WP2 AI- & HPC-Cross Methods at Exascale – Task 2.4: Software Design of a Unique AI Framework

Prof. Dr. – Ing. Morris Riedel et al.
School of Engineering & Natural Sciences, University of Iceland
2021-11-24, RAISE All Hands Meeting, Online

@ProfDrMorrisRiedel @Morris Riedel @MorrisRiedel @MorrisRiedel
https://www.youtube.com/channel/UCWC4VKHmL4NZgFfKoHtANKg morris@hi.is

WP2 Agenda & Tasks

RAISE Center of Excellence

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 2.4

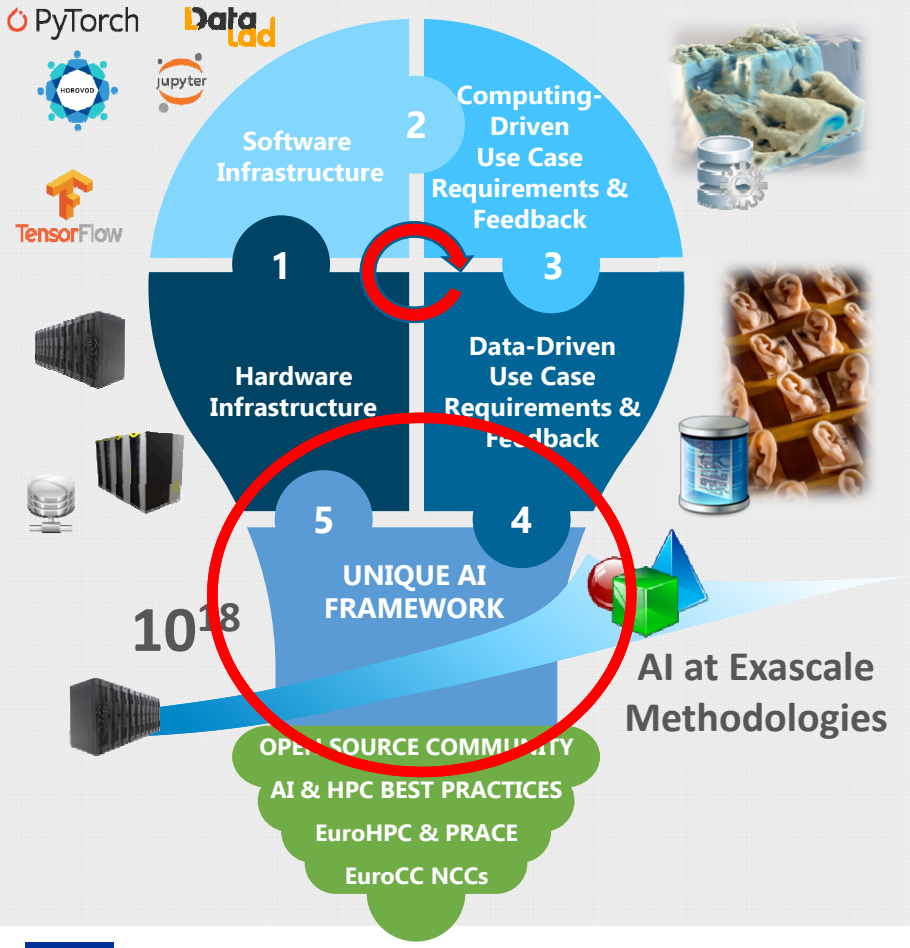
In this task, the software design of a unique use-case-driven AI framework is commenced within the frame of a planning and strategy layout phase. Therefore, the task contributors perform a use-case requirement analysis to decide on a generalized layout of the framework that includes all necessary components coming from the use-cases. It ensures that the developments in the use-cases are in line with a future integration into a generalized software framework by continuously monitoring them. A lively interaction between the framework designers and the use-case developers is necessary to find a layout, which is suitable for a generalized approach. Interfaces and APIs are described in detail together with the use-case providers to ensure the generalized approach and future sustainability of the framework as well as its easy application. It is ensured that use-case results are furthermore in line with the Design and Development of new Service prototypes task of PRACE 5IP/WP6. Suitable use-cases will be contributed to the PRACE GitLab Data Analytics project.

