



WP2 AI- & HPC-Cross Methods at Exascale – Monthly Meeting

Prof. Dr. – Ing. Morris Riedel et al.

School of Engineering & Natural Sciences, University of Iceland

2022-06-28, RAISE WP2 Monthly Meeting June 2022, Online



@ProfDrMorrisRiedel



@Morris Riedel



@MorrisRiedel



@MorrisRiedel



<https://www.youtube.com/channel/UCWC4VKHmL4NZgFfKoHtANKg>

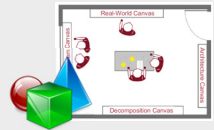
morris@hi.is



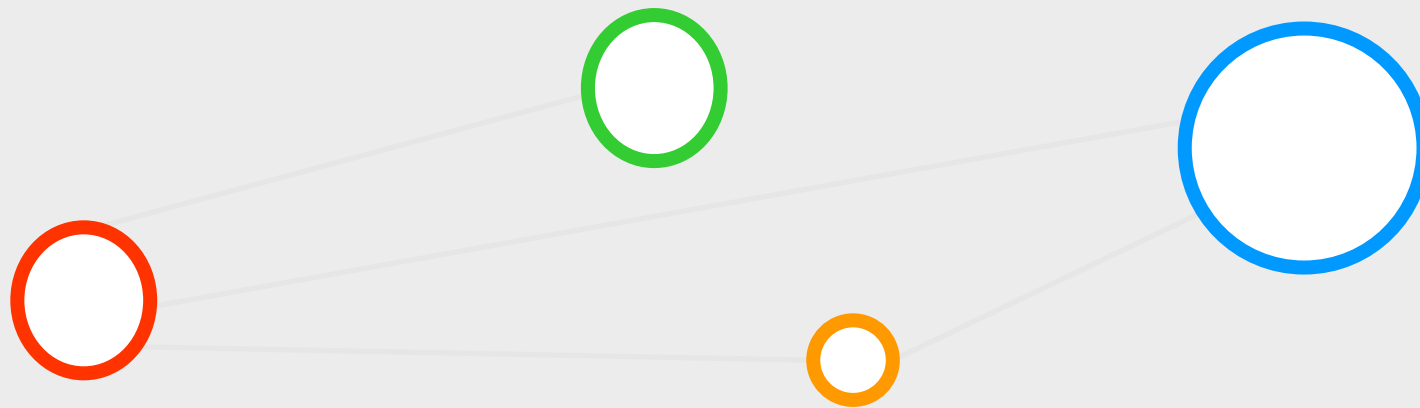
WP2 Meeting June – Welcome & Agenda



1. Approval of minutes from Monthly Meeting May 2022
 - (All), ~5 Min
2. Review WP2 Status on Interaction Rooms
 - (Morris Riedel, Matthias Book, Helmut Neukirchen), ~10 Min
3. September Review Preparation (M21)
 - (Morris, Andreas, et al.), ~20 Min
4. Status M18 Deliverables
 - (Eray, Morris et al.), ~10 Min
5. Status WP2 Training Plans
 - (Morris et al.), ~5 Min
6. Compelling Scoreboard Review & Next Steps
 - (All), ~10 Min



Agenda Item (1) – Minutes Approval – May 2022



Minutes Approval – Monthly Meeting May 2022



➤ Minutes available in BSCW

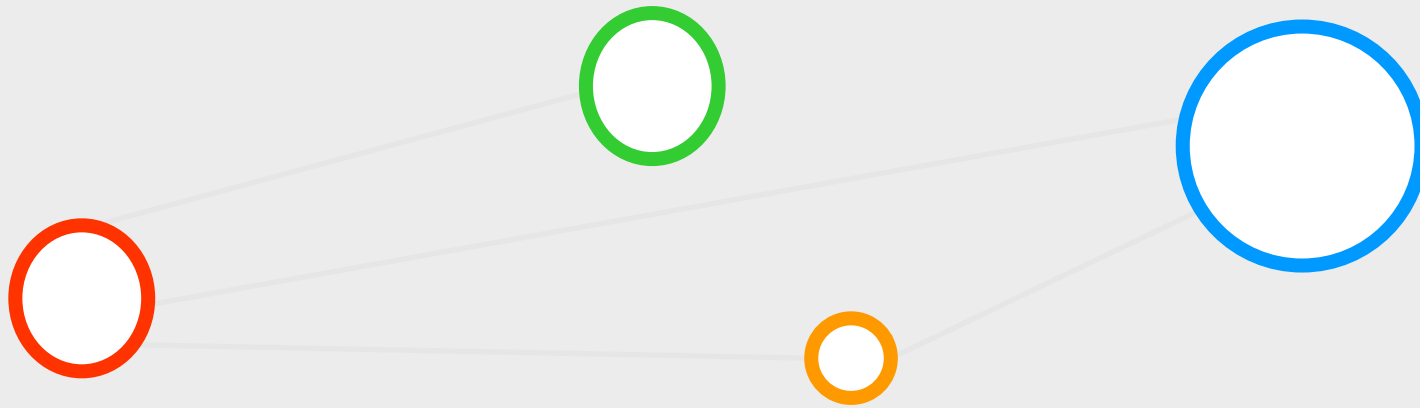
- <https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3340884>
- **TBD(all): Any objections or additions/changes?**

Open	Closed	All
Recent searches		
Search or filter results...		
Due date		
1h		
Edit issues		
New issue		
B - Create Fact Sheet Task 4.4 Sound Engineering		
#21 - created 3 minutes ago by Morris Riedel		
WP2 Fact Sheet Collection Completed		
Apr 30, 2021		
updated just now		
B - Create Fact Sheet Task 4.2 Seismic Imaging		
#20 - created 8 minutes ago by Morris Riedel		
WP2 Fact Sheet Collection Completed		
Apr 30, 2021		
updated just now		
B - Create Fact Sheet Task 4.3 Manufacturing		
#18 - created 1 month ago by Morris Riedel		
WP2 Fact Sheet Collection Completed		
Apr 30, 2021		
updated just now		
B - Create Fact Sheet Task 3.1 Turbulent Flow		
#17 - created 1 month ago by Morris Riedel		
WP2 Fact Sheet Collection Completed		
Apr 30, 2021		
updated 16 minutes ago		
B - Create Fact Sheet Task 4.1 Fundamental Physics		
#16 - created 1 month ago by Morris Riedel		
WP2 Fact Sheet Collection Completed		
Apr 30, 2021		
updated 2 weeks ago		
B - Create Fact Sheet Task 3.2 Clean Energy		
#14 - created 1 month ago by Morris Riedel		
WP2 Fact Sheet Collection Completed		
Apr 30, 2021		
updated 15 minutes ago		
B - Create Fact Sheet Task 3.5 Coating		
#13 - created 1 month ago by Morris Riedel		
WP2 Fact Sheet Collection Completed		
Apr 30, 2021		
updated just now		
B - Used Doodle for WP2 Monthly Meeting April 2021 Date & Time		
#12 - created 1 month ago by Morris Riedel		
WP2 Monthly Meeting - April 2021		
Apr 30, 2021		
updated 14 minutes ago		
B - Create Fact Sheet Task 3.3 Reacting Flows & Task 3.4 Engine Design		
#11 - created 1 month ago by Morris Riedel		
WP2 Fact Sheet Collection Completed		
Apr 30, 2021		
updated 12 minutes ago		
B - Used Doodle for WP2 Monthly Meeting May 2021 Date & Time		
#19 - created 11 minutes ago by Morris Riedel		
WP2 Monthly Meeting - May 2021		
May 31, 2021		
updated 11 minutes ago		
B - Create WP2 Expertise Matrix Draft and Circulate for WP2 Review		
#7 - created 2 months ago by Morris Riedel		
WP2 Expertise Matrix Exists		
May 31, 2021		
updated 15 minutes ago		

