



EuroHPC
Joint Undertaking



T2.5 - Cross-sectional AI methods Status & next steps – Extension Period Discussions (**M42+**)

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Lead of CoE RAISE WP2 – AI- and HPC-Cross Methods at Exascale

2023-08-28, AHM RAISE, Hveragerði, Iceland



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



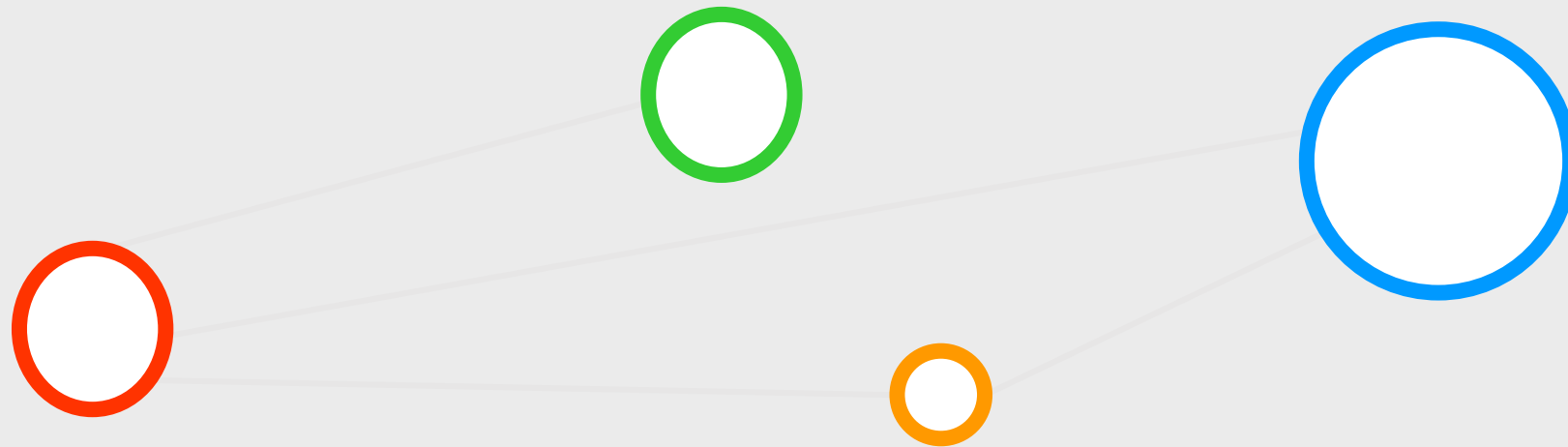
morris@hi.is



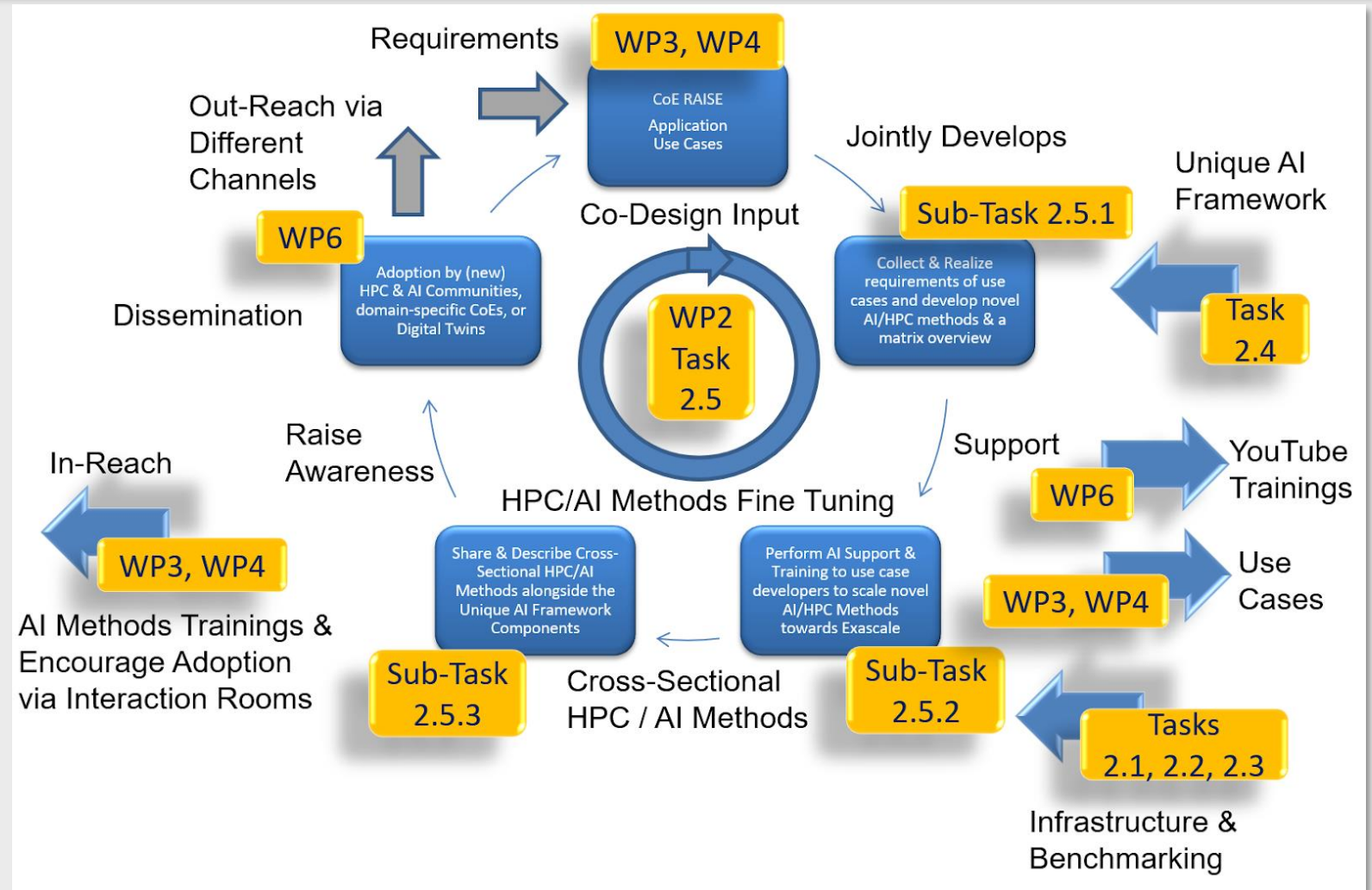
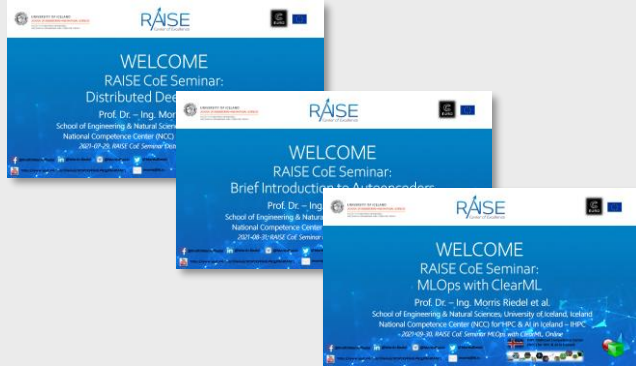
- Task 2.5 Process
 - Overview
- Challenges in using AI Methods on HPC at Scale
 - Toolset Challenges & Unique AI Framework Activities (previous talk in workshop)
 - Understanding Skillset Challenges on cross-sectional HPC/AI Methods
- Lessons Learned of HPC/AI Methods Matrix Process
 - Meetings & Interaction Room to Dive into Method Details
 - Evolution on the Adoption of HPC/AI Methods
 - Role of Hyperparameter Optimization towards Exascale
 - Role of Quantum Computing as Accelerator
 - Role of YouTube Trainings for Skillset Building
- Summary & Q&A
 - Feedback from NCCs on AI/HPC Methods
 - Additions of new use cases with new AI/HPC methods