WP2 Deliverables – Status

Del. No.	Delivery Name	Lead benificiary	Type	Dis. Level	Del mo.	WP Leader	Responsible Editor, Authors	Internal Reviewers	Reviewers from PMT	Date draft av. for int. review	Deadline subm. to EC	Submitted to EU on
D2.1	Best practice guidelines/tutorials for MSA/heterogenous systems	BSC	R	PU	2	M. Riedel/ UOI	G. Houzeaux/ BSC	S. Richard/ SAFRAN	A. Lintermann/ FZJ	08.02.2021	28.02.2021	26.02.2021
D2.5	Best practice guidelines/tutorials prototype	FZJ	R	PU	2	M. Riedel/ UOI	A. Lintermann/ FZJ	V. Khristenko/ CERN	J. Lopez/ ParTec	08.02.2021	28.02.2021	26.02.2021
D2.6	Support report	FZJ	R	PU	6	M. Riedel/ UOI	E. Inanc/ FZJ	R. Heylen/ FM	I. Schmitz/ ParTec	09.06.2021	30.06.2021	25.06.2021
D2.12	Software framework layout plan	UOI	OTHER	PU	9	M. Riedel/ UOI	M. Book/ UOI	R. Speck/ FZJ	J. Lopez/ ParTec	09.09.2021	30.09.2021	30.09.2021
D2.2	Report on porting & performance engineering	BSC	R	PU	12	M. Riedel/ UOI	G. Houzeaux/ BSC	M. Meinke/ RWTH	A. Lintermann/ FZJ	29.11.2021	31.12.2021	
D2.14	Report on novel AI technologies	UOI	R	CO	12	M. Riedel/ UOI	M. Riedel/ UOI	S. Kesselheim/ FZJ	J.Lopez/ ParTec	29.11.2021	31.12.2021	
D3.1	Report on outcomes of WP3 use-cases	RWTH	R	CO	12	W. Schröder/ RWTH	M. Meinke/ RWTH	S. Schlimpert/ FM	J.Lopez/ ParTec	29.11.2021	31.12.2021	
D4.1	Report on outcomes of WP4 use-cases	CERN	R	CO	12	M.Girone/ CERN	E. Wulff/ CERN	H. Neukirchen/ UOI	I. Schmitz/ ParTec	29.11.2021	31.12.2021	

➢ **Talk of Task 2.4 (UOI): Software design of a unique AI framework includes interaction room process for co-design & more D2.12 details**

Towards AI & HPC at Exascale with CoE RAISE Results



Hardware Infrastructure

GRAPHCORE

Prepare & Document available production systems at partners' HPC centers

Examples: JUWELS (JUELICH), LUMI (UoICELAND), DEEP Modular Prototypes, JUNIQ (JUELICH), etc.

Software Infrastructure

Prepare & Document available open source tools & libraries for HPC & AI useful for implementing use cases

Examples: DeepSpeed and/or Horovod for interconnecting N GPUs for a scalable deep learning jobs

Computing-driven Use Cases Requirements & Feedback

Use cases with emphasize on computing bring in co-design information about AI framework & hardware

Examples: Use feedback that TensorFlow does not work nicely, so WP2 works with use cases on pyTorch

Data-driven Use Cases Requirements & Feedback

Use cases with emphasize on data bring in co-design information about AI framework & hardware

