



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



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

Prof. Dr. – Ing. Morris Riedel et al.

School of Engineering & Natural Sciences, University of Iceland

2021-08-30, RAISE WP2 Monthly Meeting August 2021, Online



@ProfDrMorrisRiedel



@Morris Riedel



@MorrisRiedel



@MorrisRiedel



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

morris@hi.is

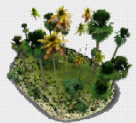
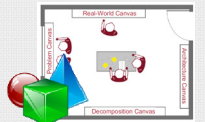


WP2 August Meeting – Welcome & Agenda

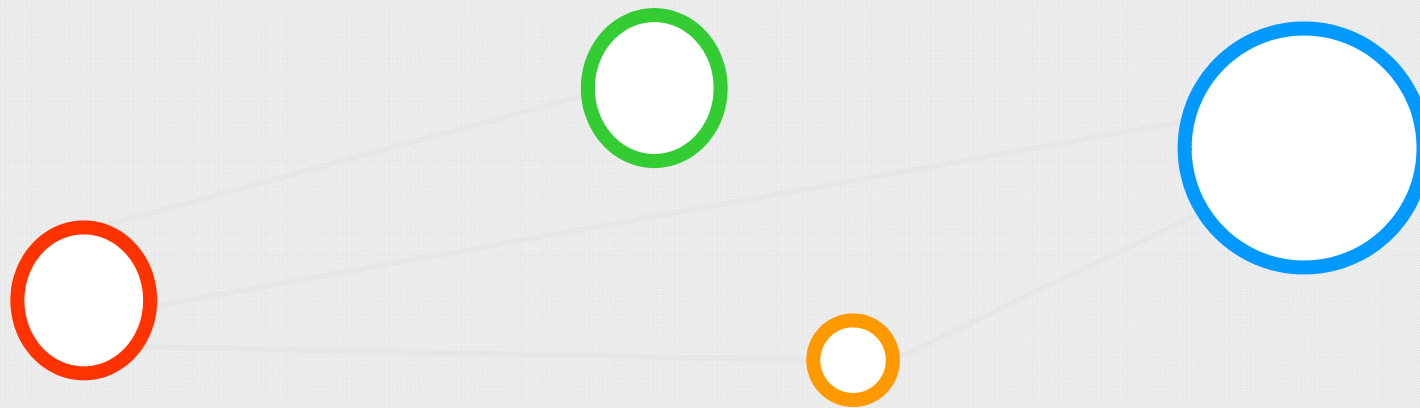


RAISE
Center of Excellence

1. Approval of minutes from Monthly Meeting July 2021
 - (All), ~5 Min
2. Review WP2 Status on Interaction Rooms
 - (Morris Riedel, Matthias Book, Helmut Neukirchen), ~10 Min
3. Achieved Milestone AI/HPC Methods (M7)
 - (Morris Riedel & Andreas Lintermann), ~30 Min
4. Plans Deliverable D2.12 Framework (M9)
 - (Morris Riedel & Andreas Lintermann), ~10 Min
5. Compelling Scoreboard Review & Next Steps
 - (All), ~5 Min