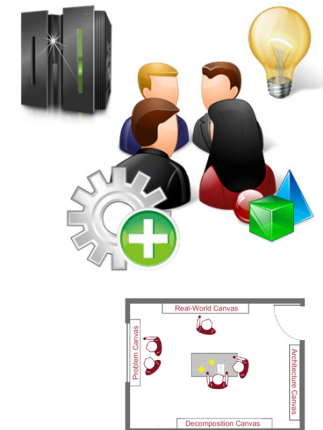
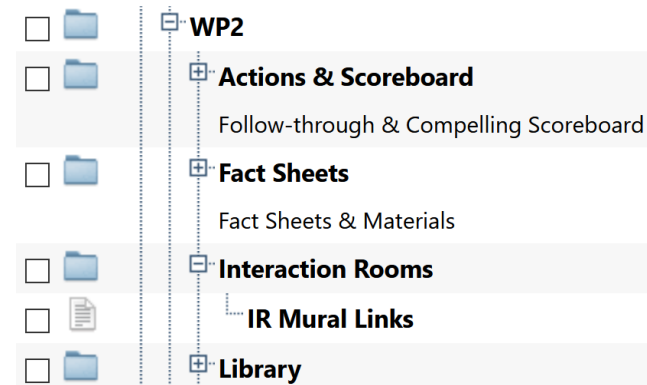
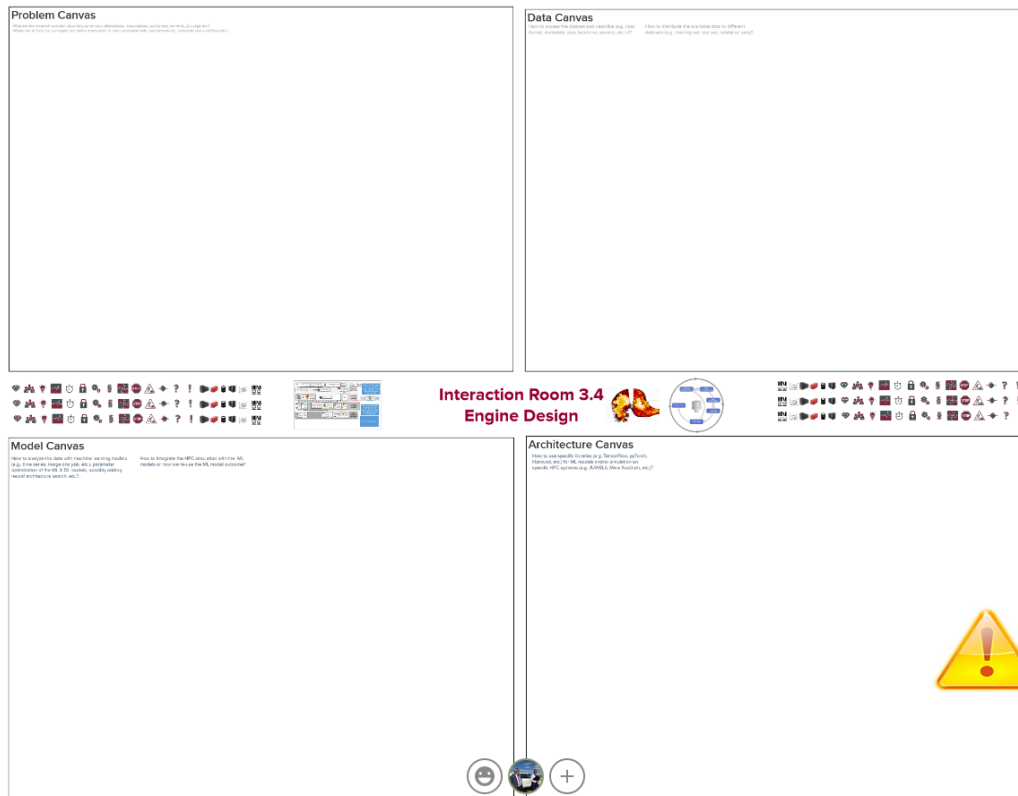
Slides & Materials from Meeting 2021-10-29			
2021_11_26_Monthly_Meeting_November_2021	2	M.Riedel	2022-01-17 12:56
Slides & Materials from Meeting 2021-11-26			
2022_01_31_Monthly_Meeting_January_2022	2	M.Riedel	2022-02-28 11:10
Slides & Materials from Meeting 2022-01-31			
2022_02_28_Monthly_Meeting_February_2022	2	M.Riedel	2022-03-30 09:41
Slides & Materials from Meeting 2022-02-28			
2022_03_30_Monthly_Meeting_March_2022	2	Katrine	2022-04-29 10:23
Slides & Materials from Meeting 2022-03-30			
2022_04_29_Monthly-Meeting_April_2022	2	M.Riedel	2022-05-31 11:23
Slides & Materials from Meeting 2022-04-29			
2022_05_31_Monthly_Meeting_May_2022	2	Katrine	2022-06-27 13:03
Slides & Materials from 2022_05_31 Monthly_Meeting May 2022			
2022_05_31_CoE-RAISE-WP2-Monthly-Meeting-Riedel-v1.pptx	26.5 M	M.Riedel	2022-06-27 13:03
WP2_MOM_May_2022.docx	14.9 K	Katrine	2022-06-16 15:25



Agenda Item (2) – Review WP2 Status on Interaction Rooms



Interaction Rooms via MURAL Boards & Milestone Inputs

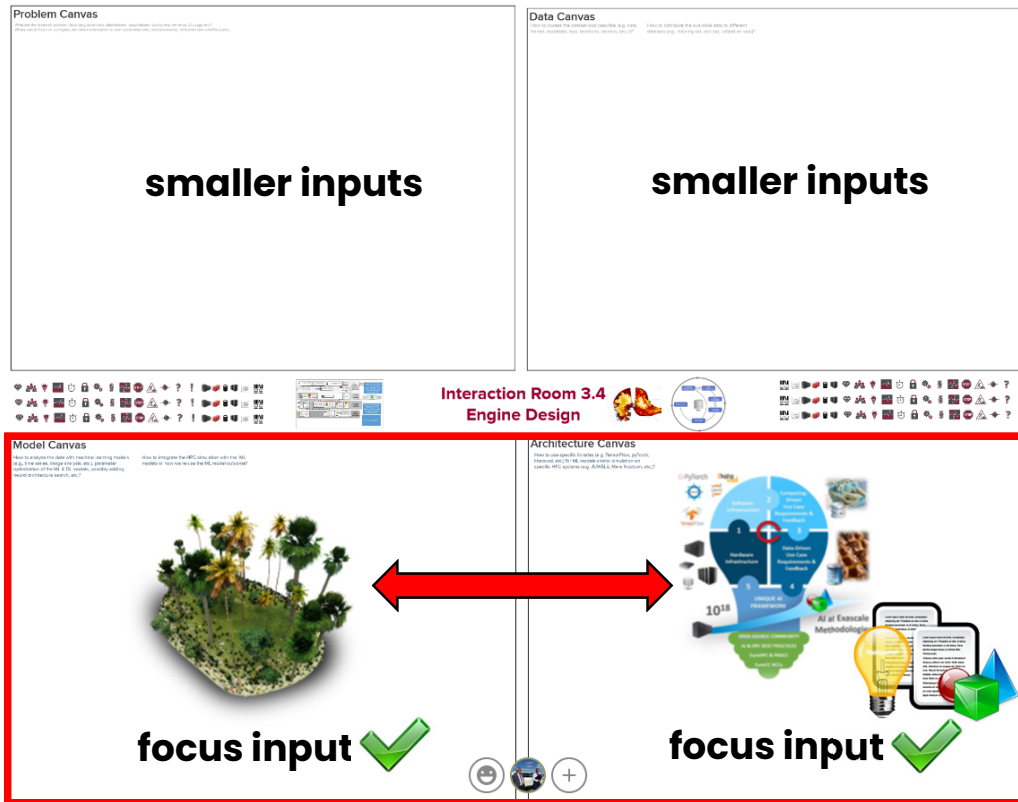


IR Mural Links

- IR3.1 Turbulent Flow: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377866397/8613c384d54f66fb5e78599ff307a4ce8a9090c0?sender=u15c3008bb41d6628a5bb5701>
- IR3.2 Clean Energy: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377887905/cb44cca3eed3bb9964fbfa36a1f6b1bfcc085f?sender=u15c3008bb41d6628a5bb5701>
- IR3.3 Reactive Flows: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377959022/0c363886f24833eeb19b025d87324b57fd50e2db?sender=u15c3008bb41d6628a5bb5701>
- IR3.4 Engine Design: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377976343/8d7aba6be09af3b2fd305d2f709c53661ac889d?sender=u15c3008bb41d6628a5bb5701>**
- IR3.5 Coating: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377991014/7a5d7e1ea7230178342d1e1d4a84d656d9055d52?sender=u15c3008bb41d6628a5bb5701>
- IR4.1 Fundamental Physics: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378007335/6f0d5285feae3eaf515bd6676e84d8b4879d39?sender=u15c3008bb41d6628a5bb5701>
- IR4.2 Seismic Imaging: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ac3e28a4bb8d9adbec33874998?sender=u15c3008bb41d6628a5bb5701>
- IR4.3 Manufacturing: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378038069/93df6fa7a41093f4eaae7bce9d72979dc2ba42b9d?sender=u15c3008bb41d6628a5bb5701>
- IR4.4 Sound Engineering: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa12219002404059f90a4bbb0101fa379a8503?sender=u15c3008bb41d6628a5bb5701>

- TBD(all): People should use the MURAL boards, maybe Task 3.3/3.4 critical in the review!
- <https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3591551>

MURAL Board contents for Deliverables & Milestones



- ☐ **WP2**
- ☐ **Actions & Scoreboard**
Follow-through & Compelling Scoreboard
- ☐ **Fact Sheets**
Fact Sheets & Materials
- ☐ **Interaction Rooms**
IR Mural Links
- ☐ **Library**



