WP2 - AI- and HPC-cross methods at exascale Overview and plans – Extension Period Discussions (→ M42+)

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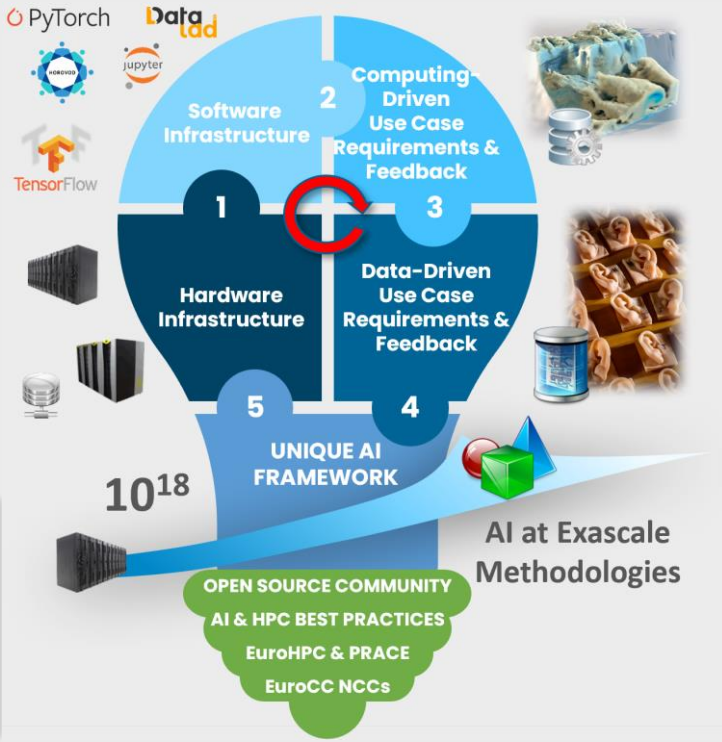
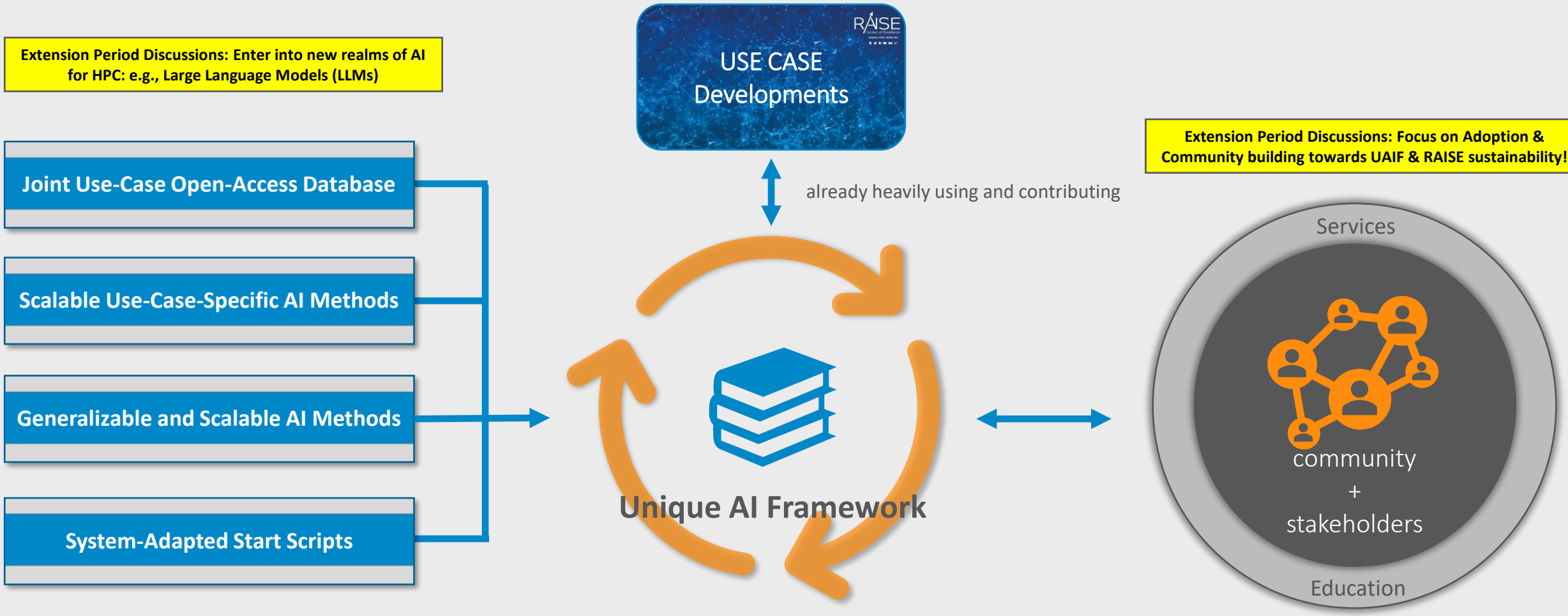
WP2 Objectives

- Build the AI / HPC Exascale backbone by providing the hardware & software infrastructure needed for the implementation of the WP3/WP4 use-cases
- Provide access to available production systems and new prototypes & disruptive technologies for testing, porting, and benchmarking
- Develop and tune cross-sectional HPC/AI methods with WP3/WP4 use cases
- Co-design, implement, and deploy a unique AI framework for Exascale



Extension Period Discussions: New AI areas, new HPC systems, new use cases for UAIF, new UAIF components?

