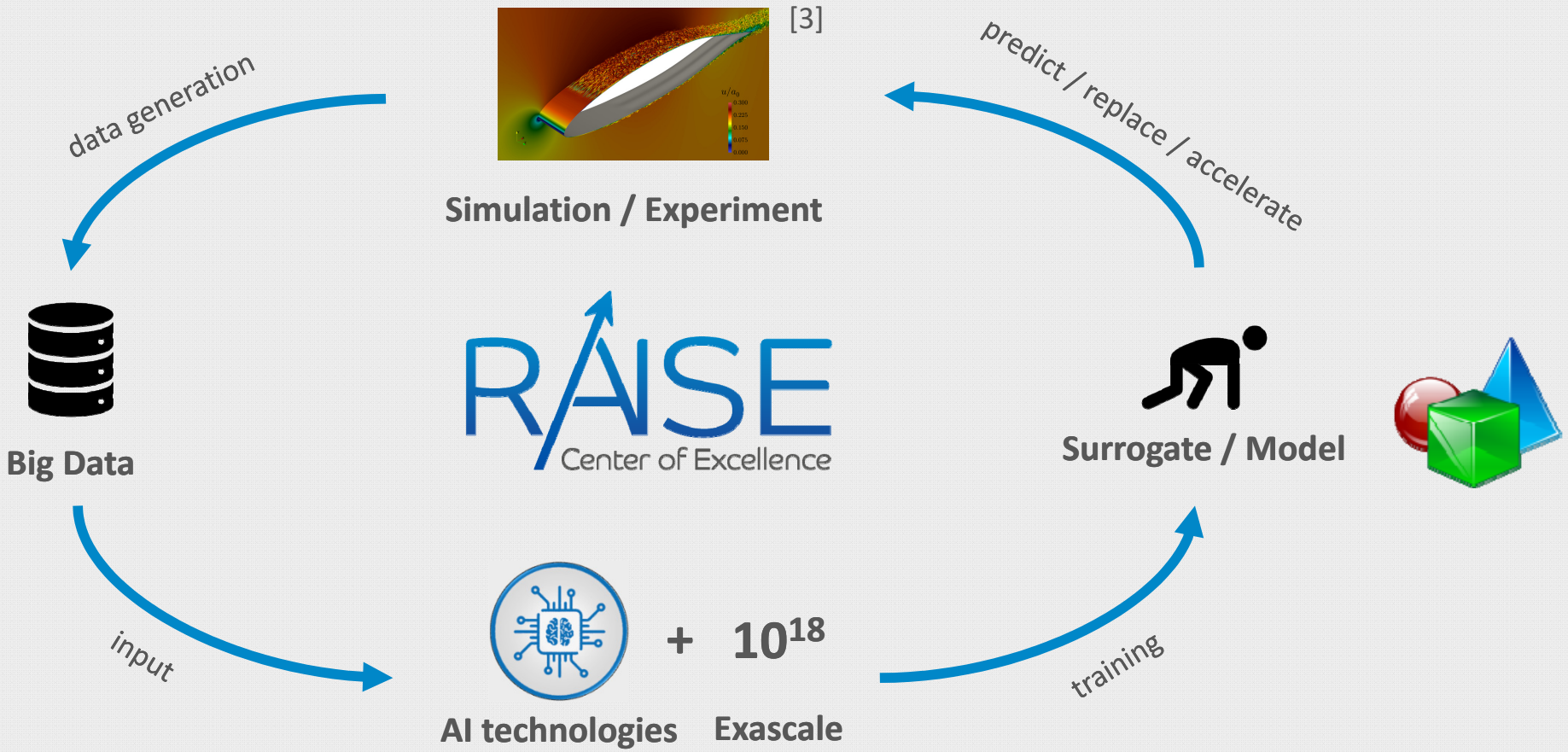


CoE RAISE Web Page & More Information



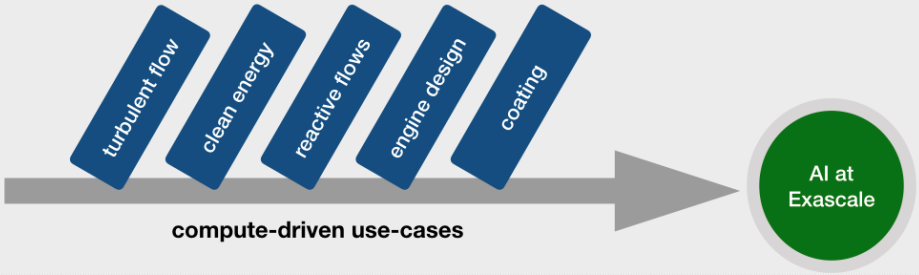
https://www.coe-raise.eu

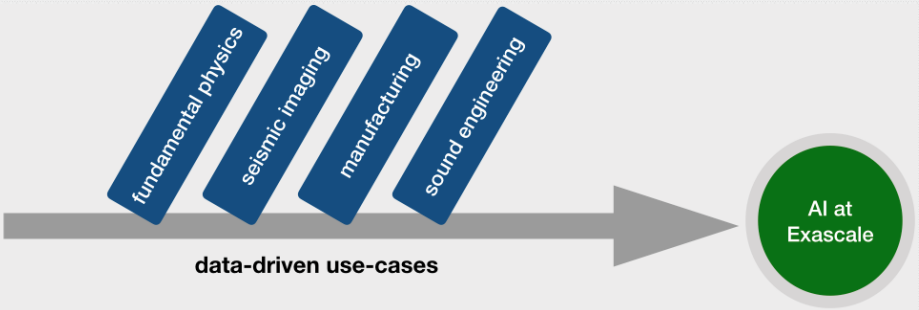