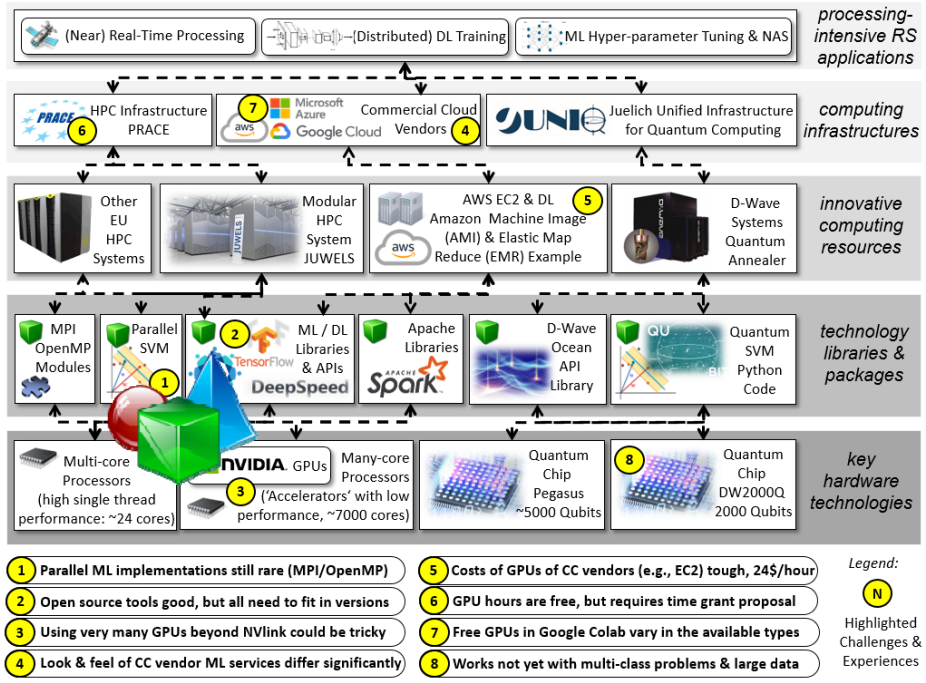
Examples: Deployment blueprint by using AI training on cluster module & inference/testing on booster

→ UNIQUE AI FRAMEWORK

Living design document & software framework blueprint for using HPC & AI offering also pretrained AI models

