Lessons Learned of applying cross-sectional AI/HPC Methods in Scientific & Engineering Applications

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2022-12-01, AI & Simulation-based Engineering Workshop, Prague

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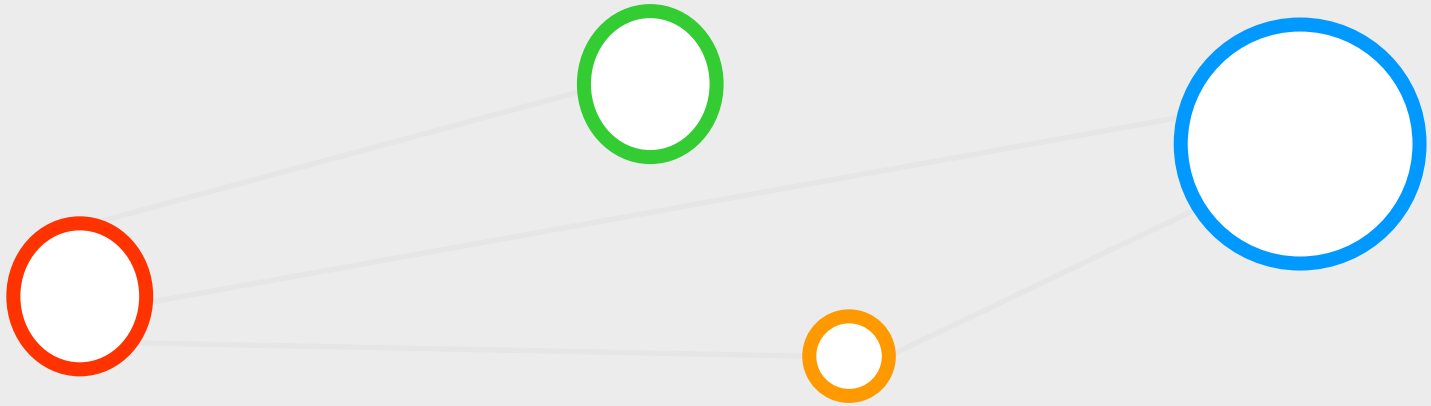
Outline

- 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
- Selected References

Challenges in using AI Methods on HPC at Scale



Complex Challenges of a wide area of Toolsets & Skillsets

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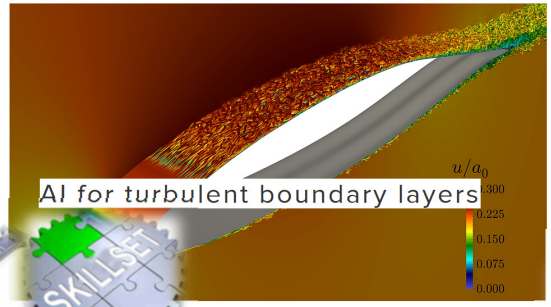
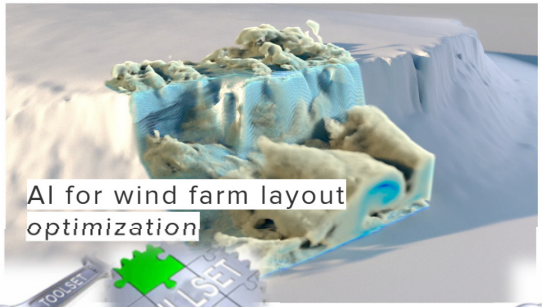
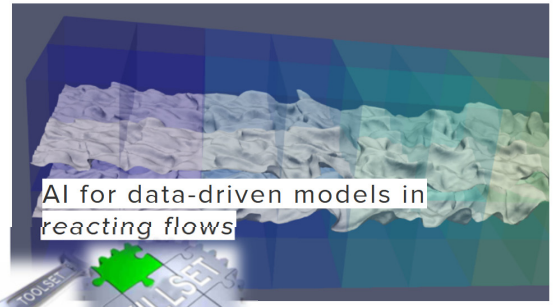


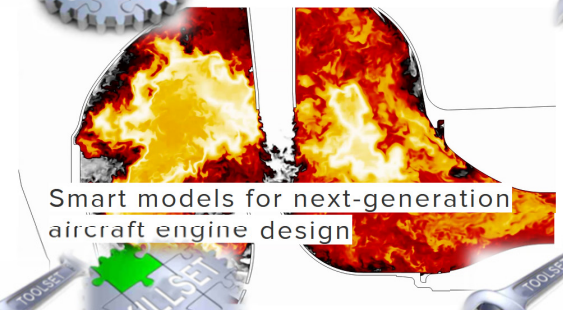
AI for turbulent boundary layers



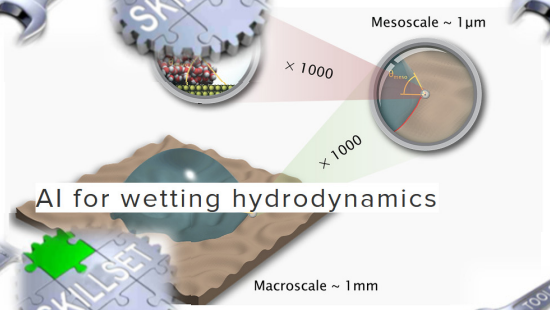
AI for wind farm layout optimization



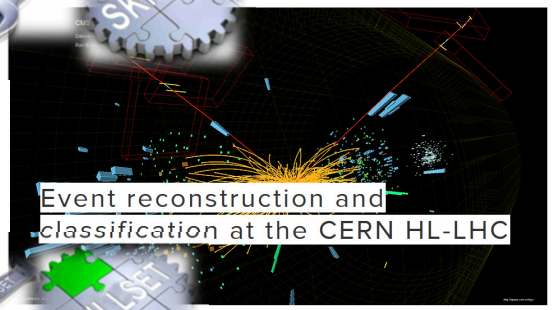
AI for data-driven models in reacting flows



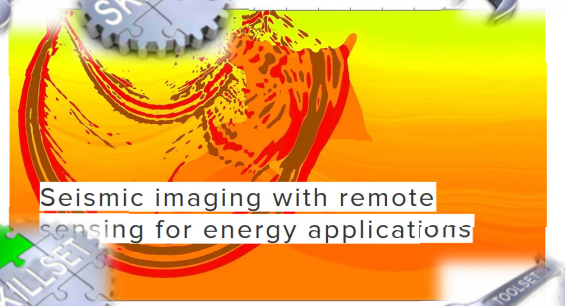
Smart models for next-generation aircraft engine design



