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

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

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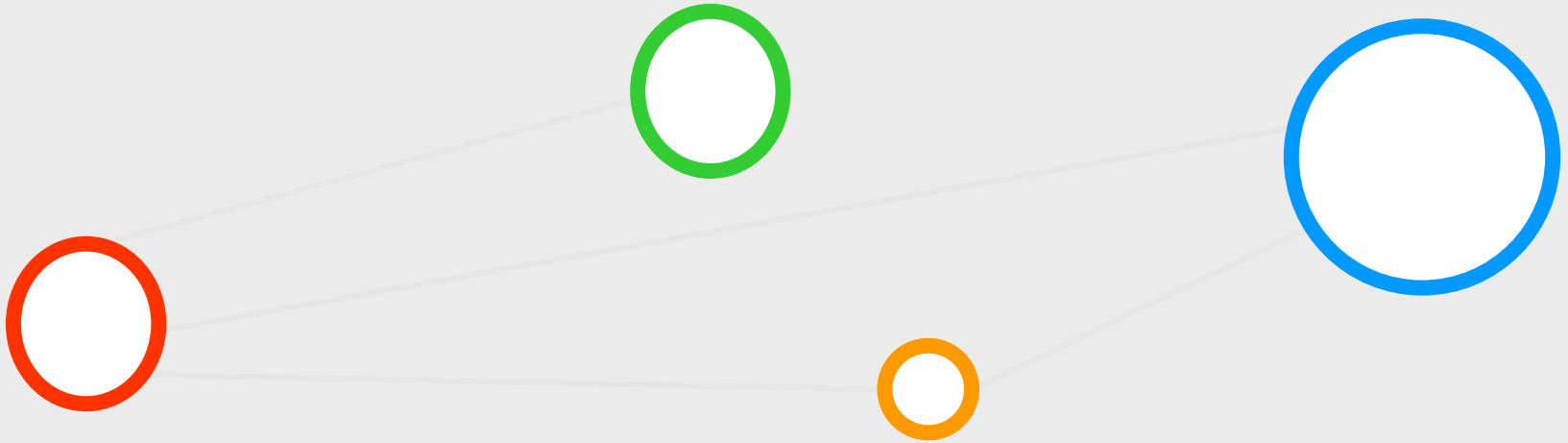
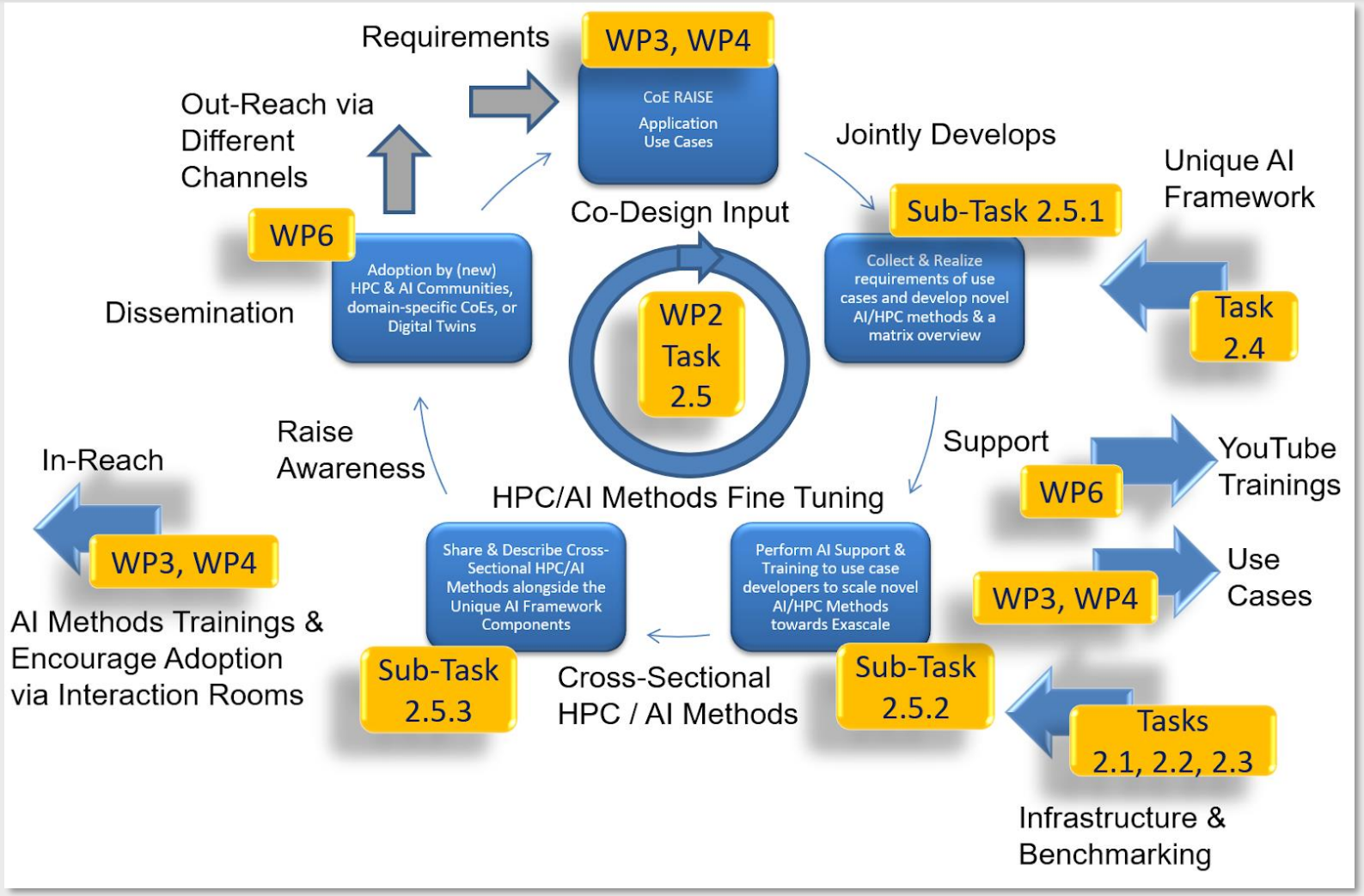
Outline

