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

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School of Engineering & Natural Sciences, University of Iceland

2022-05-31, RAISE WP2 Monthly Meeting May 2022, Online

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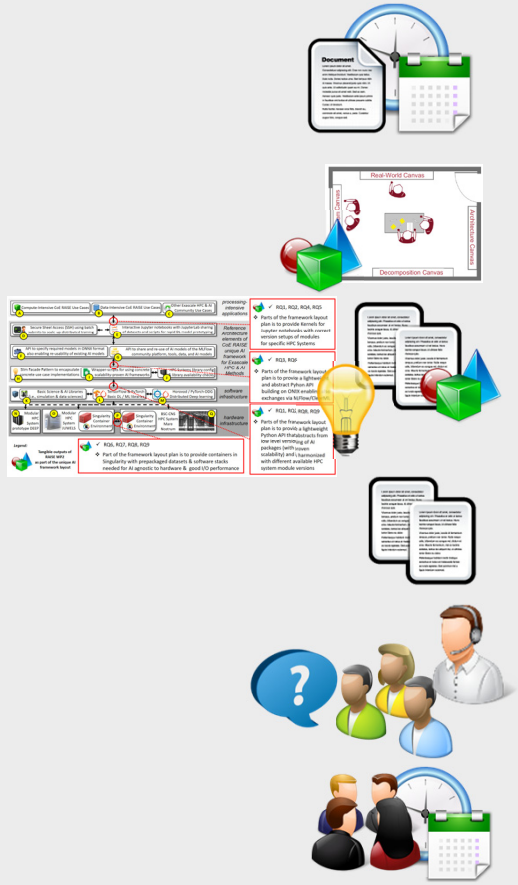
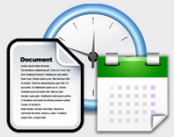
WP2 May – Welcome & Agenda

1. Approval of minutes from Monthly Meeting April 2022
   - (All), ~5 Min
2. Review WP2 Status on Interaction Rooms
   - (Morris Riedel, Matthias Book, Helmut Neukirchen), ~10 Min
3. Realization of the SW Framework
   - (Morris, Liang, Johannes et al.), ~5 Min
4. Upcoming Deliverables
   - (Eray, Morris et al.), ~20 Min
5. Status WP2 Training Plans
   - (Morris et al.), ~5 Min
6. Compelling Scoreboard Review & Next Steps
   - (All), ~15 Min