IR Mural Links

- IR3.1 Turbulent Flow: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377866397/8613c384d54f66fb5e78599ff307a4ce8a9090c0?sender=u15c3008bb41d6628a5bb5701>
- IR3.2 Clean Energy: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377887905/cb44cca3eed3bb9964fbfa36af16b1bfcc085f?sender=u15c3008bb41d6628a5bb5701>
- IR3.3 Reactive Flows: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377959022/0c363886f24833eeb19b025d87324b57fd50e2db?sender=u15c3008bb41d6628a5bb5701>
- IR3.4 Engine Design: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377976343/8d7aba6be09af3b2fd305d2f709e53661ac889d?sender=u15c3008bb41d6628a5bb5701>
- IR3.5 Coating: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377991014/7a5d7e1eaf230178342d1e1d4a84d656d9055d52?sender=u15c3008bb41d6628a5bb5701>
- IR4.1 Fundamental Physics: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378007335/6f0d3285feac3eaf315bd6676e84d8b4879d39?sender=u15c3008bb41d6628a5bb5701>
- IR4.2 Seismic Imaging: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ac3e28a4fbb8d9adbec33874998?sender=u15c3008bb41d6628a5bb5701>
- IR4.3 Manufacturing: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378038069/93df6fa7a41093f4eaae7be9d72979dc2ba42b9d?sender=u15c3008bb41d6628a5bb5701>
- IR4.4 Sound Engineering: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa12219002404059f90a4bbb0101fa379a8503?sender=u15c3008bb41d6628a5bb5701>

Interaction Room Status & Discussions – WP3/WP4 Overview

➤ WP3 (second round IRs)

- T3.1: Turbulent Flow → scheduled (25.7)
- T3.2: Clean Energy (not started) → done
- T3.3: Reactive Flows → scheduled (19.7.)
- T3.4: Engine design → scheduled (19.7.)
- T3.5: Coating → done

➤ WP4 (second round IRs)

- T4.1: Fundamental physics (asked) → done
- T4.2: Seismic imaging (started) → done
- T4.3: Manufacturing → scheduled (29.6.)
- T4.4: Sound engineering → done

➤ TBD(Katrín): Schedule meetings with Interaction Room teams (hard to find slots)

ATOS: affects of change in persons?



Use Case	AE	PIML	ANNs	CNN	NO	SMs	GNN	IN	LSTM	GRU
Details	CAE	RBP-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

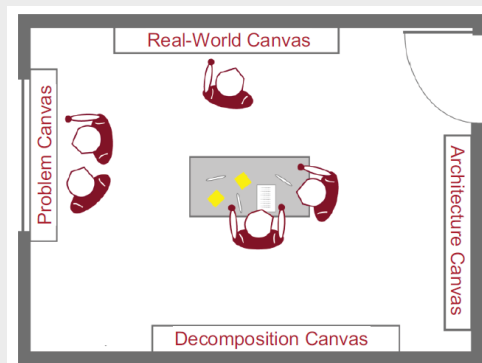
➤ Next round of Interaction Rooms with WP2

- Carve out more details on AI/HPC methods
- Contribute to the Unique AI Framework
- Update our HPC/AI Methods Matrix

Cross HPC/AI Methods Table – IR Results (D2.10)

✓ Interaction Rooms

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

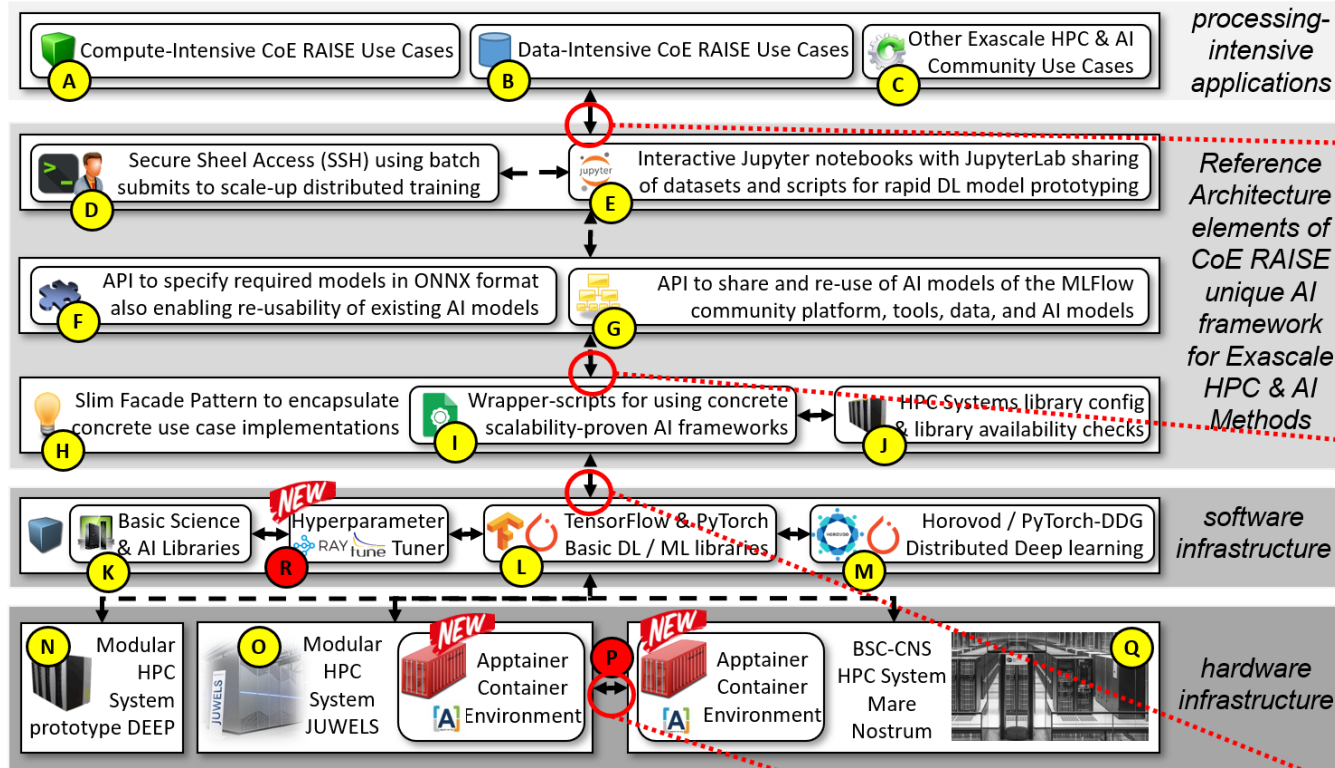


Input to Deliverable D2.10

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															



Realization of SW Framework – IR Results (D2.10)



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

processing-intensive applications

Reference Architecture elements of CoE RAISE unique AI framework for Exascale HPC & AI Methods