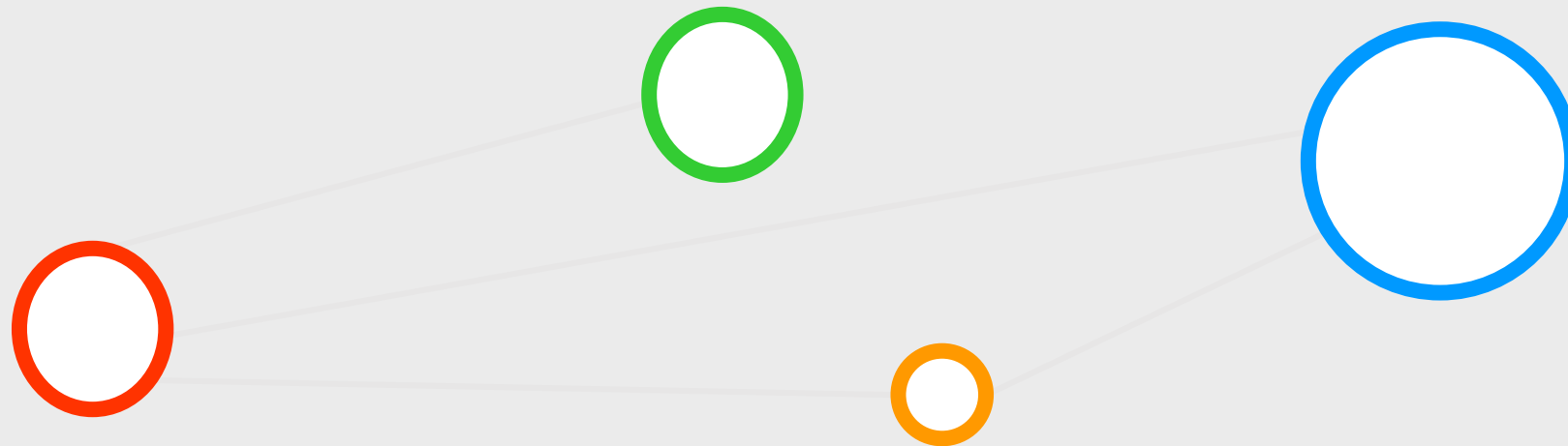
Task 2.5 Process



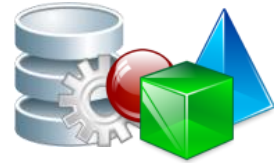
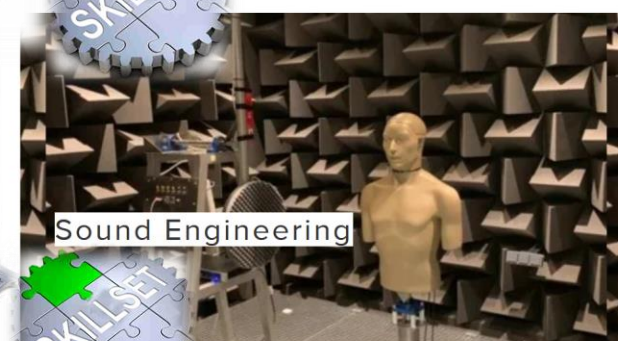
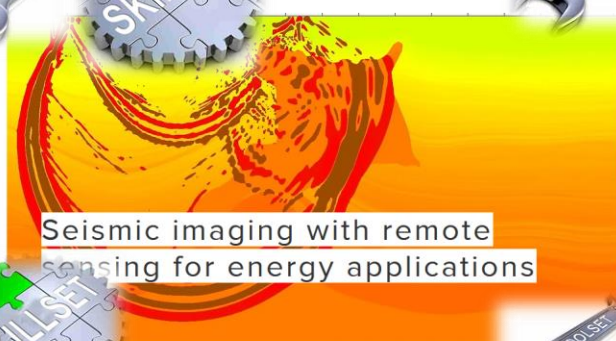
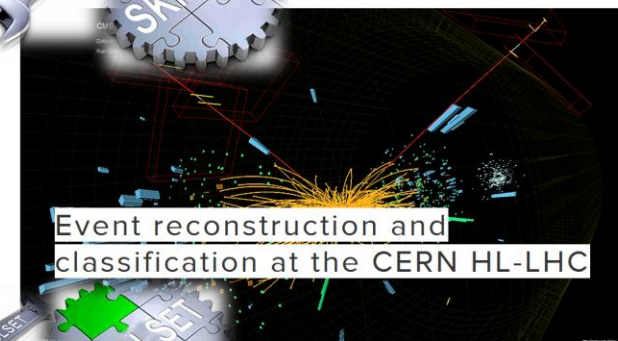
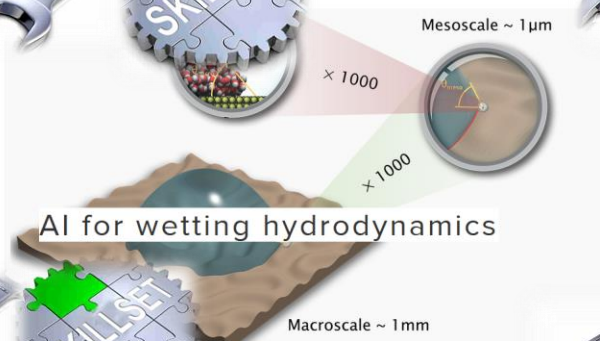
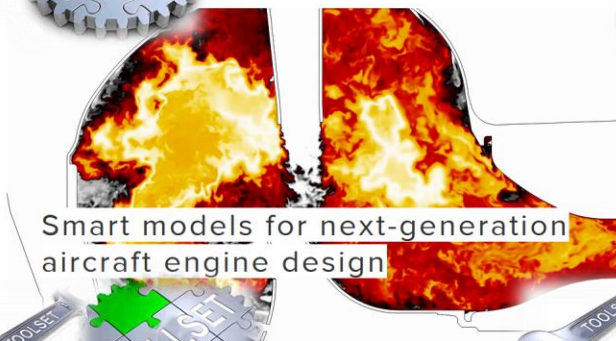
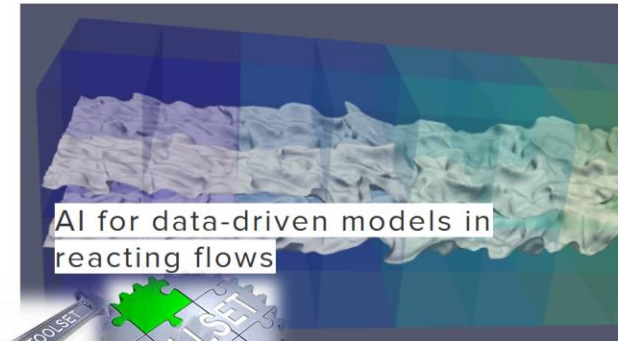
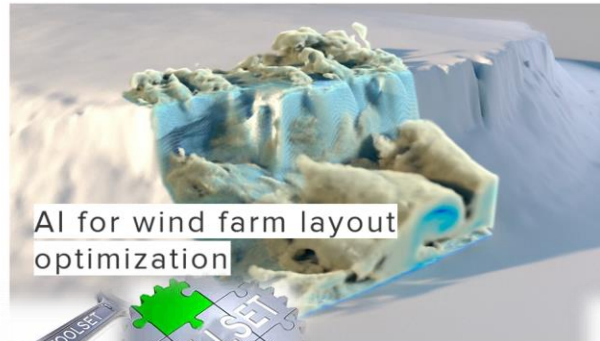
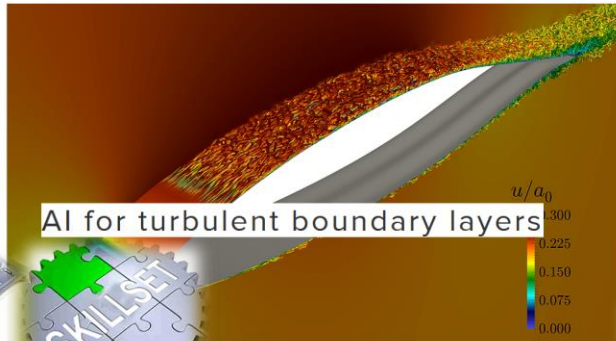
Task 2.5 Process