AI for wetting hydrodynamics

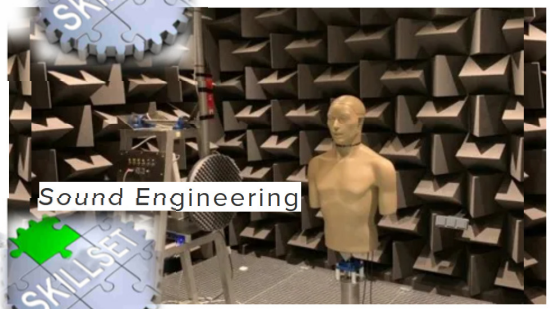


Event reconstruction and classification at the CERN HL-LHC



Seismic imaging with remote sensing for energy applications

Defect-free metal additive manufacturing



Sound Engineering

PyTorch

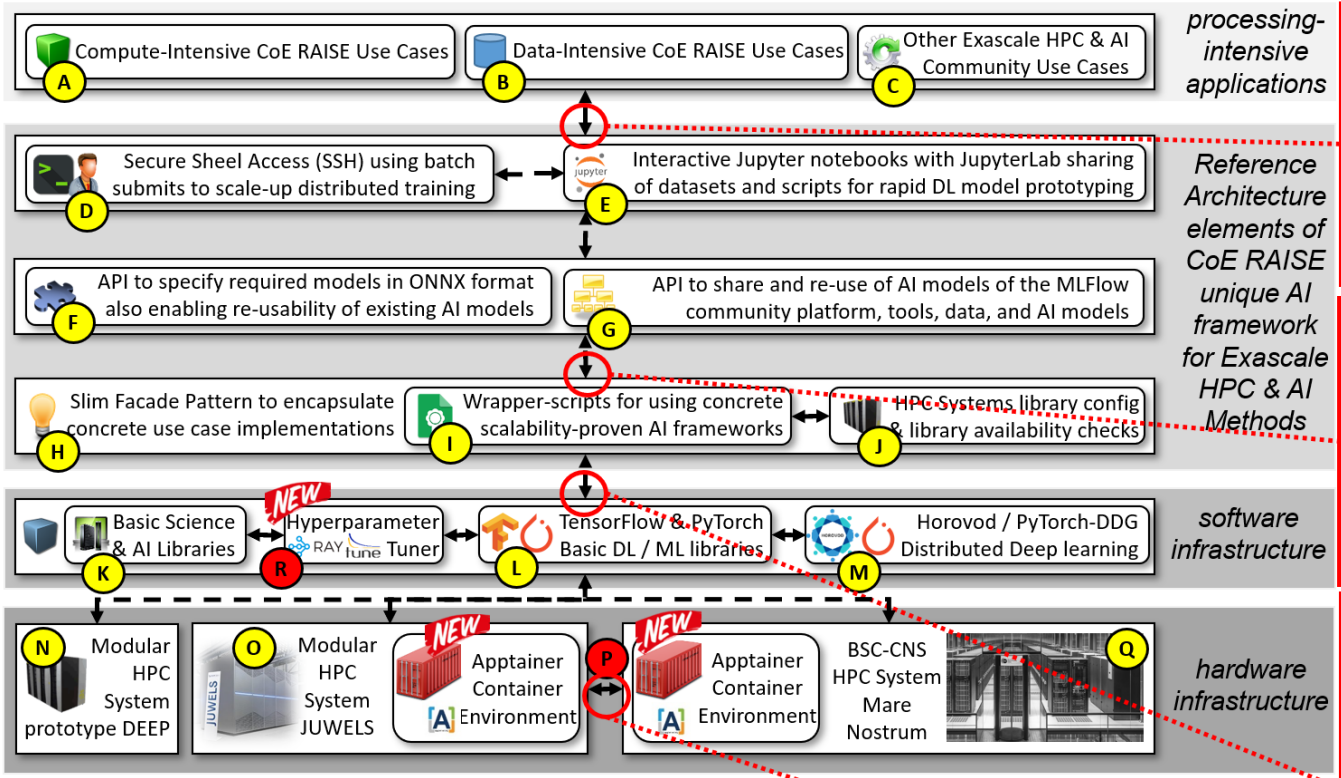
Horovod

TensorFlow

Data Lad

jupyter

Toolsets Addressed via UAIF (→ see previous talk)



✓ RQ1, RQ2, RQ4, RQ5

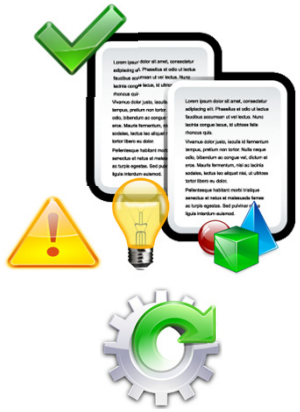
❖ Parts of the framework layout plan is to provide Kernels for Jupyter notebooks with correct version setups of modules for specific HPC Systems

✓ RQ3, RQ6 NEW

❖ Parts of the framework layout plan is to provide lightweight & abstract Python APIs building on ONNX enabling exchange with MLFlow, OpenML, ClearML, etc.

✓ RQ1, RQ2

❖ 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



Continously Updating!

Legend:

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

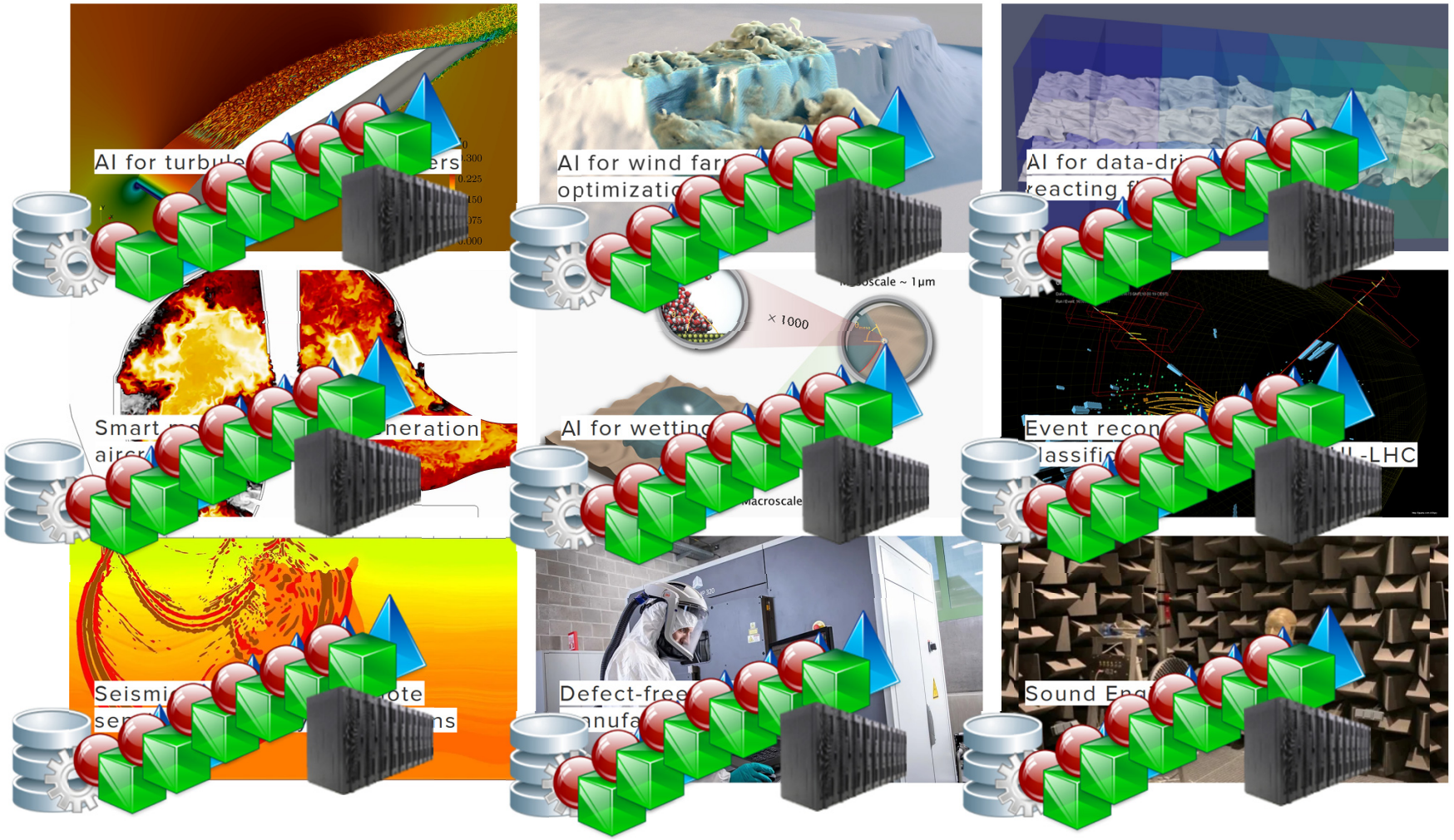
✓ RQ6, RQ7

❖ Part of the framework layout plan is to provide containers in Apptainer with prepackaged datasets and required software stacks needed for AI models