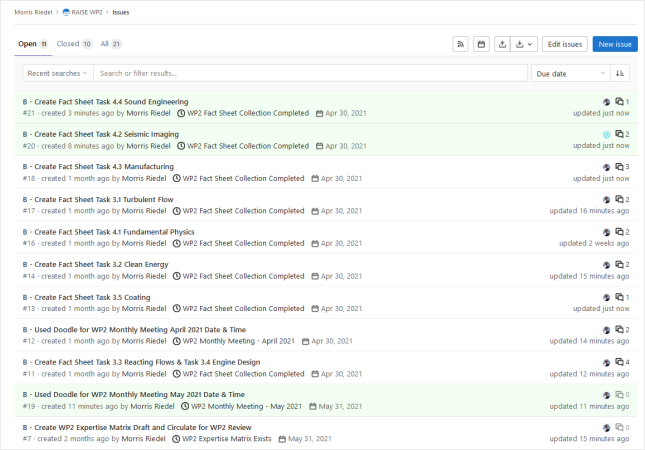


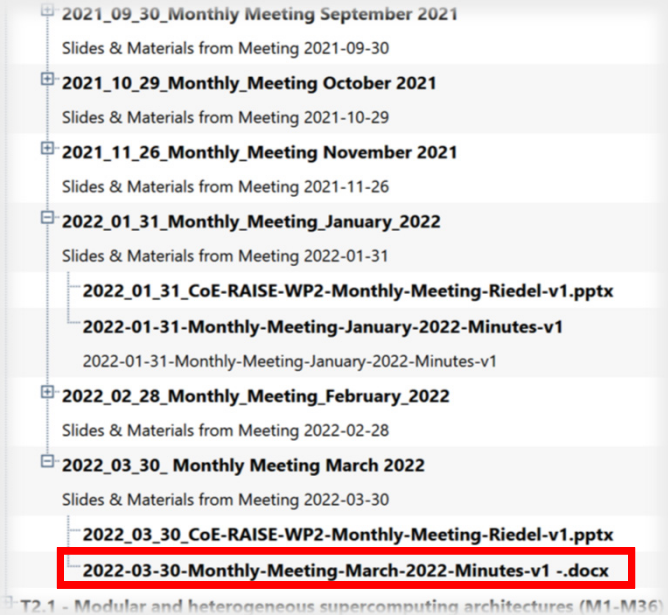
Agenda Item (1) – Minutes Approval – April 2022

Minutes Approval – Monthly Meeting April 2022



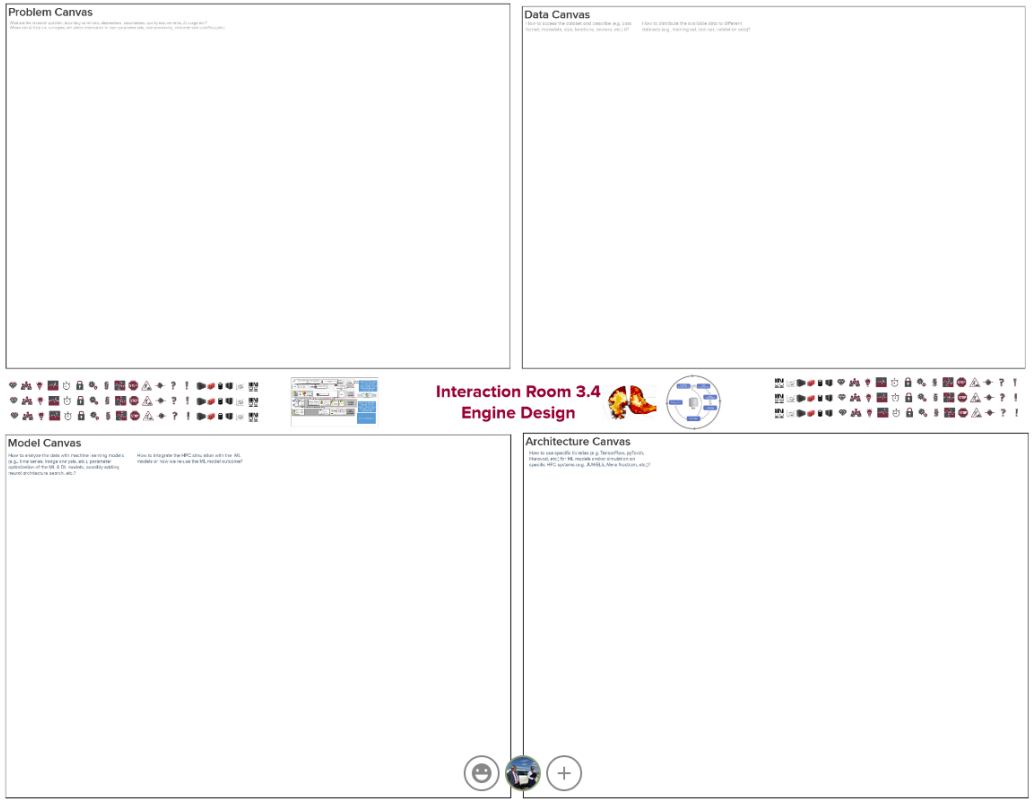
- Minutes available in BSCW
  - https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3340884
  - TBD(all): Any objections or additions/changes?