Unique AI Framework Overview



Partners and Tasks of WP2

Partner	FZJ	UOI	RWTH	BSC	CERN	BULL	RTU	FM
PM	43	13	10	8	8	8	22	12

Task	Title	Lead	Duration	Status
2.1	Modular and heterogeneous supercomputing architectures	BSC	M1 – M36	Ongoing
2.2	Hardware prototypes	FZJ	M1 – M18	Done
2.3	Benchmarking on disruptive technologies	FZJ	M19 – M36	Ongoing
2.4	Software design of a unique AI framework	UOI	M4 – M36	Ongoing
2.5	Cross-Sectional AI Methods	UOI	M3 – M36	Ongoing

Extension Period Discussions: Tasks will run longer!

Deliverables of WP2 (1/2) – Status Updates

ID	Title	Due	Lead	Status
D2.1	Best practice guidelines/tutorials for MSA/heterogeneous systems	M2	BSC	Submitted
D2.2	Report on porting and performance analysis	M12	BSC	Submitted
D2.3	Report on porting and performance analysis	M24	BSC	Submitted
D2.4	**Report on porting and performance analysis**	**M42?**	**BSC**	Not started NEW
D2.5	Best practice guidelines / tutorials prototype	M2	FZJ	Submitted
D2.6	Report on support activities	M6	FZJ	Submitted
D2.7	Report on support activities	M18	FZJ	Submitted
D2.8	Report on benchmarking AI technologies (QA) and on support activities	M24	FZJ	Submitted
D2.9	**Report on benchmarking AI technologies (QA) and on support activities**	**M42?**	**FZJ**	Not started NEW
D2.10	Monitoring Report	M18	UOI	Submitted

Extension Period Discussions: Deliverable Due Dates Shifts

Deliverables of WP2 (2/2) and Milestones

ID	Title	Due	Lead	Status
D2.11	**Monitoring Report**	**M42?**	**UOI**	**Not started** NEW
D2.12	Software Layout Plan for a unique AI Framework	M9	UOI	**Submitted**
D2.13	Software Layout Plan for a unique AI Framework	M26	UOI	**Submitted**
D2.14	Report on Novel AI Technologies	M12	UOI	**Submitted**
D2.15	Report on Novel AI Technologies	M24	UOI	**Submitted**
D2.16	**Report on Novel AI Technologies**	**M42?**	**UOI**	**Not started** NEW

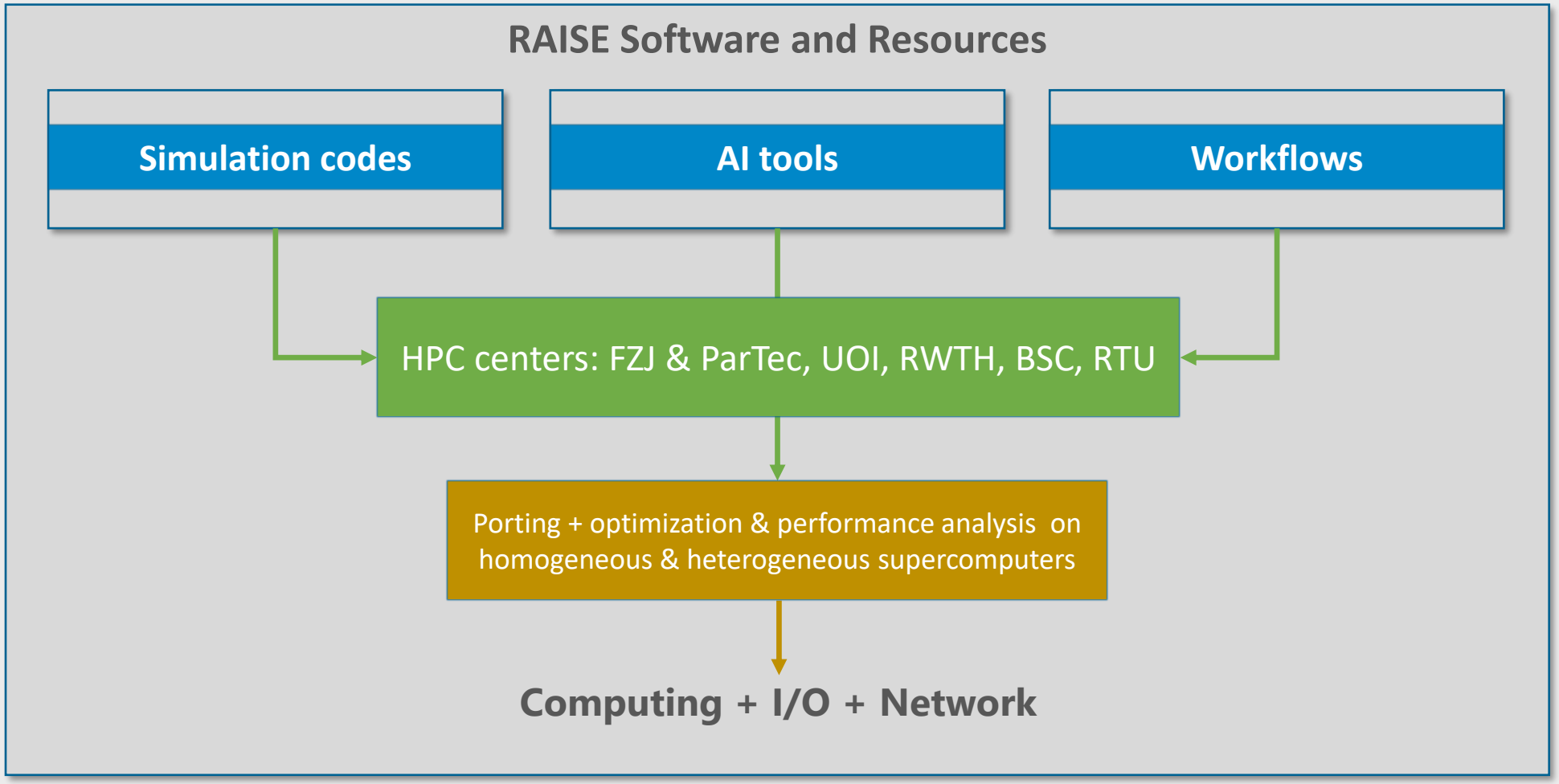
ID	Title	Due	Lead	Status
MS2	AI/HPC Methods	M7	UOI	**Achieved**
MS4	Technical implementations functional	M24	FZJ	**Achieved**
MS6	**All final reports**	**M42?**	**FZJ**	**Not yet achieved** NEW