[4] M. Riedel, M. Book, H. Neukirchen, G. Cavallaro & A. Lintermann, "Practice and Experience using High Performance Computing and Quantum Computing to Speed-up Data Science Methods in Scientific Applications, MIPRO 2022

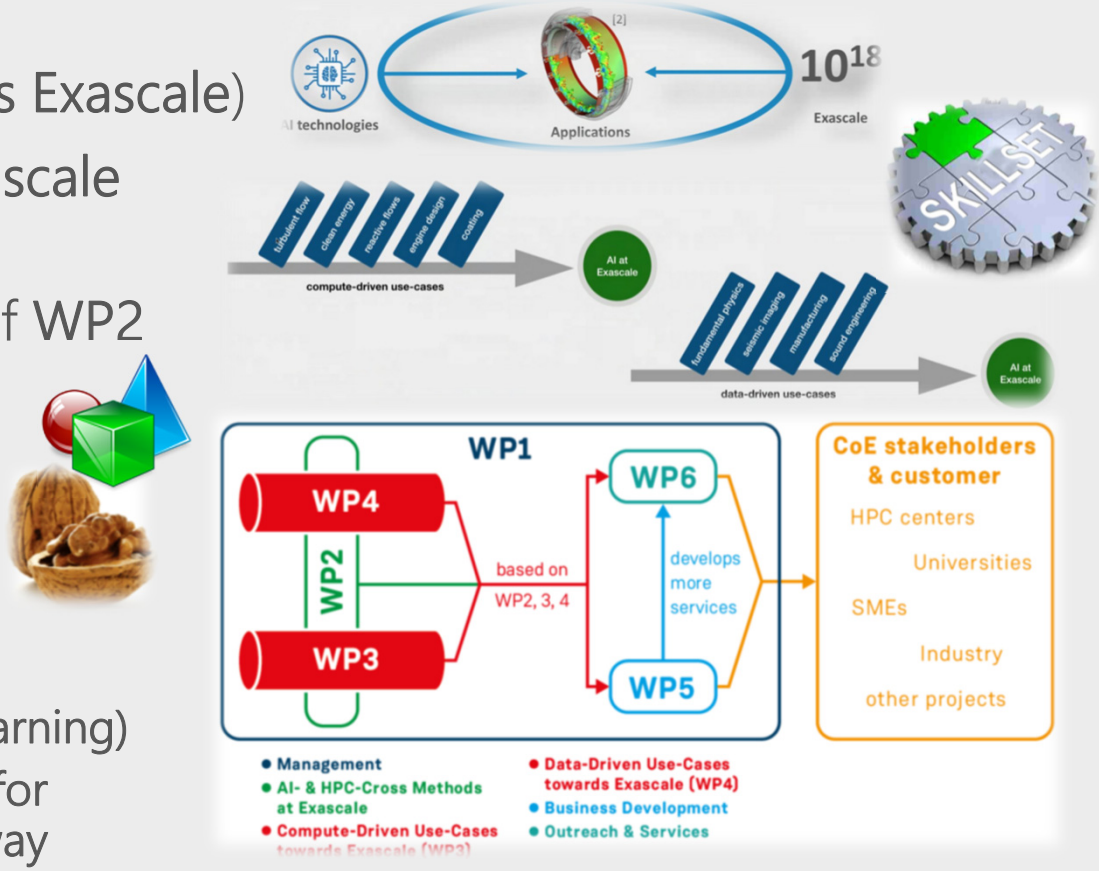
Compute- and Data-driven Use Cases – Data & Modeling

Use Cases – Many AI Models & Hyperparameter Relevance

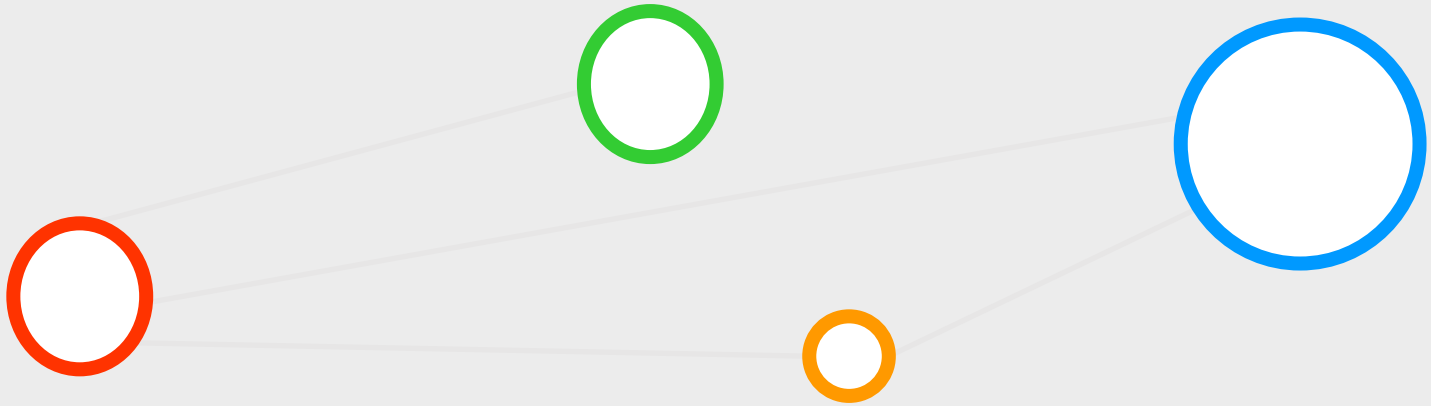


WP2 – AI- & HPC-Cross Methods at Exascale in a nutshell

- 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

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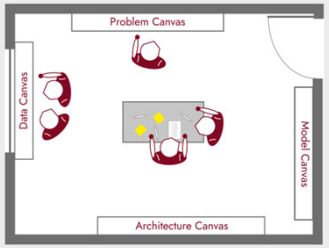
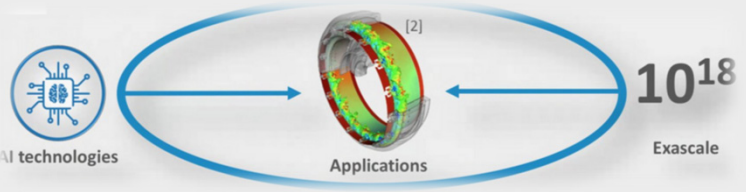
- CoR RAISE Interaction Room Process as Next Step
  - Supports the proper software engineering design of the unique AI framework blueprint
  - Expecting to work with WP3 & WP4 experts in an open minded way
  - Process will be guided by **Prof. Dr. Matthias Book** (University of Iceland)
  - Supported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