Fact Sheet Process of CoE RAISE & Early Co-Design Examples

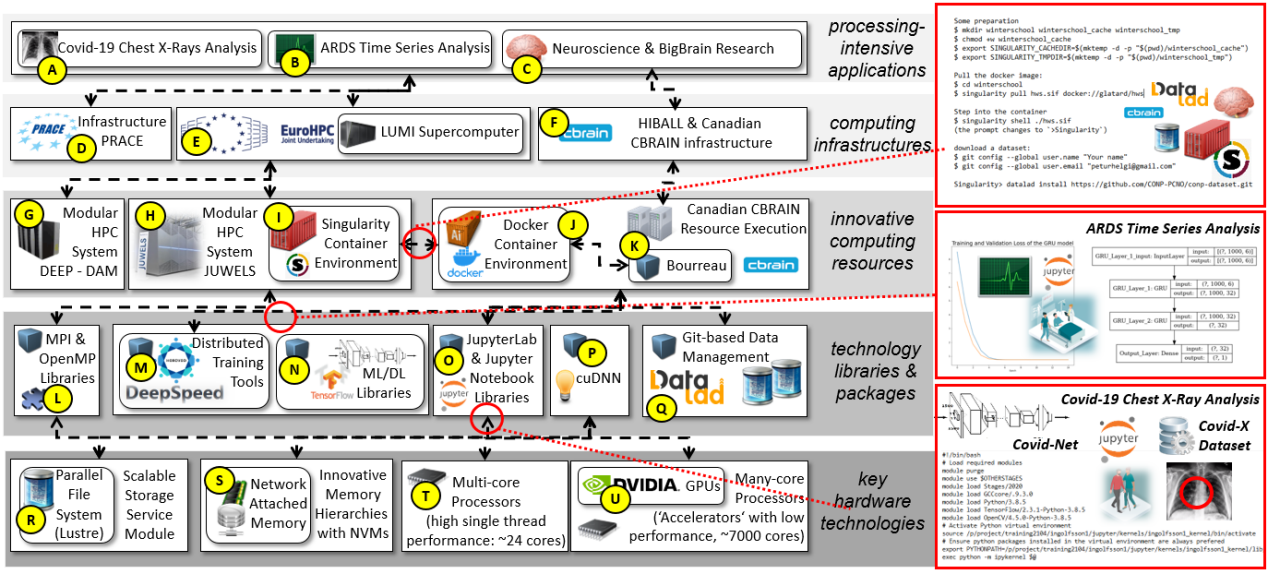
RAISE Center of Excellence



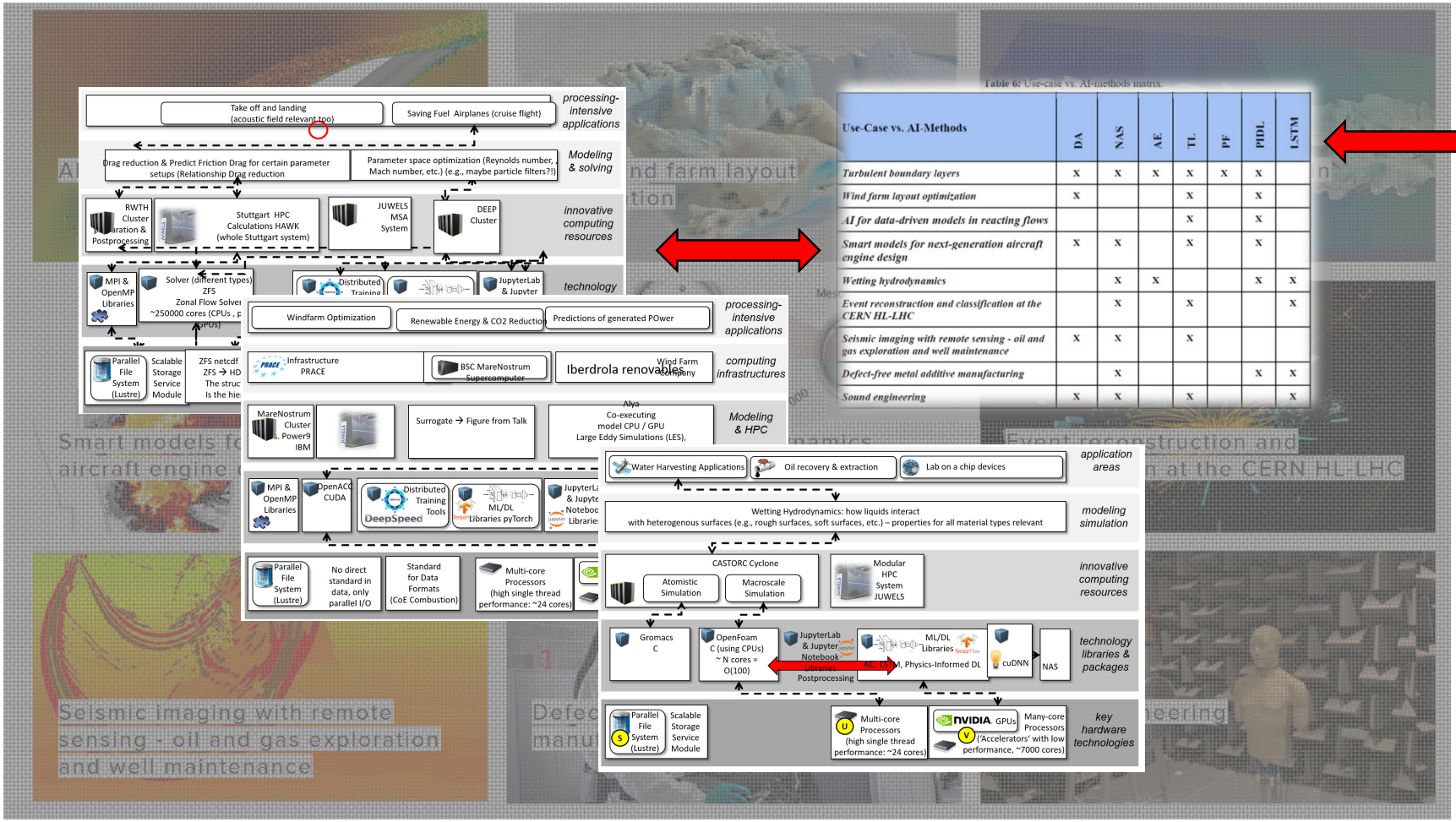
Riedel, M., Cavallaro, G., Benediktsson, J.A.: Practice and Experience in using Parallel and Scalable Machine learning in Remote Sensing from HPC over Cloud to Quantum Computing, in conference proceedings of the IEEE IGARSS Conference, Brussels, Belgium, 2021, Physical and Online event, to appear
https://igarss2021.com/