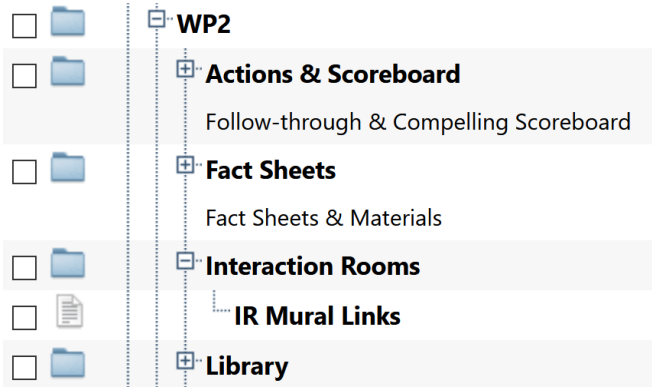


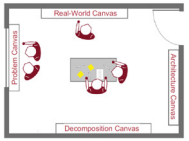


Agenda Item (2) – Review WP2 Status on Interaction Rooms

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=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/matthiasbook8855/1621378007555/6f0d5285fcacc5cafa515bd6676c84d8b4879d39?sender=u15e3008bb41d6628a5bb5701

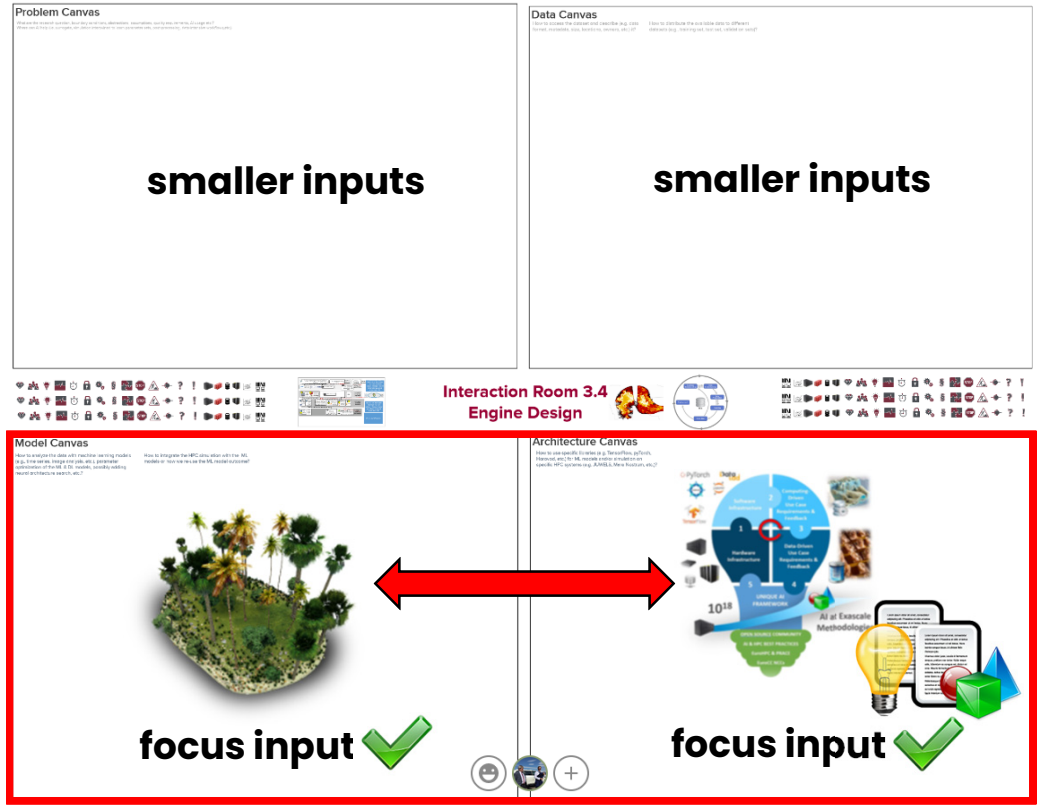
IR4.2 Seismic Imaging: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ae3e28af4bb8d9adbec33874998?sender=u15e3008bb41d6628a5bb5701

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

- TBD(all): Do people use the MURAL boards
- 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=u15e3008bb41d6628a5bb5701

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IR3.3 Reactive Flows: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377959022/0c363886f24833ecb19b025d87324b57fd50e2db?sender=u15e3008bb41d6628a5bb5701

