UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES
FACULTY OF INDUSTRIAL ENGINEERING,
MECHANICAL ENGINEERING AND COMPUTER SCIENCE

RAISE Center of Excellence

EURO

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

Prof. Dr. – Ing. Morris Riedel et al.
School of Engineering & Natural Sciences, University of Iceland

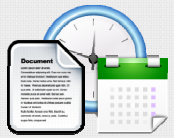
2021-09-30, RAISE WP2 Monthly Meeting September 2021, Online

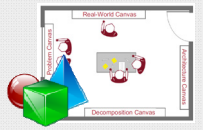
@ProfDrMorrisRiedel @Morris Riedel @MorrisRiedel @MorrisRiedel
https://www.youtube.com/channel/UCWC4VKHmL4NZgFfKoHtANKg morris@hi.is

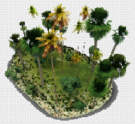
WP2 September Meeting – Welcome & Agenda

RAISE Center of Excellence

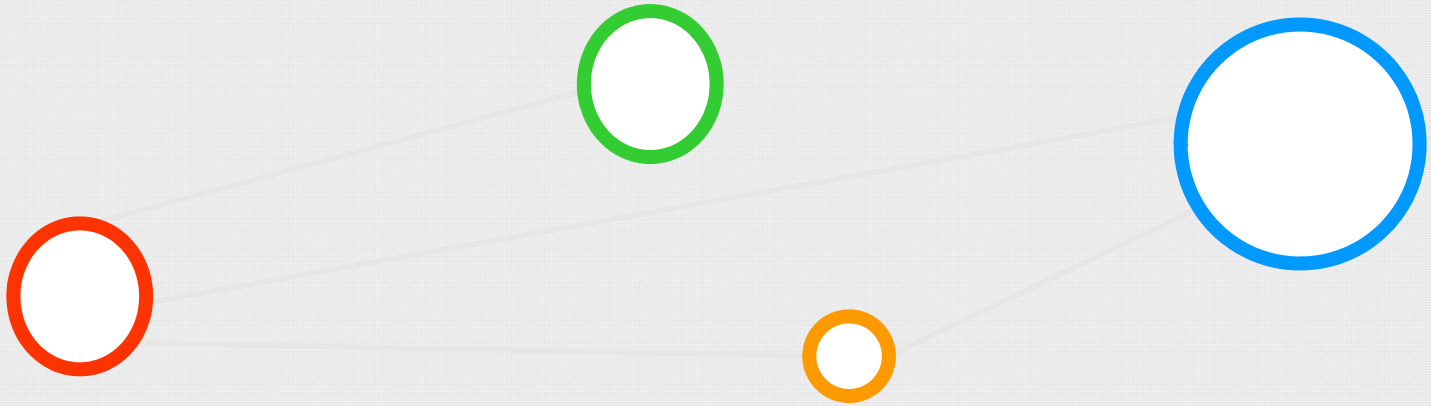
1. Approval of minutes from Monthly Meeting August 2021
   - (All), ~5 Min
2. Review WP2 Status on Interaction Rooms
   - (Morris Riedel, Matthias Book, Helmut Neukirchen), ~10 Min
3. Debrief Milestone AI/HPC Methods (M7)
   - (Morris Riedel), ~10 Min
4. Debrief Deliverable D2.12 Framework (M9)
   - (Morris Riedel & Andreas Lintermann), ~20 Min
5. Resources & Deliverable D2.2 (M12)
   - (Guillaume, Guillermo, Cristóbal), ~5 Min
6. Compelling Scoreboard Review & Next Steps
   - (All), ~10 Min





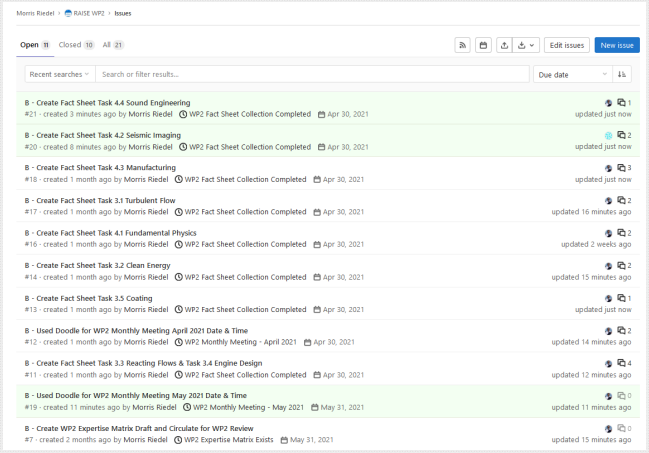


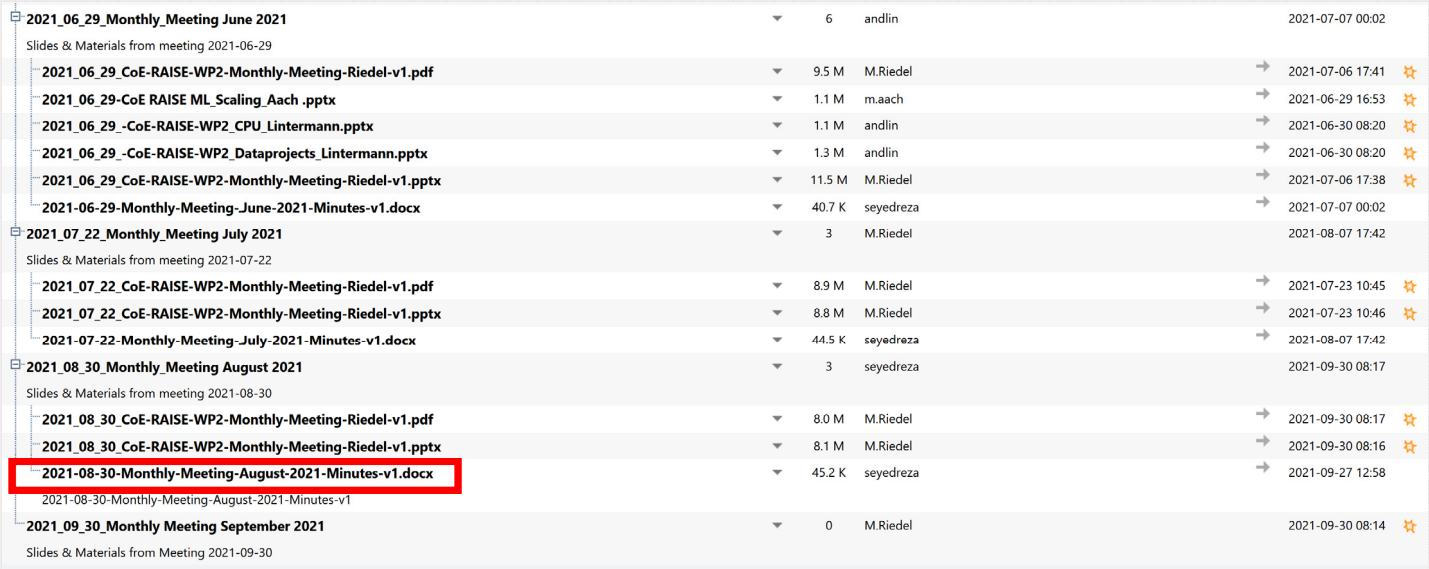
Agenda Item (1) – Minutes Approval – Meeting August 2021