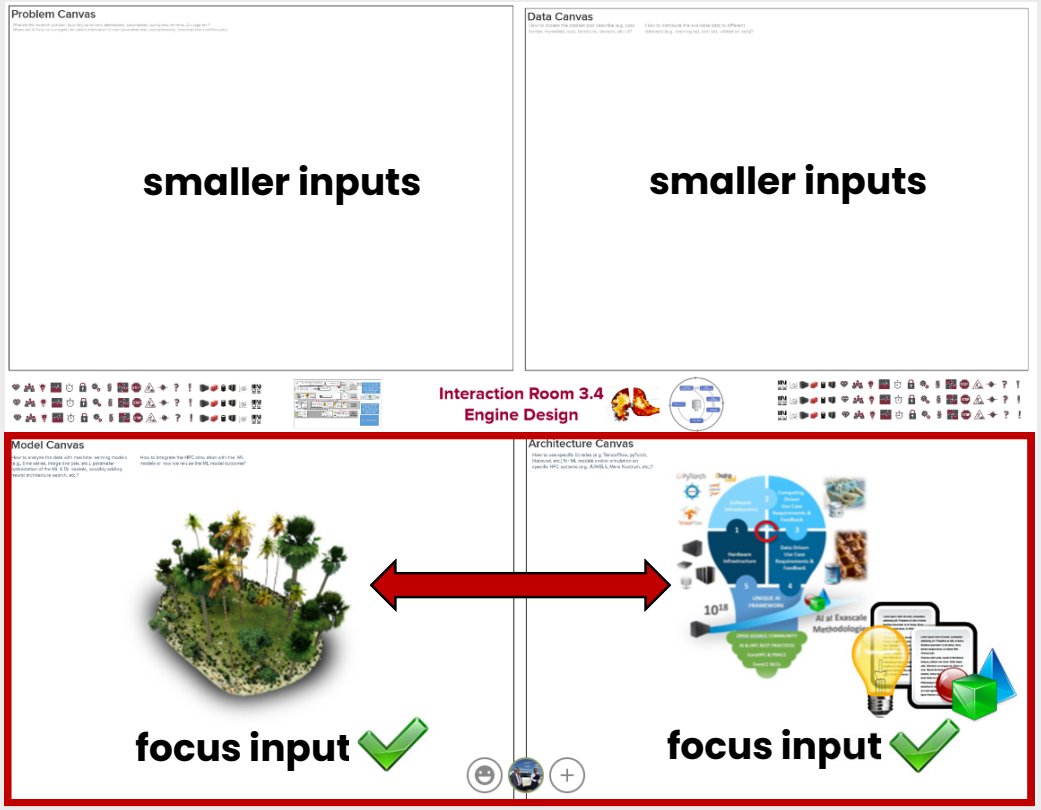
YouTube

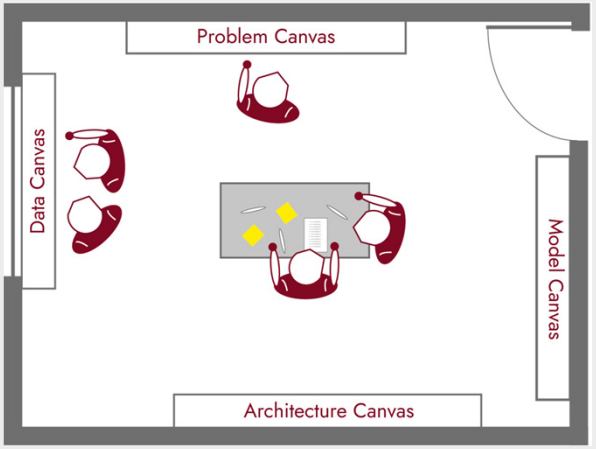


[1] Book, M., Riedel, M., Neukirchen, H., Goetz, M.: Facilitating Collaboration in High-Performance Computing Projects with an Interaction Room, in conference proceedings of the 4th ACM SIGPLAN International Workshop on Software Engineering for Parallel Systems (SEPS 2017), October 22-27, 2017, Vancouver, 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/matthiasbook8855/1621378007555/6f0d5285fcaec5eafa515bd6676e84d8b4879d39?sender=u15e3008bb41d6628a5bb5701

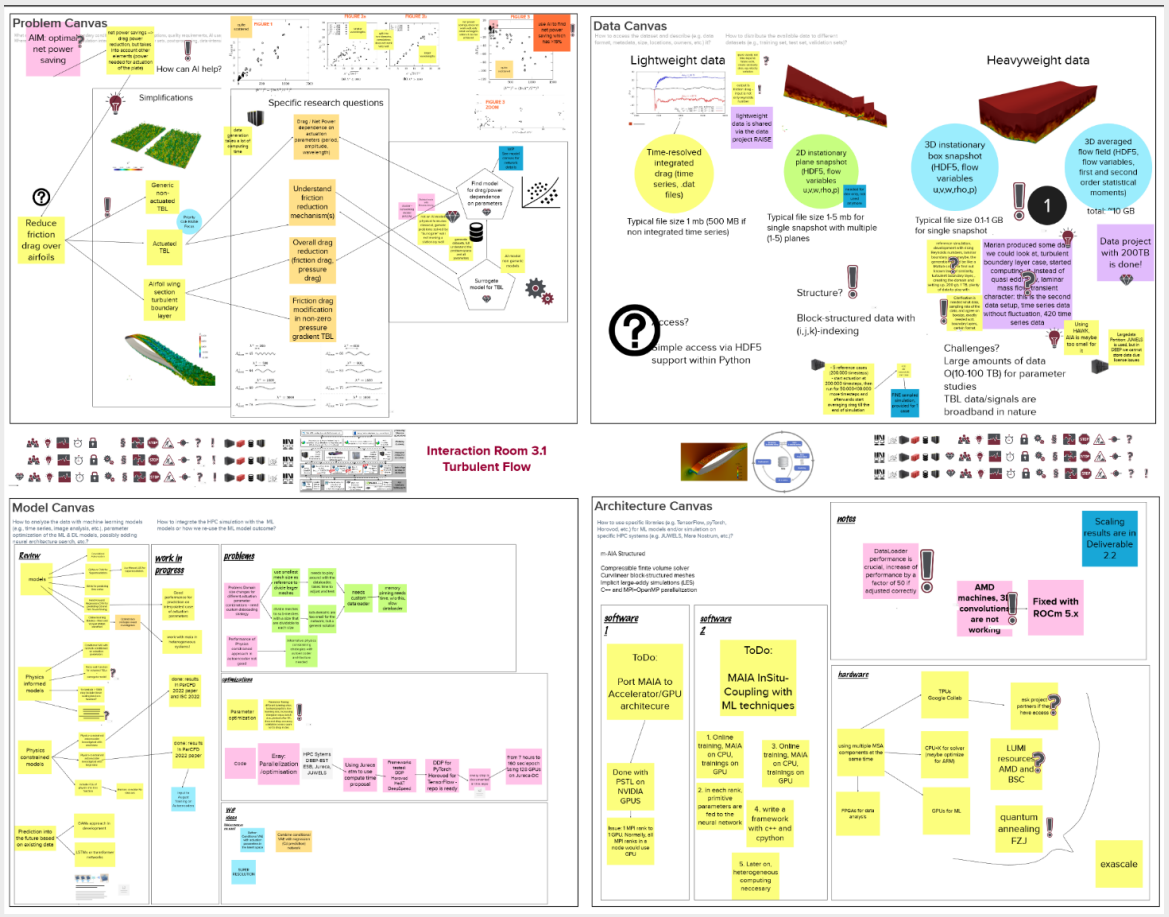
IR4.2 Seismic Imaging: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ae3e28af4bb8d9adbec33874998?sender=u15e3008bb41d6628a5bb5701

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/b5fa122190024040 59f90a4bbb0101fa379a8503?sender=u15e3008bb41d6628a5bb5701

In addition to WP2 Monthly Meetings & Monthly Trainings

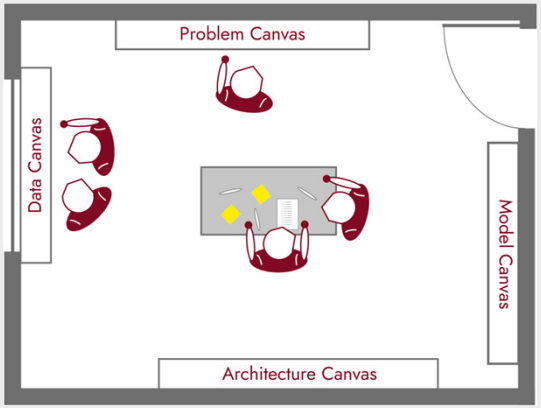
Interaction Room Example: Task 3.1 & Detail Levels



Cross HPC/AI Methods Initial Evolution (M0 → M8)

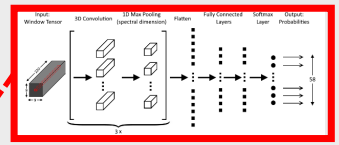
Table 6: Use-case vs. AI-methods matrix.