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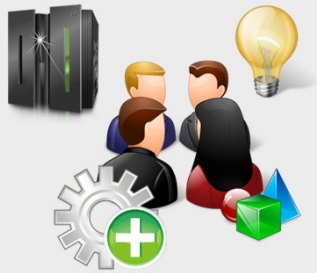
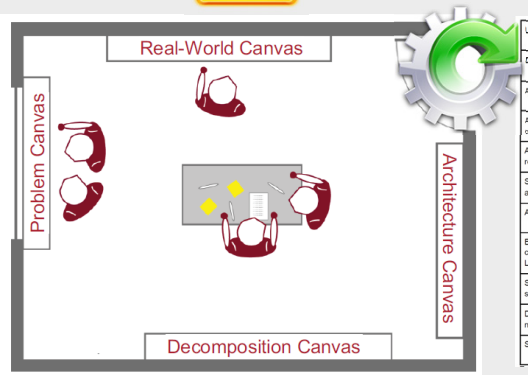
IR4.4 Sound Engineering: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa122190024040 59f90a4bbb0101fa379a8503?sender=u15e3008bb41d6628a5bb5701

Interaction Room Status & Discussions – WP3/WP4 Overview

- WP3 (second round IRs)
  - T3.1: Turbulent Flow (asked) → later, needs RWTH
  - T3.2: Clean Energy (not started) → later today!
  - T3.3: Reactive Flows (not started)
  - T3.4: Engine design (not started)
  - T3.5: Coating (not started)
- WP4 (second round IRs)
  - T4.1: Fundamental physics (asked) → done
  - T4.2: Seismic imaging (started) → done
  - T4.3: Manufacturing (not started)
  - T4.4: Sound engineering (not started)
- TBD(Katrín): Schedule meetings with Interaction Room teams (hard to find slots)



Continously Updating



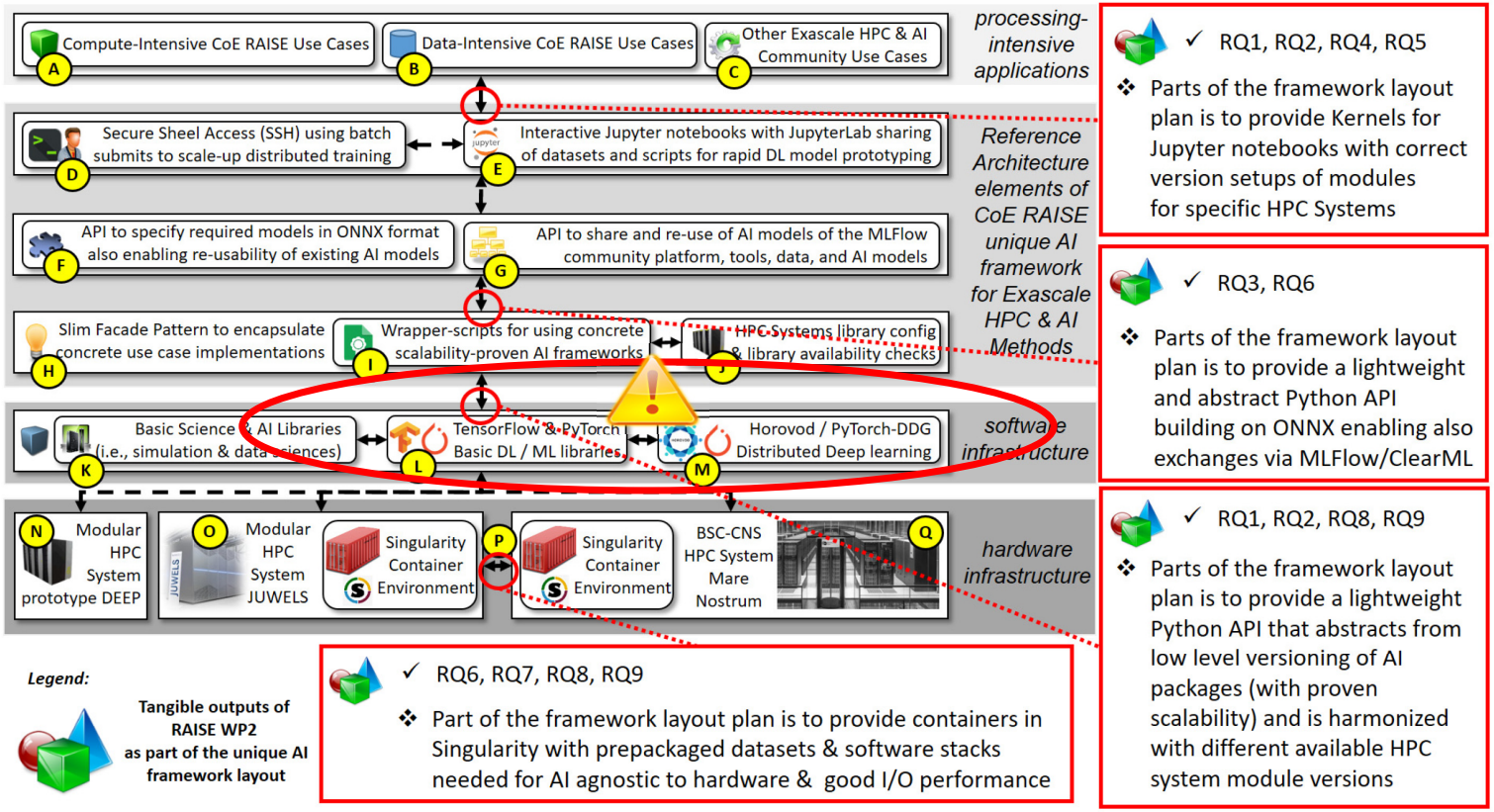
Use Case	AE	PIML	ANNs	CNN		NO	SMs			GNN	IN	LSTM	GRU
Details	*CAE*		*RBF-ANN*	*U-Net*	*RESNET*	*FNO*	*AR*	*ARMA*	*ARIMA*		*JEDI-net*		
AI for turbulent boundary layers	X	X											
AI for wind farm layout optimization			X				X	X	X				
AI for data-driven models in reacting flows				X						X			
Smart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