- 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

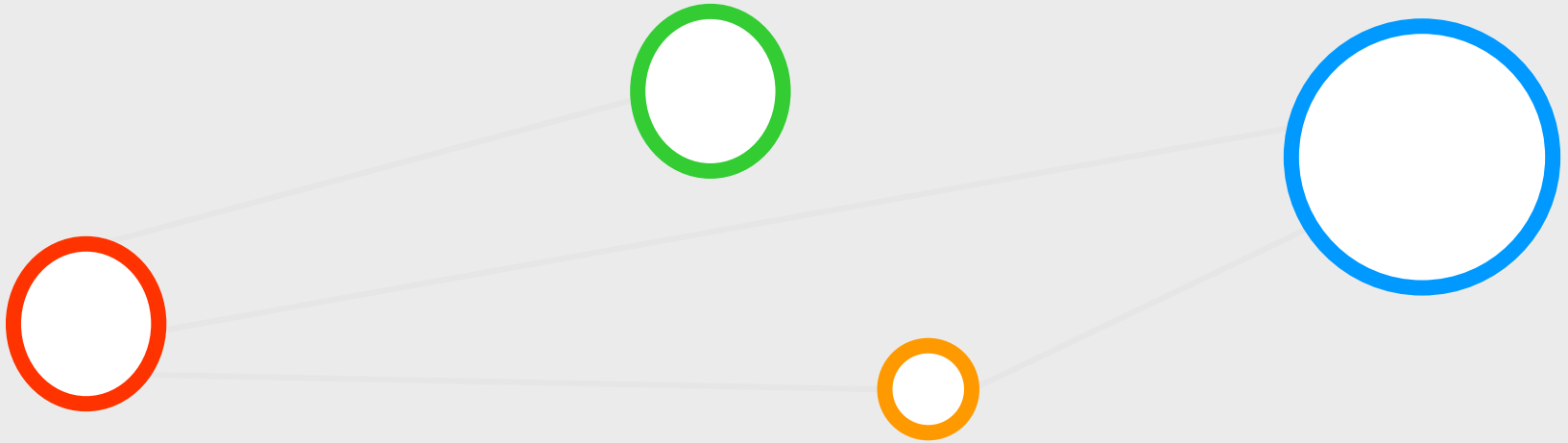
Task 2.5 Process



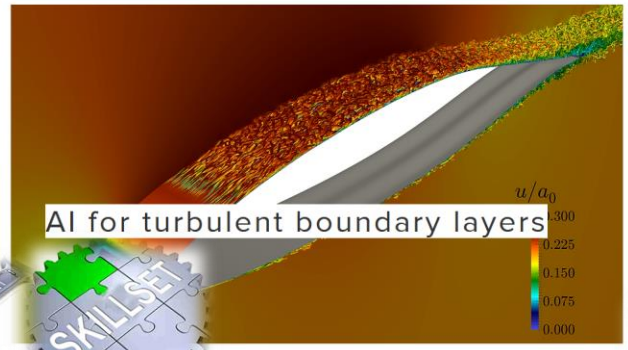
Task 2.5 Process

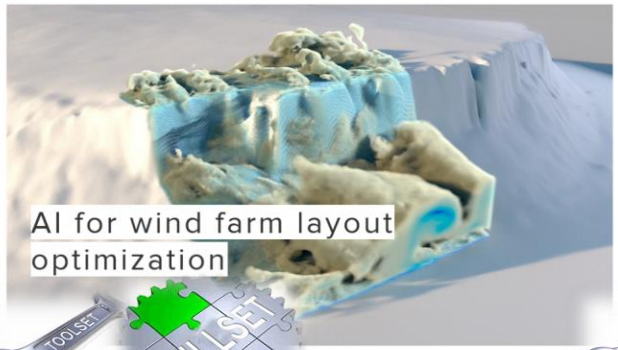


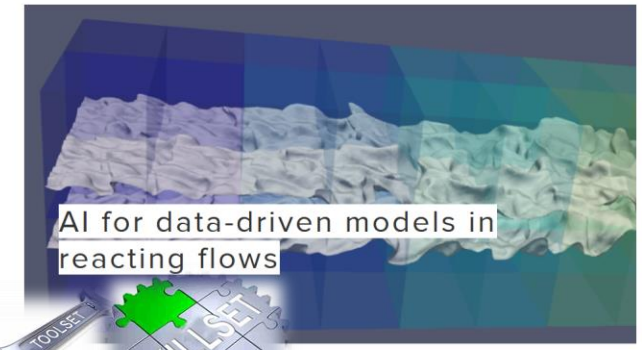
Challenges in using AI Methods on HPC at Scale

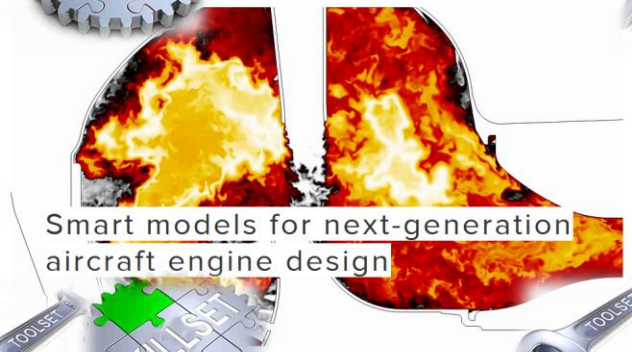


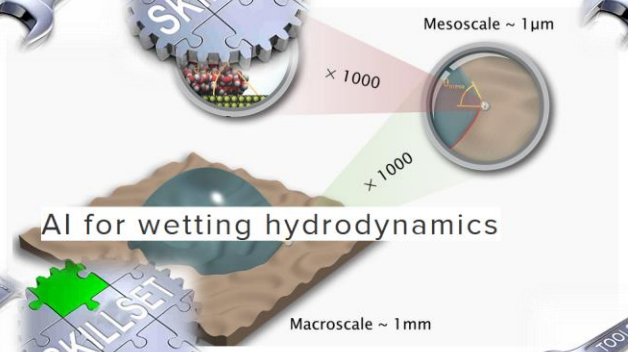
Complex Challenges of a wide area of Toolsets & Skillsets