Extension Period Discussions: Deliverable & Milestone Due Dates Shifts

Task 2.1

Modular and heterogeneous supercomputing architectures

Task 2.1 – Modular and heterogeneous supercomputing …

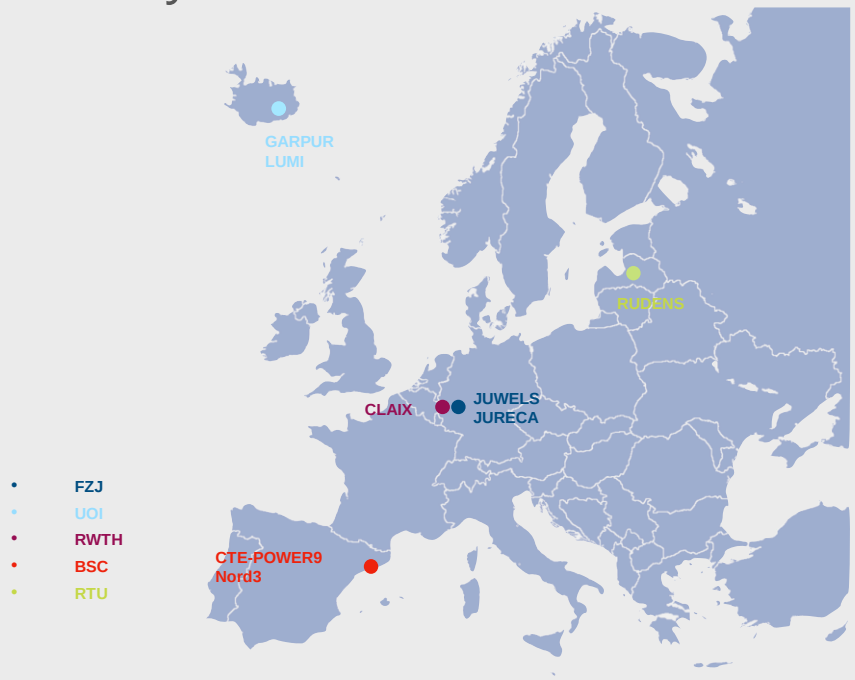


Task 2.1 – Modular and heterogeneous supercomputing …

Deliverable D2.1: Best practice guidelines and tutorials for the various HPC systems

- 4 countries
- 8 systems

Extension Period Discussions: What systems are important for UAIF uptake?



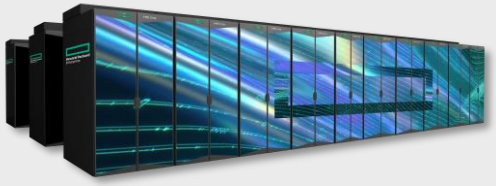
CTE-Power, Nord3

JUWELS

JURECA

RUDENS

CLAIX



GARPUR & LUMI

Task 2.2 (M1-M18 DONE)

Extension Period Discussions: new prototypes?