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!

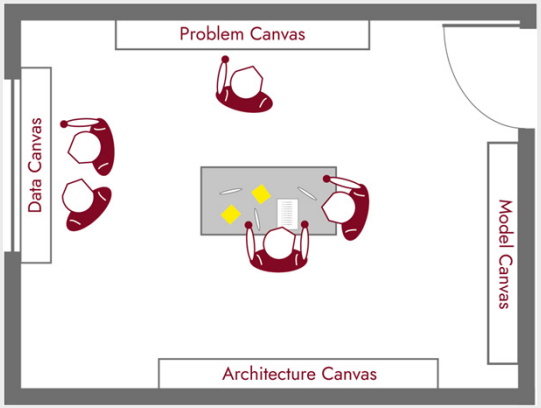


Use Case	AE	PIML	ANNs	CNN		NO	SMs			GNN	IN	LSTM	GRU
Details	*CAE*		*RBF-ANN*	*U-Net*	*RESNET*	*FNO*	*AR*	*ARMA*	*ARIMA*		*JEDI-net*		
AI for turbulent boundary layers	X	X											
AI for wind farm layout optimization			X				X	X	X				
AI for data-driven models in reacting flows				X						X			
Smart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

Latest-Greatest: Cross HPC/AI Methods Table (M18)

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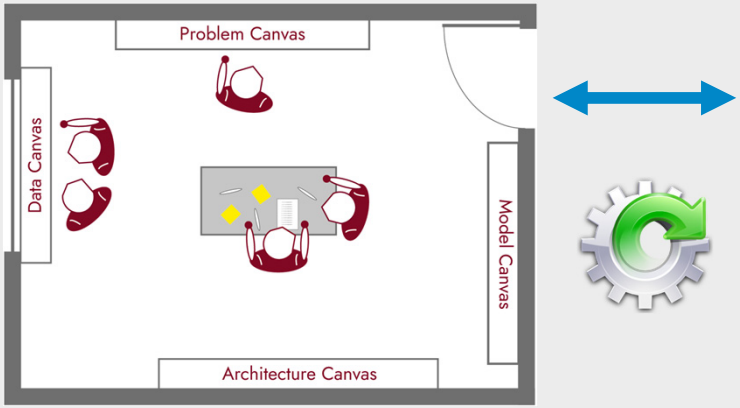
Interaction Room results:

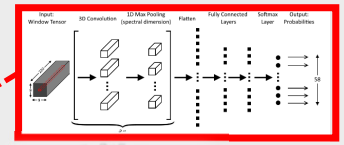
- Update of Matrix
- Components relatively constant & common
- Methods change & new methods added (e.g., Transformers, RFs)



Use Case	AE	PINN	ANNs		CNN		NO	GNN		RNN		GAN	TF				SVM	RF
Details	*CAE*		*ANN*	*RBF-ANN*	*U-Net*	*RESNET*	*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

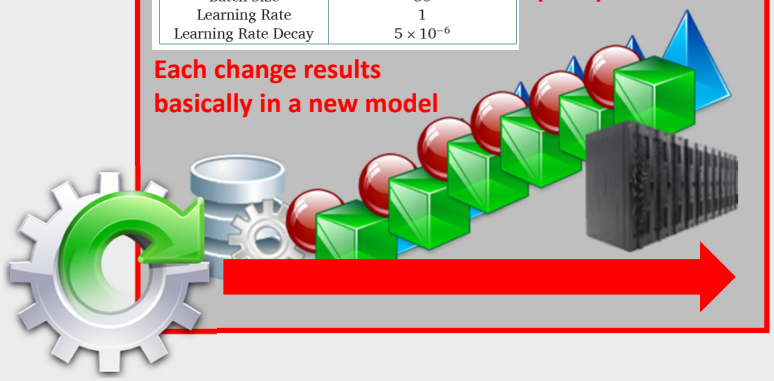
Use Case	AE	PINN	ANNs		CNN		NO	GNN		RNN		GAN	TF				SVM	RF
Details	*CAE*		*ANN*	*RBF-ANN*	*U-Net*	*RES NET*	*FNO*	*MLPF*	*GAT*	*LSTM*	*GRU*	*WGAN*	*MViT*	*ViViT*	*Swin*			
AI for turbulent boundary layers	X	X	X									X						
AI for wind farm layout optimization				X												X		
AI for data-driven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



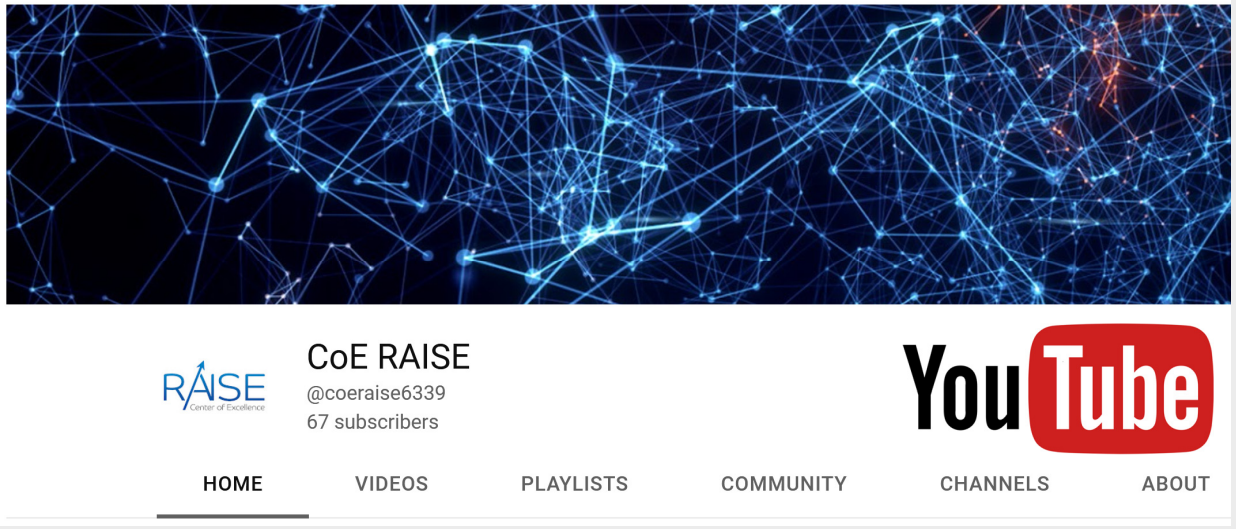
Feature	Representation / Value
Conv. Layer Filters	48, 32, 32
Conv. Layer Filter size	(3,3,5), (3,3,5), (3,3,5)
Dense Layer Neurons	128, 128
Optimizer	SGD
Loss Function	mean squared error
Activation Functions	ReLU
Training Epochs	600
Batch Size	50
Learning Rate	1
Learning Rate Decay	5×10^{-6}