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



Minutes Approval – Monthly Meeting July 2021



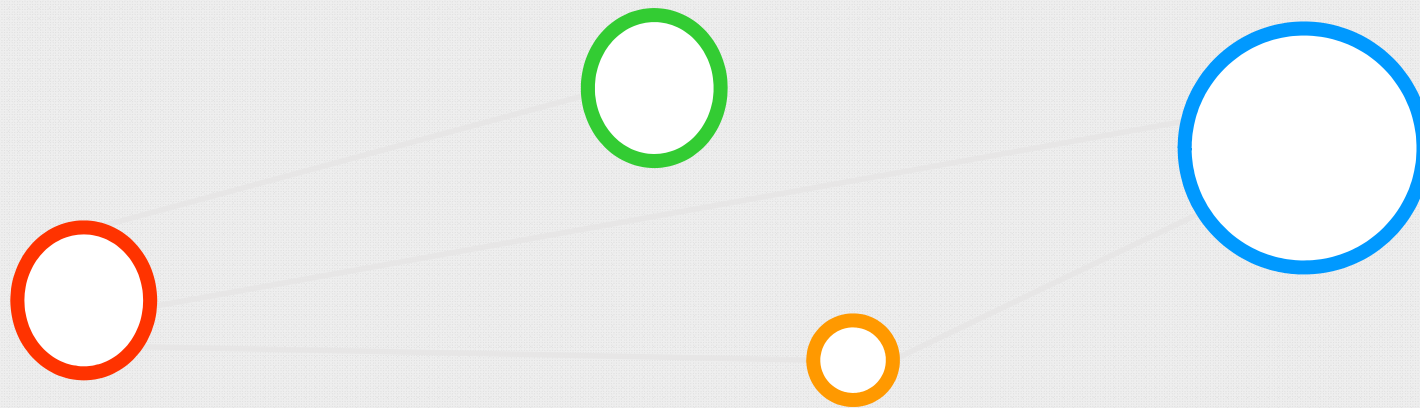
1. Minutes available in BSCW

- <https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/d3650527/2021-06-29-Monthly-Meeting-%d9%80June-2021-Minutes-v1.docx>
- TBD(all): Any objections or additions/changes?
- None in the call!

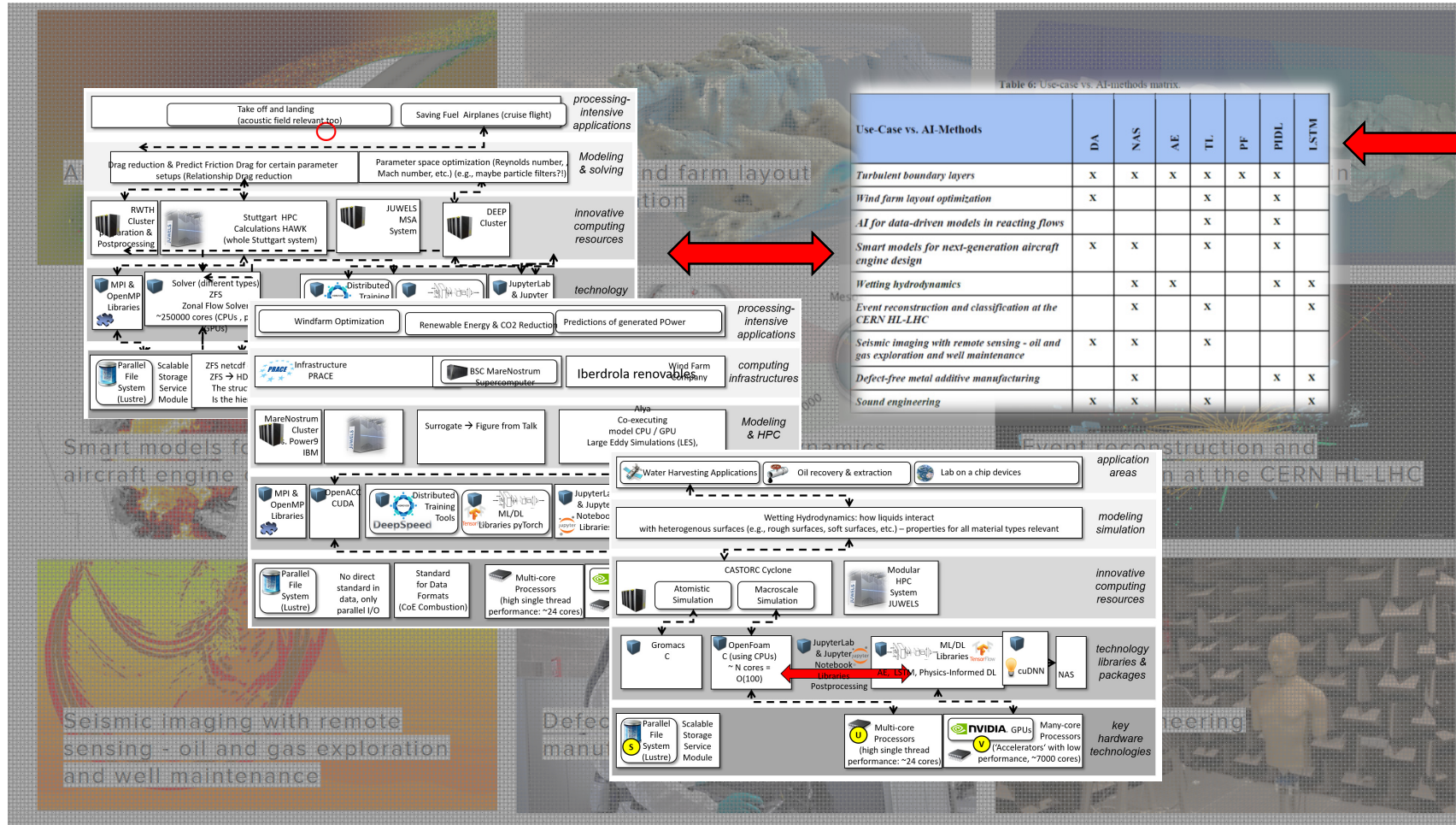
Morris Riedel - RAISE WP2 - Issues		
Open	Closed	All
Recent searches - Search or filter results...		
Due date		
B - Create Fact Sheet Task 4.4 Sound Engineering		
#21 - created 3 minutes ago by Morris Riedel	WP2 Fact Sheet Collection Completed	Apr 30, 2021
B - Create Fact Sheet Task 4.2 Seismic Imaging		
#20 - created 8 minutes ago by Morris Riedel	WP2 Fact Sheet Collection Completed	Apr 30, 2021
B - Create Fact Sheet Task 4.3 Manufacturing		
#18 - created 1 month ago by Morris Riedel	WP2 Fact Sheet Collection Completed	Apr 30, 2021
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
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
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
B - Create Fact Sheet Task 3.5 Coating		
#13 - created 1 month ago by Morris Riedel	WP2 Fact Sheet Collection Completed	Apr 30, 2021
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
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
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
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