CoE RAISE – Motivation & Approach

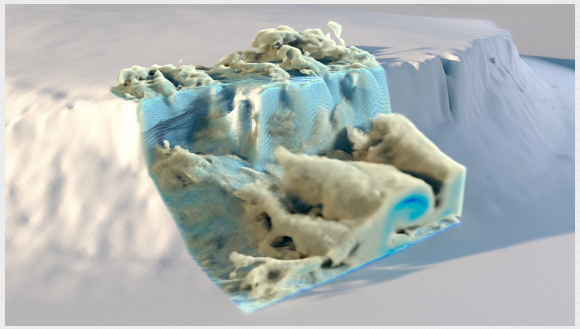


Use Cases in CoE RAISE

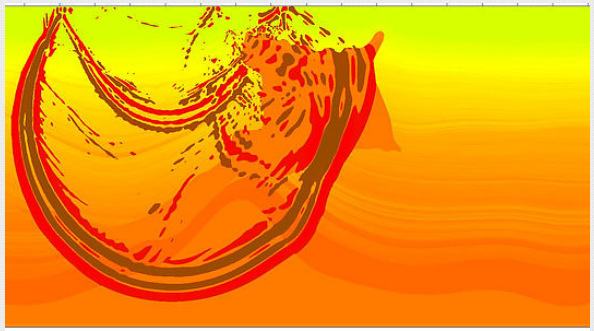
- Two kinds of use cases:





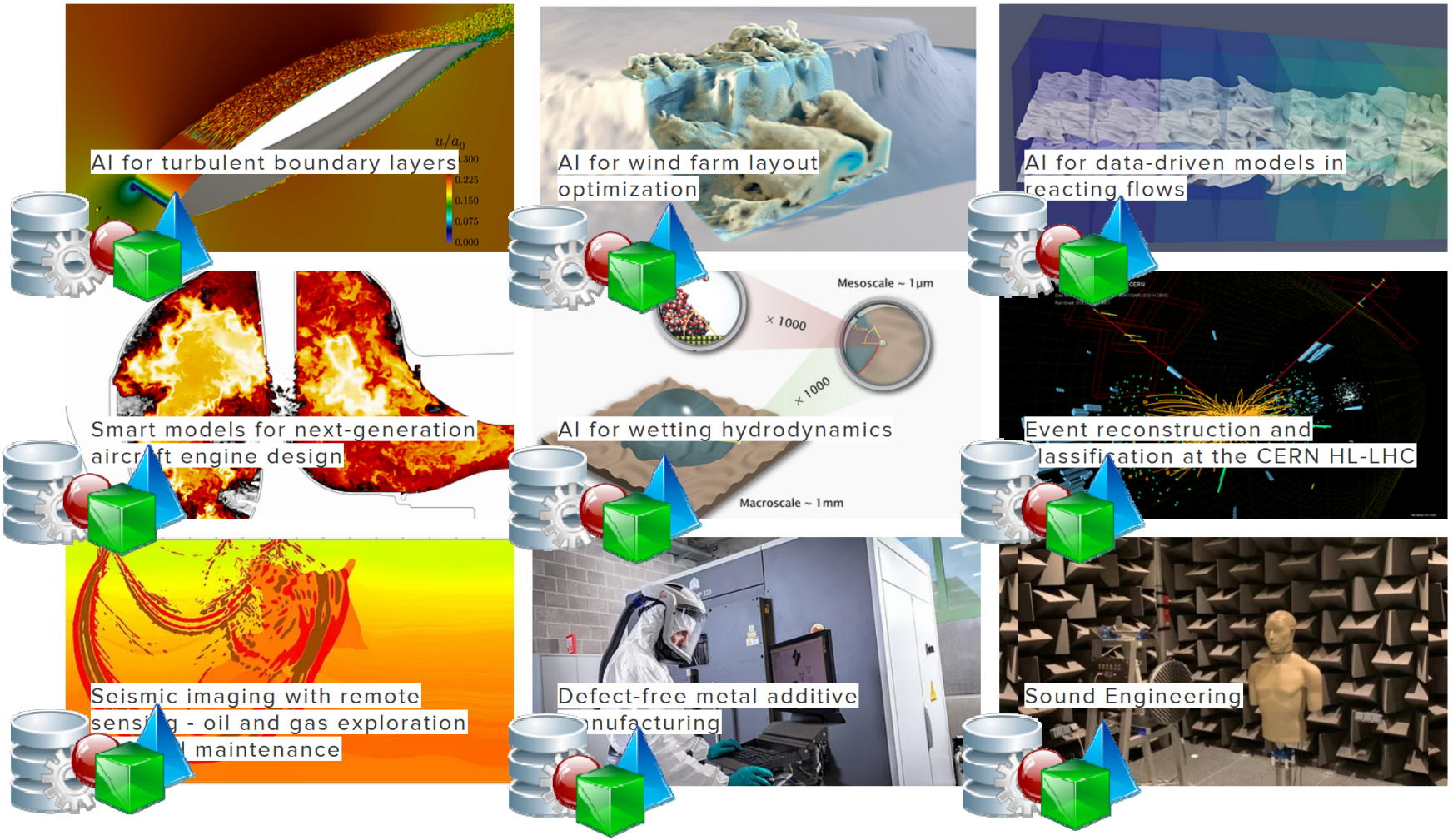


Example from use case "AI for wind farm layout": Turbulence generated by a cliff on Bolund Island, Denmark.



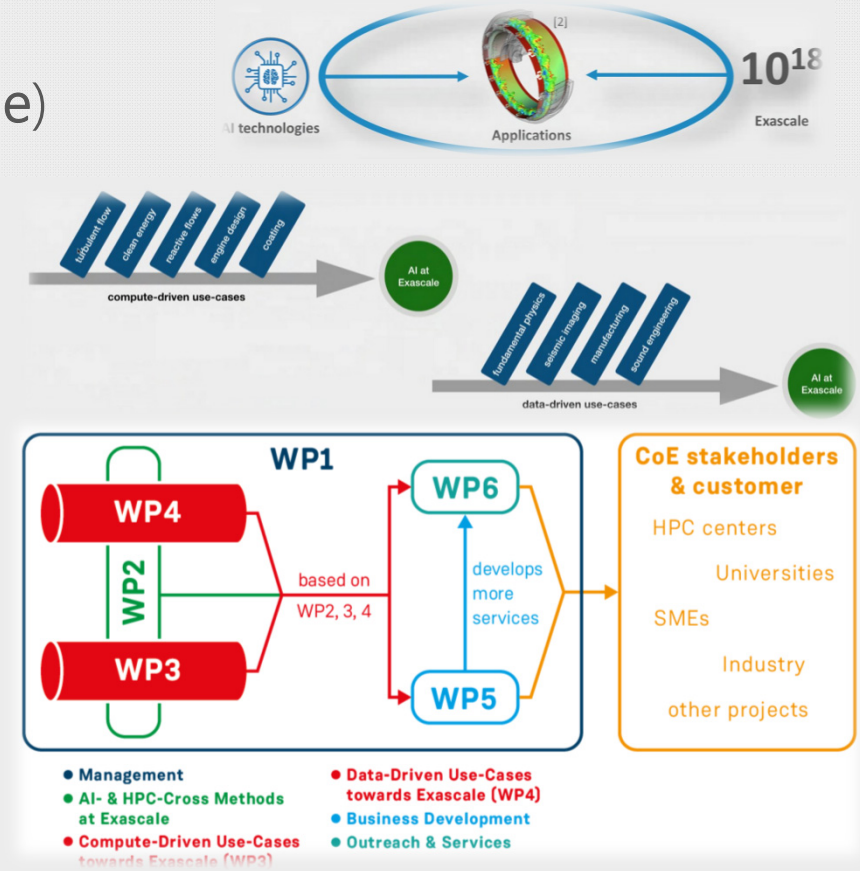
Example from use case " Seismic imaging with remote sensing - oil and gas exploration and well maintenance": Snapshot from a wavefield.