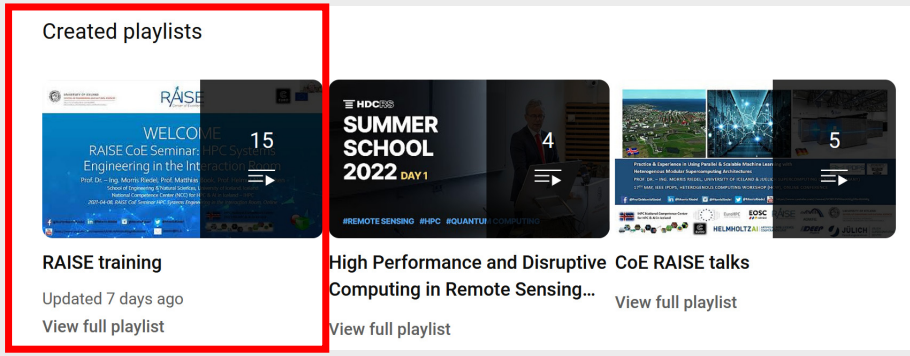
Examples of Hyperparameters for a Convolutional Neural Network (CNN)

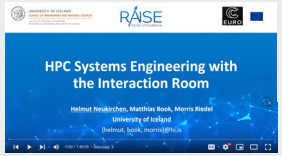
Each change results basically in a new model

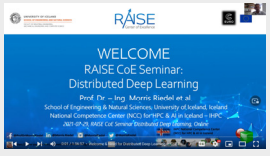


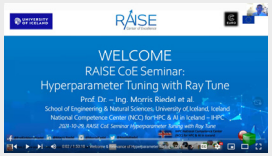
Lessons Learned Example: Role of YouTube Trainings

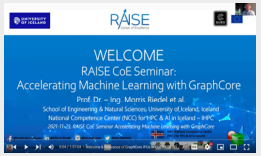


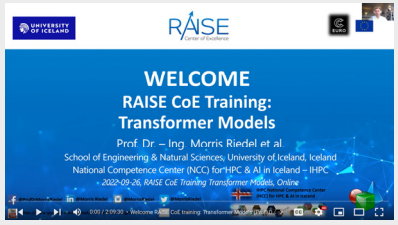


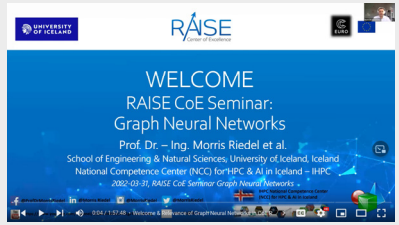












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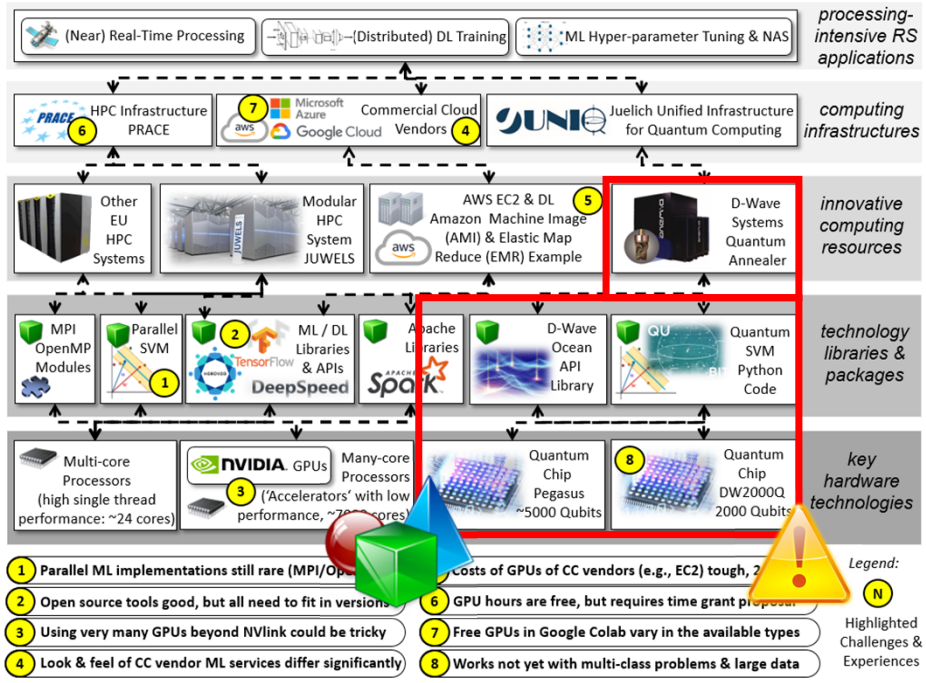
Lessons Learned Example: Role of Quantum Computing