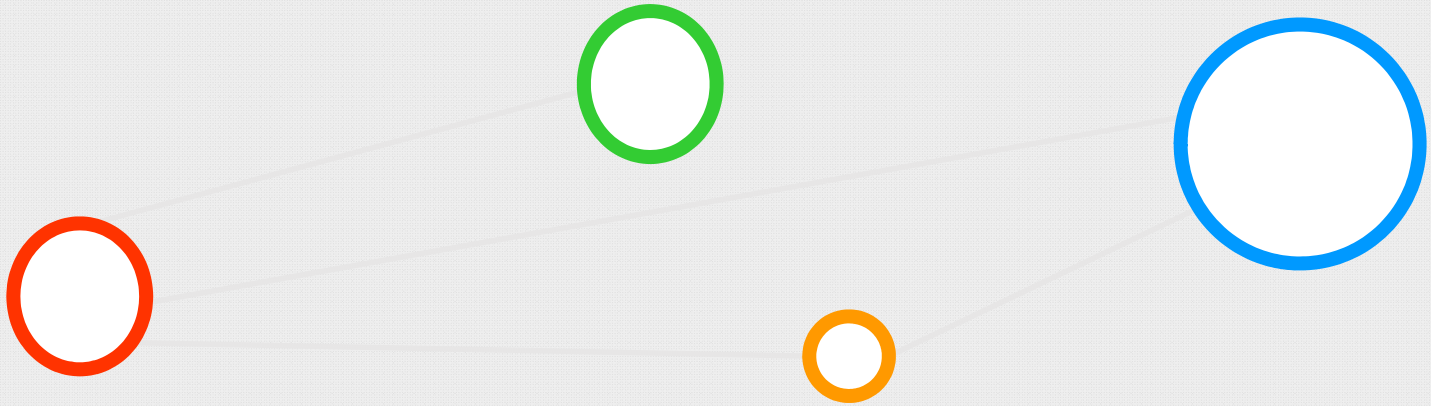
Minutes Approval – Monthly Meeting August 2021

- Minutes available in BSCW
  - https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3704758
  - TBD(all): Any objections or additions/changes?





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



WP2 Updates – Action Item Fact Sheets (refinement started)

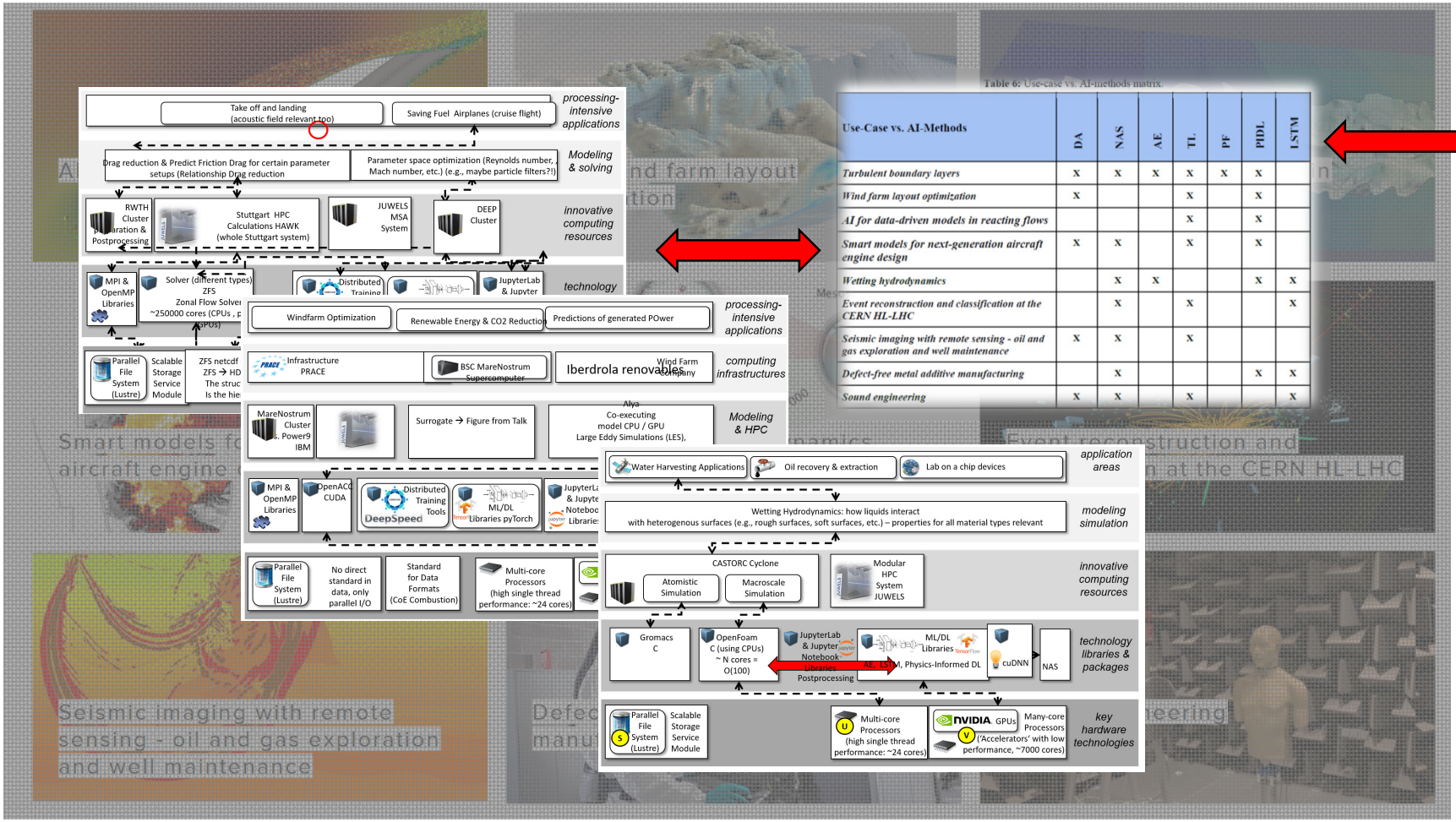
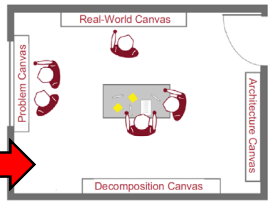


Table 6: Use-case vs. AI-methods matrix.