Compute- and Data-driven Use Cases – Use & Generate Data

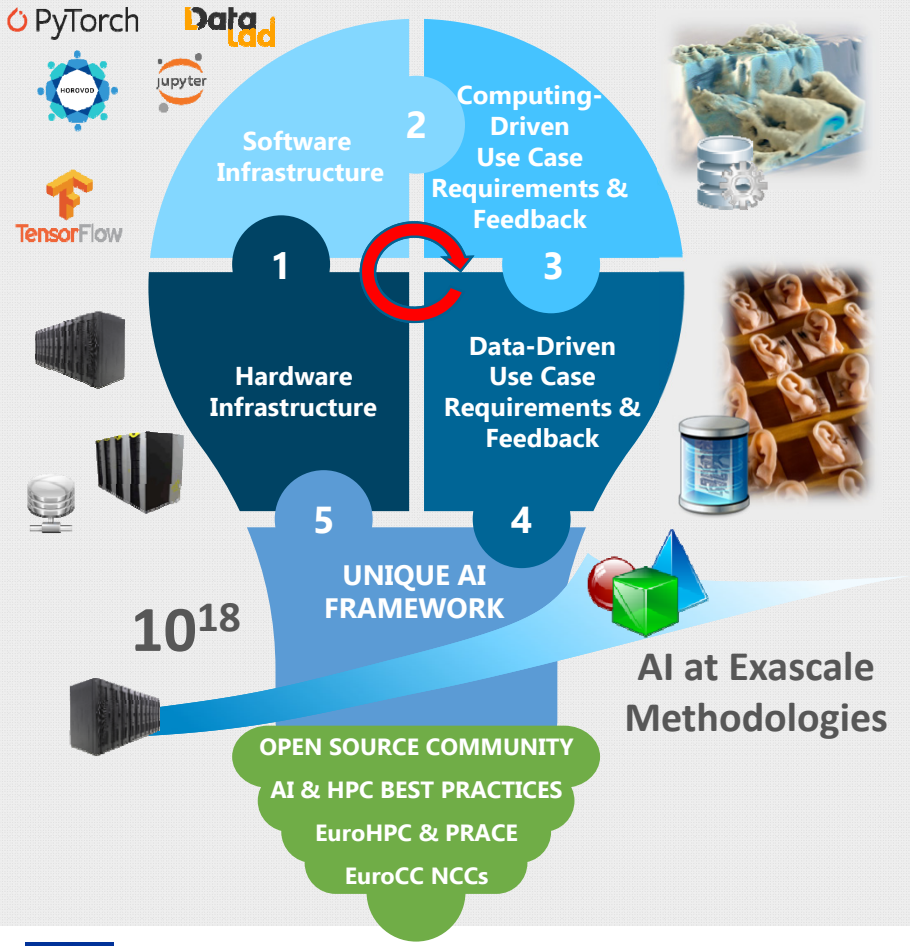


WP2 – AI- & HPC-Cross Methods at Exascale in a nutshell

- 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



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 pyTorch

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

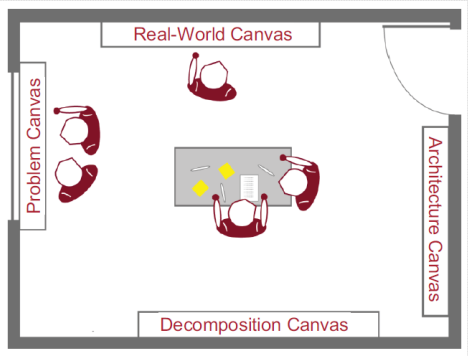
Selected Techniques to Identify Cross-Methods for HPC & AI

- Fact Sheets
  - Foster initial understanding
  - Living document & each Fact Sheet per WP3/WP4 Use Case
  - *(Experience from many other EU projects)*