Challenges in using AI Methods on HPC at Scale



Complex Challenges of a wide area of Toolsets & Skillsets



PyTorch

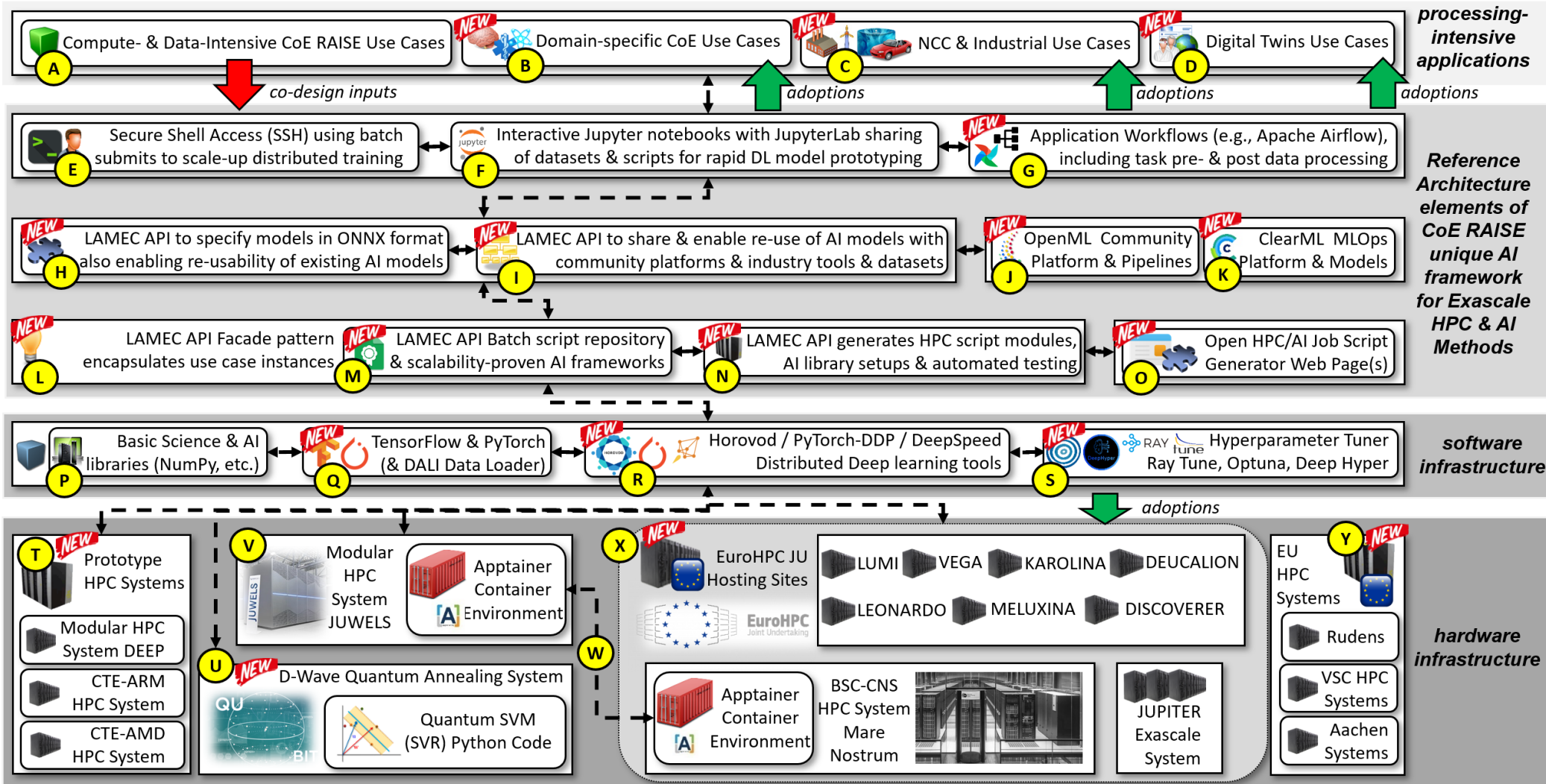


TensorFlow

DataLad



Realization of SW Framework – Task 2.4 Achievements



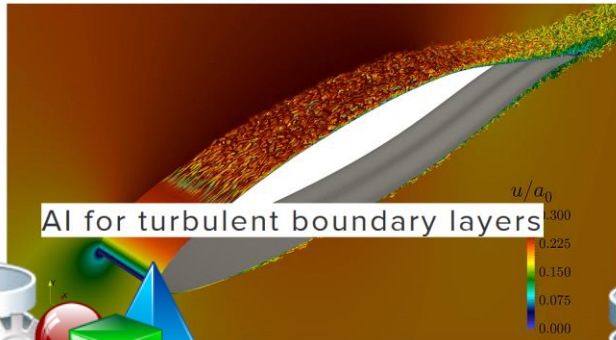
The strategy of “ready-to-run toolsets” Presented at CASTIEL Code of the Month event (2023-07-26 public Webinar), where to put the tools in the overview, e.g. HPC4AI, PhzDLL, etc.?



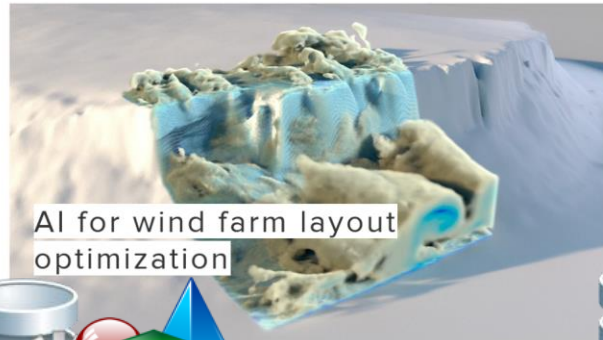
Continuously Updating!

Extension Period Discussions: LAMEC = Load AI Modules, Environments, and Containers – How far can we go? How many systems to add? What happens at M43? Sustainability? Calls?

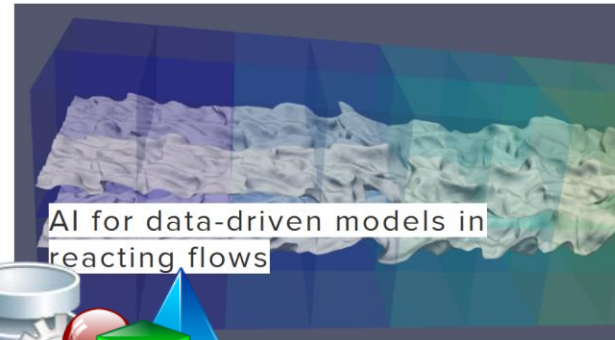
Compute- and Data-driven Use Cases – Data & Modeling



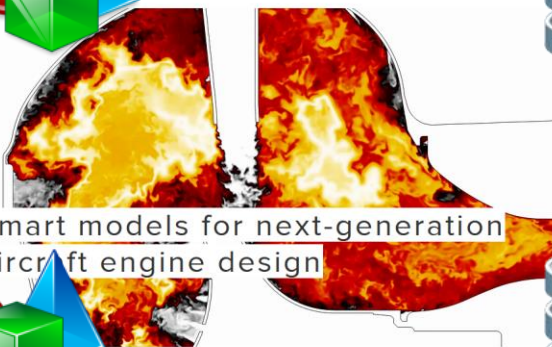
AI for turbulent boundary layers



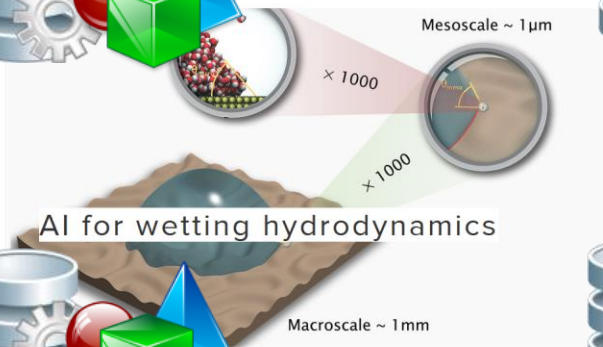
AI for wind farm layout optimization



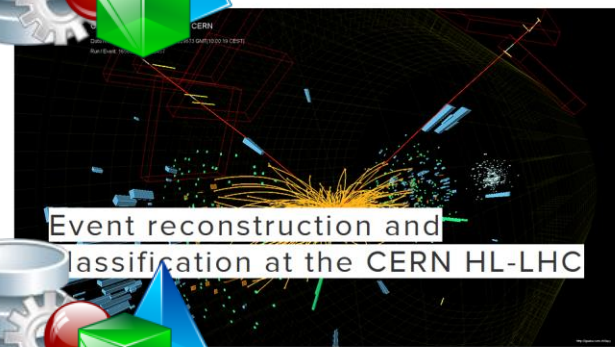
AI for data-driven models in reacting flows



Smart models for next-generation aircraft engine design



AI for wetting hydrodynamics



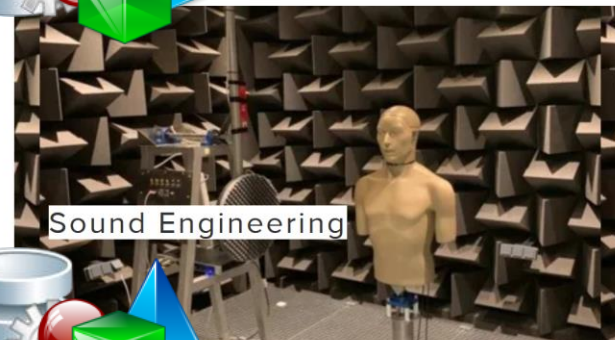
Event reconstruction and classification at the CERN HL-LHC