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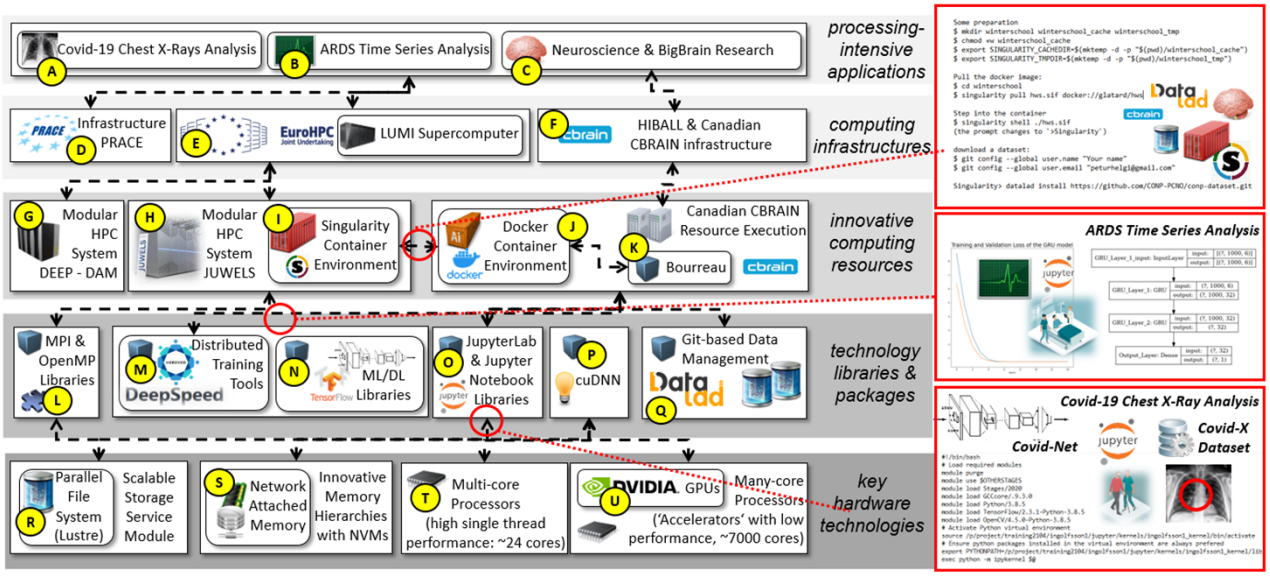
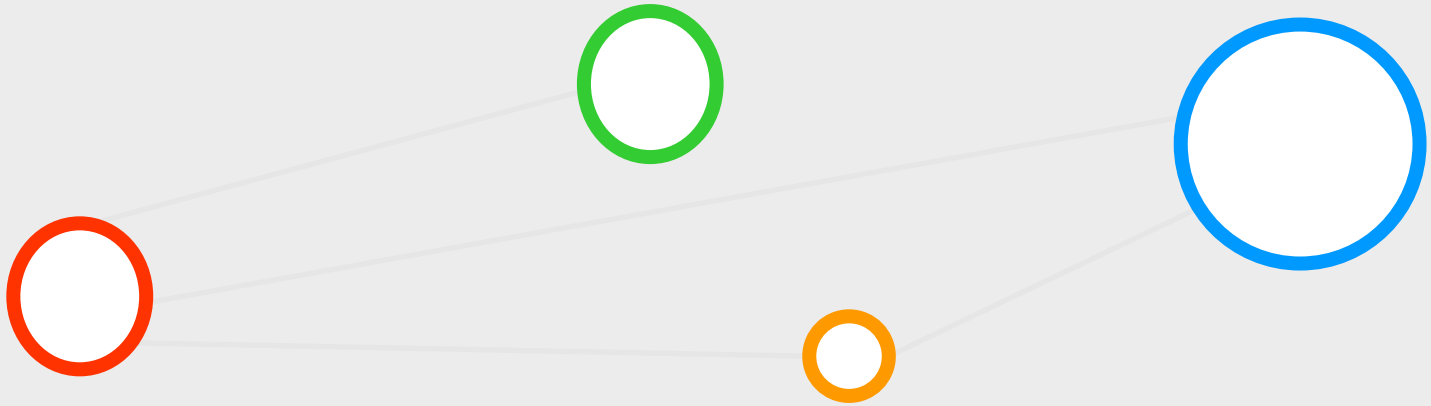
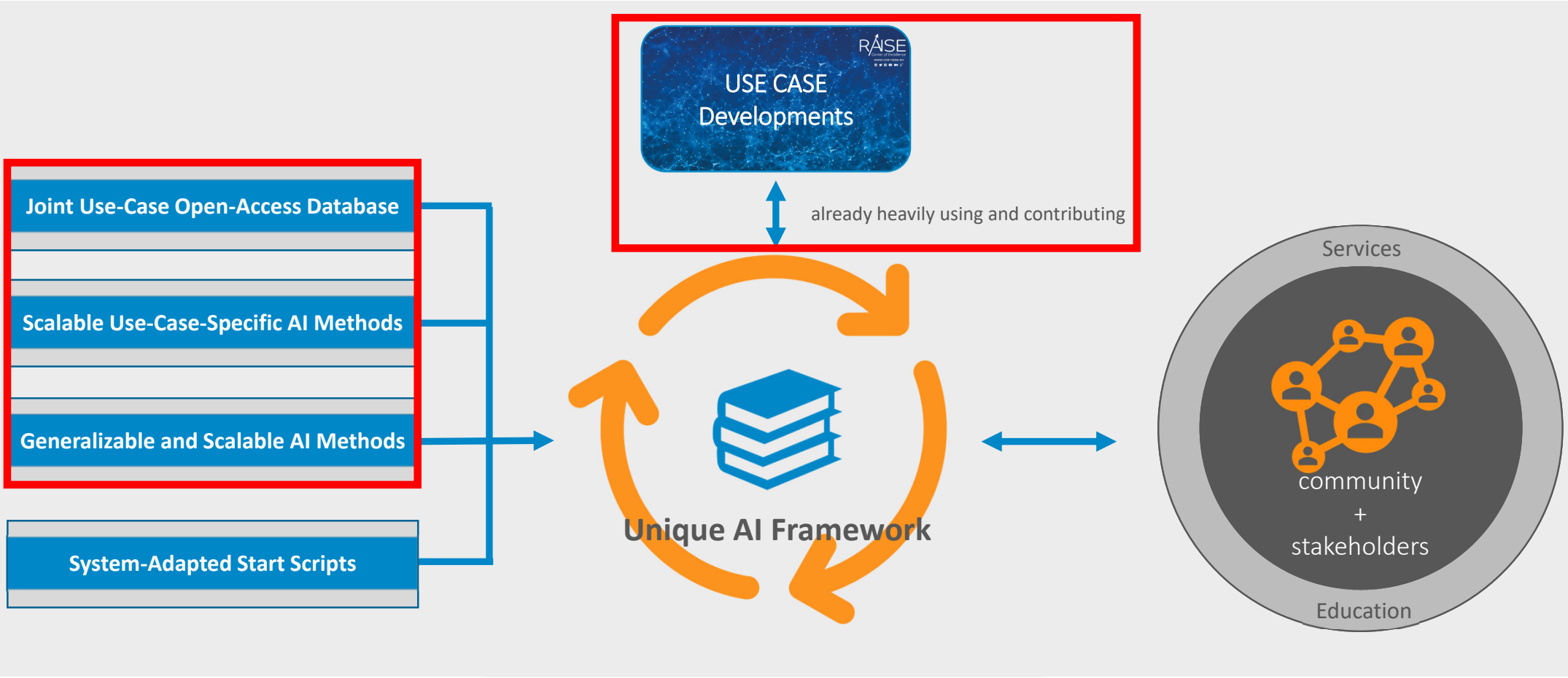
IPDPS 2021 Portland