software infrastructure

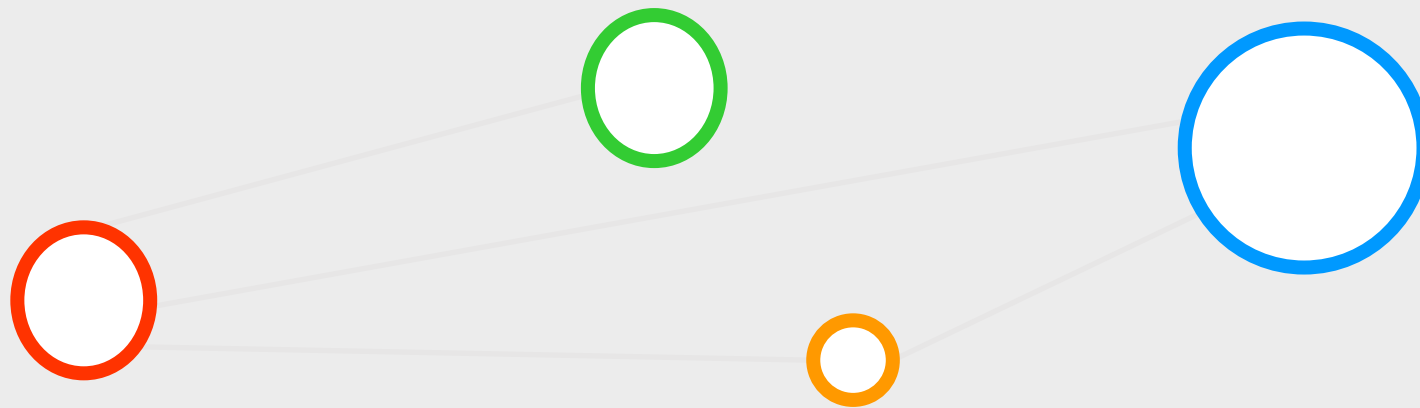
hardware infrastructure

- ✓ 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

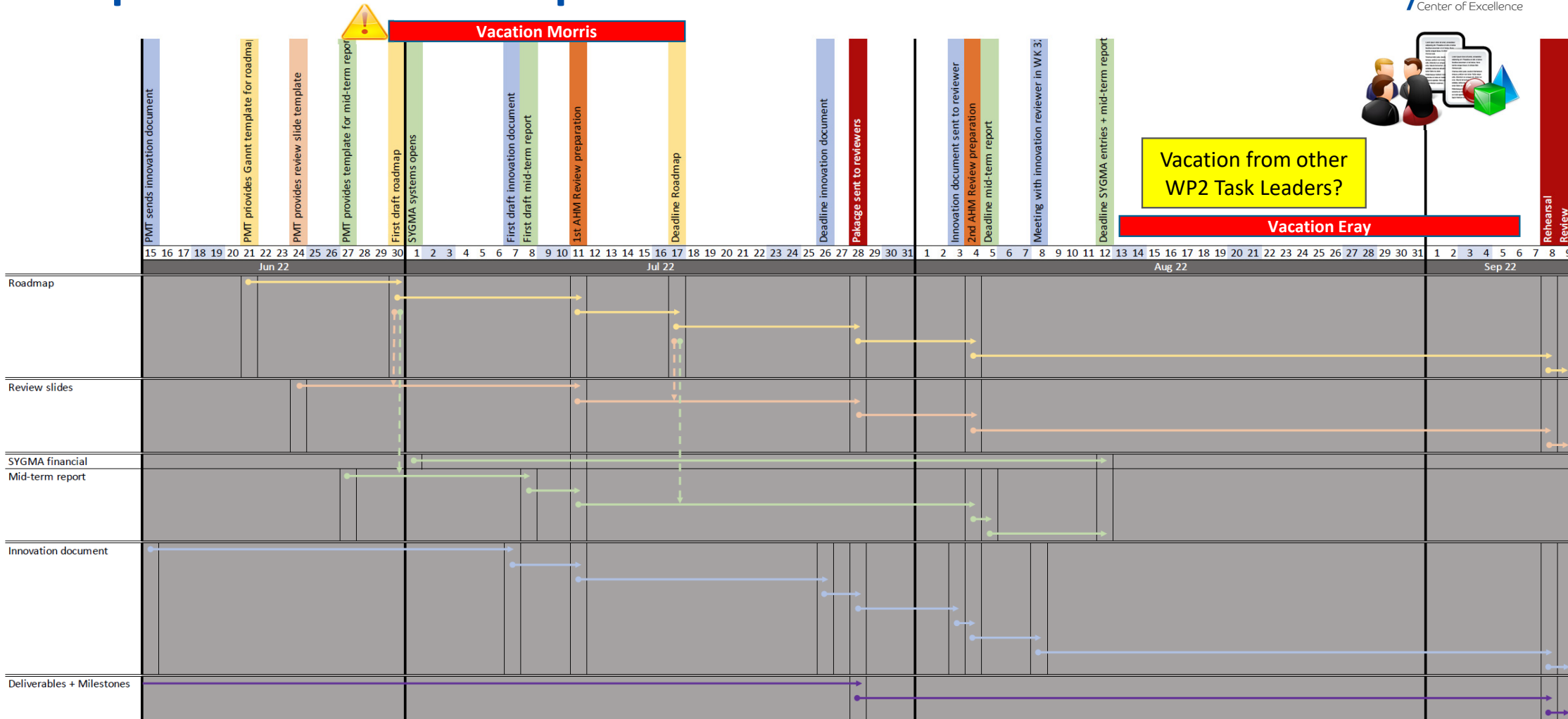


Continously Updating!

Agenda Item (3) – September Review Preparation (M21)



September Review Preparation: 08.09. + 09.09.



September Review Preparation: Roadmap Document

H2020-INFRAEDI-2018-2020



CoE RAISE

Center of Excellence "Research on AI- and Simulation-Based Engineering at Exascale"

Grant Agreement Number: 951733

Roadmap

Draft

Version: 0.1
Author(s): A. Lintermann (FZJ)
Contributor(s):
Date: 17.05.2022

How can we prepare?

- A roadmap document is currently in preparation
 - It aims at
 - self-reflecting our activities
 - inspiring us to think about further requirements to fulfill our promises
 - inspiring us to think about our next steps
 - Basic structure:
 - Status of the various domains before the start of CoE RAISE
 - Changes achieved so far (impact)
 - Future plans



- Contents of the WP presentations
 - Overview of the Tasks and details on what has happened in the WP (requires input from the task leaders)
 - Slides will be finalized on the day of the rehearsal (there will only be a single presenter)



10.06.2022 – TCB Meeting – Andreas Lintermann

12

➤ TBD (Task Leaders): https://docs.google.com/document/d/1eJ5sV6Ubr_prHt80PJAmnB4fWEK6Kyvh/edit



September Review Preparation: Roadmap T2.1

Morris, Matthias, Helmut

H2020-INFRAEDI-2018-2020



CoE RAISE

Center of Excellence "Research on AI- and
Simulation-Based Engineering at Exascale"

Grant Agreement Number: 951733

Roadmap

Draft

Version: 0.1
Author(s): A. Lintermann (FZJ)
Contributor(s):
Date: 17.05.2022

Roadmap

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Porting of HPC codes to GPUs

Task objectives

[TODO Task leader]: Present the objectives and how they go beyond the SoA

Strategy to reach the objectives including already accomplished work

[TODO Task leader]: Present the strategy to reach the goals and what has already been done. Provide a detailed Gantt chart including the major milestone (project) + mini self-given milestones. What are the requirements? Where do they come from? Provide a flow chart (together with the Gantt) with inputs and outputs to and from this task. What external input is required? Are results required in other tasks? Place dependencies etc. into the Gantt chart (create temporal dependencies).

Who?

4.2 Work Package 2 - AI- and HPC-Cross Methods at Exascale

[TODO WP leader]: Introduction WP, structure of the WP, overview of objectives, tasks, participants, high-level Gantt, and interaction and dependencies and synergies with other WPs

4.2.1 Task 2.1 - Modular and heterogeneous supercomputing architectures

[TODO Task leader]: General introduction to the task

The fundamental objective of RAISE is To develop innovative AI methods on heterogeneous HPC architectures capable of scaling towards Exascale. To this end, task 2.1 provides all the necessary support for the porting of the codes and their optimizations on heterogeneous architectures, while ensuring constant availability of Tier-3 to Tier-0 supercomputers.

For this, the HPC centers of RAISE provide their computational resources for development and testing of RAISE's software. This includes the homogeneous and heterogeneous HPC systems found at the Tier-2 and Tier-3 centers of the consortium (UOI, RWTH, and RTU) as well as the cutting-edge HPC systems of the Tier-0 and Tier-1 providers (FZJ and BSC). That is, FZJ and BSC give access to their MSA/heterogeneous supercomputers JUWELCA, JUWELS, and MareNostrum 4 (MN4) general cluster and its three prototypes. Together with the use-case providers, the representative applications, where necessary, are jointly prepared for such heterogeneous systems together with the HPC centers of the consortium.

The AI experts further exploit the HPC architectures and file systems for relevant algorithms, i.e., they work on the enhancement of the scalability of existing ML/DL methods on dedicated or shared HPC components using, e.g., GPGPUs or other accelerator platforms, and test I/O performance.

The developers are supported by the HPC experts by means of performance engineering activities, best practice guidelines, and system-specific tutorials and manuals. The training courses of the HPC centers are offered to the use-case providers in line with Task 6.1.

Status at the beginning of the project (SoA)

[TODO Task leader]: Provide the state-of-the-art, or the general status of the domain, if applicable

➤ TBD (Task Leaders): https://docs.google.com/document/d/1eJ5sV6Ubr_prHt80PJAmnB4fWEK6Kyvh/edit

September Review Preparation: Roadmap T2.2 + T2.3



H2020-INFRAEDI-2018-2020



CoE RAISE

Center of Excellence "Research on AI- and Simulation-Based Engineering at Exascale"

Grant Agreement Number: 951733

Roadmap

Draft

Version: 0.1
Author(s): A. Lintermann (FZJ)
Contributor(s):
Date: 17.05.2022

4.2.2 Task 2.2 - Hardware prototypes

Eray

[TODO Task leader]: General introduction to the task

Status at the beginning of the project (SoA)

[TODO Task leader]: Provide the state-of-the-art, or the general status of the domain, if applicable

Task objectives

[TODO Task leader]: Present the objectives and how they go beyond the SoA

Strategy to reach the objectives including already accomplished work

[TODO Task leader]: Present the strategy to reach the goals and what has already been done. Provide a detailed Gantt chart including the major milestone (project) + mini self-given milestones. What are the requirements? Where do they come from? Provide a flow chart (together with the Gantt) with inputs and outputs to and from this task. What external input is required? Are results required in other tasks? Place dependencies etc. into the Gantt chart (create temporal dependencies).