Riedel, M., Sedona, R., Barakat, C., Einarsson, P., Hassanian, R., Cavallaro, G., Book, M., Neukirchen, H., Lintermann, A.: Practice and Experience in using Parallel and Scalable Machine learning with Heterogenous Modular Supercomputing Architectures, in conference proceedings of the IEEE IDPDS Conference, Heterogenous Computing Workshop (HCW), Portland, USA, 2021, Online, to appear
https://www.ipdps.org/

IPDPS 2021 Portland



WP2 – Fact Sheets in Close Collaboration with WP3/4



WP2 Fact Sheets Iteration – Next Steps: Interaction Rooms

- Follow-Through
  - Fact Sheet actions done → Closing
  - Interaction Rooms done → Closing
    (continue within tasks, plan another round now)
  - Task-wise Interaction Rooms started

B - Create WP2 Expertise Matrix Draft and Circulate for WP2 Review
#7 · created 4 months ago by Morris Riedel · WP2 Expertise Matrix Exists · Aug 31, 2021

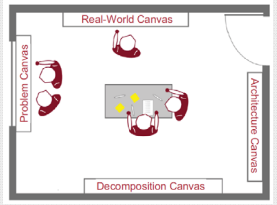
B - Perform Interaction Room Task 4.2 Seismic Imaging
#31 · created just now by Morris Riedel

B - Perform Interaction Room Task 3.3 Reacting Flows & Task 3.4 Engine Design
#30 · created 1 minute ago by Morris Riedel

B - Perform Interaction Room Task 4.1 Fundamental Physics
#29 · created 2 minutes ago by Morris Riedel

initial steps

input to Interaction Room process



input to Milestone (M7) AI/HPC Methods

input to Deliverable D2.12 (M9) Layout plan AI Framework

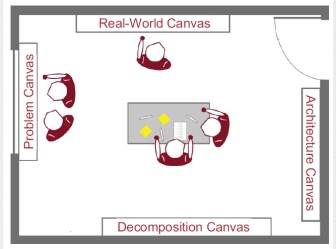
Plan for next 12 Month
- **Use interaction room more often and have more meetings with WP3/WP4**

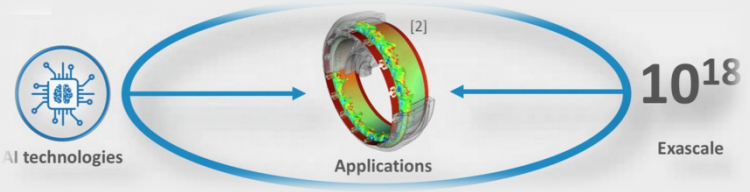
B - Create Deliverable D2.12 - Software layout plan for a unique AI framework (M9)
#33 · created 19 hours ago by Morris Riedel

B - Create Milestone M2 - AI/HPC Methods (M7)
#32 · created 19 hours ago by Morris Riedel

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: https://www.youtube.com/channel/UCAdIZ-v6cWwGdapwYxdN7dg
  - Methology as one CoE RAISE outcome