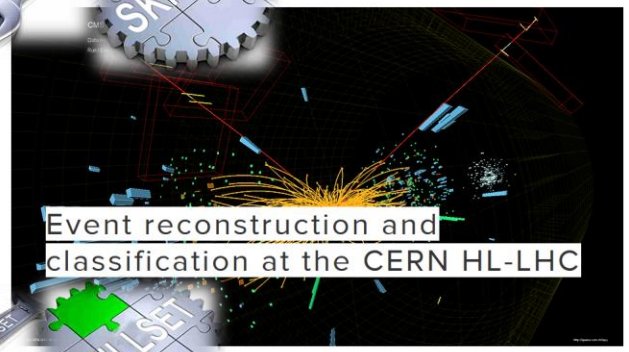


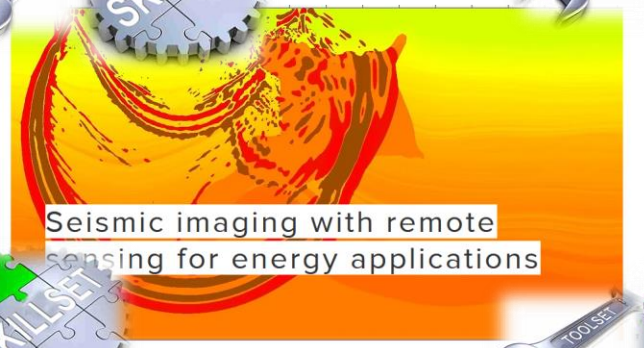


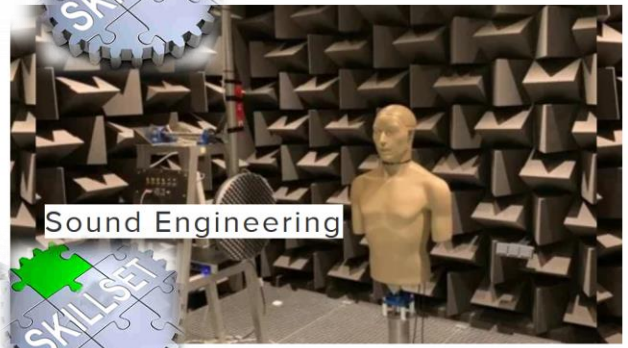




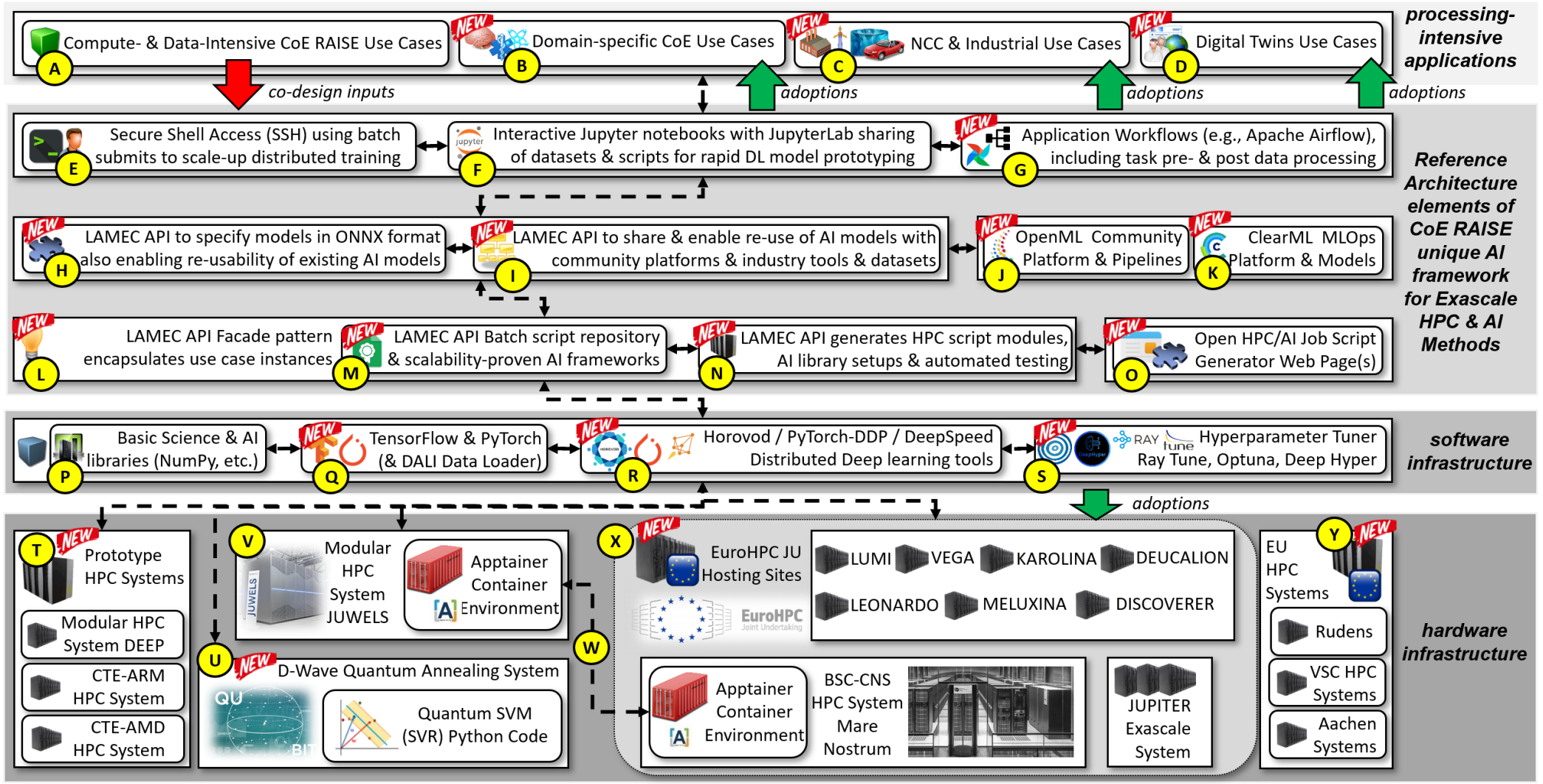








Realization of SW Framework – Task 2.4 Achievements

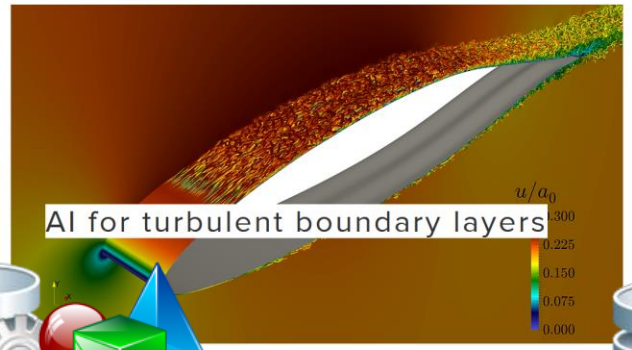


The strategy of "ready-to-run toolsets" Presented at CASTIEL Code of the Month event (2023-07-26 public Webinar), where to put the tools in the overview, e.g. HPC4AI, PhzDLL, etc.?

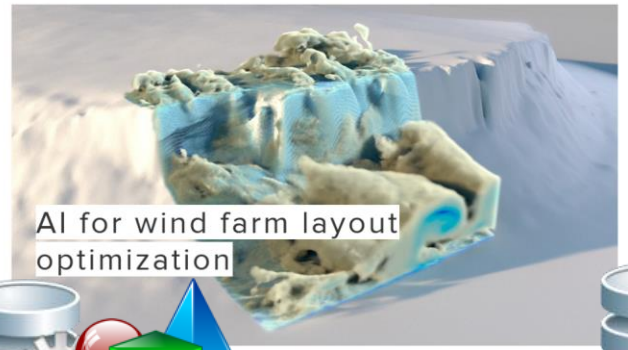
Continously Updating!

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?

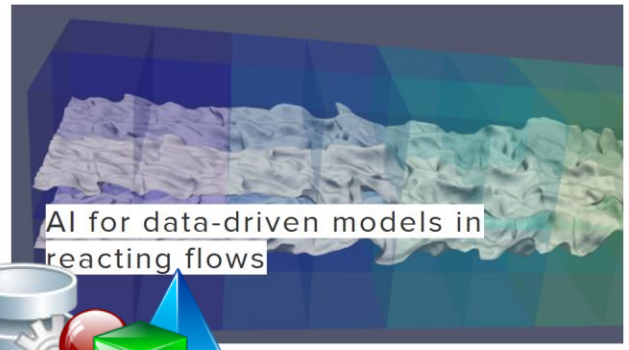
Compute- and Data-driven Use Cases – Data & Modeling



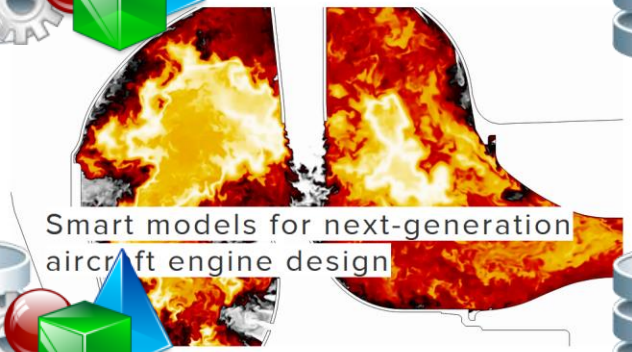
AI for turbulent boundary layers



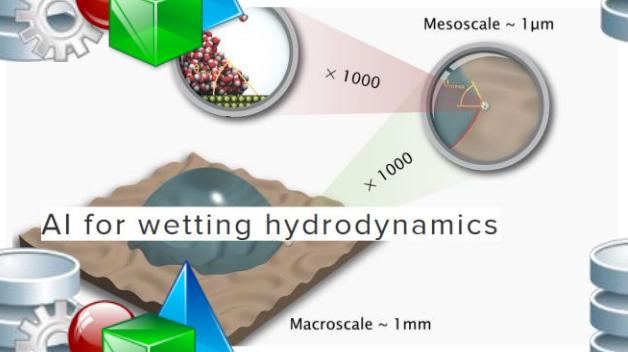
AI for wind farm layout optimization



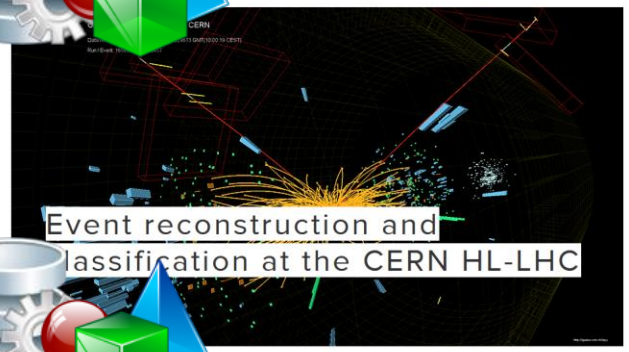
AI for data-driven models in reacting flows



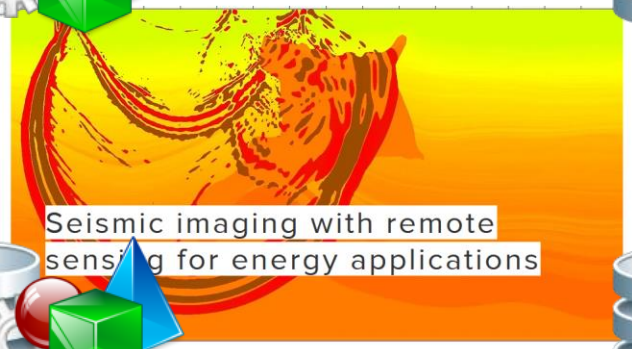
Smart models for next-generation aircraft engine design