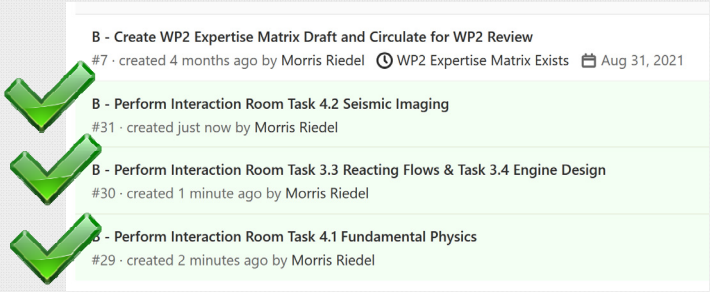
Use-Case vs. AI-Methods	DA	NAS	AE	TL	PF	PIDL	LSTM
Turbulent boundary layers	X	X	X	X	X	X	
Wind farm layout optimization	X			X		X	
AI for data-driven models in reacting flows				X		X	
Smart models for next-generation aircraft engine design	X	X		X		X	
Wetting hydrodynamics		X	X			X	X
Event reconstruction 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



WORK IN PROGRESS

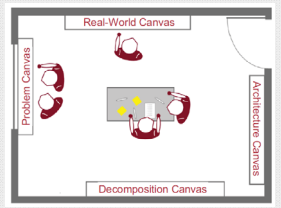
WP2 Updates – Action Items Tracker & Status Updates

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



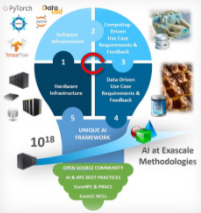
initial steps

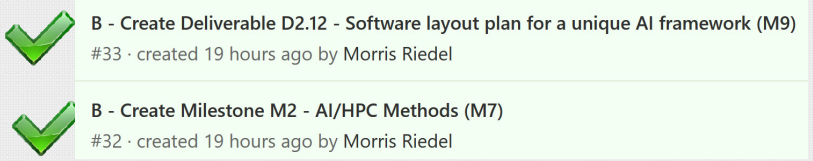
input to Interaction Room process



input to Milestone (M7) AI/HPC Methods

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

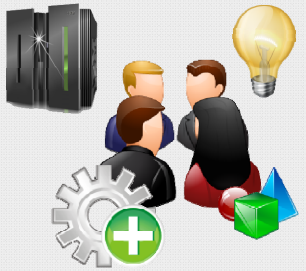




- https://gitlab.version.fz-juelich.de/riedel1/raise-wp2/-/issues

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)



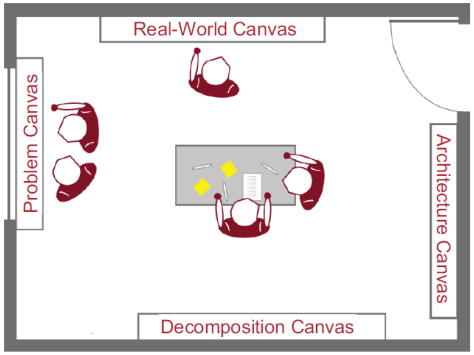
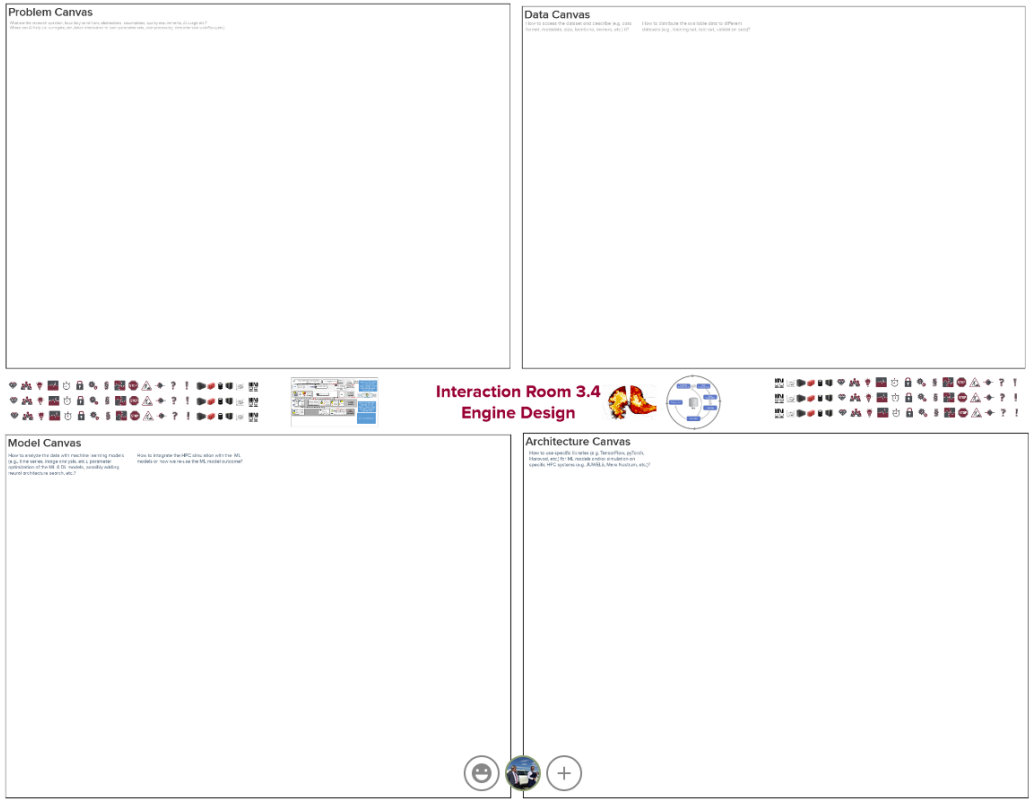


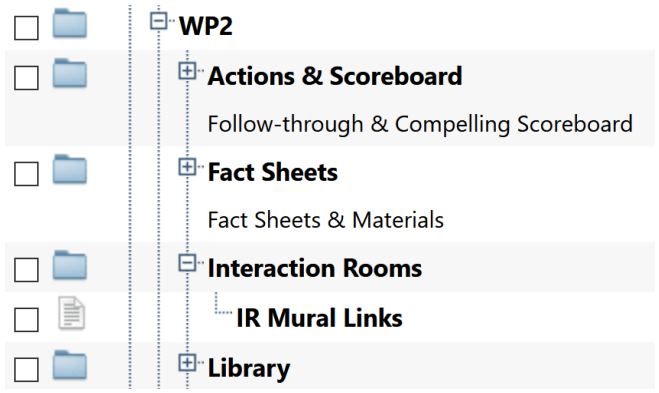
Table 6: Use-case vs. AI-methods matrix.

