WP2 AI- & HPC-Cross Methods at Exascale – Task 2.5: Cross-Sectional AI Methods

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WP2 Agenda & Tasks

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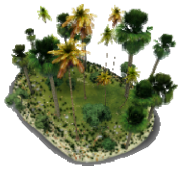
Work package 2 presentations		13:15 – 14:25
13:15 – 13:25	WP2 (UOI): Introduction AI- and HPC-Cross Methods at Exascale	M. Riedel
13:25 – 13:40	Task 2.1 (BSC): Modular and heterogeneous supercomputing architectures	G. Houzeaux
13:40 – 13:55	Task 2.2 (FZJ): Hardware prototypes	E. Inanc
13:55 – 14:10	Task 2.4 (UOI): Software design of a unique AI framework NEW	M.Riedel
14:10 – 14:25	Task 2.5 (UOI): Cross-Sectional AI Methods	M. Riedel

WP2 Task 2.5

The aim of this task is to complement the domain-specific application approaches in **WP3** and **WP4** with complementary general ML/DL and statistical methods. In-depth discussions with use-cases raised the requirements for the following initial set of methods (see Sec. 1.4.2): (i) feature selection/engineering methods, e.g., POD or dynamic mode decomposition, (ii) DA techniques, since the involved simulation science applications are computational very expensive and as a consequence lack enough data to learn from, (iii) PF methods to reduce parameter spaces in simulations, (iv) TL methods to transfer existing NN to novel problems, (v) NAS methods adapting their data acquisition and learning methods to systematically search parameter spaces of DL networks, (vi) PIDL techniques using constraints from physics in **WP3** simulations, (vii) AE techniques to partly replace coarse-grained elements, (viii) LSTM models for sequence problems in **WP4** use-cases. These methods are developed towards their Exascale-readiness.

WP2 Task 2.5 Key AI Methods to Consider form WP3/4



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MS2 - AI/HPC Methods (M7)

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Plan for next 12 Month

- **Revise factsheets over time & WP2 AI/HPC Methods matrix**

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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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

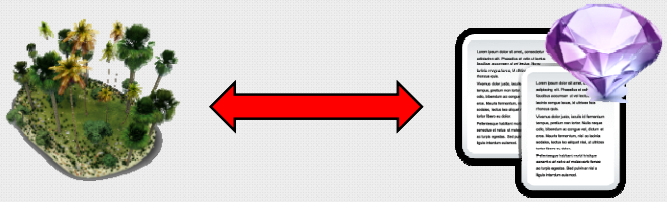
Use Case	AE	PIML	ANNs	CNN		NO	SMs			GNN	IN	LSTM	GRU
Details	*CAE*		*RBF-ANN*	*U-Net*	*RESNET*	*FNO*	*AR*	*ARMA*	*ARIMA*		*JEDI-net*		
AI for turbulent boundary layers	X	X											
AI for wind farm layout optimization			X				X	X	X				
AI for data-driven models in reacting flows				X						X			
Smart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

➢ **Talk of Task 2.5 (UOI): Cross-Sectional AI Methods includes details on how to move ahead with identifying cross-sectional techniques**

WP2 AI/HPC Methods – Identify Cross-Sectional AI Methods

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

- D2.14 Report on novel AI technologies (M12)



Continously Updating

Plan for next 12 Month

- Identify commonalities across AI methods in use cases
- Can we learn something from the common approaches?
- Can we identify and introduce common approaches to other use cases via lessons learned?

WP2 Framework with cross-sectional AI Methods & Techniques

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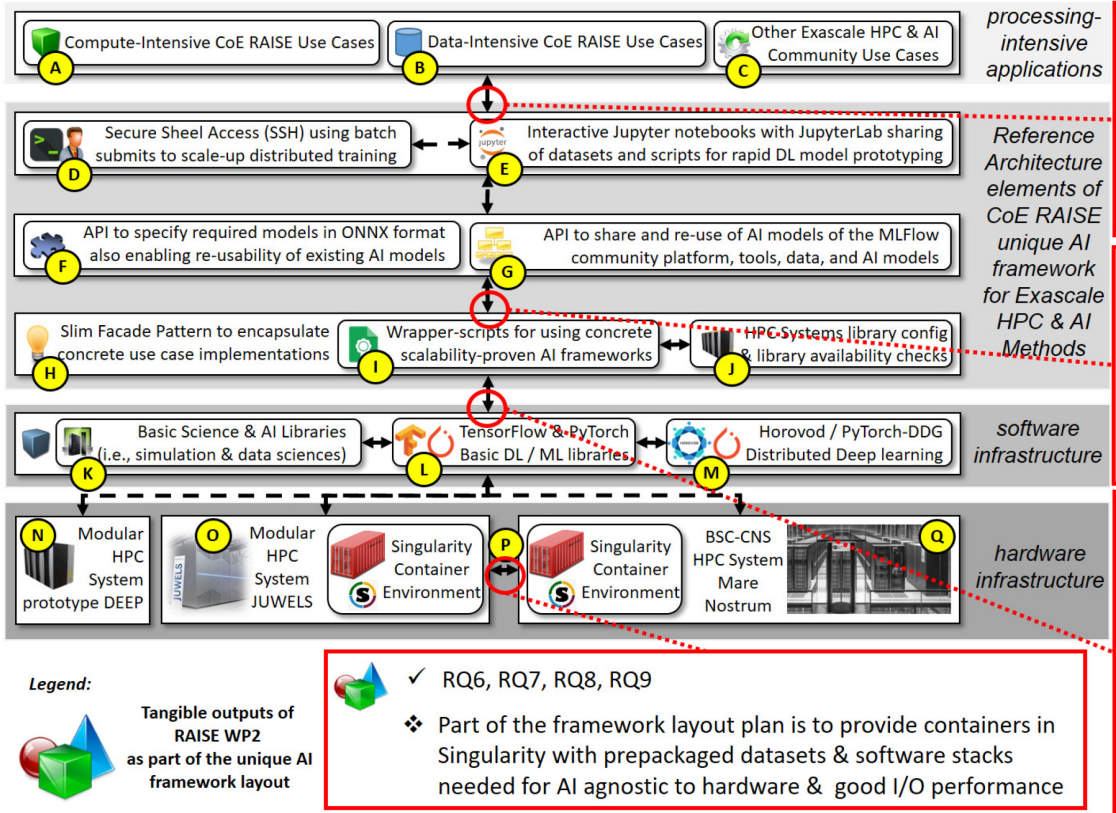
- Available in BSCW: https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3694045



Continously Updating

Plan for next 12 Month

- **Providing solutions for these requirements w.r.t. code, data, guidelines, descriptions, etc.**
- **Revise framework (e.g., add hyperparameter tuning) with WP3/WP4 and check the adoption of solutions**

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