Hardware prototypes

Task 2.3

Benchmarking on disruptive technologies

Task 2.3 – Benchmarking on disruptive technologies

First 5,000 Qubits Quantum Annealer (JUPSI) in Europe (FZJ)

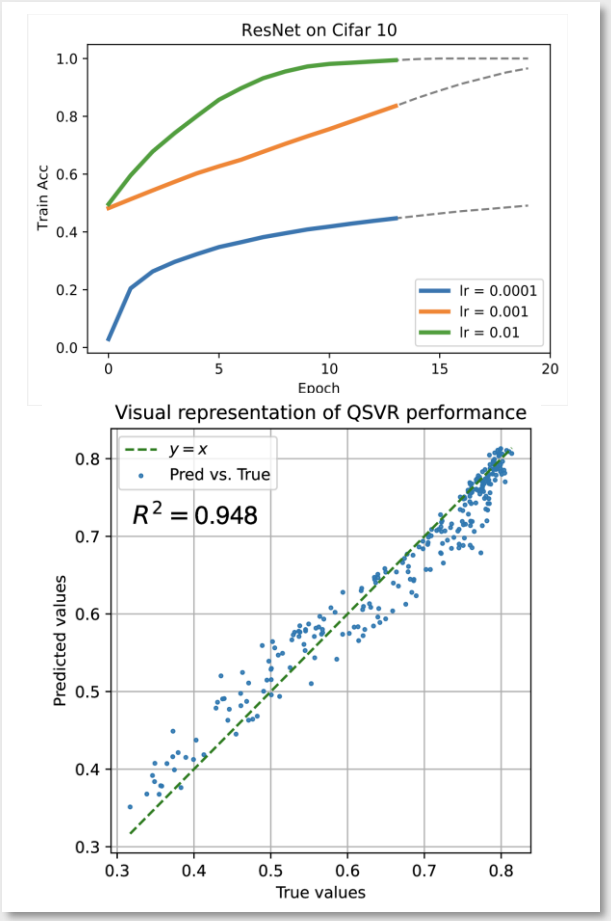
- 5 hours of compute time for RAISE project
- problem size still very limited -> hybrid/modular supercomputing approach

Applications:

- Quantum accelerated hyperparameter tuning
- Quantum clustering of energy particles
- Quantum classification of satellite images

First results:

- predicting the learning curves of neural network training with Quantum Support Vector Regression



Solution

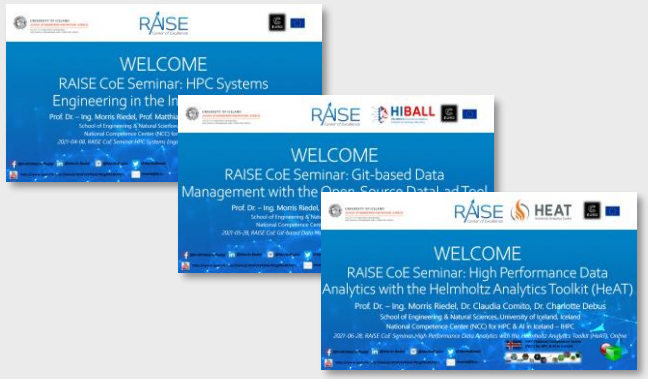
Data problem

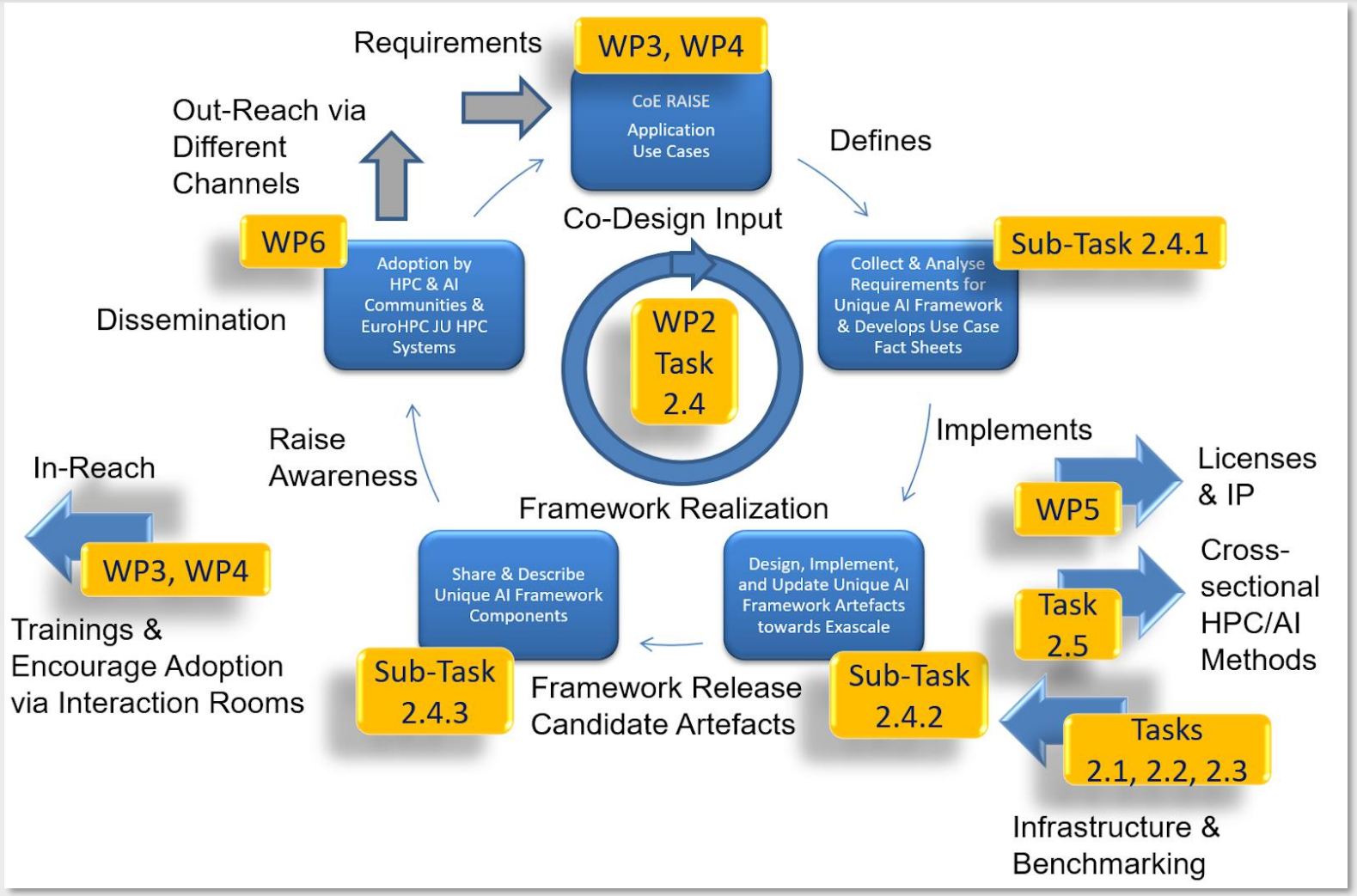
Extension Period Discussions: Quantum important – other Quantum systems?