AI for wetting hydrodynamics

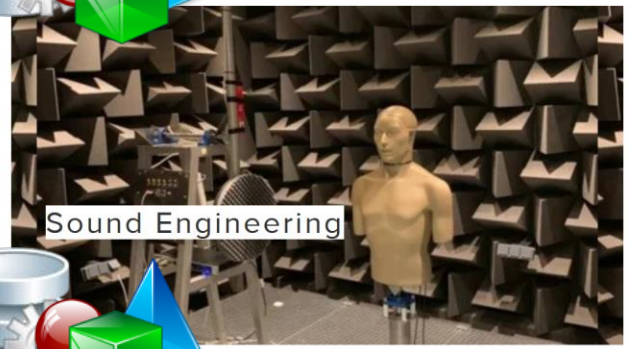


Event reconstruction and classification at the CERN HL-LHC



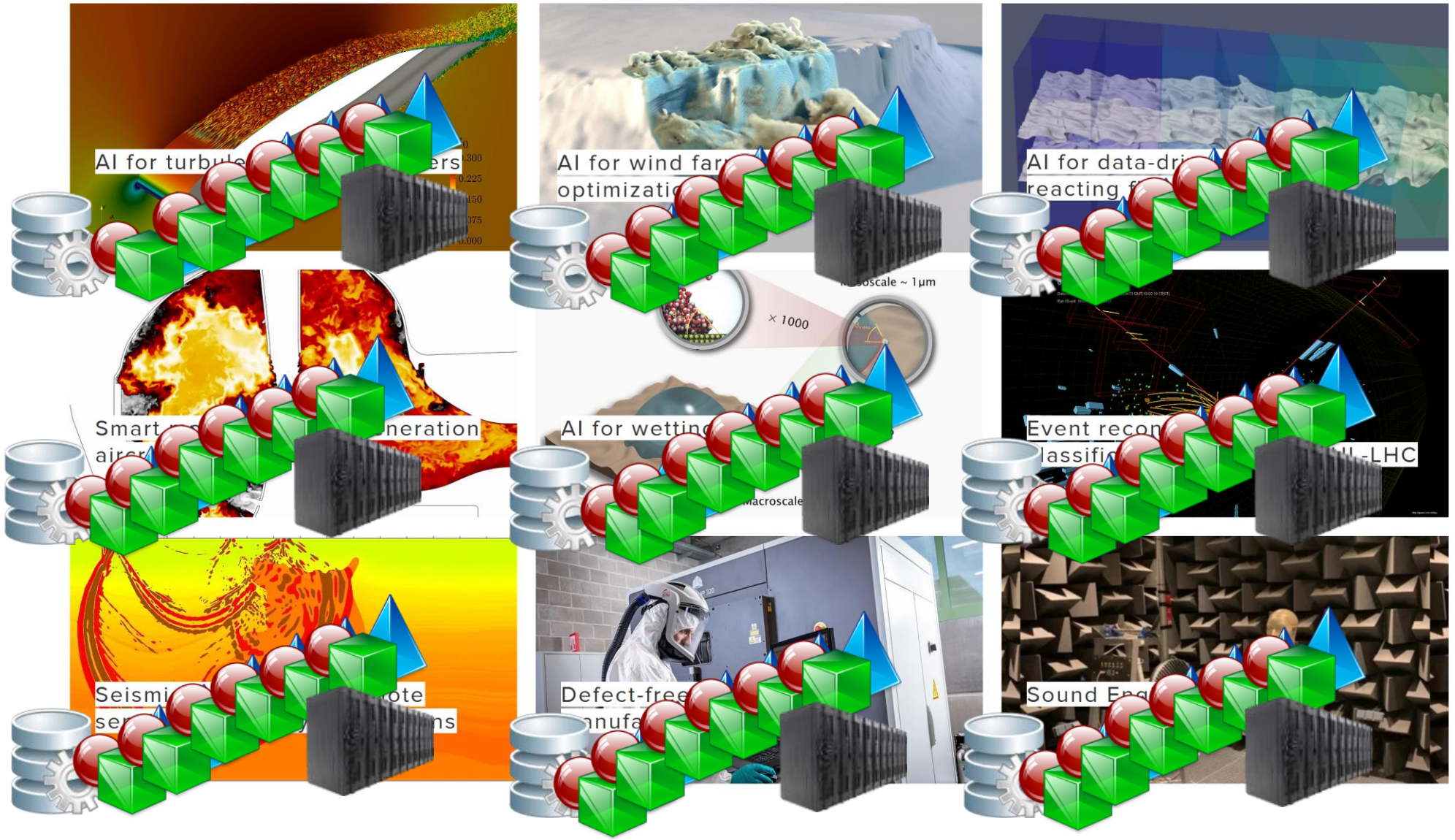
Seismic imaging with remote sensing for energy applications

Defect-free metal additive manufacturing



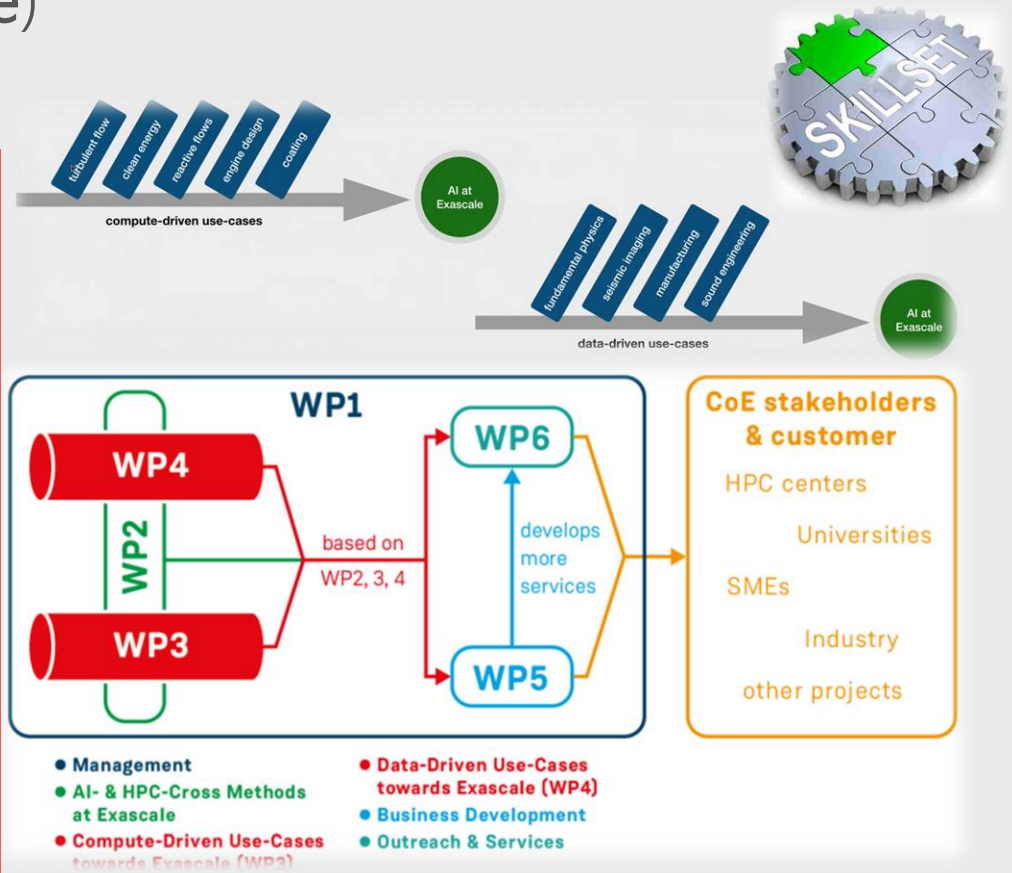
Sound Engineering

Use Cases – Many AI Models & Hyperparameter Relevance

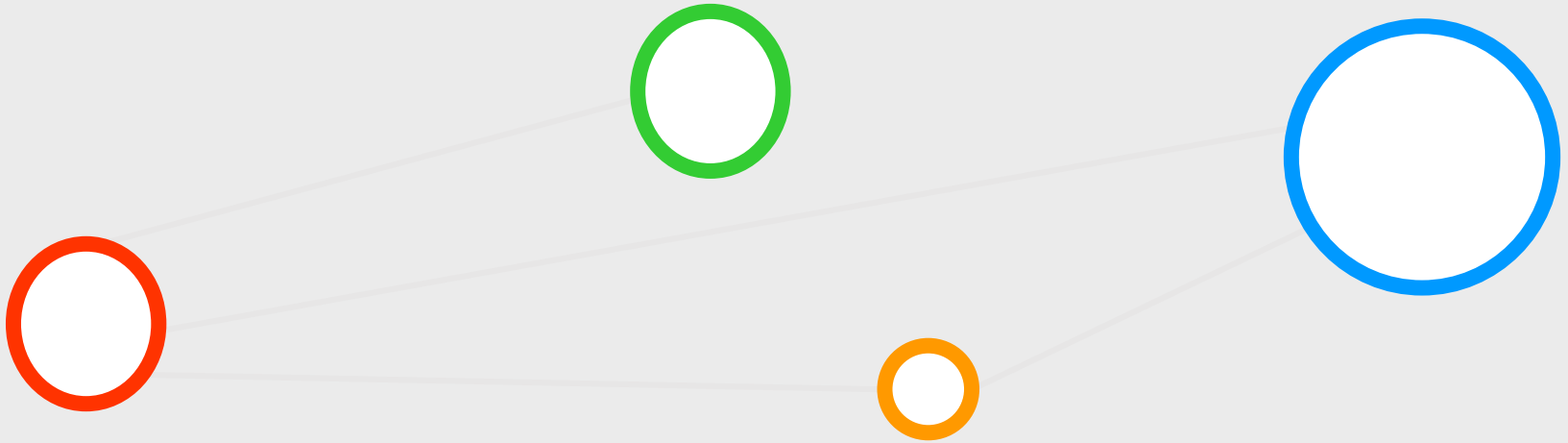


WP2 – AI- & HPC-Cross Methods at Exascale in a nutshell

- 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

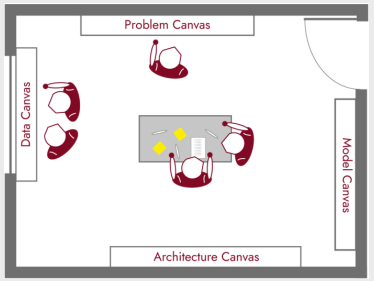


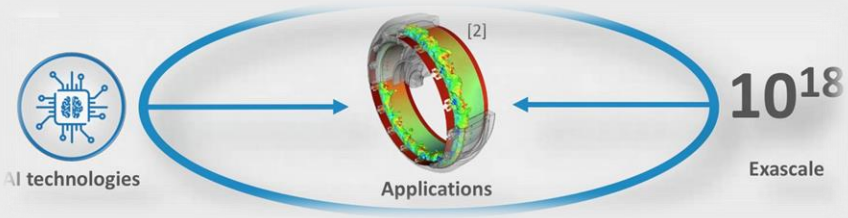
Lessons Learned of HPC/AI Methods Matrix Process