Seismic imaging with remote sensing for energy applications

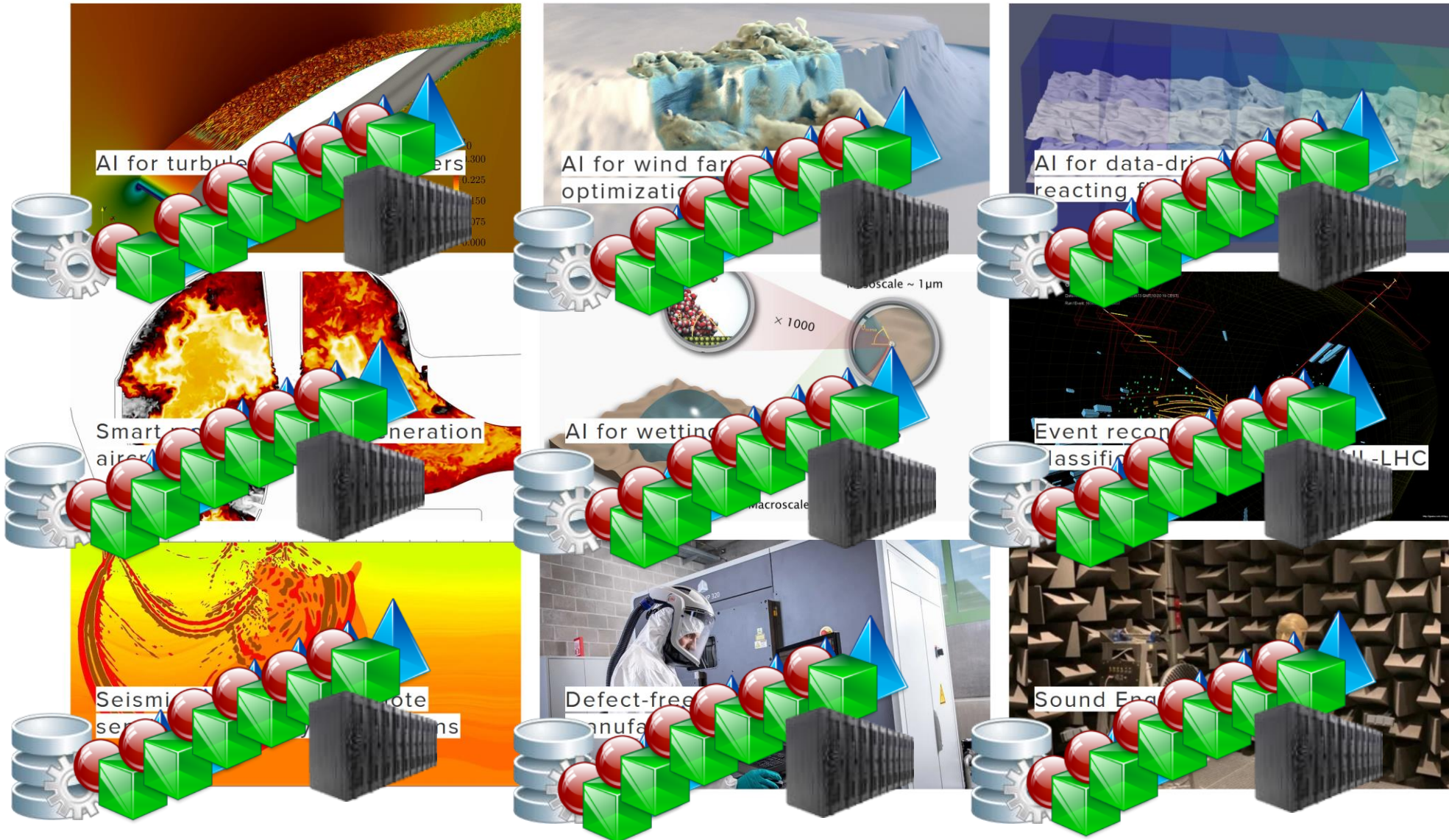


Defect-free metal additive manufacturing



Sound Engineering

Use Cases – Many AI Models & Hyperparameter Relevance

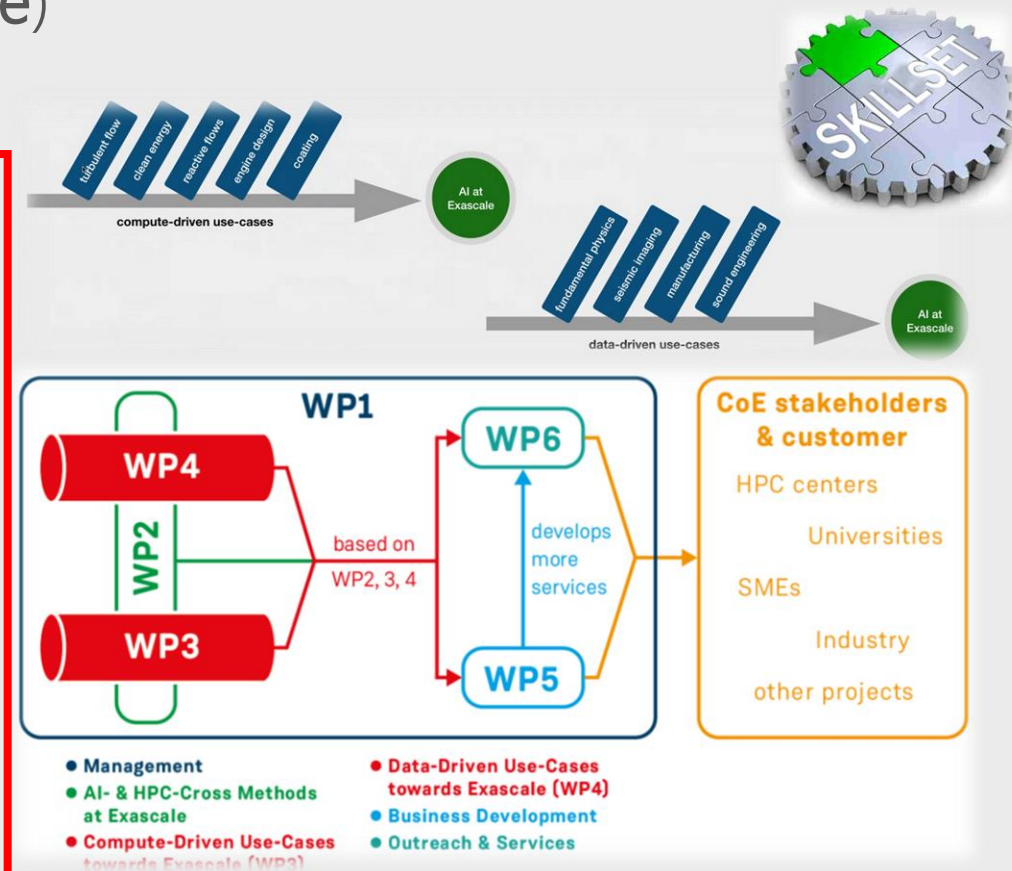


WP2 – AI- & HPC-Cross Methods at Exascale in a nutshell

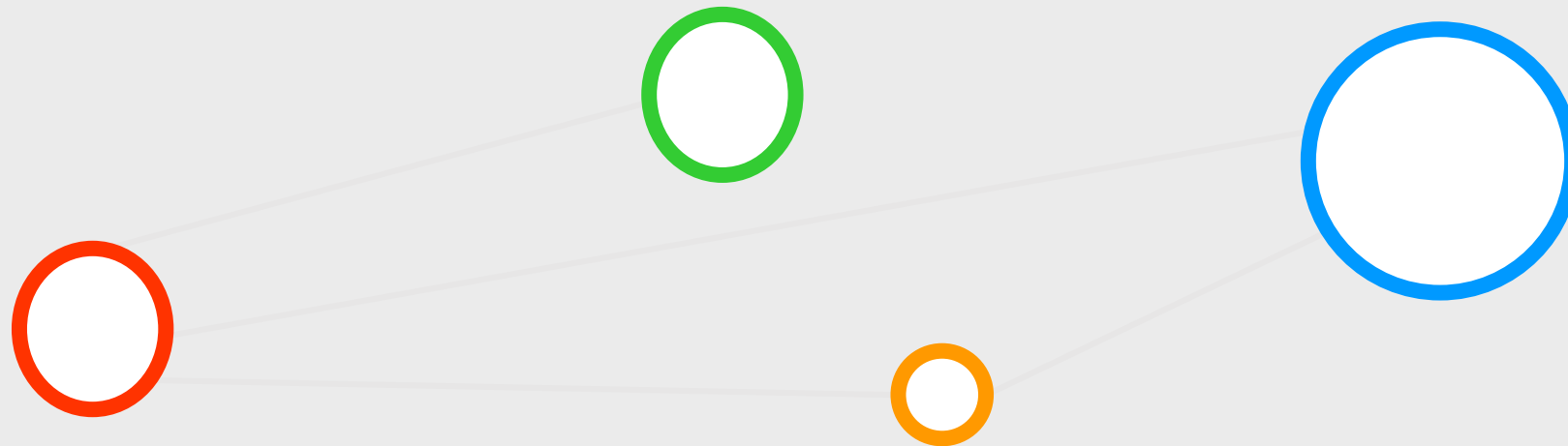
- WP3 (Compute-Driven Use-Cases towards Exascale)
- WP4 (Data-Driven Use-Cases towards Exascale)

➤ 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

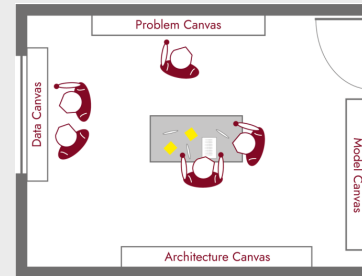


Lessons Learned of HPC/AI Methods Matrix Process



➤ CoR RAISE Interaction Room Process as Next Step

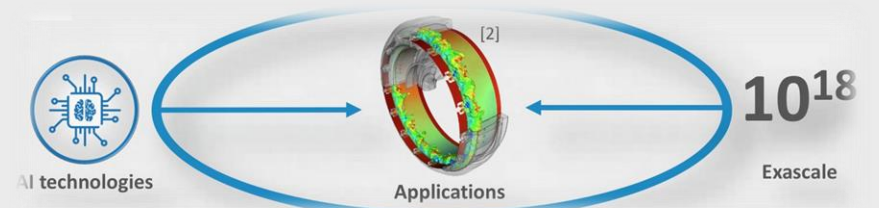
- Supports the proper software engineering design of the unique AI framework blueprint
- Expecting to work with WP3 & WP4 experts in an open minded way
- Process will be guided by **Prof. Dr. Matthias Book** (University of Iceland)
- Supported by Software Engineering & testing expert **Prof. Dr. Helmut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



HPC Systems Engineering in the Interaction Room

Matthias Book

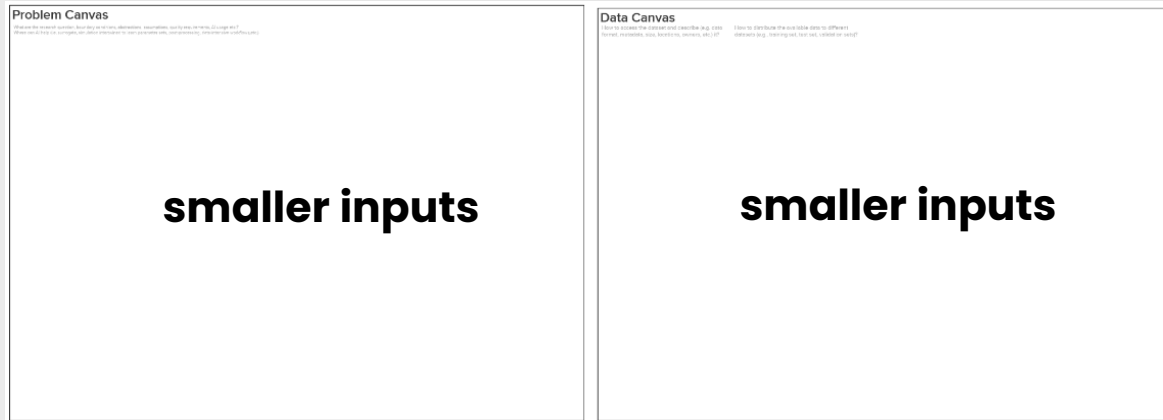
with Morris Riedel, Jülich Supercomputing Centre / UoI and Helmut Neukirchen, University of Iceland



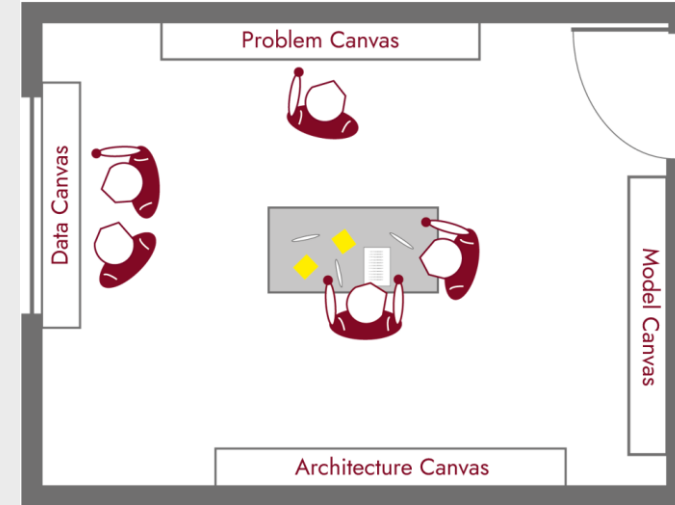
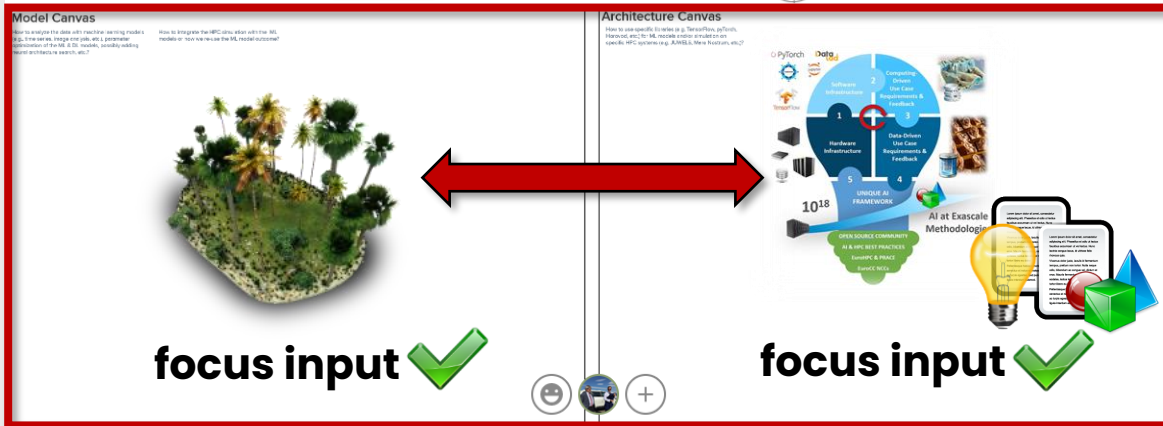
[1] Book, M., Riedel, M., Neukirchen, H., Goetz, M.: Facilitating Collaboration in High-Performance Computing Projects with an Interaction Room, in conference proceedings of the 4th ACM SIGPLAN International Workshop on Software Engineering for Parallel Systems (SEPS 2017), October 22-27, 2017, Vancouver,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