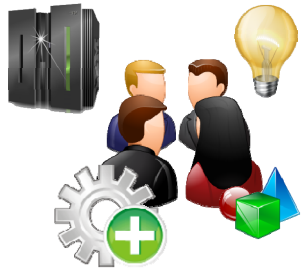
Use-Case vs. AI-Methods	DA	NAS	AE	TL	PF	PIDL	LSTM
Turbulent boundary layers	x	x	x	x	x	x	
Wind farm layout optimization	x			x		x	
AI for data-driven models in reacting flows				x		x	
Smart models for next-generation aircraft engine design	x	x		x		x	
Wetting hydrodynamics		x	x			x	x
Event reconstruction 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

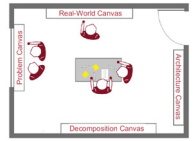
- Continuing Steps
  - Carve out more details on AI/HPC methods
  - Identify concrete detailed algorithms
  - Evaluate and benchmark scalability of methods

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/matthiasbook8855/1621378007555/6f0d5285fcaec5eafa515bd6676c84d8b4879d39?sender=u15e3008bb41d6628a5bb5701

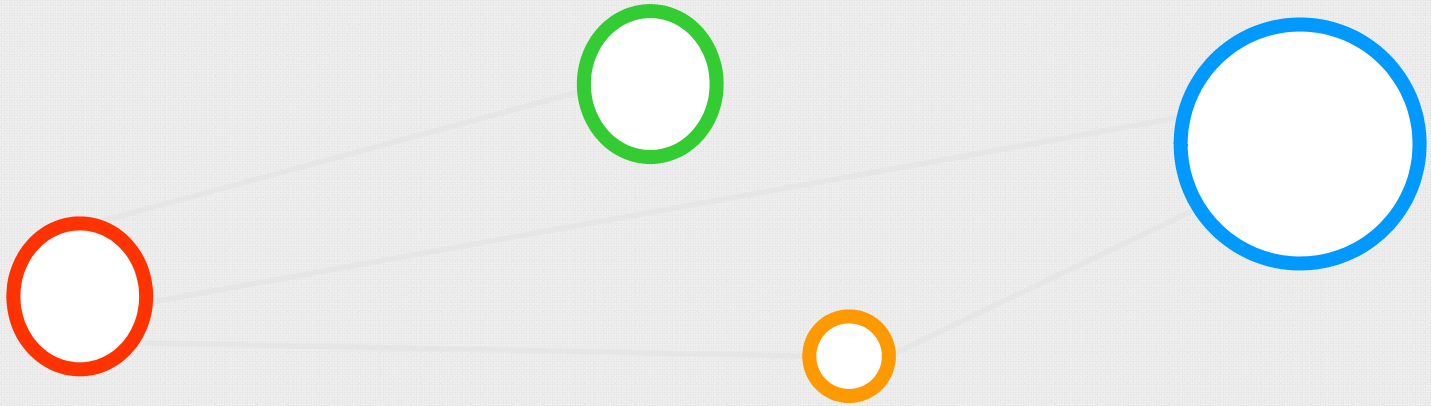
IR4.2 Seismic Imaging: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ae3e28af4bb8d9adbec33874998?sender=u15e3008bb41d6628a5bb5701

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/b5fa12219002404059f90a4bbb0101fa379a8503?sender=u15e3008bb41d6628a5bb5701

- TBD(all): Do people use the MURAL boards (e.g., Task 3.4 is pretty empty but with Task 3.3)?
- https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3591551

Agenda Item (3) – Debrief Milestone AI/HPC Methods (M7)

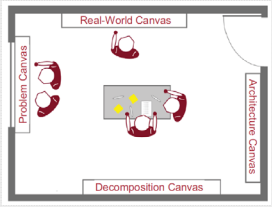


Achieved Milestone MS2 AI/HPC Methods (M7)

Milestones

Number	Name	Lead Beneficiary	Delivery Date (Annex I)	Achieved	Delivery Date (actual)	Comments
1	Project kick-off	FZJ	31 Jan 2021	☑	22 Jan 2021	The kick-off took place online via video conference with >40 participants coming from all partners, linked third-parties and third-parties. The kick-off included a keynote
2	AI/HPC methods	UOI	31 Jul 2021	☑	31 Jul 2021	The software engineering process driven by WP2 in collaboration with all WP3/WP4 use cases started with the development of Use Case Fact Sheets. This was
3	Training courses	BSC	30 Apr 2022	☐		
4	Use-cases / technical developments	UOI	31 Dec 2022	☐		
5	Business plan	FLANDERS MAKE	30 Jun 2023	☐		
6	All final reports	FZJ	31 Dec 2023	☐		

- Discussions with PMO
  - Should be not a formal report (not too long, not too short)
  - Optional document (not required to send to EC)
  - Links to MURAL Boards included
  - Summarizes findings of MURAL Board discussions (w.r.t. Model/Data/Architecture Canvas)
  - Refining our initial Matrix of Methods & identify common methods
  - Means of Verification ('practical use' in use cases):
    '*First set of AI and HPC methods is ready to be used in the use-cases*'



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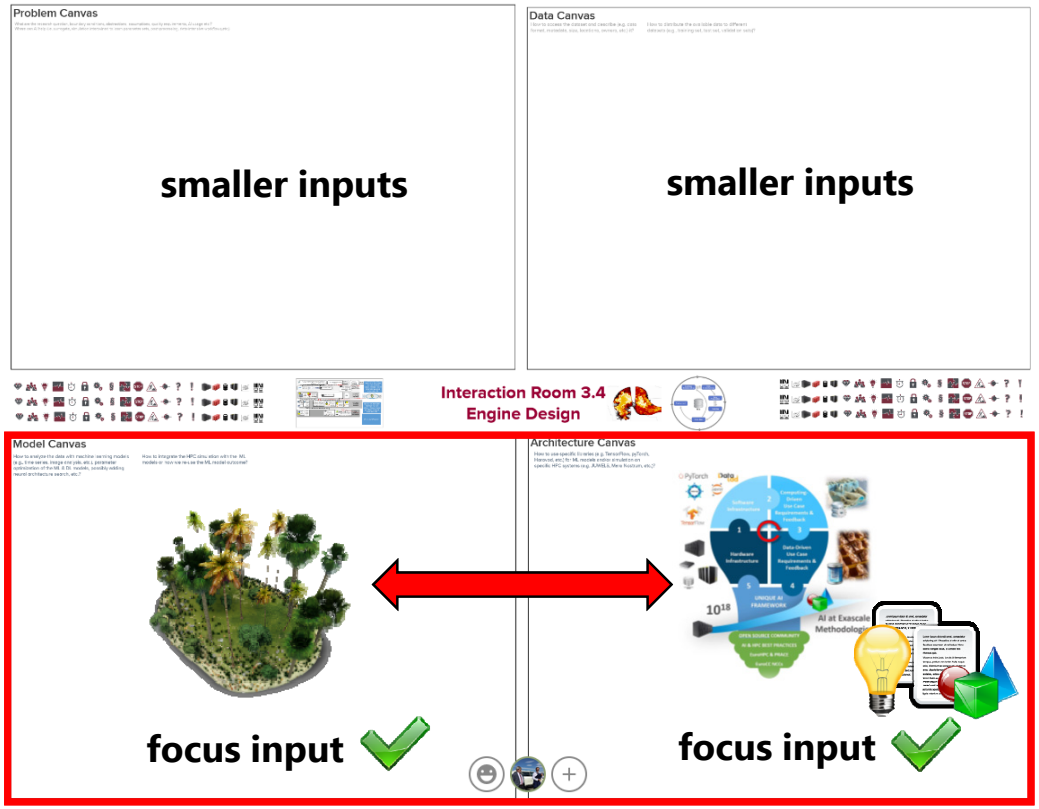
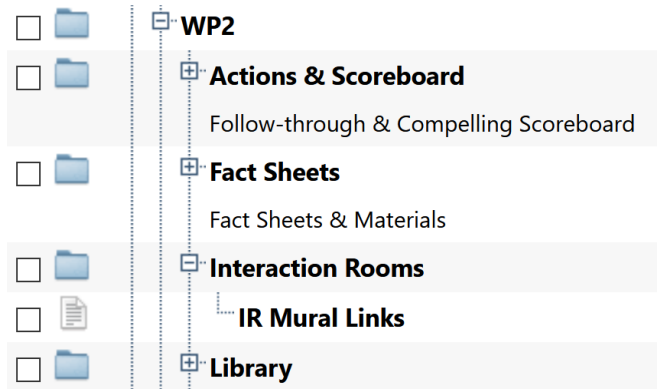
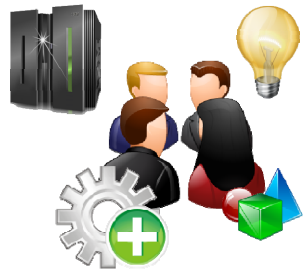
Turbulent boundary layers	X	X	X	X	X	X	
Wind farm layout optimization	X			X		X	
AI for data-driven models in reacting flows				X		X	
Smart models for next-generation aircraft engine design	X	X		X		X	
Wetting hydrodynamics		X	X			X	X
Event reconstruction and classification at the CERN HL-LHC		X		X			X
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