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
  - Methology as one CoE RAISE outcome

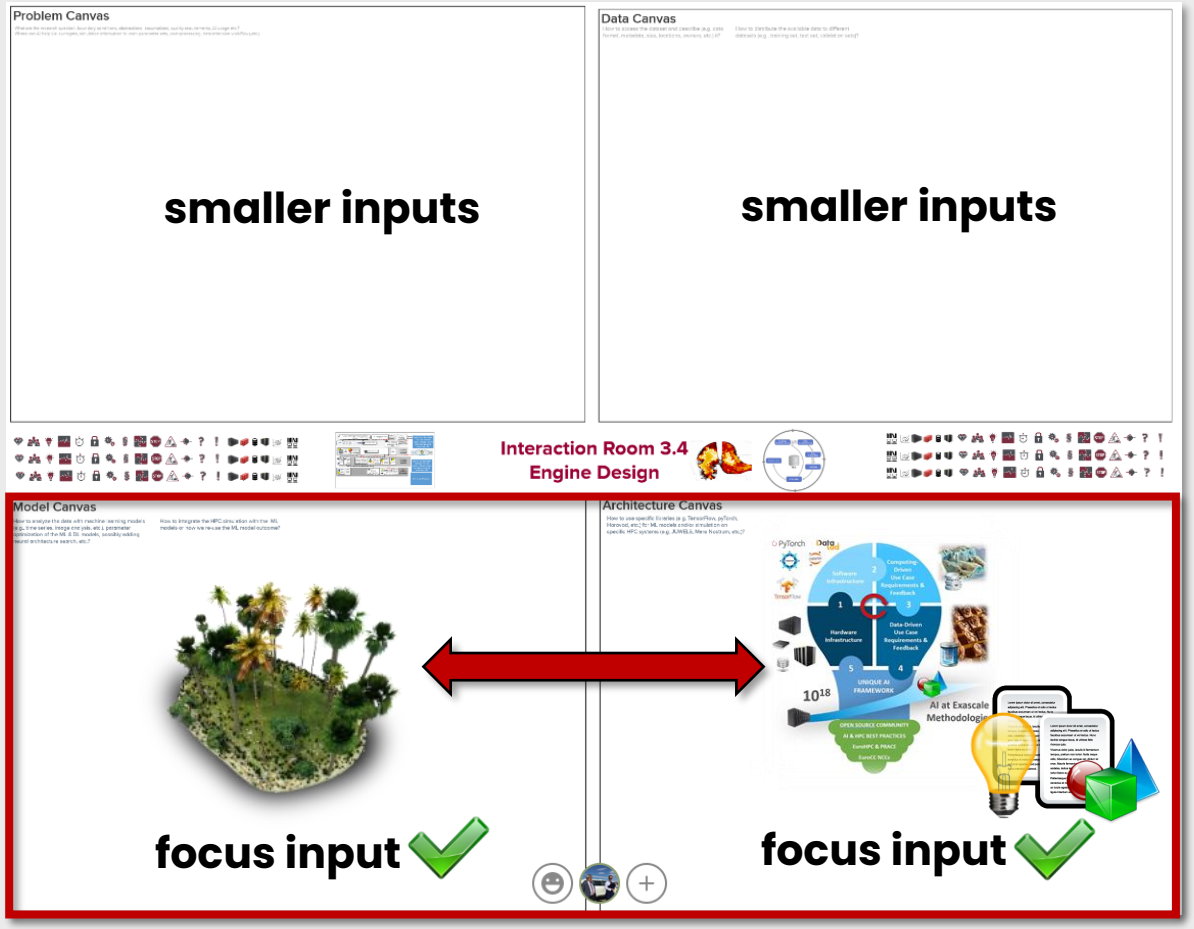


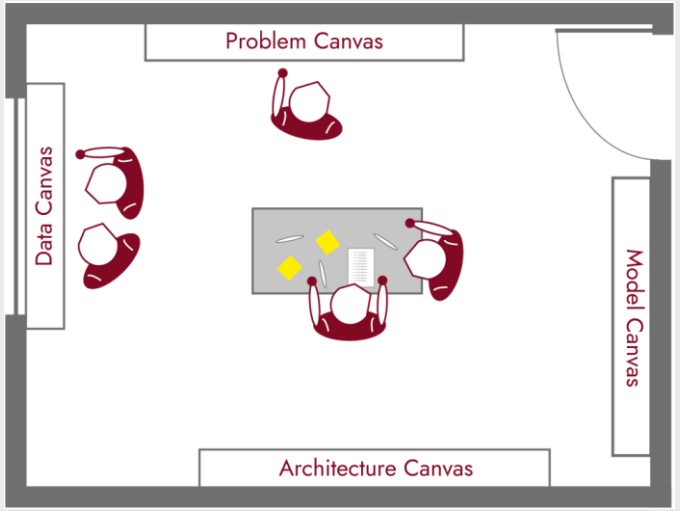


[1] Book, M., Riedel, M., Neukirchen, H., Goetz, M.: Facilitating Collaboration in High-Performance Computing Projects with an Interaction Room, in conference proceedings of the 4th ACM SIGPLAN International Workshop on Software Engineering for Parallel Systems (SEPS 2017), October 22-27, 2017, Vancouver,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





IR Mural Links

IR3.1 Turbulent Flow: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377866397/8613c384d54f66fb5e78599ff307a4ce8a9090c0?sender=u15e3008bb41d6628a5bb5701

IR3.2 Clean Energy: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377887905/cb44cca3eedd3bb9964fbfa36af16b1bfcce085f?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/matthiasbook8855/1621377976343/8d7aba6be09af3b2ffd305d2f709c53661ac889d?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

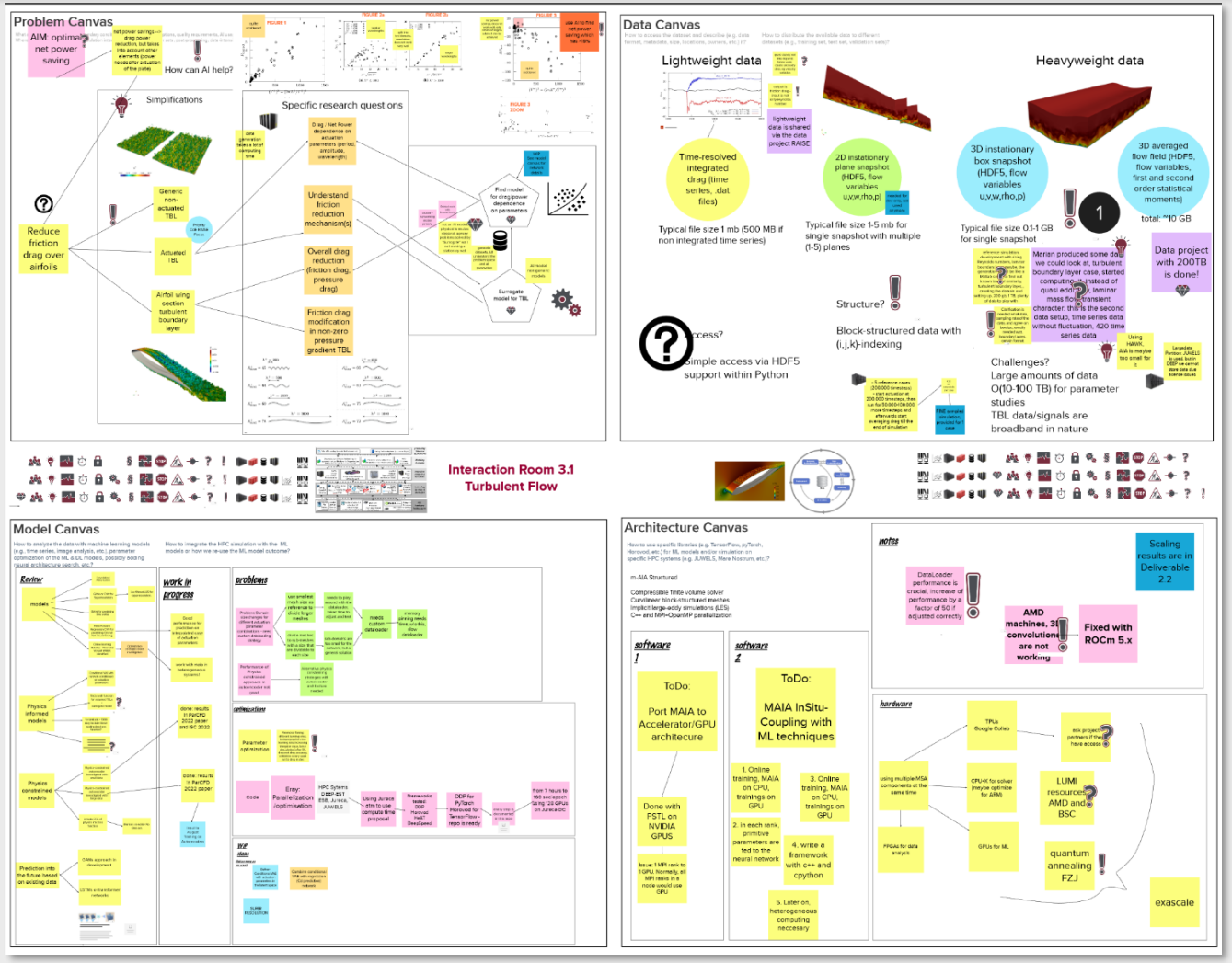
IR4.2 Seismic Imaging: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ae3e28af4bb8d9adbec33874998?sender=u15e3008bb41d6628a5bb5701