Task 2.4

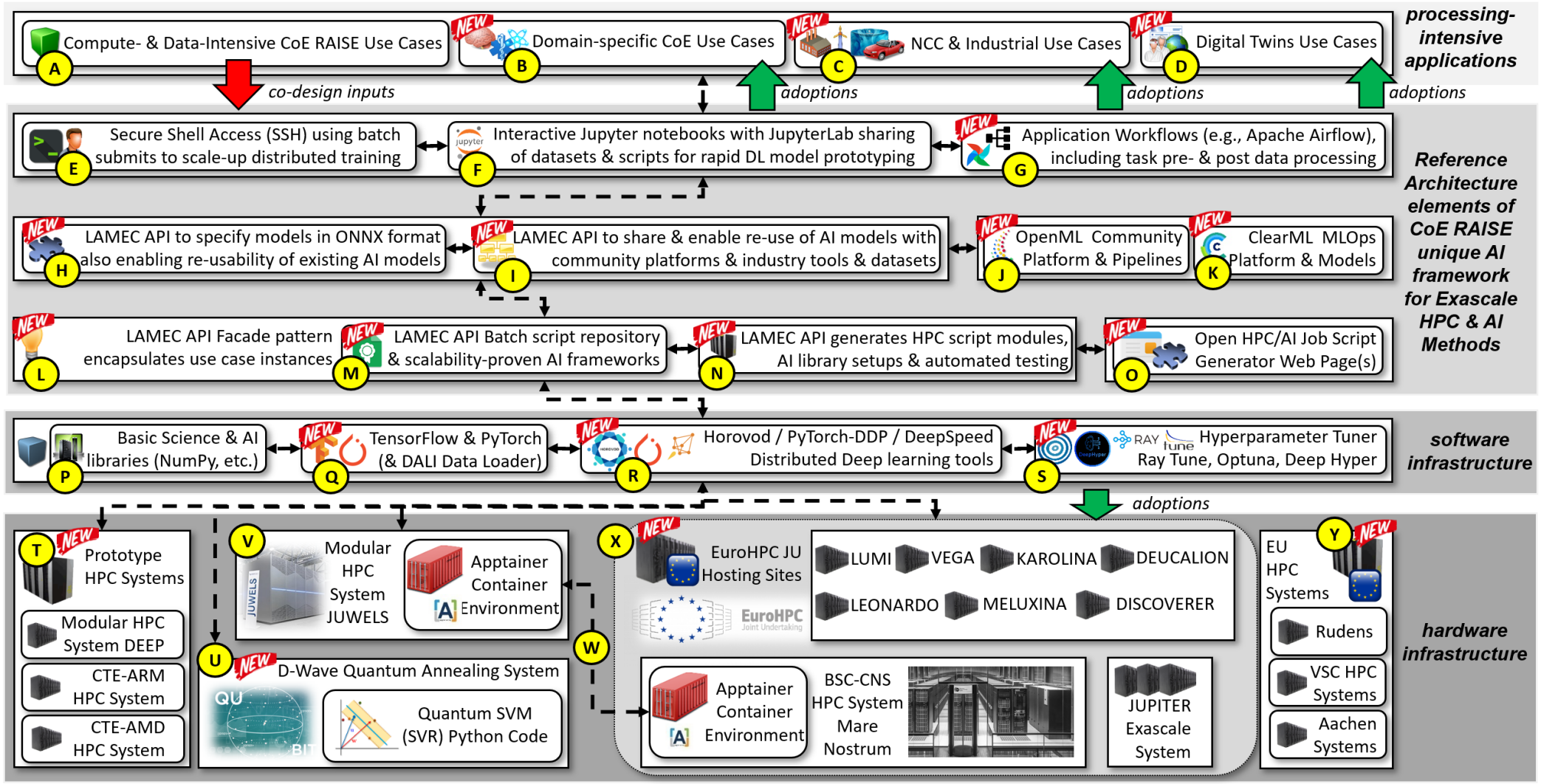
Software design of a unique AI framework

Task 2.4 – Status: Process towards Framework Realization





Realization of SW Framework



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.?