Interaction Rooms via MURAL Boards & Milestone / Deliverable







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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

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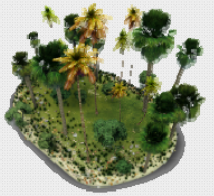
IR4.2 Seismic Imaging: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ae3e28af4bb8d9adbec33874998?sender=u15e3008bb41d6628a5bb5701

IR4.3 Manufacturing: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378038069/93df6fa7a41093f4eaae7be9d72979dc2ba42b9d?sender=u15e3008bb41d6628a5bb5701

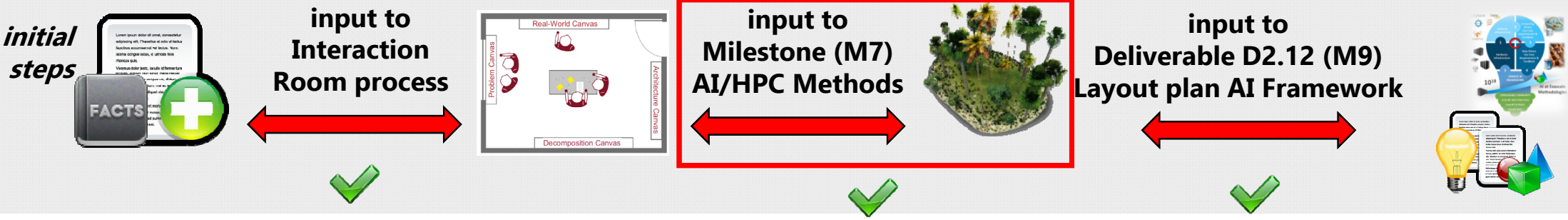
IR4.4 Sound Engineering: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa122190024040 59f90a4bbb0101fa379a8503?sender=u15e3008bb41d6628a5bb5701

- https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3591551

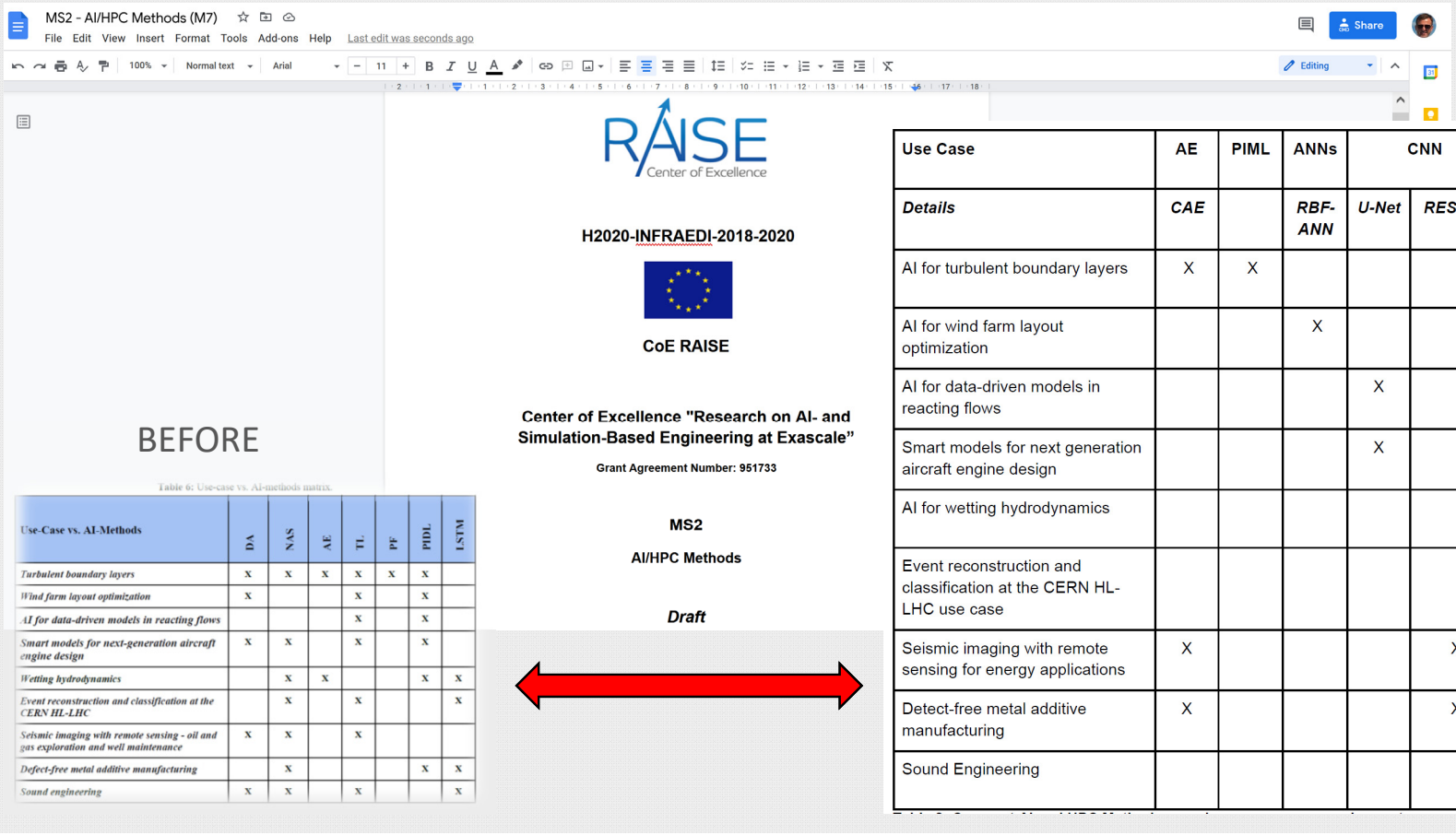
WP2 Updates – Location Milestone MS2 AI/HPC Methods (M7)