- Selected Contents
  - Short Application Introduction
  - Clarify Primary Contacts
  - Codes/Libraries/Executables
  - HPC System Usage Details
  - Specific Platforms & 'where is what data'?
  - Machine/Deep Learning Approaches of Interest

initial steps

Driven by
Prof. Matthias Book &
Prof. Helmut Neukirchen



interaction room process

Fact Sheet Process of CoE RAISE & Early Co-Design Examples

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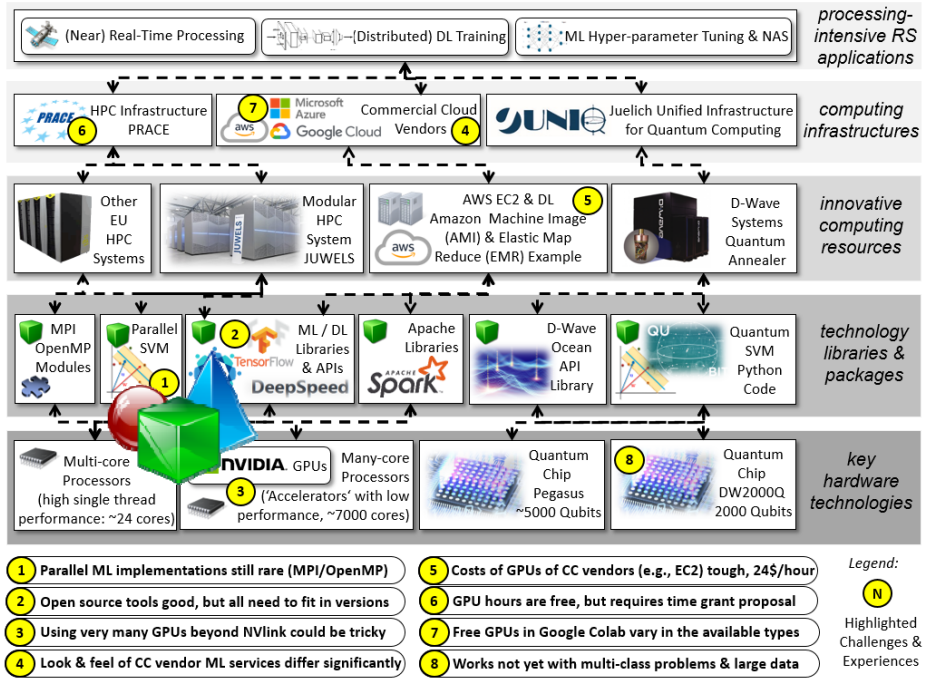
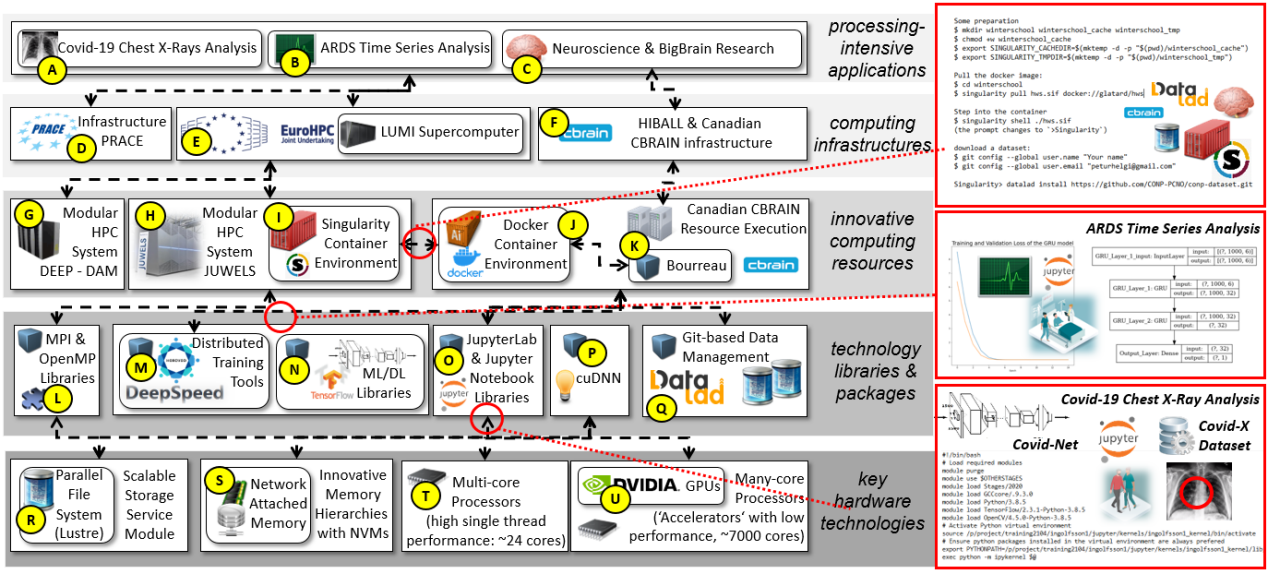