4.2.3 Task 2.3 - Benchmarking on disruptive technologies

Rakesh

[TODO Task leader]: General introduction to the task

Status at the beginning of the project (SoA)

[TODO Task leader]: Provide the state-of-the-art, or the general status of the domain, if applicable

Task objectives

[TODO Task leader]: Present the objectives and how they go beyond the SoA

Strategy to reach the objectives including already accomplished work

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➤ TBD (Task Leaders): https://docs.google.com/document/d/1eJ5sV6Ubr_prHt80PJAmnB4fWEK6Kyvh/edit



September Review Preparation: Roadmap T2.4 + T2.5



H2020-INFRAEDI-2018-2020



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Grant Agreement Number: 951733

Roadmap

Draft

Version: 0.1
Author(s): A. Lintermann (FZJ)
Contributor(s):
Date: 17.05.2022

4.2.4 Task 2.4 - Software design of a unique AI framework

Morris, Matthias, Helmut

[TODO Task leader]: General introduction to the task

Status at the beginning of the project (SoA)

[TODO Task leader]: Provide the state-of-the-art, or the general status of the domain, if applicable

Task objectives

[TODO Task leader]: Present the objectives and how they go beyond the SoA

Strategy to reach the objectives including already accomplished work

[TODO Task leader]: Present the strategy to reach the goals and what has already been done. Provide a detailed Gantt chart including the major milestone (project) + mini self-given milestones. What are the requirements? Where do they come from? Provide a flow chart (together with the Gantt) with inputs and outputs to and from this task. What external input is required? Are results required in other tasks? Place dependencies etc. into the Gantt chart (create temporal dependencies).

Approach: Summarizing D2.10

4.2.5 Task 2.5 - Cross-Sectional AI Methods

Morris, Matthias, Helmut

[TODO Task leader]: General introduction to the task

Status at the beginning of the project (SoA)

[TODO Task leader]: Provide the state-of-the-art, or the general status of the domain, if applicable

Task objectives

[TODO Task leader]: Present the objectives and how they go beyond the SoA

Strategy to reach the objectives including already accomplished work

[TODO Task leader]: Present the strategy to reach the goals and what has already been done. Provide a detailed Gantt chart including the major milestone (project) + mini self-given milestones. What are the requirements? Where do they come from? Provide a flow chart (together with the Gantt) with inputs and outputs to and from this task. What external input is required? Are results required in other tasks? Place dependencies etc. into the Gantt chart (create temporal dependencies).

➤ TBD (Task Leaders): https://docs.google.com/document/d/1eJ5sV6Ubr_prHt80PJAmnB4fWEK6Kyvh/edit



September Review Preparation: Roadmap GANTT Example



H2020-INFRAEDI-2018-2020



CoE RAISE

Center of Excellence "Research on AI- and Simulation-Based Engineering at Exascale"

Grant Agreement Number: 951733

Roadmap

Draft

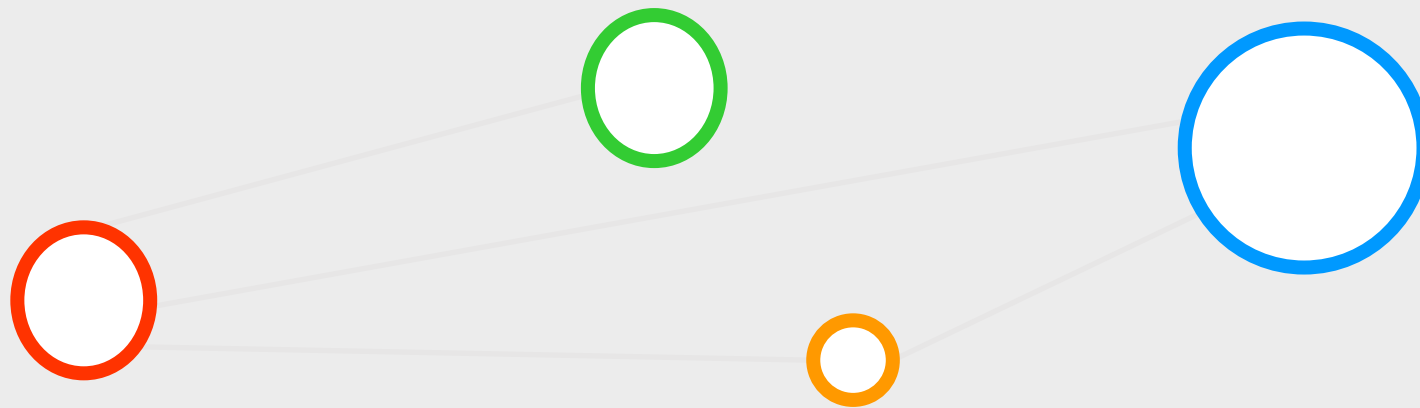
Version: 0.1
Author(s): A. Lintermann (FZJ)
Contributor(s):
Date: 17.05.2022



➤ TBD (Task Leaders): https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/d3937966/CoE_RAISE_Gantt_Roadmap_TX.Y.xlsx



Agenda Item (4) – Status M18 Deliverables



Status M18 Deliverables

- Selected deliverables → PMT Reviews finished → PMT Feedback Addressed
 - TBD(Morris, Eray): Short Summary for deliverables for PMT



D2.7	Support report	FZJ	R	PU	18	M. Riedel/ UOI	E. Inanc/ FZJ	Thomas Jaravel/ CERFACS	I. Schmitz/ ParTec	09.06.2022	30.06.2022
D2.10	Monitoring report	UOI	R	CO	18	M. Riedel/ UOI	M. Book/ UOI	M. Nicolaou/ CYI	A. Lintermann/ FZJ	09.06.2022	30.06.2022
D5.1	Market analysis report; innovation plan	FM	R	CO	18	W. Lammens/ FM	W. Lammens/ FM	A. Lektuers/ RTU	K. Pausch / FZJ	09.06.2022	30.06.2022
D6.6	Network evaluation document	BSC	R	PU	18	R. Gregorio/ BSC	G. Houzeaux/ BSC	R. Heylen/ FM	J. Lopez/ ParTec	09.06.2022	30.06.2022
D2.3	Report on porting & performance engineering	BSC	R	PU	24	M. Riedel/ UOI	G. Houzeaux/ BSC	L. Nicoletti/ BULL	A. Lintermann/ FZJ	28.11.2022	31.12.2022
D2.8	Benchmarking & support report	FZJ	R	PU	24	M. Riedel/ UOI	K. Michielsen/ FZJ	Guillermo Oyarzun/ BSC	J.Lopez/ ParTec	28.11.2022	31.12.2022
D2.15	Report on novel AI technologies	UOI	R	CO	24	M. Riedel/ UOI	M. Riedel/ UOI	C. Lapeyre/ CERFACS	I. Schmitz/ ParTec	28.11.2022	31.12.2022
D3.2	Report on outcomes of WP3 use-cases	RWTH	R	CO	24	C. Lapeyre/ CERFACS	M. Meinke/ RWTH	Matthias Book/ UOI	A. Lintermann/ FZJ	28.11.2022	31.12.2022

Status M18 Deliverables

▪ Update selected deliverables



Task 2.2 Hardware prototypes <Leader: FZJ> <M1-M18>

Contributors: FZJ & ParTec, UOI, RTU Outputs: **D2.5, D2.6, D2.7**



FZJ gives access to hardware prototypes that are developed in the DEEP-projects via corresponding “Early Access Programs”. At FZJ, this means provision of access to the DEEP-EST prototype, which consist of a x86-based Cluster module, an NVIDIA-GPGPU-based Booster module, and a x86-, NVIDIA-GPGPU-, and FPGA-based Data Analytics module. The prototypes also include technologies for NAMs, NVMs, and non-x86-based solutions like ARM architectures. Furthermore, the D-Wave Quantum Annealing machine is integrated into FZJ’s MSA environment when it becomes available. At BSC, other prototype facilities, described in Sec. 4.1.5, are available for running the use-cases proposed by BSC. In case of additional user-requirements, FZJ & ParTec, and BSC provide solutions for integrating the aforementioned technologies as well as support, training, best practice guidelines, and manuals in using these new technologies for the AISE partners.

Eray et al.

Task 2.4 Software design of a unique AI framework <Leader: UOI> <M7-M36>

Contributors: FZJ, UOI, RTU Outputs: **D2.10, D2.11, D2.12**



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.

Morris, Matthias,
Helmut et al.

Status M18 Deliverables - D2.7 Support Report

▪ Update deliverable status



Task 2.2 Hardware prototypes <Leader: FZJ> <M1-M18>

*Contributors: FZJ & ParTec, UOI, RTU Outputs: **D2.5, D2.6, D2.7***

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Eray et al.



Status M18 Deliverables – D2.10 Monitoring Report

■ Update deliverable status



Task 2.4 Software design of a unique AI framework <Leader: UOI> <M7-M36>

*Contributors: FZJ, UOI, RTU Outputs: **D2.10, D2.11, D2.12***

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.

**Morris, Matthias,
Helmut et al.**

Deliverable Outline & Content Plan

(term 'monitoring' interpreted as 'progress monitoring'?!)