- 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

Agenda Item (3) – Realization of the SW Framework

Realization of SW Framework – Ideas of Web Page & Git Links

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



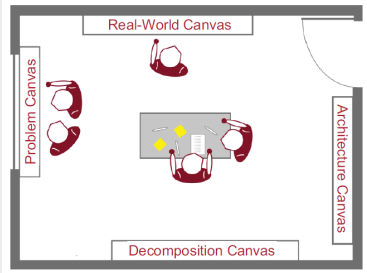
Continously Updating: e.g., add hyper-parameter optimization tools, pipelines?!

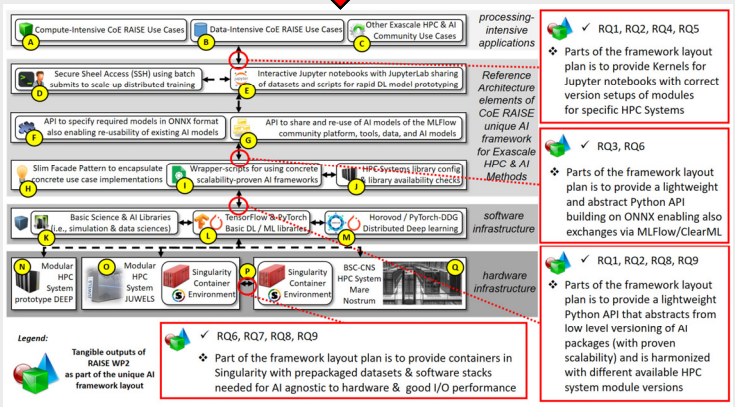
Realization of SW Framework – Interaction Room Results (1)

RAISE Center of Excellence

- ✓ Interaction Room Seismic Imaging
  - Pipeline activities relevant for the SW Framework Co-Design
  - Updates from Johannes (WP2) & Liang (WP4)
- ✓ Interaction Room Event Reconstruction & Classification at the CERN-LHC
  - Official Repository exists, no need to put elements into github
  - Includes also job scripts, AI model scripts, etc.
  - Very specific model in the community „MLPF“, perhaps limited use for other communities
  - Good to share for world-wide LHC collaboration
  - TBD(): Adding Raytune to SW framework relevant and Rapids.AI (e.g., for memory management)