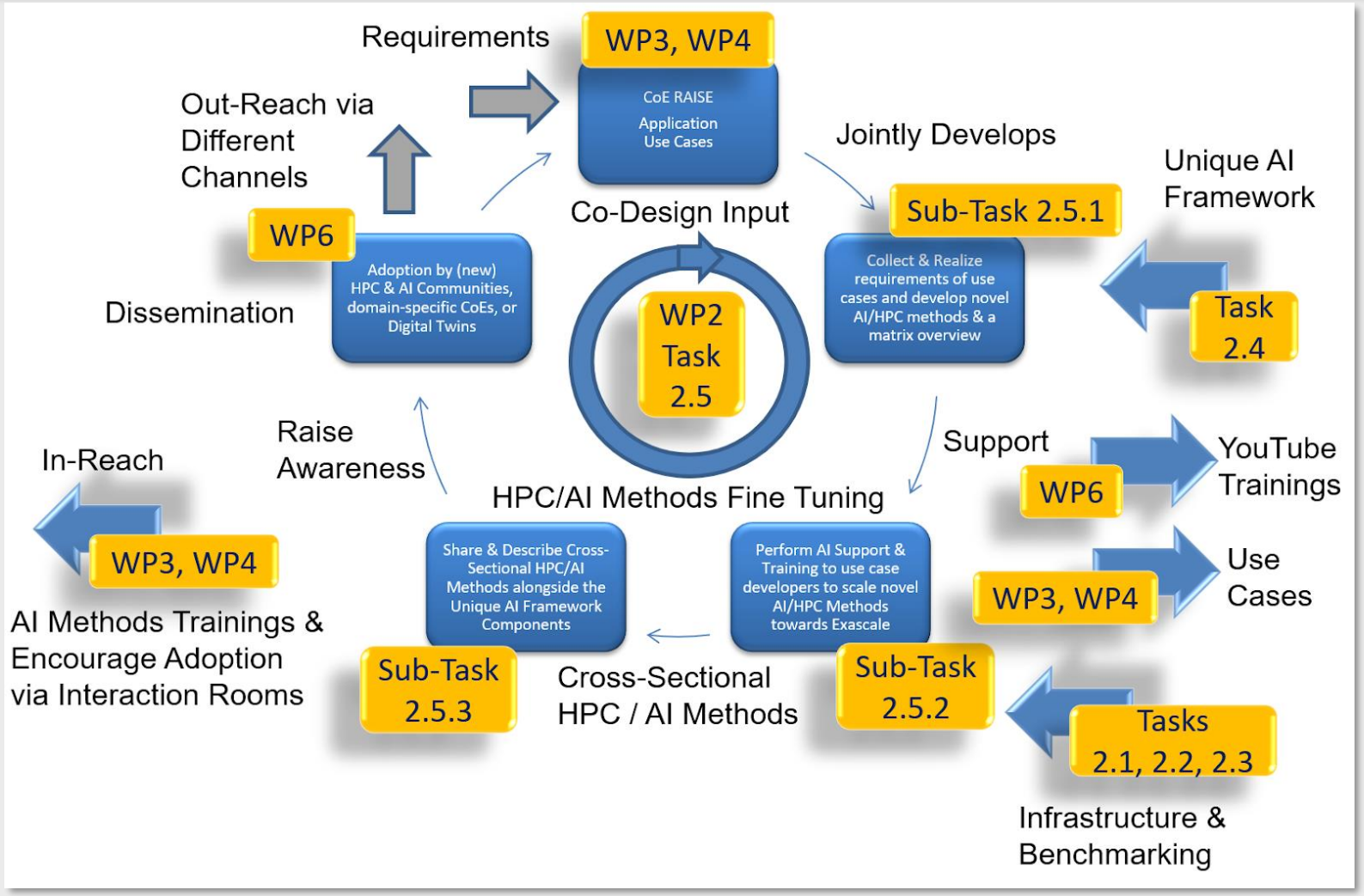
Continously Updating!

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?