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



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

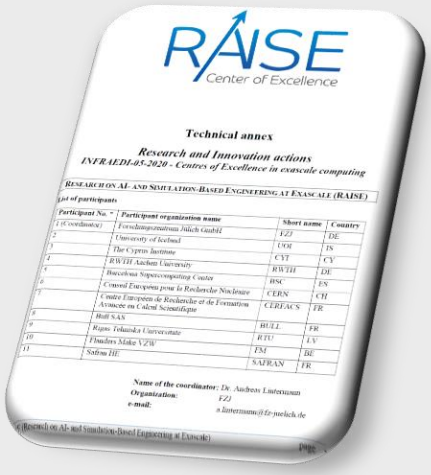
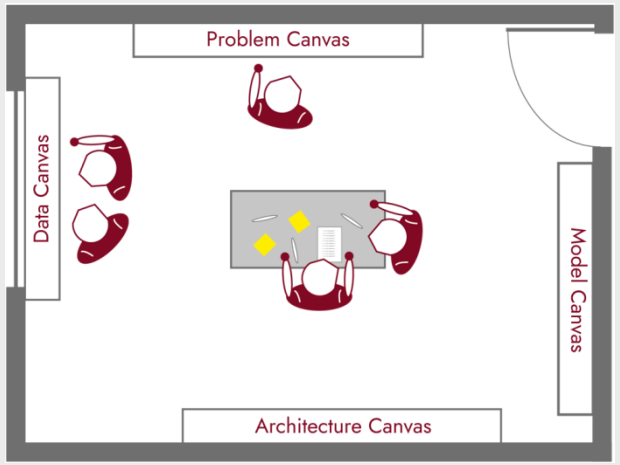


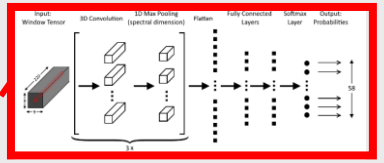
Table 6: Use-case vs. AI-methods matrix.

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



Month 0

Continously Updating!

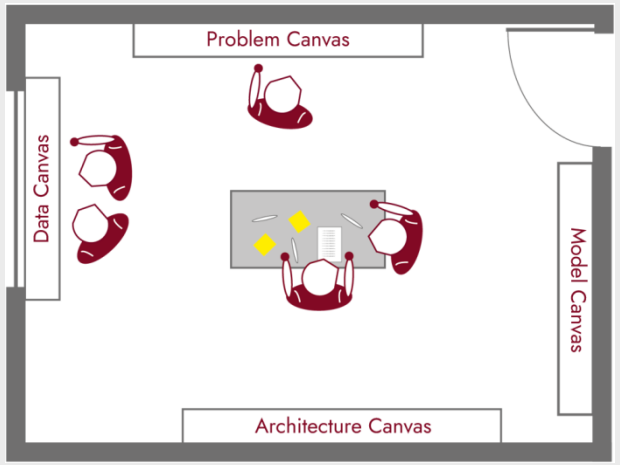


Use Case	AE	PIML	ANNs	CNN		NO	SMs			GNN	IN	LSTM	GRU
Details	***CAE***		***RBF-ANN***	***U-Net***	***RESNET***	***FNO***	***AR***	***ARMA***	***ARIMA***		***JEDI-net***		
AI for turbulent boundary layers	X	X											
AI for wind farm layout optimization			X				X	X	X				
AI for data-driven models in 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

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



Month 7

Continously Updating!

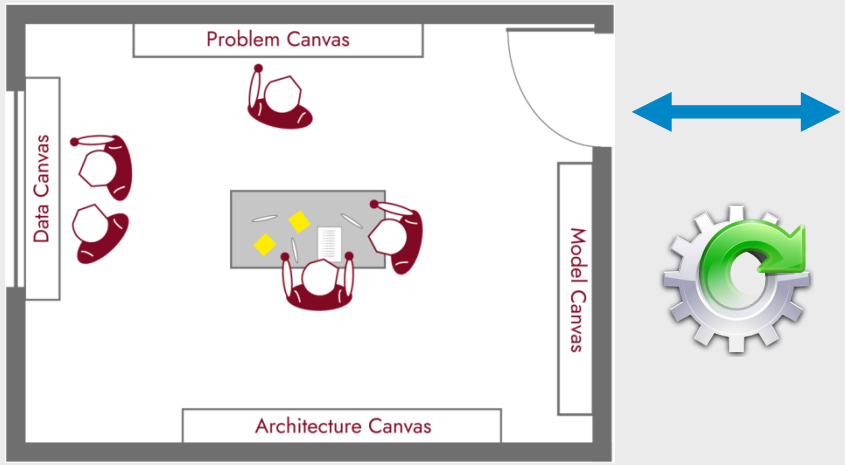
Use Case	AE	PINN	ANNs		CNN		NO	SMs			GNN		RNN		GAN	SVM
Details	*CAE*		*ANN*	*RBF-ANN*	*U-Net*	*RES NET*	*FNO*	*AR*	*ARMA*	*ARIMA*	*MLPF*	*JEDI-net*	*LSTM*	*GRU*	*WGAN*	
AI for turbulent boundary layers	X															
AI for wind farm layout optimization				X				X	X	X						
AI for data-driven models 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:

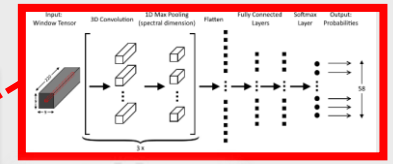
- Update of Matrix
- Components relatively constant & common
- Methods change & new methods added (e.g., Transformers, RFs)



Use Case	AE	PINN	ANNs		CNN		NO	GNN		RNN		GAN	TF				SVM	RF
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	X
Detect-free metal additive manufacturing	X		X									X	X	X	X			
Sound Engineering	X		X															

Lessons Learned Example: Role of Hyperparameters

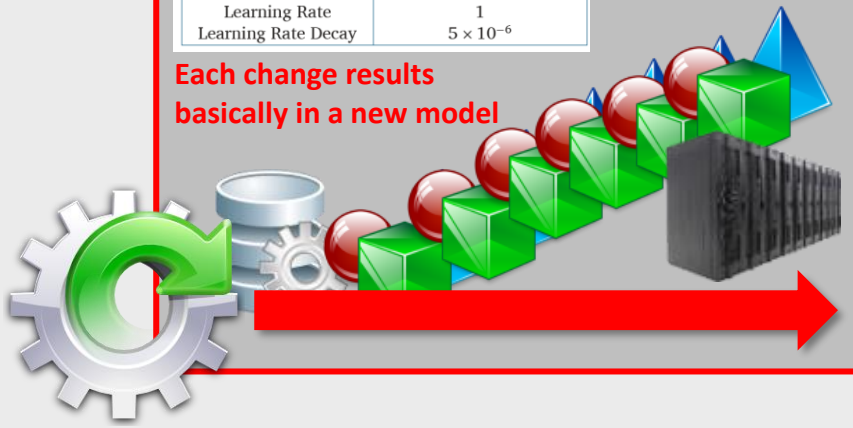
Use Case	AE	PINN	ANNs		CNN		NO	GNN		RNN		GAN	TF				SVM	RF
Details	*CAE*		*ANN*	*RBF-ANN*	*U-Net*	*RES NET*	*FNO*	*MLPF*	*GAT*	*LSTM*	*GRU*	*WGAN*	*MViT*	*ViViT*	*Swin*			
AI for turbulent boundary layers	X	X	X									X						
AI for wind farm layout optimization				X												X		
AI for data-driven 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	X
Detect-free metal additive manufacturing	X		X									X	X	X	X			
Sound Engineering	X		X															