Riedel, M., Cavallaro, G., Benediktsson, J.A.: Practice and Experience in using Parallel and Scalable Machine learning in Remote Sensing from HPC over Cloud to Quantum Computing, in conference proceedings of the IEEE IGARSS Conference, Brussels, Belgium, 2021, Physical and Online event, to appear
https://igarss2021.com/

Riedel, M., Sedona, R., Barakat, C., Einarsson, P., Hassanian, R., Cavallaro, G., Book, M., Neukirchen, H., Lintermann, A.: Practice and Experience in using Parallel and Scalable Machine learning with Heterogenous Modular Supercomputing Architectures, in conference proceedings of the IEEE IDPDS Conference, Heterogenous Computing Workshop (HCW), Portland, USA, 2021, Online, to appear
https://www.ipdps.org/

IPDPS 2021 Portland



Compute- and Data-driven Use Cases Fact Sheets – Drafts(!)

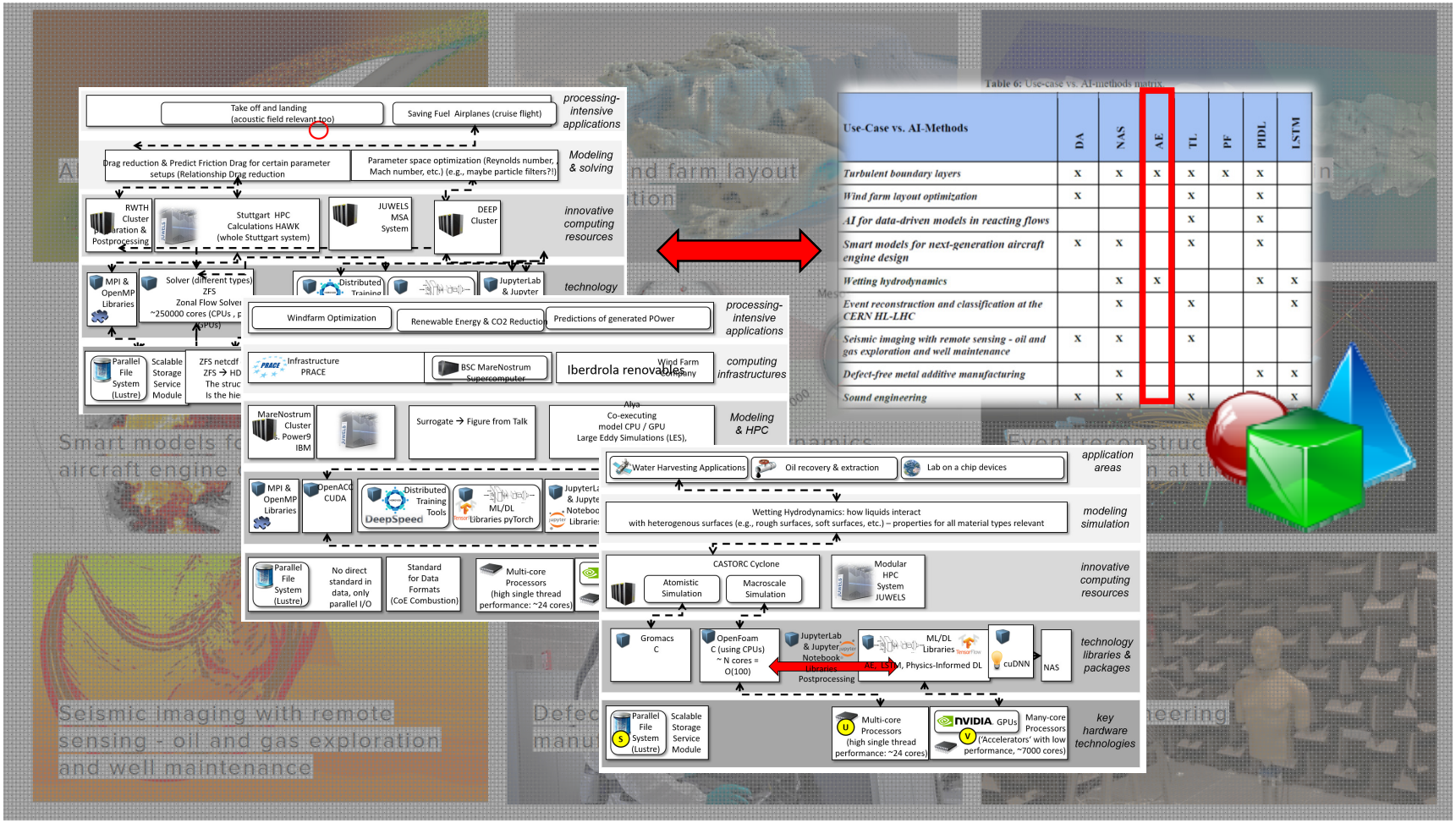


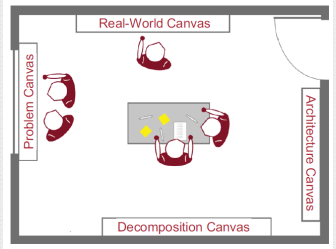
Table 6: Use-case vs. AI-methods matrix

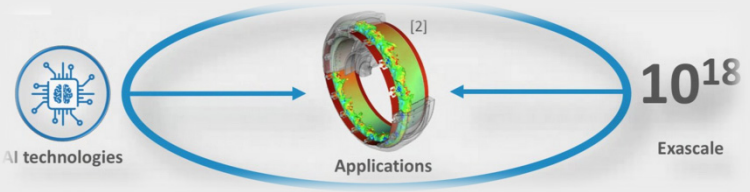
Use-Case vs. AI-Methods	DA	NAS	AE	TL	PF	PIDL	LSTM
Turbulent boundary layers	X	X	X	X	X	X	
Wind farm layout optimization	X			X		X	
AI for data-driven models in reacting flows				X		X	
Smart models for next-generation aircraft engine design	X	X		X		X	
Wetting hydrodynamics		X	X			X	X
Event reconstruction and classification at the CERN HL-LHC		X		X			X
Seismic imaging with remote sensing - oil and gas exploration and well maintenance	X	X		X			
Defect-free metal additive manufacturing		X				X	X
Sound engineering	X	X		X			X

WORK IN PROGRESS

HPC Systems Engineering in the Interaction Room Seminar

- CoR RAISE Interaction Room Process as Next Step
  - 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)
  - 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