[5] Book, Riedel, Neukirchen, Erlingsson: Facilitating Collaboration in Machine Learning and High-Performance Computing Projects with an Interaction Room, International Workshop on Software Engineering for eScience, IEEE 2022

Interaction Rooms with WP3/WP4 Teams



Interaction Room 3.4
Engine Design



IR Mural Links

- IR3.1 Turbulent Flow: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377866397/8613c384d54f66fb5e78599f307a4ce8a9090c0?sender=u15e3008bb41d6628a5bb5701>
- IR3.2 Clean Energy: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377887905/cb44cca3eedd3bb9964fba36af16b1bfcee085f?sender=u15e3008bb41d6628a5bb5701>
- IR3.3 Reactive Flows: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377959022/0c363886f24833ecb19b025d87324b57fd50e2db?sender=u15e3008bb41d6628a5bb5701>
- IR3.4 Engine Design: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377976343/8d7aba6be09af3b2ff2305d2f709c53661ac889d?sender=u15e3008bb41d6628a5bb5701>
- IR3.5 Coating: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377991014/7a5d7e1eaf230178342d1e1d4a84d656d9055d52?sender=u15e3008bb41d6628a5bb5701>
- IR4.1 Fundamental Physics: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378007555/6f0d5285feaec5eafa515bd6676e84d8b4879d39?sender=u15e3008bb41d6628a5bb5701>
- IR4.2 Seismic Imaging: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ac3e28af4bb8d9adbec33874998?sender=u15e3008bb41d6628a5bb5701>
- IR4.3 Manufacturing: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378038069/93df6fa7a41093f4eaae7be9d72979de2ba42b9d?sender=u15e3008bb41d6628a5bb5701>
- IR4.4 Sound Engineering: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa12219002404059f90a4bbb0101fa379a8503?sender=u15e3008bb41d6628a5bb5701>

In addition to WP2 Monthly Meetings & Monthly Trainings

Interaction Room Example: Task 3.1 & Detail Levels



Problem Canvas

AIM: optimize net power saving

How can AI help?