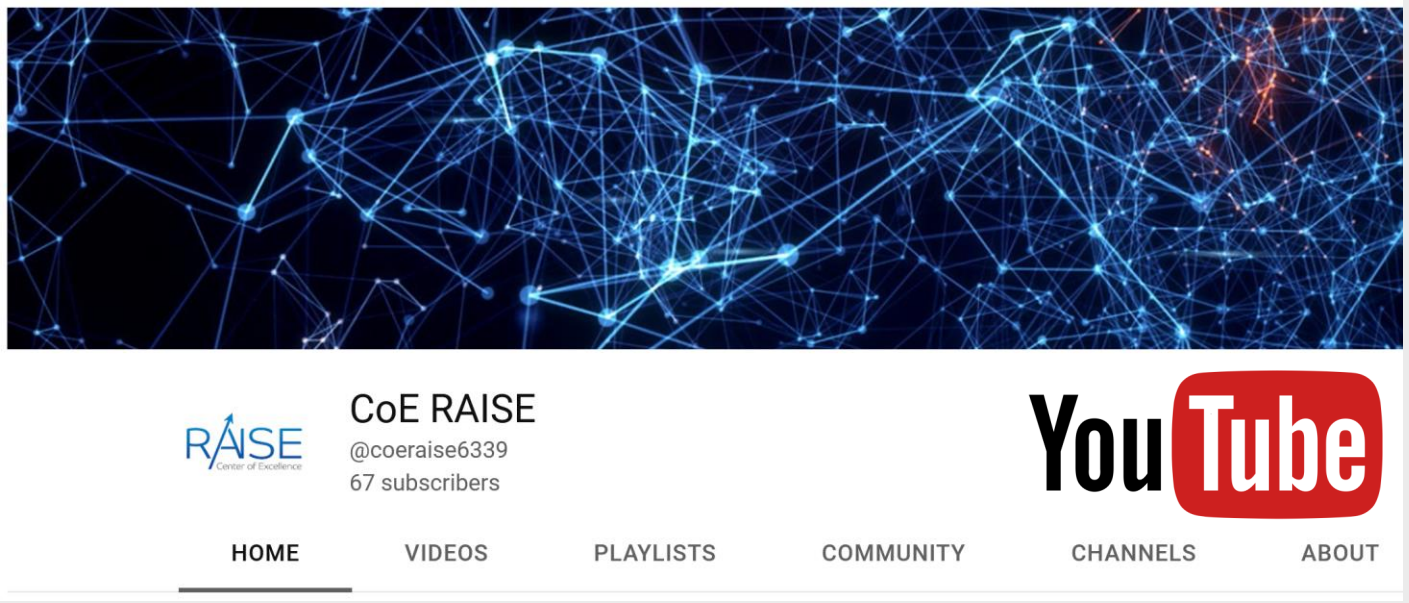
Feature	Representation / Value
Conv. Layer Filters	48, 32, 32
Conv. Layer Filter size	(3,3,5), (3,3,5), (3,3,5)
Dense Layer Neurons	128, 128
Optimizer	SGD
Loss Function	mean squared error
Activation Functions	ReLU
Training Epochs	600
Batch Size	50
Learning Rate	1
Learning Rate Decay	5×10^{-6}

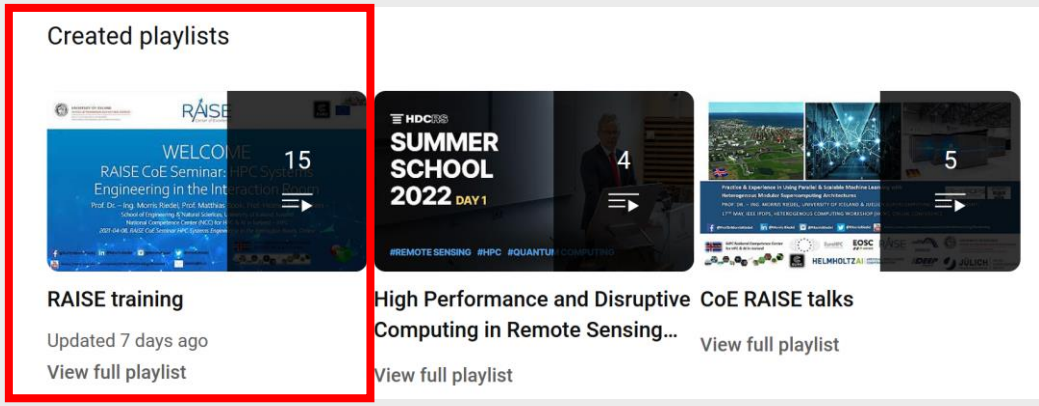
Examples of Hyperparameters for a Convolutional Neural Network (CNN)

Each change results basically in a new model



Lessons Learned Example: Role of YouTube Trainings





Please follow us on YouTube to get Informed about New Trainings

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

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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)