RAISE Initial Identified AI/HPC Methods (Milestone M7)

MS2 - AI/HPC Methods (M7)

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BEFORE

Table 6: Use-case vs. AI-methods matrix.

Use-Case vs. AI-Methods	DA	NAS	AE	TL	PF	PIDL	LSTM
Turbulent boundary layers	X	X	X	X	X	X	
Wind farm layout optimization	X			X		X	
AI for data-driven models in reacting flows				X		X	
Smart models for next-generation aircraft engine design	X	X		X		X	
Wetting hydrodynamics		X	X			X	X
Event reconstruction and classification at the CERN HL-LHC		X		X			X
Seismic imaging with remote sensing - oil and gas exploration and well maintenance	X	X		X			
Defect-free metal additive manufacturing		X				X	X
Sound engineering	X	X		X			X

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NEW

H2020-INFRAEDI-2018-2020

CoE RAISE

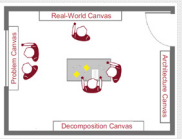
Center of Excellence "Research on AI- and Simulation-Based Engineering at Exascale"

Grant Agreement Number: 951733

MS2

AI/HPC Methods

Draft



Continously Updating

Use Case	AE	PIML	ANNs	CNN		NO	SMs			GNN	IN	LSTM	GRU
Details	***CAE***		***RBF-ANN***	***U-Net***	***RESNET***	***FNO***	***AR***	***ARMA***	***ARIMA***		***JEDI-net***		
AI for turbulent boundary layers	X	X											
AI for wind farm layout optimization			X				X	X	X				
AI for data-driven models in reacting flows				X						X			
Smart models for next generation aircraft engine design				X						X			
AI for wetting hydrodynamics						X							
Event reconstruction and classification at the CERN HL-LHC use case										X	X		
Seismic imaging with remote sensing for energy applications	X				X								
Detect-free metal additive manufacturing	X				X								
Sound Engineering												X	X