- Milestone MS2 – AI/HPC Methods (M7)
  - Format and Template clarified with PMO: https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/d3657643/CoE%20RAISE_MS_Template.docx
  - Not an official document, maybe only useful in the review;
  - Summary (1/4 page) provided as comment in EU portal by clicking the checkbox for MS2
  - Google Document to keep it as a living document with important updates from Mural over time
  - TBD: Snapshot at end of August for archiving via Word document as MS2 document (optional)
  - Location (shared for everyone to edit): https://docs.google.com/document/d/1Az88KP9Z4USFA5hPMnqRhCE_8I9IzxnnvsYIhE2UXzc/edit?usp=sharing



Google Doc Milestone AI/HPC Methods (M7) – Living Document



BEFORE

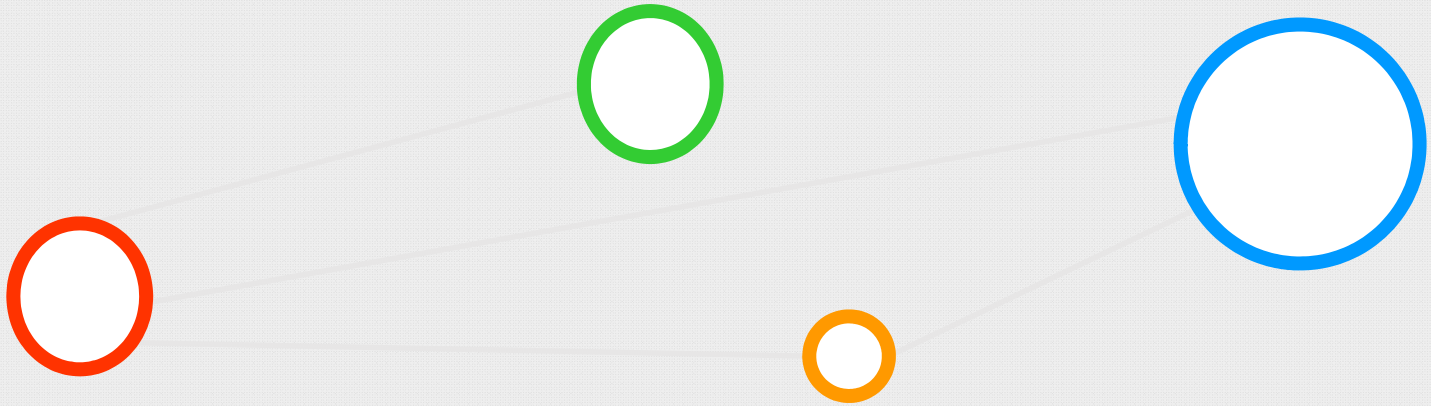
Table 6: Use-case vs. AI-methods matrix.

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

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

Agenda Item (4) – Debrief Deliverable D2.12 (M9)

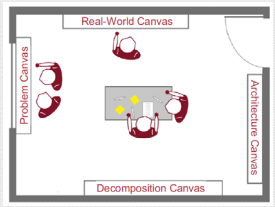


Debrief Deliverable D2.12 Framework (M9)

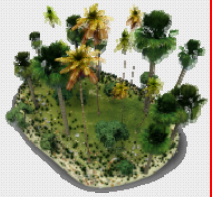
- Deliverable D2.12 - Software layout plan for a unique AI framework
  - Initial ideas around a comprehensive set of tools, also consider OpenML.org work
  - Challenge: massive toolsets available (e.g., distributed training tools via GPUs are ~10, etc.)
  - No need to re-invent the wheel, consider ONNX and other interoperable ML model formats
  - Library: Google document as initial start to collectively better work on it, interface (Matthias?, OpenML?), Meta-API library ideas: how can I link and integrate it, import coe_raise_lib, etc.?
  - Initial version in the word document as official document D2.12, but will be updated over time
  - TBD(all): Discussions between Gael (ATOS) and Matthias (UoI)