1. Progress: Finalized FactSheets

1. Content out of Mural Board sessions & dedicated meetings in next two weeks to craft FactSheet 'final versions'
2. Can be updated later of course, but should be really usable
3. Reasonable final for review in Sep

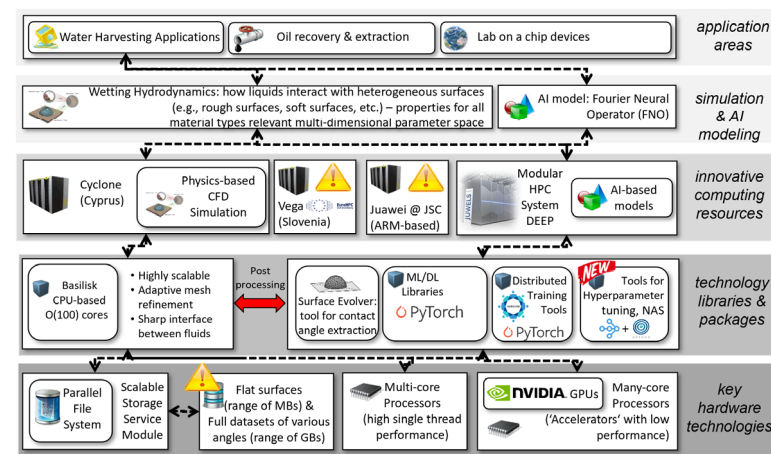
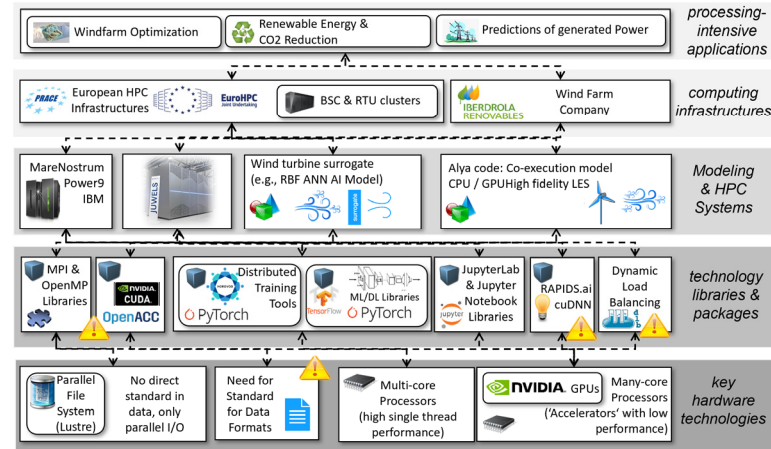
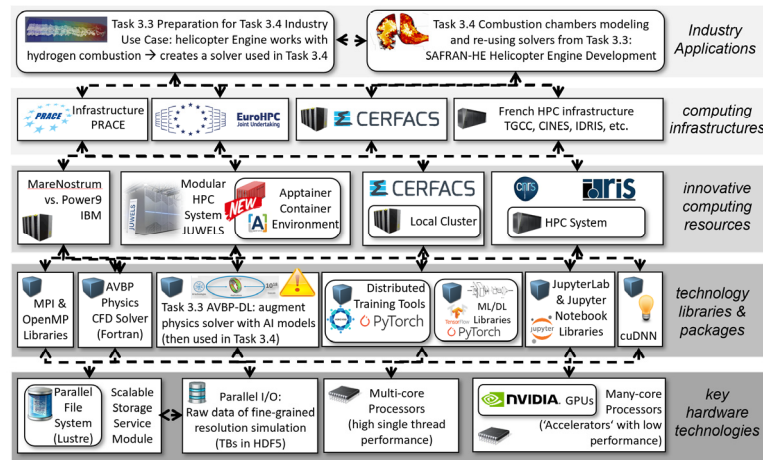
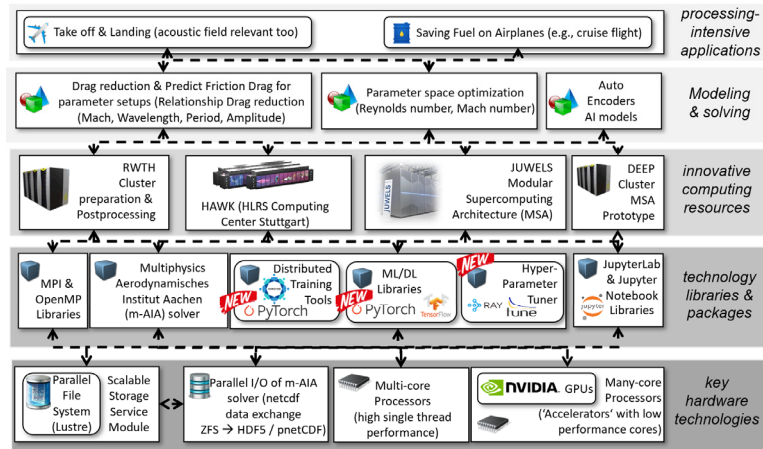
2. Progress: Updates to the AI Matrix

1. Mural boards already revealed changes and updates in AI methods
2. E.g., no statistical methods used anymore, drop of JEDI-Net, etc.
3. Additions of selected approaches

3. Progress: Updates of the AI Unique Framework Design

1. Initial downloadable material on Website (→ WP6 Web page part) linking to Git materials
2. Updates on Tools identified, e.g., RayTune, others
3. Other community sharing channels: e.g., OpenML, PRACE GitLab Data Analytics project (EuroHPC transition?), etc. EuroAccess Portal, EOSC git, FAIR data sharing → Channel 3rd
4. Link to 2.7 modules, etc. (Eray)

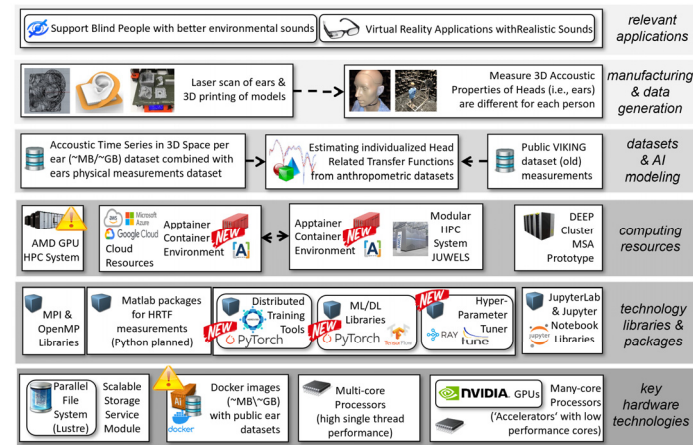
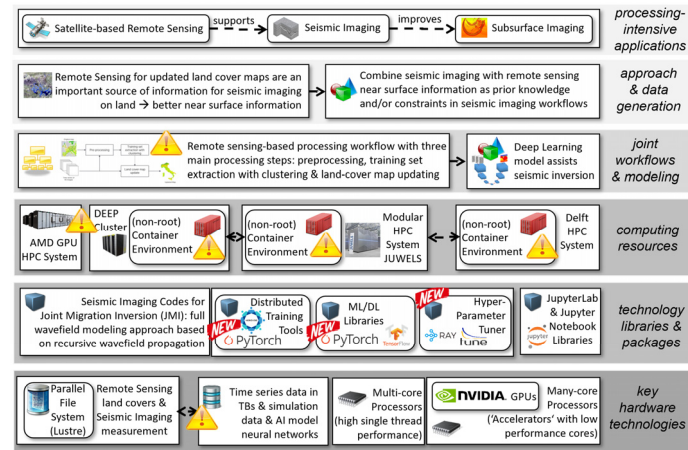
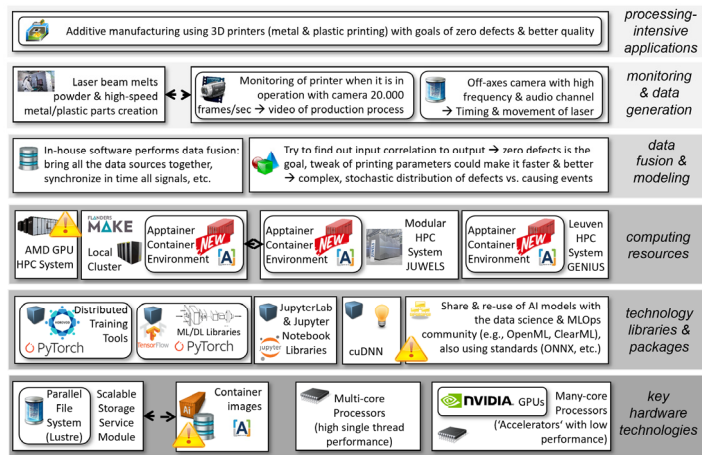
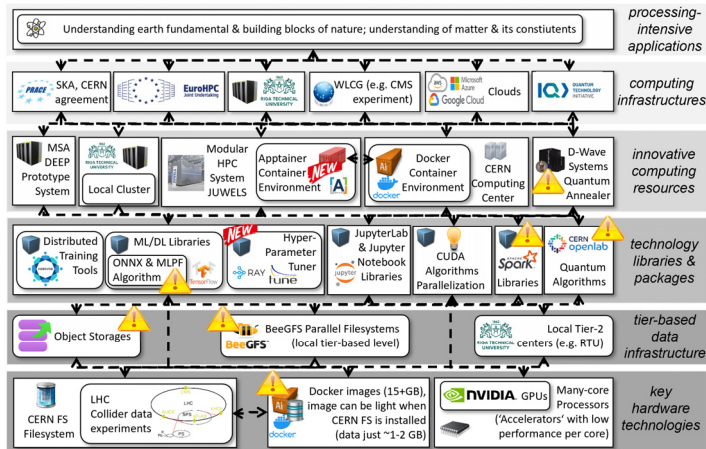
Status M18 Deliverables – D2.10 Monitoring Report WP3