MLOps Platforms relevant in RAISE Unique AI Framework for Exascale

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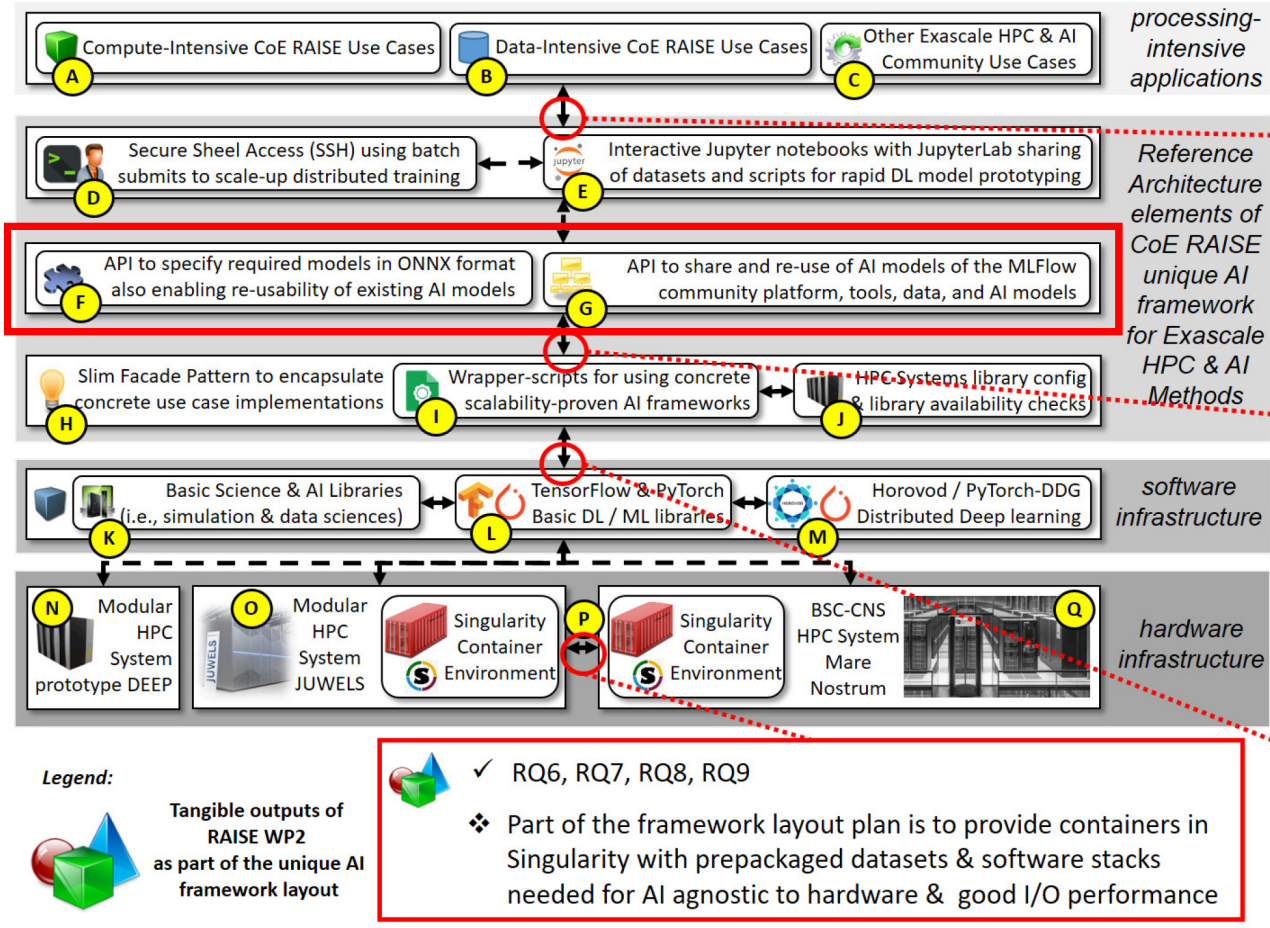

✓ RQ1, RQ2, RQ4, RQ5

❖ Parts of the framework layout plan is to provide Kernels for Jupyter notebooks with correct version setups of modules for specific HPC Systems

✓ RQ3, RQ6

❖ Parts of the framework layout plan is to provide a lightweight and abstract Python API building on ONNX enabling also exchanges via MLFlow/ClearML

✓ RQ1, RQ2, RQ8, RQ9

❖ Parts of the framework layout plan is to provide a lightweight Python API that abstracts from low level versioning of AI packages (with proven scalability) and is harmonized with different available HPC system module versions

✓ RQ6, RQ7, RQ8, RQ9

❖ Part of the framework layout plan is to provide containers in Singularity with prepackaged datasets & software stacks needed for AI agnostic to hardware & good I/O performance

Legend:

Tangible outputs of RAISE WP2 as part of the unique AI framework layout

Continously Updating

drive. enable. innovate.

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