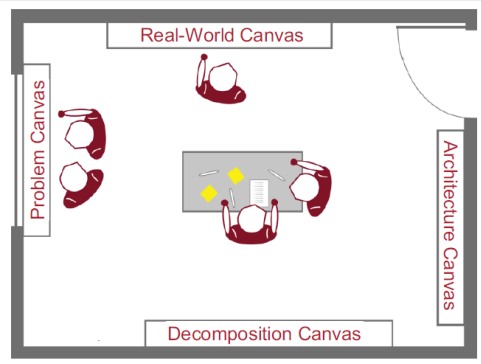
Input to Deliverable D2.10





Realization of SW Framework – Interaction Room Results (2)

- ✓ Interaction Room Event Reconstruction & Classification at the CERN-LHC
  - ✓ Initial set of models analyzed, but not used in RAISE
  - ➢ Removal of Statistical Methods
  - ➢ Removal of Jedi-NET
  - ➢ Update of Matrix



Input to Deliverable D2.10

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

Agenda Item (4) – Upcoming Deliverables

Upcoming Deliverables

- Time to start with selected deliverables

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. Lektauers/ 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

Upcoming Deliverables

- Time to start with 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 AISee 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.

Upcoming Deliverables D2.7 Support Report

- Time to start with selected deliverables

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.

Upcoming Deliverables – D2.10 Monitoring Report

- Time to start with selected deliverables

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

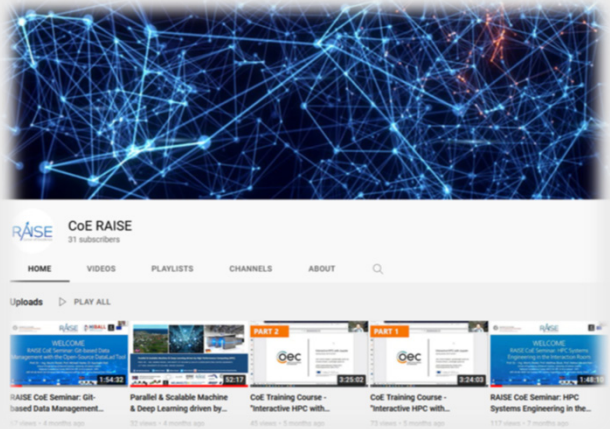
(term 'monitoring' interpreted as 'progress monitoring'?!)

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)**

Agenda Item (5) – Status WP2 Training Plans

WP2 Monthly Trainings – Review & Plan

- 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/UCAdIZ-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**

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

WP2 Monthly Trainings – Review & Plan

WP2 Monthly Trainings – Review & Plan

December:
No Seminar

January:
RTU CUDA Seminar
(THANKS!)

February:
none

2022-03-31 14:00 GMT
Graph Neural Network
Morris: Intro GNNs (30 min)
Leo from Atos (45 min)
Eric from Cern (20 min)

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

April:
Quantum Annealing
Maybe Gabriele Examles 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 (?)
→ Katrin : check and schedule

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

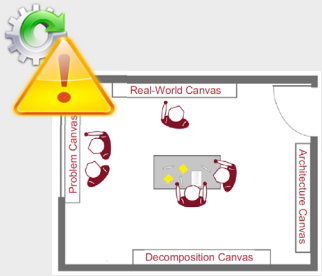
September:
EOSC – NI4OS-Europe
→ Katrin: check and schedule

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

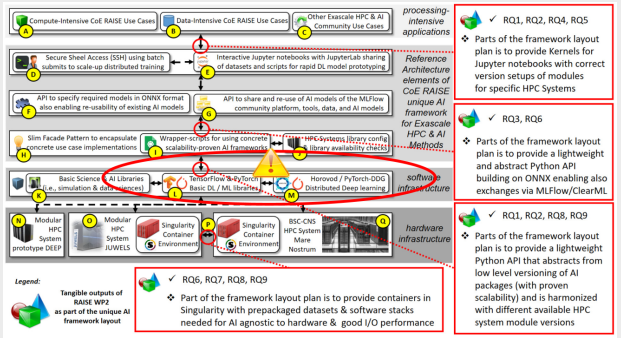
Compelling Scoreboard Review – Use Case Progress