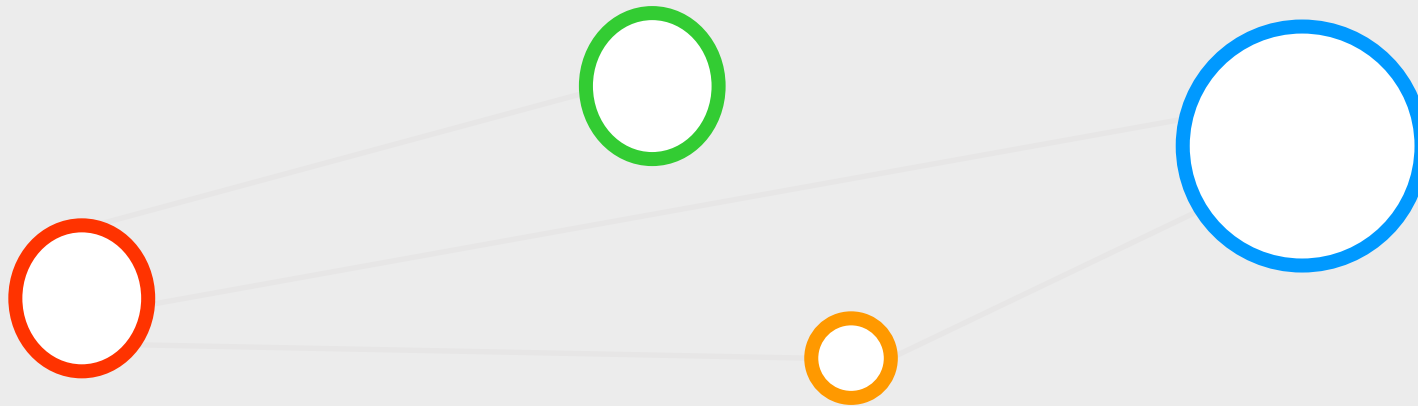
Fact Sheets
available for
each use case
(Task 3.3 /
Task 3.4 in
one)

Status M18 Deliverables – D2.10 Monitoring Report WP4

Fact Sheets
available for
each use case



Agenda Item (5) – Status WP2 Training Plans



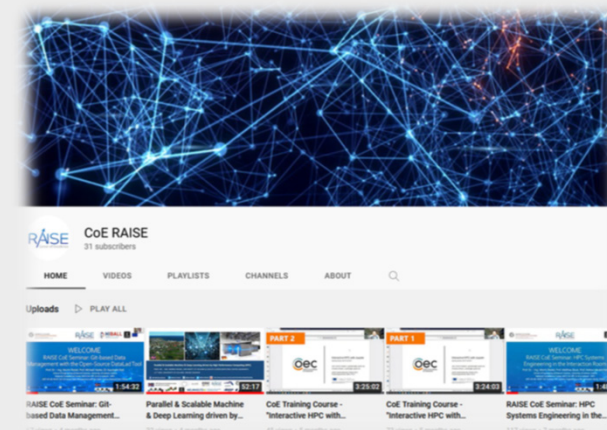
WP2 Monthly Trainings – Review & Plan



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➤ Monthly WP2 Trainings

- Co-organized with Icelandic National Competence Center (NCC) funded by the EuroCC project: <http://ihpc.is>
- Performed since Quarter 2 of the project (April 2021)
- Selected dates via agreement of availability of speakers
- Used as major AI/HPC methods information/training for WP3/WP4
- Contributed to outreach via YouTube Channel recordings: <https://www.youtube.com/channel/UCAdlZ-v6cWwGdapwYxdN7dg>
- TBD(Katrín): Schedule the YouTube Training series with speakers

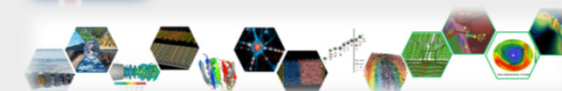


Plan for next months

- Carry on with monthly WP2 trainings in the same style, but schedule on 3-4 month horizons
- Repeat certain trainings with advanced content and updates of activities
- Work better together with WP6 on releasing seminars on YouTube channel more regularly
- Collect slides of speakers and make them available on BSCW and/or on the RAISE Web Page



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WP2 Monthly Trainings – Review & Plan



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UNIVERSITY OF ICELAND

SCHOOL OF ENGINEERING AND NATURAL SCIENCES

DEPARTMENT OF PHYSICS, MATHEMATICS AND CHEMISTRY



Center of Excellence




WELCOME

RAISE CoE Seminar: HPC Systems Engineering in the Interaction Room

Prof. Dr. – Ing. Morris Riedel, Prof. Matthias Book, Prof. Helmut Neukirchen

School of Engineering & Natural Sciences, University of Iceland, Iceland

National Competence Center (NCC) for HPC & AI in Iceland – IHPC

2021-04-08, RAISE CoE Seminar HPC Systems Engineering in the Interaction Room, Online






<https://www.youtube.com/watch?v=3C9N4X95W0g>

morris@hi.is



IHPC National Competence Center (NCC) for HPC & AI in Iceland




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HIBALL
 HPC & AI
High-Performance Computing & Artificial Intelligence


EUROPEAN COMMISSION
EUROPEAN COMMISSION

WELCOME

RAISE CoE Seminar: Git-based Data Management with the Open-Source DataLad Tool

Prof. Dr. Ing. Morris Riedel, Prof. Michael Hanke, Dr. Kaustubh Patil
 School of Engineering & Natural Sciences, University of Iceland, Iceland
 National Competence Center (NCC) for HPC & AI in Iceland – IHPC
 2021-05-28, RAISE CoE Git-based Data Management with the Open-Source DataLad Tool, Online

@ProfDrMorrisRiedel in @MorrisRiedel @MorrisRiedel
 <https://www.github.com/morris/COE-OPEN-SCIENCE-TOOLBOX> morris@hi.is


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[illegible]


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WELCOME

RAISE CoE Seminar: Distributed Deep Learning

Prof. Dr. – Ing. Morris Riedel et al.

School of Engineering & Natural Sciences, University of Iceland, Iceland
 National Competence Center (NCC) for HPC & AI in Iceland – IHPC
 2021-07-29, RAISE CoE Seminar: Distributed Deep Learning, Online

 @ProfDrMorrisRiedel
  in @MorrisRiedel
  @MorrisRiedel
  morris@hi.is


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 HPC & AI in Iceland



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JÓHANNAKVEÐI, HÖFÐI 101, REYKJAVÍK, ICELAND

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WELCOME

RAISE CoE Seminar: Brief Introduction to Autoencoders

Prof. Dr. – Ing. Morris Riedel et al.

School of Engineering & Natural Sciences, University of Iceland, Iceland
National Competence Center (NCC) for HPC & AI in Iceland – IHPC
2021-08-31: RAISE CoE Seminar Brief Introduction to Autoencoders, Online

 @ProfDrMorrisRiedel  @MorrisRiedel  @MorrisRiedel
<https://www.youtube.com/channel/UCVC0w0H0W4ALQZf0C7H9A5g>  morris@fs.is

 **HPC National Competence Center**
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HAFNARHÁLSVEGUR 1, 101 REYKJAVIK, ICELAND



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WELCOME

RAISE CoE Seminar: MLOps with ClearML

Prof. Dr. – Ing. Morris Riedel et al.

School of Engineering & Natural Sciences, University of Iceland, Iceland
National Competence Center (NCC) for HPC & AI in Iceland – IHPC

2021-09-30, RAISE CoE Seminar MLOps with ClearML, Online



[@MorrisRiedel](https://www.facebook.com/morrisriedel)



[@Morris Riedel](https://www.linkedin.com/company/morrisriedel)



[@MorrisRiedel](https://twitter.com/morrisriedel)



[@MorrisRiedel](https://www.youtube.com/channel/UCQWv9v8a4G2gTnAA9g5)



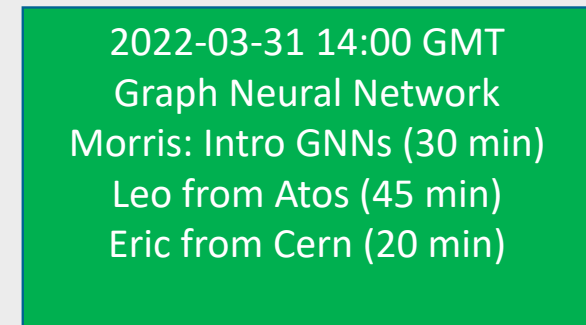
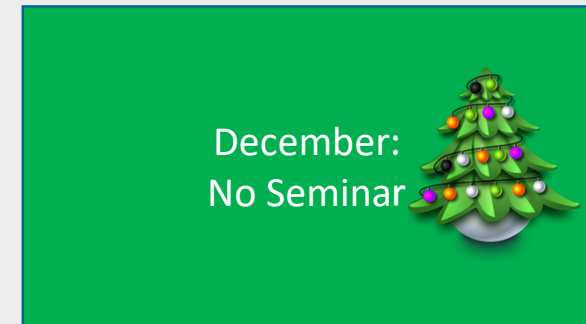
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WP2 Monthly Trainings – Review & Plan



TBD (all): Please suggest further training & teaching seminars for YouTube channel on our WP2 mailing list to plan better ahead



WP2 Monthly Trainings – Review & Plan



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April:
Quantum Annealing
Maybe Gabriele Examples from
SVMs, Amer SVR

May:
Using OpenML for sharing
datasets, algorithms, and
experiments

9th of June:
Morris: GPUs in general
Arnis & Cuda @ RTU

July:
TREX Project (in scheduling)
→ Katrin : check and schedule



August:
Request Project Partners?
Gael (continuous integration
ATOS)???
Eray: Tooling with modules???