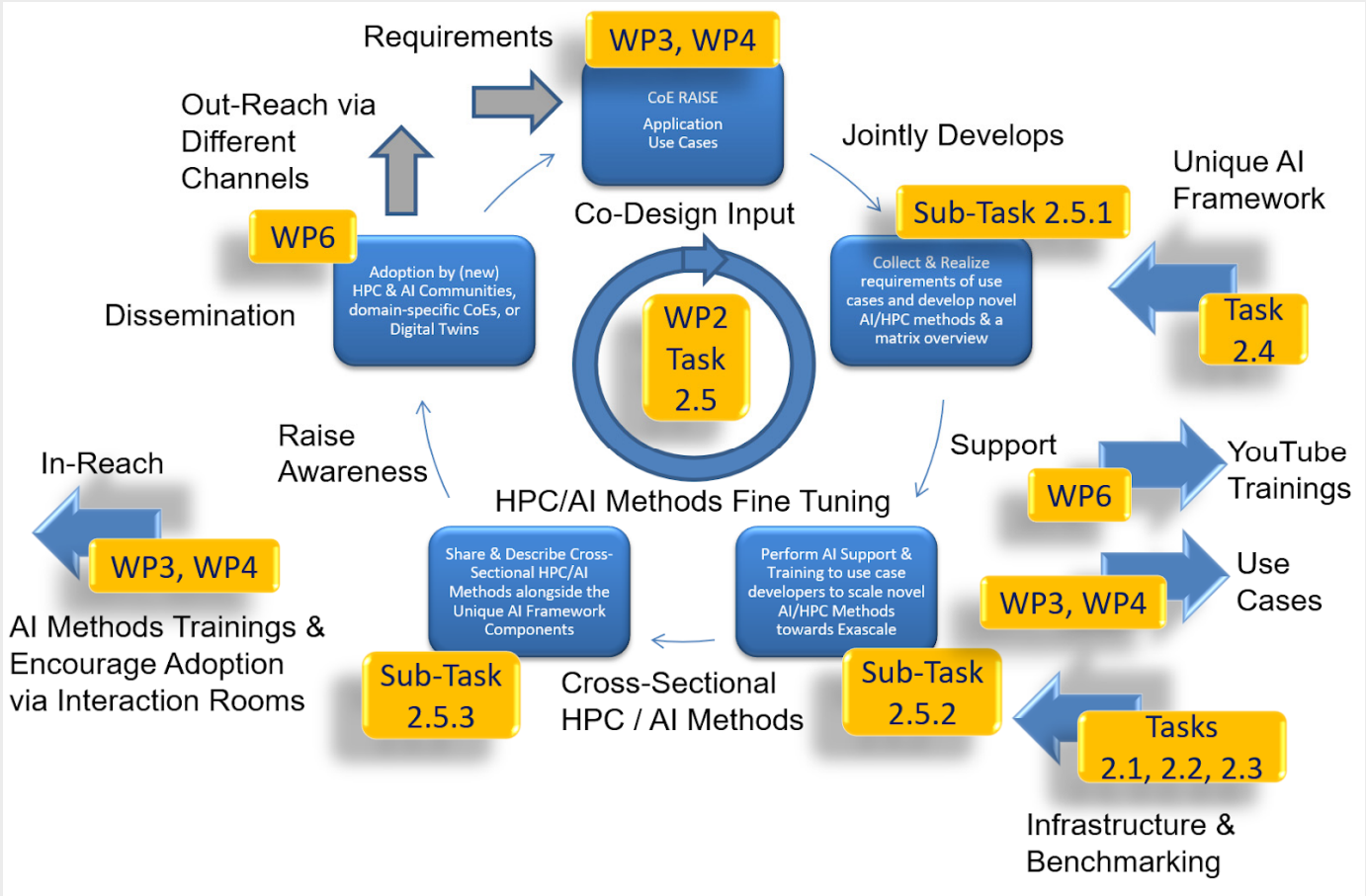
Summary & Q&A



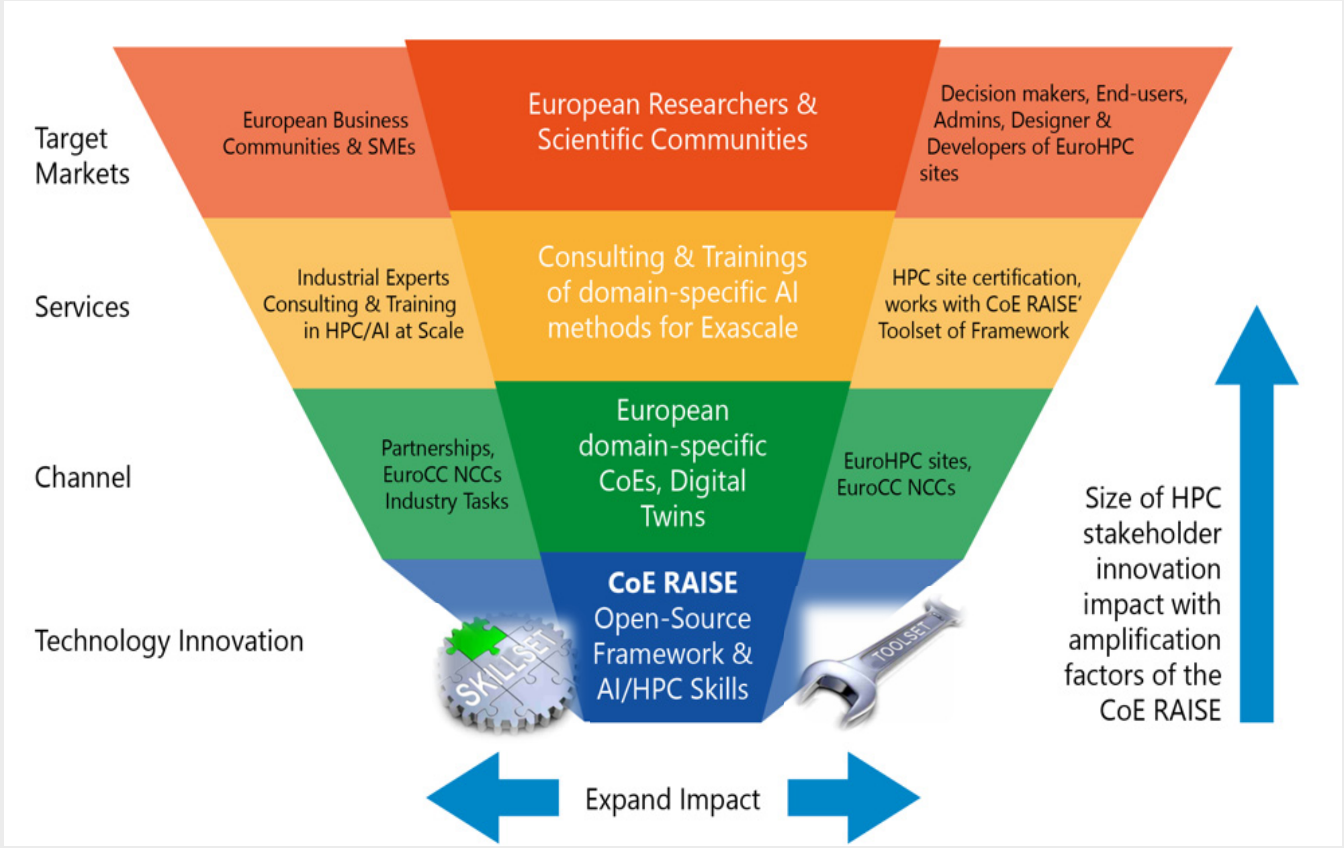
Summary: Unique AI Framework Overview



Summary: Working on Cross-Sectional HPC / AI Methods

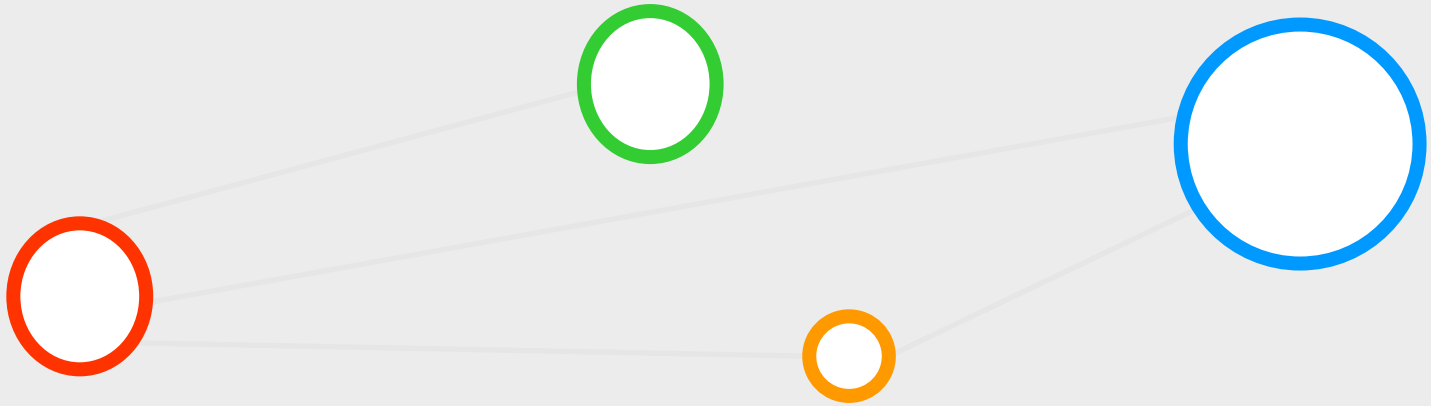


Q&A: NCC Feedback for Adoption?



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															

Selected References



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