initial steps

input to Interaction Room process



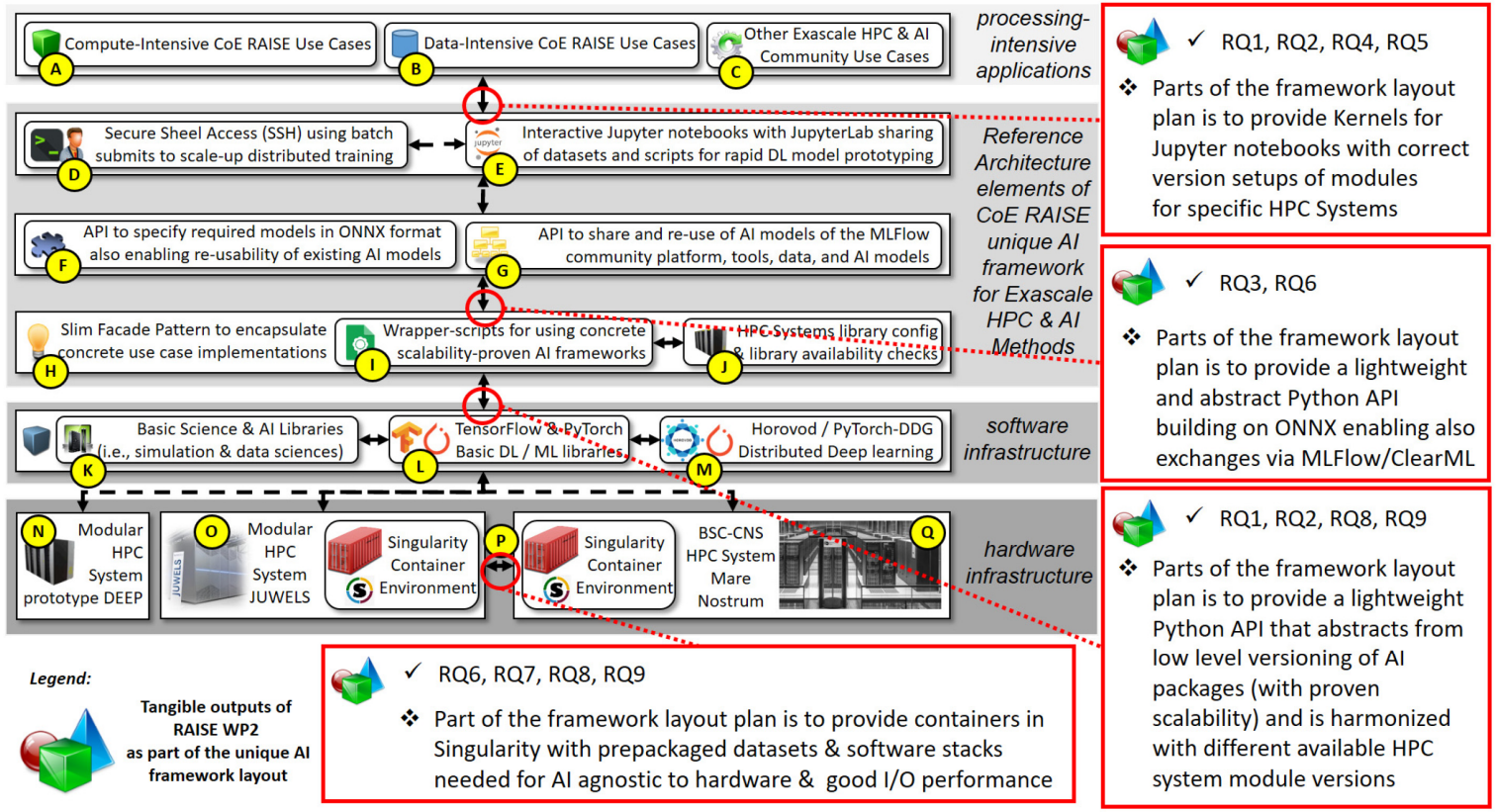
input to Milestone (M7) AI/HPC Methods



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

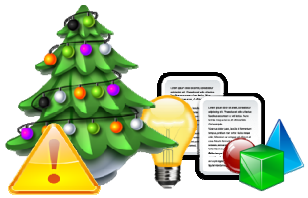
Debrief Deliverable D2.12 Framework (M9) – Initial Blueprint

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



Continously Updating

Changed Time Schedule for M12/December Deliverables (1)



- TBD(all): check your involvement for producing & reviewing
- https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/d3287337/CoE%20RAISE_Deliverables_Status.xls

As we have 8 deliverables coming up and with the Christmas holidays in mind, we would like to start with the preparation of the deliverables earlier. We are now looking at the following time schedule:

- 29.11.2021:
The author(s)upload(s)the Deliverable to the BSCW server to CoE RAISE / Reports and Deliverables / In progress / DX.Y. The author(s)inform(s)the WP leader the internal reviewer and the PMT about the uploaded document. The document name includes the term “Draft”.

- 06.12.2021:
The internal reviewer returns the document with comments and suggestions in track-changes mode to the author(s). The reviewed document is placed into the same folder on the BSCW as the original document and the PMT and WP leaders are informed in addition to the author(s).

- 06.12.2021 - 14.12.2021:
Continuous exchange between the author(s) and the reviewer (the PMT can already be involved). When a final version is ready for the PMT to review, the author(s) uploads the revised Deliverable to the BSCW server and informs the WP leader, the internal reviewer, and the PMT. The PMT starts to review the Deliverable and keeps track of all changes.

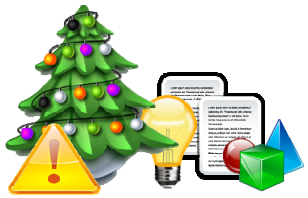
- 14.12.2021:
The PMT uploads the commented version to the BSCW server and informs the author(s) and the WP leader.

- 14.12.2021 - 21.12.2021:
Continuous exchange between the author(s), the reviewer, and the author(s). At the end, all corrections requested by the PMT have been included and the document is uploaded to the BSCW server. The file name includes the term “Final”.

- 21.12.2021 - 22.12.2021:
The PMT generates the final PDF.

- 23.12.2021:
The Coordinator submits the Deliverable to the EC and places the finally submitted version into the BSCW folder CoE RAISE / Reports and Deliverables / EC submitted.

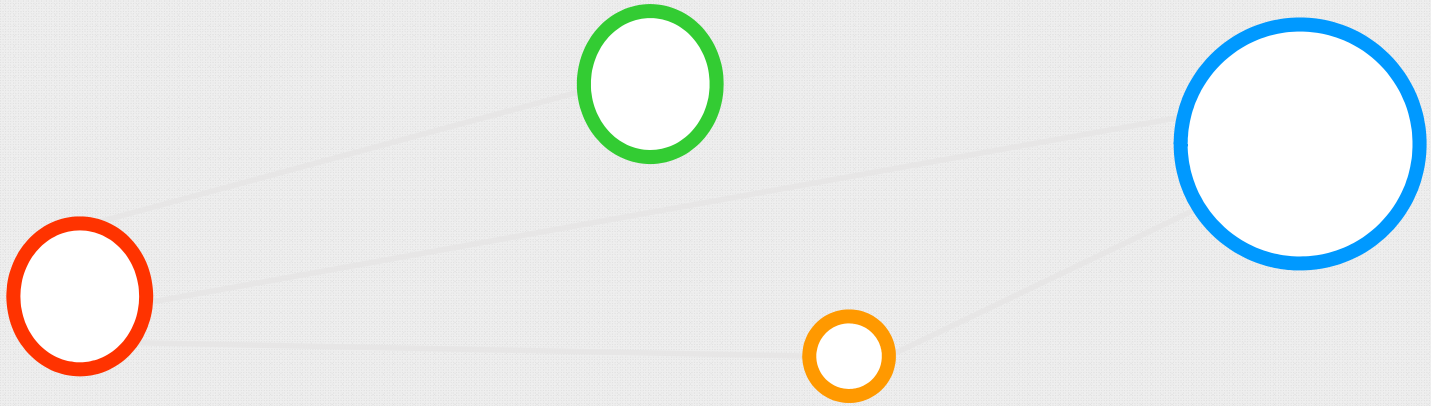
Changed Time Schedule for M12/December Deliverables (2)



- TBD(Guillaume, Morris): Start preparing D2.2 & D2.14 directly after the call
- TBD(all): note that WP2 members are also involved in WP3/WP4 use cases