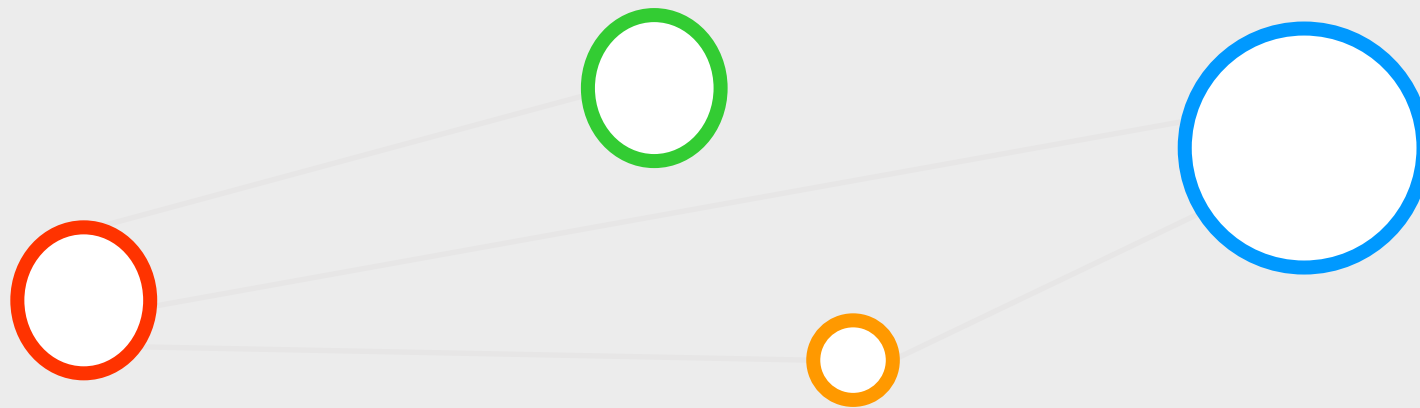
ATOS: affects of
change in persons?

September:
EOSC – NI4OS-Europe
→ Katrin: check and schedule

TBD (all): Please suggest further training & teaching seminars for YouTube channel on our WP2 mailing list to plan better ahead



Agenda Item (6) – Compelling Scoreboard Review



Compelling Scoreboard Review – Use Case Progress



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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



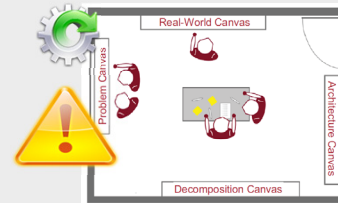
T4.4

Fact Sheet Drafts

Interaction Rooms

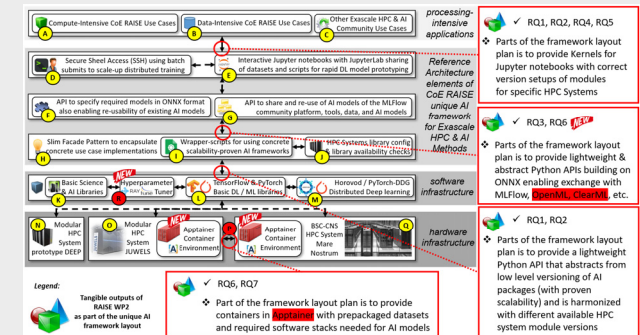
AI Methods Exploration

- ❖ Performing joint Interaction Room sessions: to identify novel AI methods and build unique AI framework parts
- ❖ Realization of SW framework design started → initial collection in WP2 Wiki page RAISE (Jupyter notebooks, etc.)
- ❖ Identified lots of problems → SW framework concept required
- ❖ Collection of software artefacts started for the realization of the framework design bottom-up by use case elements



Lessons Learned from IR Rooms with use cases:
Agreement & common components between use cases realistic → Framework Co-Design ok

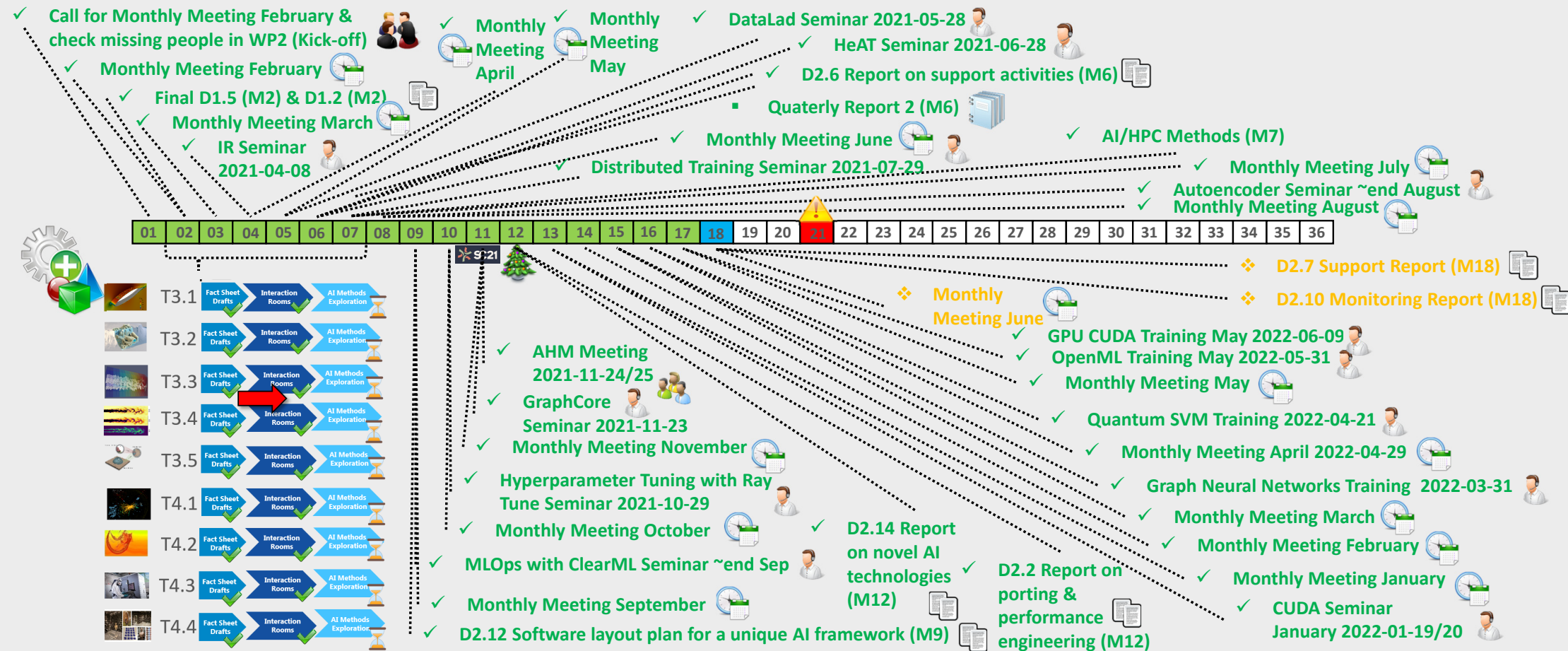
Use Case	AE	PINN	ANNs		CNN		NO	GNN		RNN		GAN	TP				SVM	RF
Details	CAE		ANN	RBF-ANN	U-Net	RES NET	FNO	MLPF	GAT	LSTM	GRU	WGAN	MVIT	VIVIT	Swin			
AI for turbulent boundary layers	X	X	X									X						
AI for wind farm layout optimization				X											X			
AI for data-driven models in reacting flows					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															



Compelling Scoreboard Review & Next Steps



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Agenda Item (6) – Next Steps & Follow-Through

➤ 08.09 - 09.09.2022 (Review Preparations start)

- One day in-person rehearsal
- One day full event in Juelich
- WP leaders, not really task leaders
- Every Organization takes part
- Instructions & schedule given by PMT

➤ Other items?

- Task 2.1
 - LUMI (get access via UICE), Puhuri access
 - Mare Nostrum (machine end of the year)



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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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