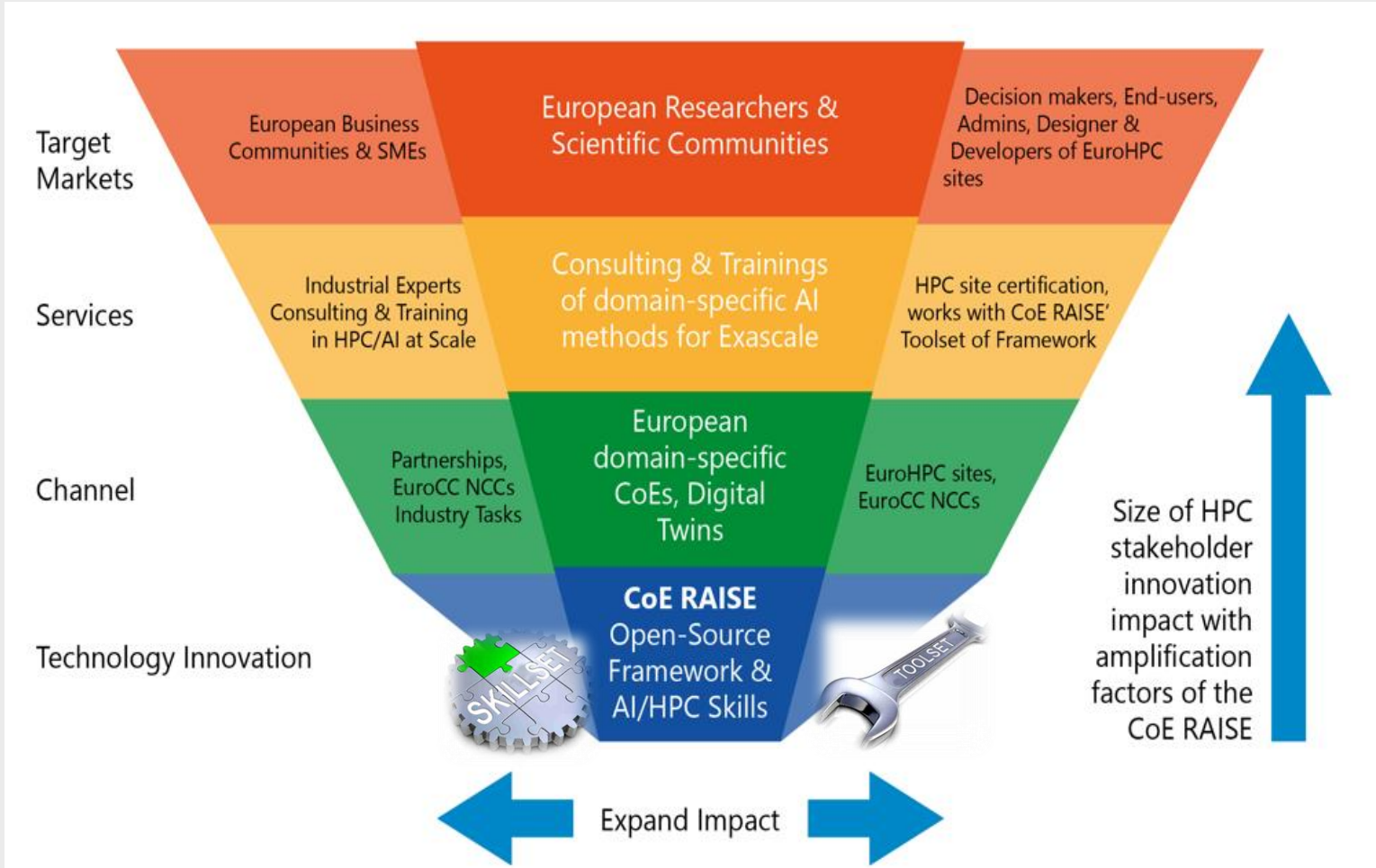
Task 2.5

Cross-Sectional AI Methods

Task 2.5 – Status: Process building AI/HPC Methods



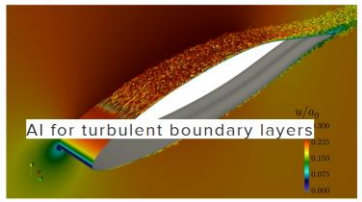
Q&A: NCC Feedback for Adoption & New RAISE Use Cases

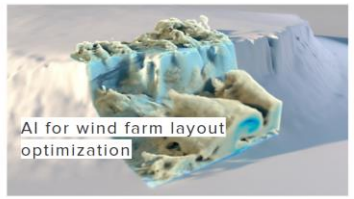


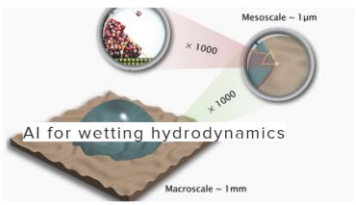
Extension Period: Addition of new stakeholders (e.g., NHR4CES Project, ARDS/Covid-19 use cases SMITH, etc.) – more needed → input to deliverables at M42!

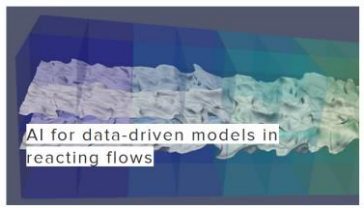
Use Case	Task	AE		PINN	ANNs		CNN			NO	GNN		RNN		GAN		TF				QC SVM	RF	CP
Details	#	CAE	VQ-VAE	PINN	ANN	RBF-ANN	U-Net	RES NET	CNN	FNO	MLPF	GAT	LSTM	GRU	WGAN	CGAN	MViT	ViViT	Swin	TF			
AI for turbulent boundary layers	3.1	X		X	X										X								
AI for wind farm layout optimization	3.2					X			X											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									
Event reconstruction and classification at the CERN HL-LHC use case	4.1																				X		
Seismic imaging with remote sensing for energy applications	4.2	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