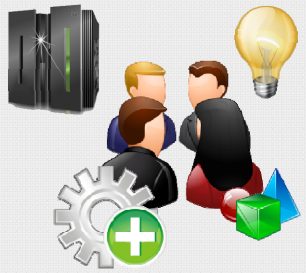


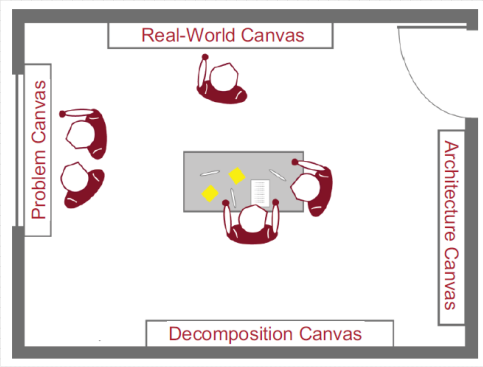


Book, M., **Riedel, M.**, **Neukirchen, H.,** Goetz, M.: Facilitating Collaboration in High-Performance Computing Projects with an Interaction Room, in conference proceedings of the 4th ACM SIGPLAN International Workshop on Software Engineering for Parallel Systems (SEPS 2017), October 22-27, 2017, Vancouver,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

Interaction Room Status & Discussions – WP3/WP4 Overview

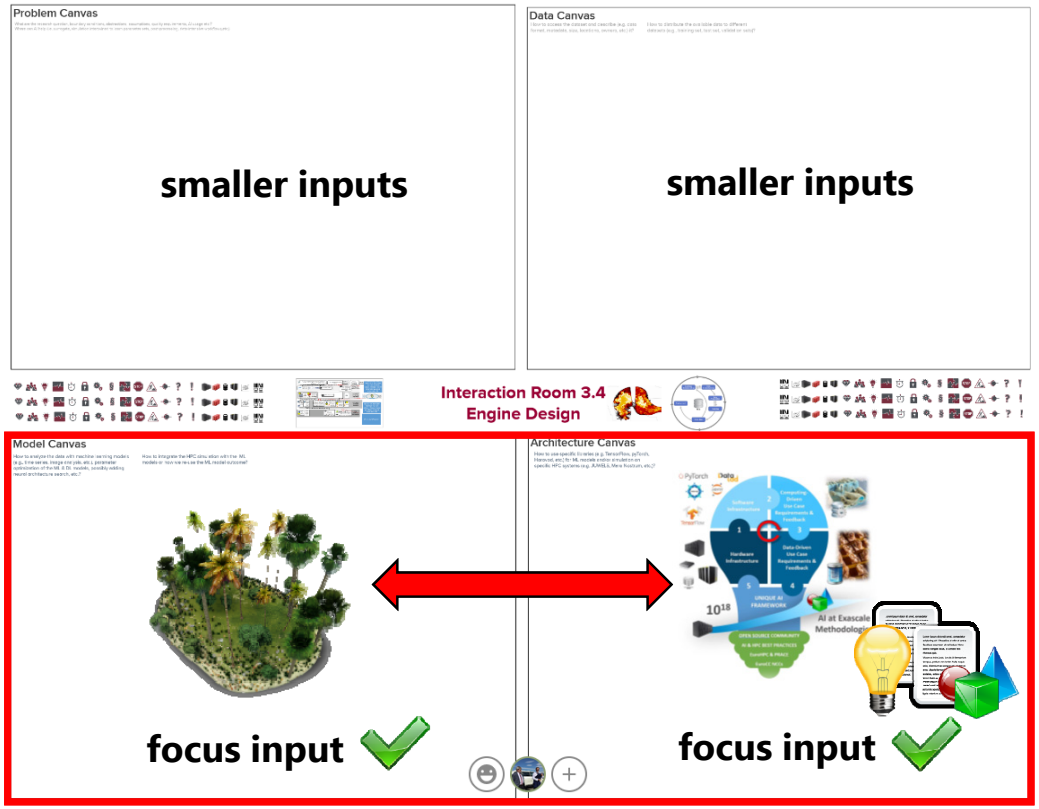
- WP3
  - T3.1: Turbulent Flow (started)
  - T3.2: Clean Energy (started)
  - T3.3: Reactive Flows (started)
  - T3.4: Engine design (started)
  - T3.5: Coating (started)
- WP4
  - T4.1: Fundamental physics (started)
  - T4.2: Seismic imaging (started)
  - T4.3: Manufacturing (started)
  - T4.4: Sound engineering (started)