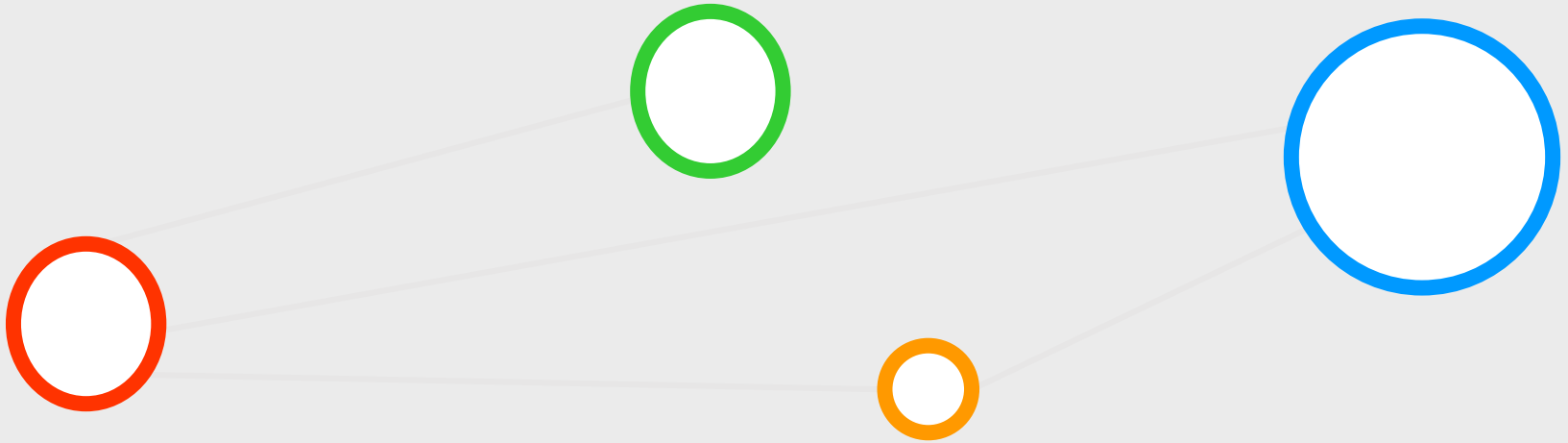
Final

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

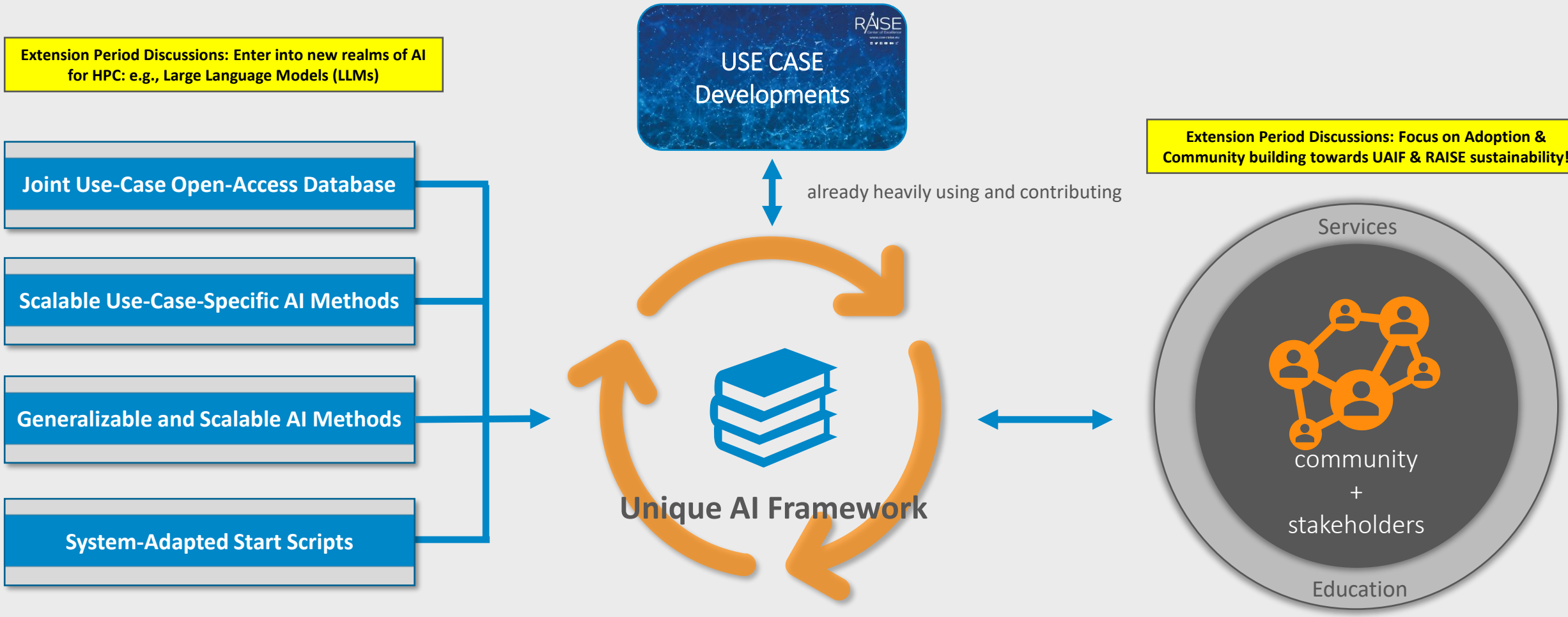
Use Case	Task	AE		PINN	ANNs		CNN			NO	GNN		RNN		GAN		TF				QC SVM	RF	CP
Details	#	*CAE*	*VQ-VAE*	*PINN*	*ANN*	*RBF-ANN*	*U-Net*	*RES NET*	*CNN*	*FNO*	*MLPF*	*GAT*	*LSTM*	*GRU*	*WGAN*	*CGAN*	*MViT*	*ViViT*	*Swin*	*TF*			
AI for turbulent boundary layers	3.1	X		X	X										X								
AI for wind farm layout 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.)

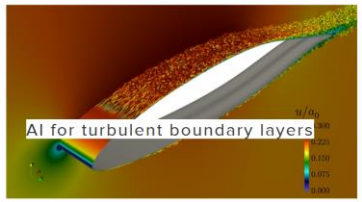
Summary & Q&A

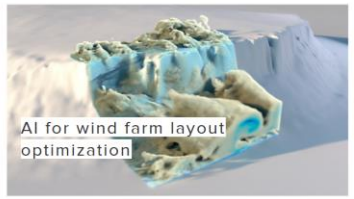


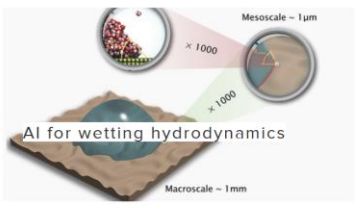
Unique AI Framework Overview

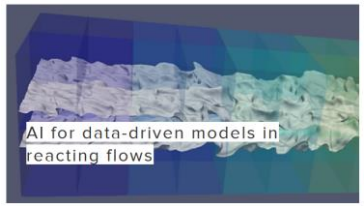


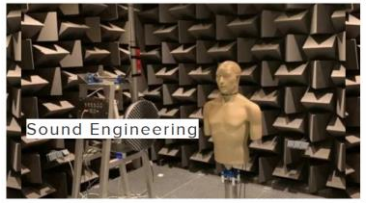
Compute & Data-Driven Use Cases of HPC/AI Methods

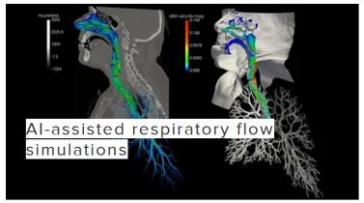


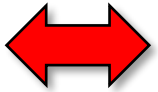








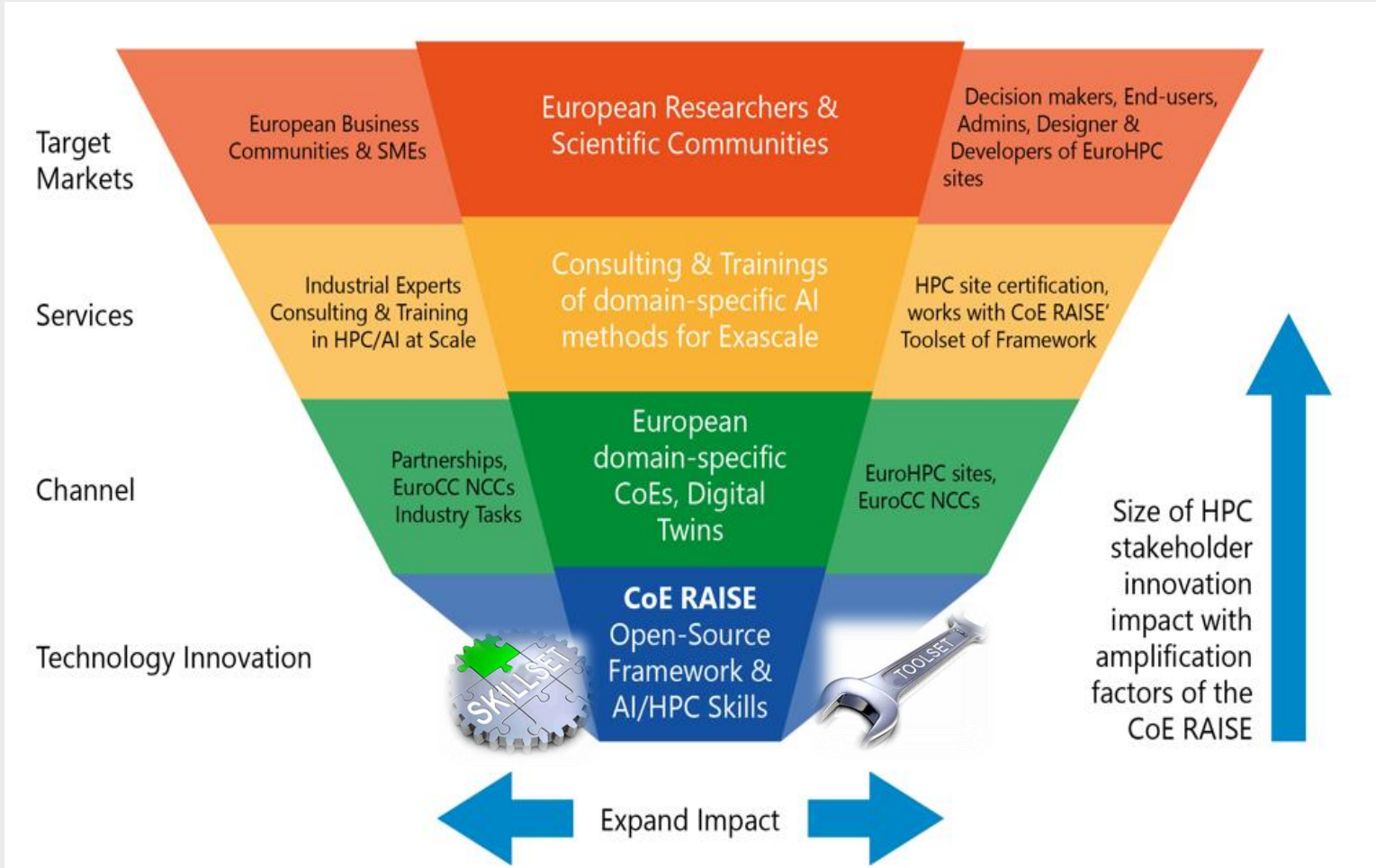




Extension Period Discussions: Update of our use cases – but what new external use cases can we add, e.g. TrustLLM?, interTwin?, NCCs?

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*	*MViT*	*ViViT*	*Swin*	*TF*			
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
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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

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

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