Simplifications

- Generic non-actuated TBL
- Actuated TBL
- Airfoil wing section turbulent boundary layer

Specific research questions

- Drag, see how dependence on actuation parameters (pressure, velocity)
- Understand friction reduction mechanism
- Overall drag reduction (friction drag, pressure drag)
- Friction drag modification in non-zero pressure gradient TBL

Find model for drag power dependence on parameters

Surrogate model for TBL

Data Canvas

How to access the dataset and describe its structure? metadata, size, location, version, etc. (if possible) e.g., training set, test set, validation set?

How to distribute the available data to different users?

Lightweight data

- Time-resolved integrated drag (time-series, .dat files)
- Typical file size 1 mb (500 MB if non-integrated time series)

Heavyweight data

- 2D instantaneous plane snapshot (HDF5, few variables u(x,y), rho(p))
- Typical file size 1-5 mb for single snapshot with multiple (1-5) planes
- 3D instantaneous box snapshot (HDF5, flow variables u(x,y,w,p))
- Typical file size 0.5-1 GB for single snapshot
- 3D averaged flow field (HDF5, flow variables, first and second order statistical moments)
- total: ~10 GB

Challenges? Large amounts of data (10-100 TB) for parameter studies

TBL data/signals are broadband in nature

Block-structured data with (i,j,k)-indexing

Simple access via HDF5 support within Python

Interaction Room 3.1 Turbulent Flow

Model Canvas

How to analyze the data with machine learning methods (e.g., 3D feature, image analysis, etc.) parameter optimization of the ML, EoS, models, anomaly spotting, neural architecture search, etc.?

How to integrate the HPC simulation with the ML model or how we reuse the ML model outcome?

Review

work in progress

problems

architecture

code

ML data

Architecture Canvas

How to use specific libraries (e.g., TensorFlow, PyTorch, Horovod, etc.) for ML, model, and/or simulation in specific HPC systems (e.g., AURELIS, New Horizon, etc.)?

in MAIA Structured

Compatible from volume solver

Container block-structured meshes

implicit large-scale solvers (EoS)

C++-enabled OpenMP parallelization

software 1

software 2

hardware

notes

Scaling results are in Deliverable 2.2

AMD machines, 31 convolutions are not working. Fixed with ROCm 5.x

quantum annealing FZJ

exascale

Cross HPC/AI Methods Initial Evolution (M0 → M7)

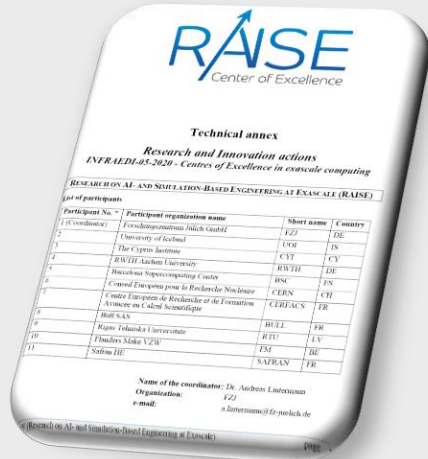
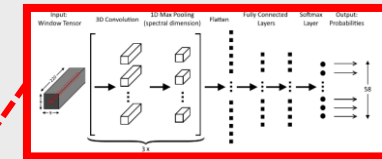
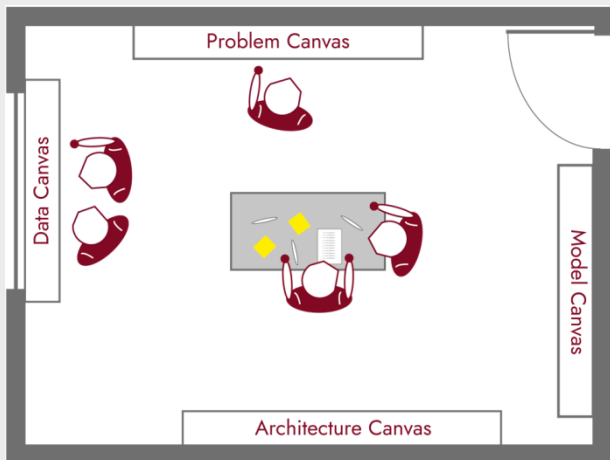


Table 6: Use-case vs. AI-methods matrix.

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



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

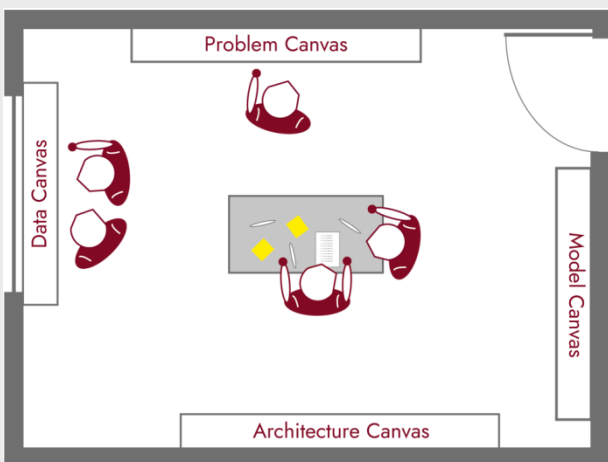


Month 7

Cross HPC/AI Methods Initial Evolution (M12)

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	

Use Case	AE	PINN	ANNs		CNN		NO	SMs			GNN		RNN		GAN	SVM
Details	CAE		ANN	RBF-ANN	U-Net	RESNET	FNO	AR	ARMA	ARIMA	MLPF	JEDI-net	LSTM	GRU	WGAN	
AI for turbulent boundary layers	X															
AI for wind farm layout optimization			X					X	X	X						
AI for data-driven models in reacting flows					X											
Smart models for next generation aircraft engine design					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				X							X	X		X
Detect-free metal additive manufacturing	X		X												X	
Sound Engineering	X		X													

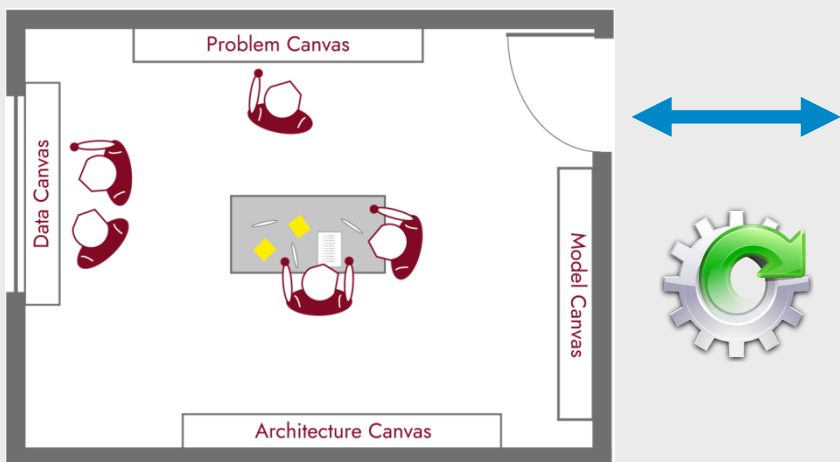


Month 12

Next Evolution: Cross HPC/AI Methods Table (M18)

Interaction Room results:

- Update of Matrix
- Components relatively constant & common
- Methods change & new methods added (e.g., Transformers, RFs)