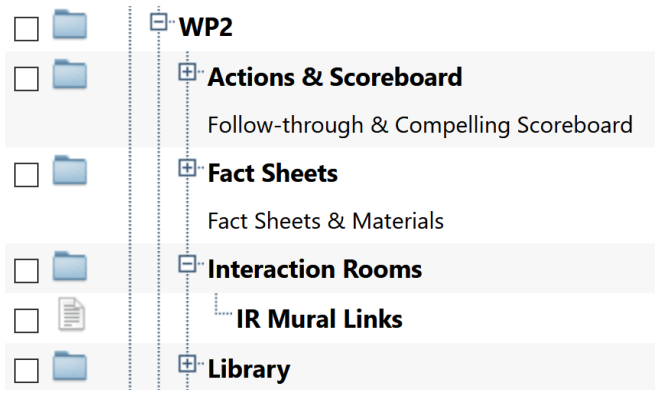


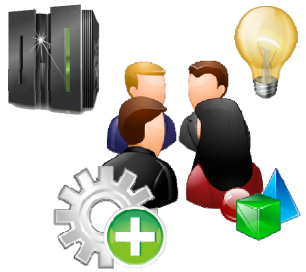


Use Case	AE	PIML	ANNs	CNN		NO	SMs			GNN	IN	LSTM	GRU
Details	*CAE*		*RBF-ANN*	*U-Net*	*RESNET*	*FNO*	*AR*	*ARMA*	*ARIMA*		*JEDI-net*		
AI for turbulent boundary layers	X	X											
AI for wind farm layout optimization			X				X	X	X				
AI for data-driven models in reacting flows				X						X			
Smart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

Interaction Rooms via MURAL Boards & Refinements for D2.14







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/matthiasbook8855/1621378007555/6f0d5285fcaec5eafa515bd6676c84d8b4879d39?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/matthiasbook8855/1621378038069/93df6fa7a41093f4eaae7be9d72979dc2ba42b9d?sender=u15e3008bb41d6628a5bb5701

IR4.4 Sound Engineering: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa122190024040 59f90a4bbb0101fa379a8503?sender=u15e3008bb41d6628a5bb5701

- TBD(Morris & use cases): another round of Mural board sessions

Compelling Scoreboard Status – Month 9

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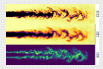
01	02	03	04	05	06	07	08	09	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36

❖ Based on initial work on MS2 and D2.12 we perform again joint Interaction Room session to identify novel AI methods

T3.1 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

T3.2 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

T3.3 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration



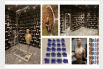
T3.4 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

T3.5 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

T4.1 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

T4.2 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

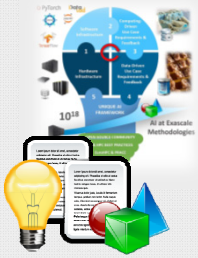
T4.3 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration



T4.4 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

based on Milestone (M7) AI/HPC Methods

Based on Deliverable D2.12 (M9) Layout plan AI Framework

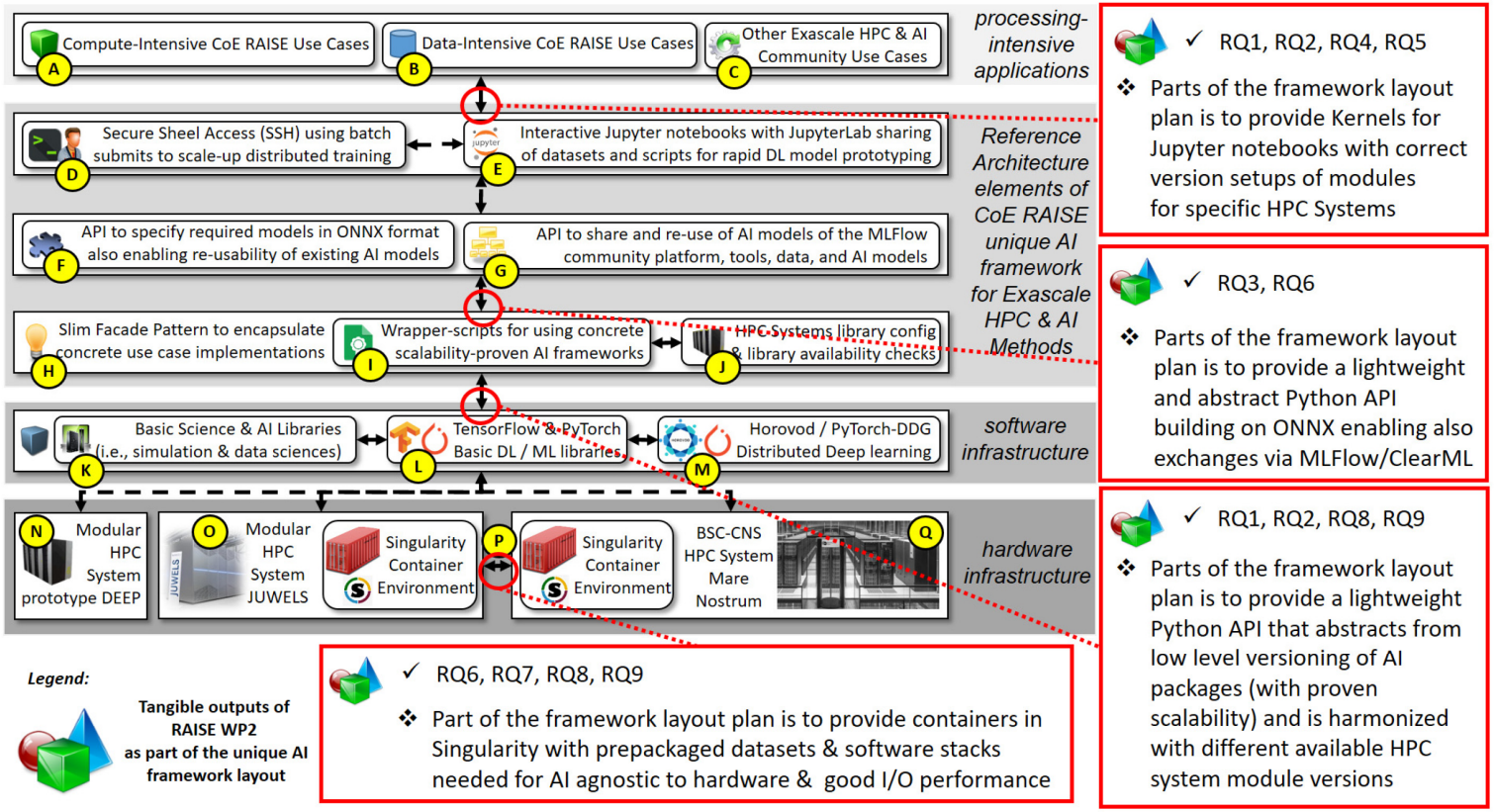


Plan for next 12 Month

- **Revise the matrix and framework and start implementing the framework core building blocks**
- **Create WP6 November News Item on Framework and updated AI/HPC Matrix**

D2.12 Framework (M9) – Initial Blueprint for Discussions

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



Continously Updating in another round of interaction rooms + adoption

drive. enable. innovate.

RAISE Center of Excellence

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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