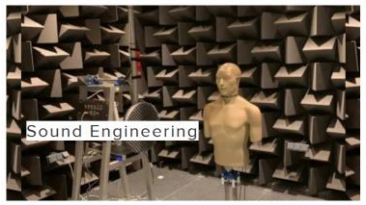
Compute & Data-Driven Use Cases of HPC/AI Methods

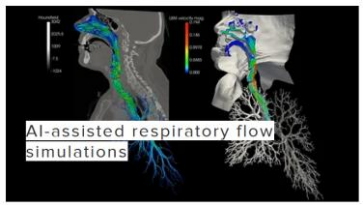


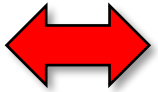












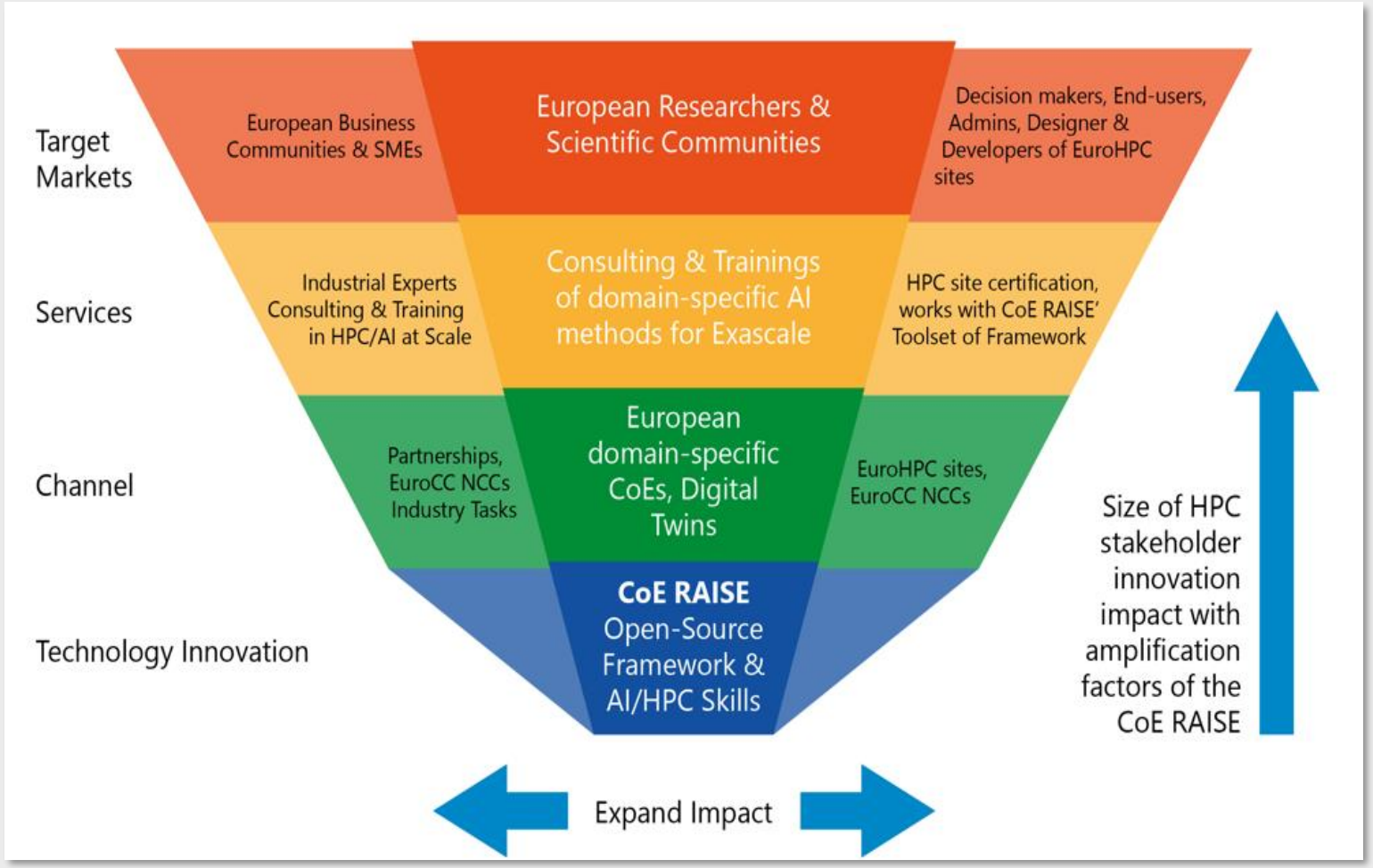
Extension Period Discussions: Update of our use cases – but what new external use cases can we add, e.g. TrustLLM?, interTwin?, NCCs?

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

WP2

Summary & Next Steps

WP 2 – Summary, Conclusions, and Next Steps



- **Working with new RAISE stakeholders (e.g., NHR4CES Project, ARDS/Covid-19 use cases SMITH, TrustLLM, etc.)**
- **Adopt framework components where possible in NCCs & EuroHPC JU Hosting Sites – use cases to add to our matrix**
- **Working on final Deliverables D2.4, D2.11, D2.16 together – shifted to M42?**
- **More YouTube trainings & WP6 News**

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