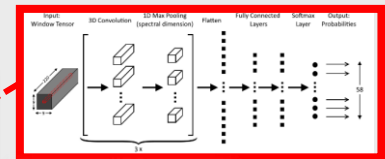


Use Case	AE	PINN	ANNs		CNN		NO	GNN		RNN		GAN	TF			SVM	RF	
	CAE		ANN	RBF-ANN	U-Net	RES NET	FNO	MLPF	GAT	LSTM	GRU	WGAN	MViT	ViViT	Swin			
AI for turbulent boundary layers	X	X	X									X						
AI for wind farm layout optimization				X												X		
AI for data-driven models in reacting flows					X				X									
Smart models for next generation aircraft engine design					X				X									
AI for wetting hydrodynamics	X	X					X			X								
Event reconstruction and classification at the CERN HL-LHC use case								X										
Seismic imaging with remote sensing for energy applications	X	X				X	X			X	X					X	X	X
Detect-free metal additive manufacturing	X		X									X	X	X	X			
Sound Engineering	X		X															



Lessons Learned Example: Role of Hyperparameters

Use Case	AE	PINN	ANNs		CNN		NO	GNN		RNN		GAN	TF			SVM	RF
Details	CAE		ANN	RBF-ANN	U-Net	RES NET	FNO	MLPF	GAT	LSTM	GRU	WGAN	MVIT	VIVIT	Swin		
AI for turbulent boundary layers	X	X	X									X					
AI for wind farm layout optimization				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	X					X			X							
Event reconstruction and classification at the CERN HL-LHC use case								X									
Seismic imaging with remote sensing for energy applications	X	X			X	X		X	X							X	X
Detect-free metal additive manufacturing	X		X									X	X	X			
Sound Engineering	X		X														



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}


Examples of Hyperparameters for a Convolutional Neural Network (CNN)

Each change results basically in a new model


Lessons Learned Example: Role of YouTube Trainings




Created playlists



RAISE training
Updated 7 days ago
[View full playlist](#)



High Performance and Disruptive Computing in Remote Sensing...
[View full playlist](#)



CoE RAISE talks
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Lessons Learned Example: Matrix Updates (D2.15 – M24)



H2020-INFRAEDI-2018-2020



CoE RAISE

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

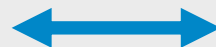
Grant Agreement Number: 951733

D2.15

Novel AI Methods Report (Update)

Final

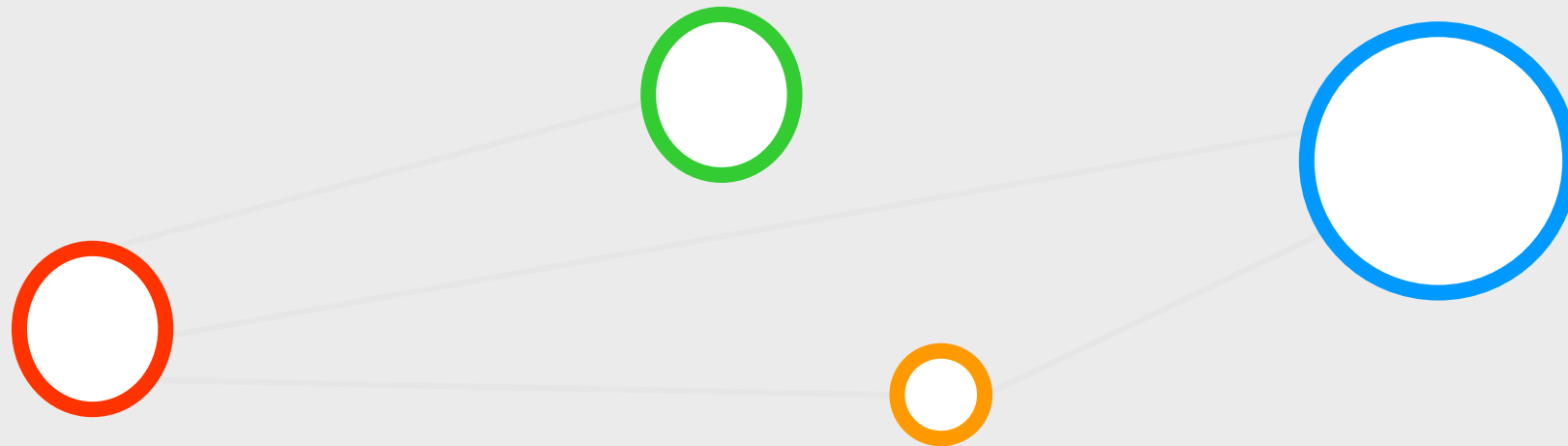
Version: 1.0
 Author(s): M. Riedel (UOI)
 Contributor(s): H. Neukirchen (UOI), M. Book (UOI)
 Date: 23.12.2022



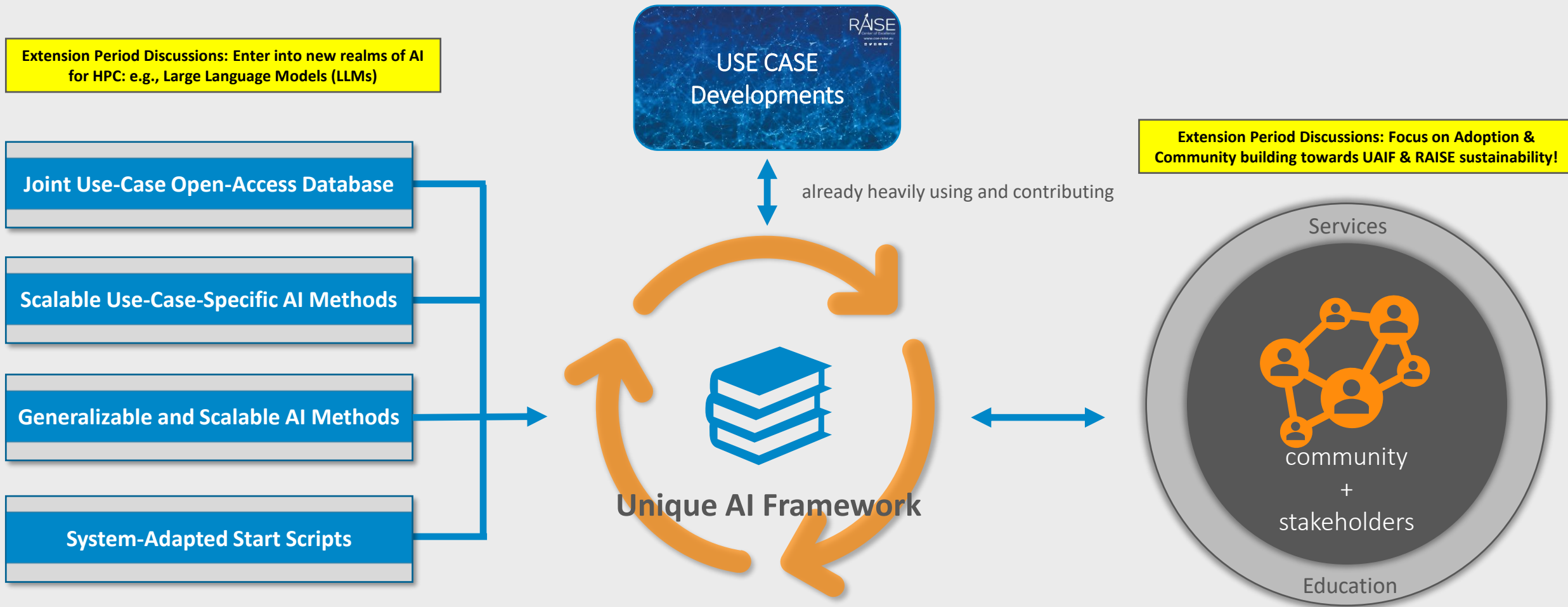
Use Case	Task	AE		PINN	ANNs			CNN			NO	GNN		RNN		GAN		TF			QC SVM	RF	CP
		CAE	VQ-VAE	PINN	ANN	RBF-ANN	U-Net	RES NET	CNN	FNO	MLPF	GAT	LSTM	GRU	WGAN	CGAN	MVIT	VIVIT	SwIn	T F			
AI for turbulent boundary layers	3.1	X		X	X										X								
AI for wind farm layout optimization	3.2					X		X											X				
AI for data-driven models in reacting flows	3.3						X					X											X
Smart models for next generation aircraft engine design	3.4						X					X											X
AI for wetting hydrodynamics	3.5	X		X						X			X										
Event reconstruction and classification at the CERN HL-LHC use case	4.1										X										X		
Seismic imaging with remote sensing for energy applications	4.2	X		X				X					X	X		X				X	X	X	
Defect-free metal additive manufacturing	4.3	X	X		X											X	X	X					
Sound Engineering	4.4	X			X																		
NHR4CES Project	ext.				X																		X



Next Steps also include the addition of new stakeholders (e.g., NHR4CES Project, ARDS/Covid-19 use cases SMITH, etc.)