⏳	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	V. Khristenko/ CERN	H. Neukirchen/ UOI	I. Schmitz/ ParTec	29.11.2021	31.12.2021
	D5.4	IP document and services	FZJ	R	CO	12	K. De Grave/ FM	M. Himmelsbach/ ParTec	I. Slaidins/ RTU	A. Lintermann/ FZJ	29.11.2021	31.12.2021
	D6.2	Educational portfolio document	RTU	R	PU	12	R. Gregorio/ BSC	I. Slaidins/ RTU	V. Harmandaris/ CYI	K. Pausch/ FZJ	29.11.2021	31.12.2021
	D6.9	Visual identity	FZJ	DEC	PU	12	R. Gregorio/ BSC	M. Bresser/ FZJ	G. Exilard/ SAFRAN	I. Schmitz/ ParTec	29.11.2021	31.12.2021
	D6.10	Communication and dissemination plan	FZJ	R	PU	12	R. Gregorio/ BSC	M. Bresser/ FZJ	D. Southwick/ CERN	J. Lopez/ ParTec	29.11.2021	31.12.2021

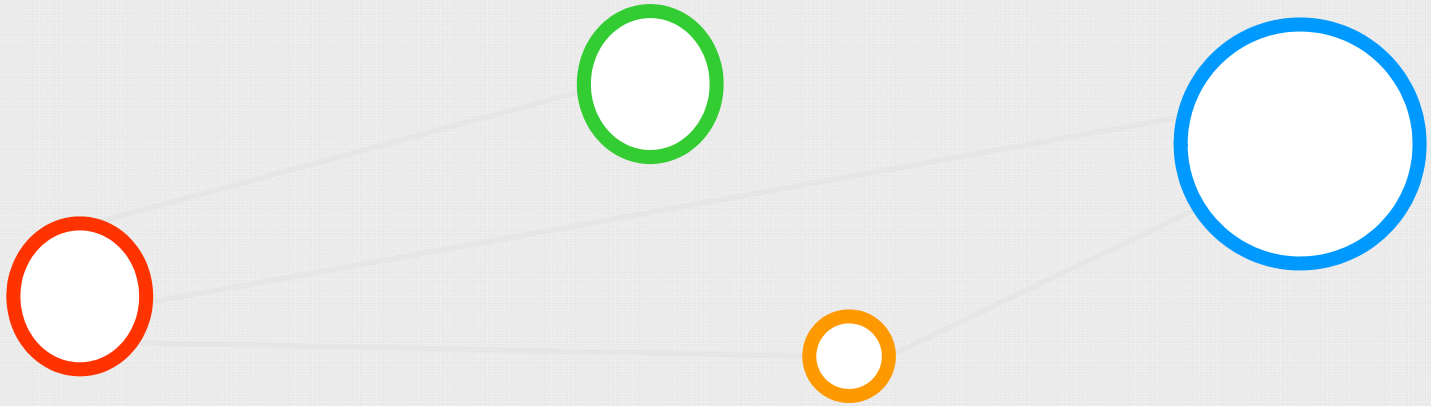
Agenda Item (5) – Resources & Deliverable D2.2 (M12)



Agenda Item (5) – Resources & Deliverable D2.2 (M12)

- (Guillaume, Guillermo, Cristóbal), ~5 Min

Agenda Item (6) – Compelling Scoreboard Review & Next Steps



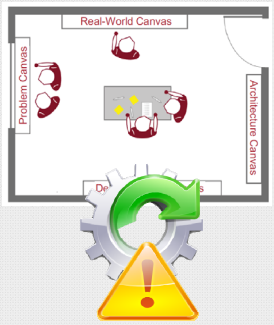
Compelling Scoreboard Review – Use Case Progress

RAISE Center of Excellence

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

- 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

❖ Fact Sheet Process & Interaction Room (started): revision & refinement process more dense (initial round)



input to Milestone (M7) AI/HPC Methods

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

RAISE Center of Excellence

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

RAISE Center of Excellence

H2020-INFRAEDI-2018-2020

CoE RAISE

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

Grant Agreement Number: 951733

D2.12

Software Layout Plan for a unique AI Framework

Draft

Version: 0.12
Author(s): M. Riedel (UOI)
Contributor(s): M. Book (UOI), H. Neukirchen (UOI)
Date: 28.09.2021

Compelling Scoreboard Review & Next Steps

RAISE Center of Excellence

✓ Call for Monthly Meeting February & check missing people in WP2 (Kick-off)

✓ Monthly Meeting February

✓ Final D1.5 (M2) & D1.2 (M2)

✓ Monthly Meeting March

✓ IR Seminar 2021-04-08

✓ Monthly Meeting April

✓ Monthly Meeting May

✓ DataLad Seminar 2021-05-28

✓ HeAT Seminar 2021-06-28

✓ D2.6 Report on support activities (M6)

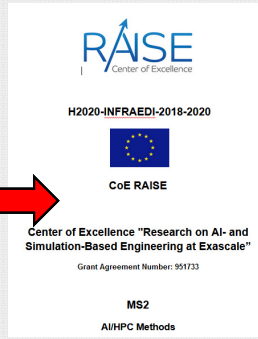
▪ Quaterly Report 2 (M6)

✓ Monthly Meeting June

✓ Distributed Training Seminar 2021-07-29

✓ AI/HPC Methods (M7)

✓ Monthly Meeting July



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

SC21

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

❖ AHM Meeting 2021-11-24/25

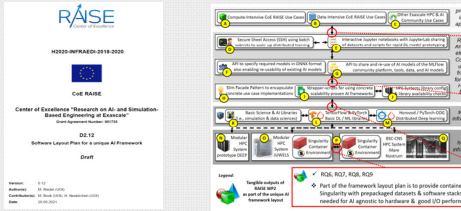
❖ MLOps with ClearML Seminar 2021-09-30

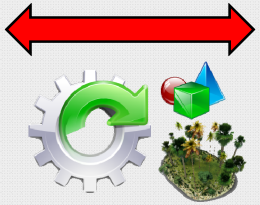
❖ Monthly Meeting September

✓ D2.12 Software layout plan for a unique AI framework (M9)

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

❖ D2.2 Report on porting & performance engineering (M12)





✓ Monthly Meeting August

✓ Autoencoder Seminar ~end August

Next Steps

- Work on Deliverables D2.2 & D2.14
- Support WP3 & WP4 Use case deliverables

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

1. AOB: All-Hands Meeting
    1. Once initial version of software layout plan is ready, maybe in Fall 2021, we present across all use cases the Milestone and Deliverable contents and new ideas and revise
    2. TBD(Andi): AHM Meeting
2. AOB: Seminar on OpenML & Interopable Formats
    1. TBD (Morris): Andi made contact and we have to follow-up on a date, probably later in the year
3. AOB: September/October Seminar with Graphcore maybe?
    1. TBD(Gael, Andi): Check benchmarking, etc.
    2. Future of HPC miletone document w.r.t. scaling: meeting
    3. U-Net benchmark data from CERFACS on real use case data
    4. ATOS has a machine: NVIDIA A100 vs. GraphCore (another project)
    5. Andi: access might be possible with a driving use case
4. AOB: Data transfers RTU, JSC, BSC?
    1. TBD(Lauris, Andi): check status
5. AOB: Data Project
    1. Data project was accepted (200 TB) → also open data is provided there

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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