- 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

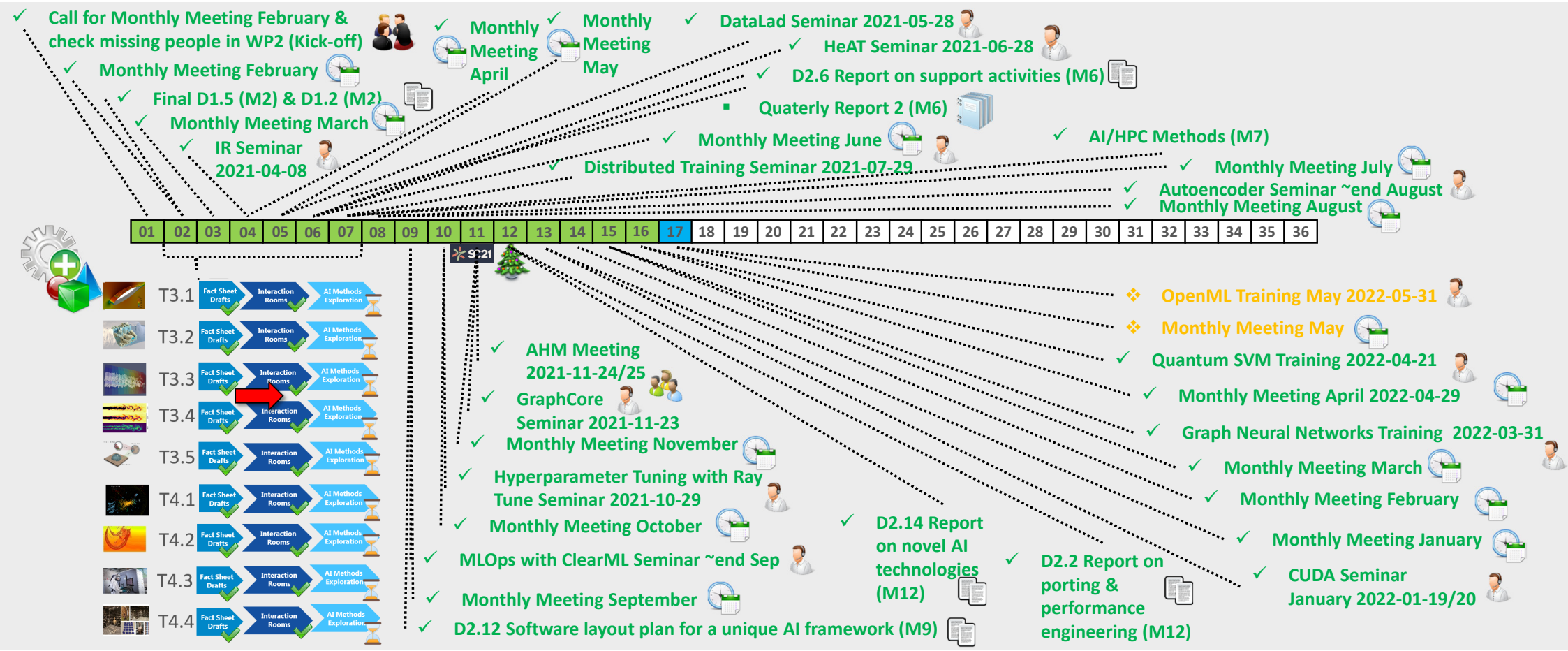


Lessons Learned:
Massive amount of post Covid-19 in-person events & travel prevents fast progress

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



Compelling Scoreboard Review & Next Steps



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

- 09.06.2022
  - Training RTU
- 08.09 - 09.09.2022 (Review)
  - One day in-person rehearsal
  - One day full event in Juelich
  - WP leaders, not really task leaders
  - Every Organization takes part

drive. enable. innovate.

RAISE Center of Excellence

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