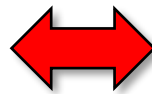


Unique AI Framework Overview

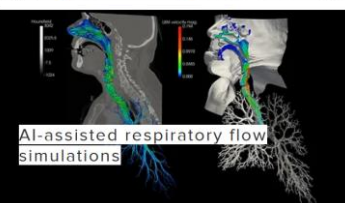
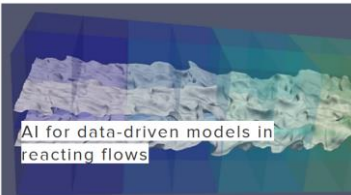
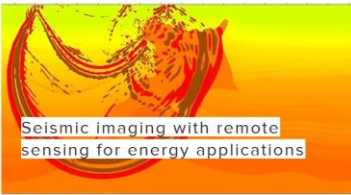
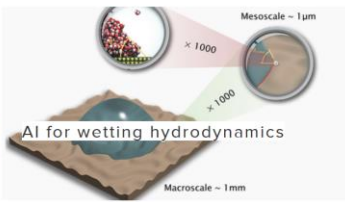
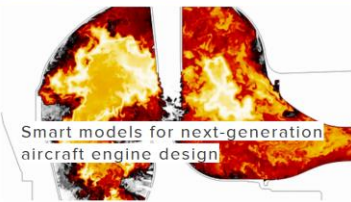
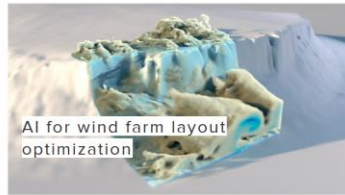
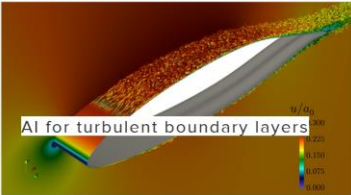


Compute & Data-Driven Use Cases of HPC/AI Methods

Extension Period Discussions: Update of our use cases – but what new external use cases can we add, e.g. TrustLLM?, interTwin?, NCCs?

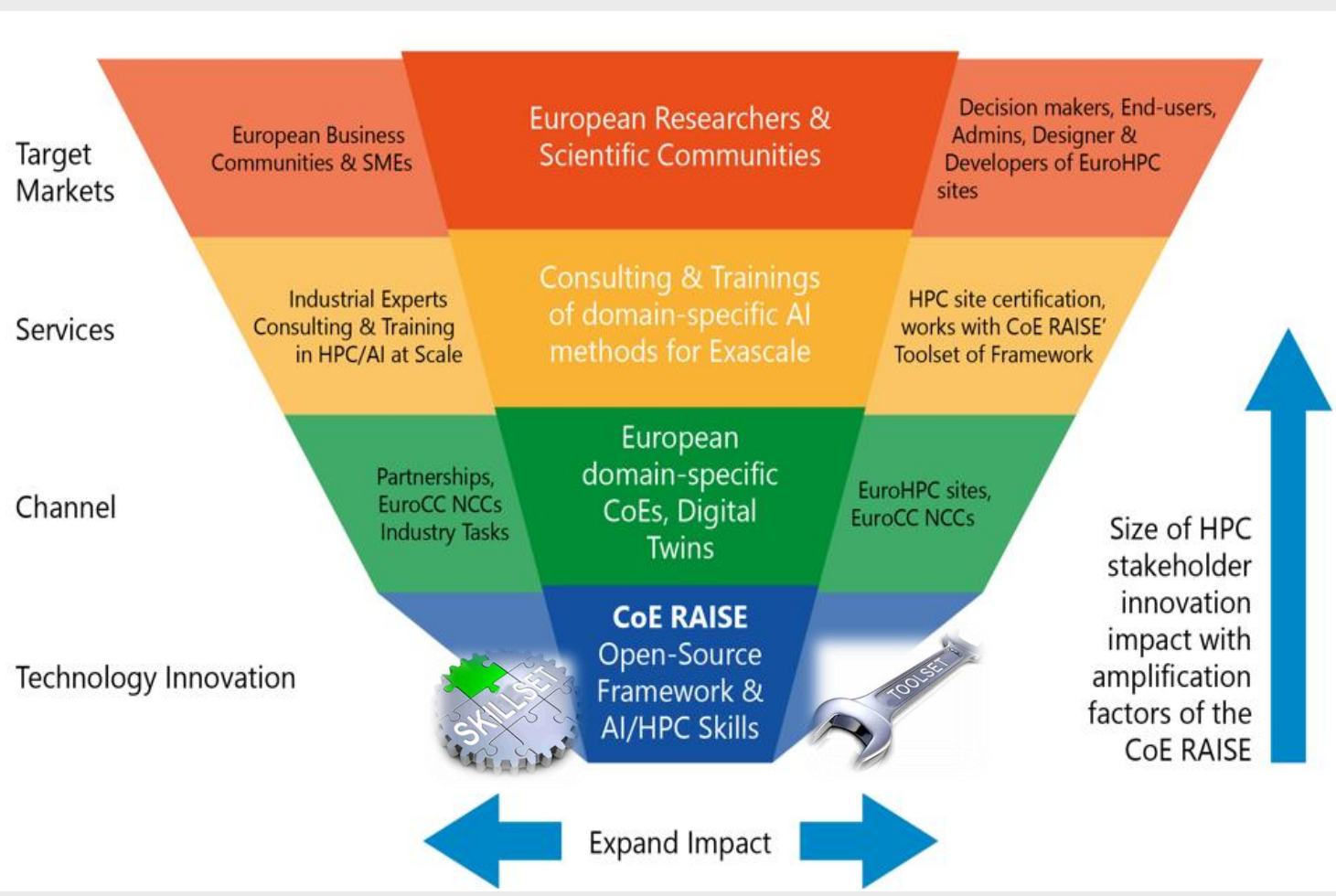


NEW



Use Case	Task	AE		PINN		ANNs		CNN			NO		GNN		RNN		GAN				TF		QC SVM	RF	CP
		CAE	VQ-VAE	PINN	ANN	RBF-ANN	U-Net	RES NET	CNN	FNO	MLPF	GAT	LSTM	GRU	WGAN	CGAN	MVIT	VIVIT	Swin	T F					
AI for turbulent boundary layers	3.1	X		X	X										X										
AI for wind farm layout optimization	3.2					X		X													X				
AI for data-driven models in reacting flows	3.3						X				X													X	
Smart models for next generation aircraft engine design	3.4						X				X													X	
AI for wetting hydrodynamics	3.5	X		X					X			X													
Event reconstruction and classification at the CERN HL-LHC use case	4.1										X												X		
Seismic imaging with remote sensing for energy applications	4.2	X		X				X				X	X		X					X	X	X			
Defect-free metal additive manufacturing	4.3	X	X		X											X	X	X							
Sound Engineering	4.4	X			X																				
NHR4CES Project	ext.				X																			X	

Q&A: NCC Feedback for Adoption & New RAISE Use Cases



Addition of new stakeholders (e.g., NHR4CES Project, ARDS/Covid-19 use cases SMITH, etc.)

Use Case	Task	AE	PINN	ANNs	CNN	NO	GNN	RNN	GAN	TF	QC SVM	RF	CP										
Details	#	CAE	VQ-VAE	PINN	ANN	RBF-ANN	U-Net	RES NET	CNN	FNO	MLPF	GAT	LSTM	GRU	WGAN	CGAN	MVT	VVT	SwIn	T	F		
A for turbulent boundary layers	3.1	X		X	X										X								
A for wind farm layout optimization	3.2				X			X												X			
A for data-driven models in reacting flows	3.3					X						X											X
Smart models for next generation aircraft engine design	3.4					X						X											X
A for wetting hydrodynamics	3.5	X		X						X				X									
Event reconstruction and classification at the CERN HL-LHC use case	4.1										X											X	
Seismic imaging with remote sensing for energy applications	4.2	X		X				X					X	X		X				X	X	X	
Defect-free metal additive manufacturing	4.3	X	X		X											X	X	X	X				
Sound Engineering	4.4	X			X																		
NHR4CES Project	ext.				X																		X

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