2021_05_28_Monthly_Meeting May 2021	4	M.Riedel	2021-06-29 15:32
Slides & Materials from meeting 2021-05-28			
2021_05_28_CoE-RAISE-WP2-Monthly-Meeting-Riedel-v1.pdf	11.6 M	M.Riedel	2021-06-29 15:32
2021_05_28_CoE-RAISE-WP2-Monthly-Meeting-Riedel-v1.pptx	14.6 M	M.Riedel	2021-06-29 15:31
T2.2 Support activities	1.2 M	eray	2021-05-28 17:01
by Marcel Aach and Eray Inanc			
2021-05-28-Monthly-Meeting-Minutes	40.6 K	seyedreza	2021-06-07 15:36
2021_06_29_Monthly_Meeting June 2021	6	andlin	2021-07-07 00:02
Slides & Materials from meeting 2021-06-29			
2021_06_29_CoE-RAISE-WP2-Monthly-Meeting-Riedel-v1.pdf	9.5 M	M.Riedel	2021-07-06 17:41
2021_06_29_CoE-RAISE-ML_Scaling_Aach .pptx	1.1 M	m.aach	2021-06-29 16:53
2021_06_29_CoE-RAISE-WP2_CPU_Lintermann.pptx	1.1 M	andlin	2021-06-30 08:20
2021_06_29_CoE-RAISE-WP2_Dataprojects_Lintermann.pptx	1.3 M	andlin	2021-06-30 08:20
2021_06_29_CoE-RAISE-WP2-Monthly-Meeting-Riedel-v1.pptx	11.5 M	M.Riedel	2021-07-06 17:38
2021-06-29-Monthly-Meeting-June-2021-Minutes-v1.docx	40.7 K	seyedreza	2021-07-07 00:02
2021_07_22_Monthly_Meeting July 2021	3	M.Riedel	2021-08-07 17:42
Slides & Materials from meeting 2021-07-22			
2021_07_22_CoE-RAISE-WP2-Monthly-Meeting-Riedel-v1.pdf	8.9 M	M.Riedel	2021-07-23 10:45
2021_07_22_CoE-RAISE-WP2-Monthly-Meeting-Riedel-v1.pptx	8.8 M	M.Riedel	2021-07-23 10:46
2021-07-22-Monthly-Meeting-July-2021-Minutes-v1.docx	44.5 K	seyedreza	2021-08-07 17:42

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




WP2 Updates – Action Item Fact Sheets (refinement started)




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




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



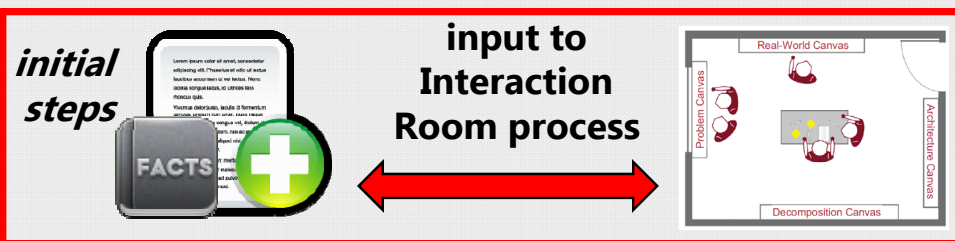
B - Perform Interaction Room Task 4.2 Seismic Imaging
#31 · created just now by Morris Riedel



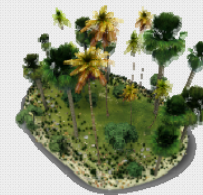
B - Perform Interaction Room Task 3.3 Reacting Flows & Task 3.4 Engine Design
#30 · created 1 minute ago by Morris Riedel



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



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>



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

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)

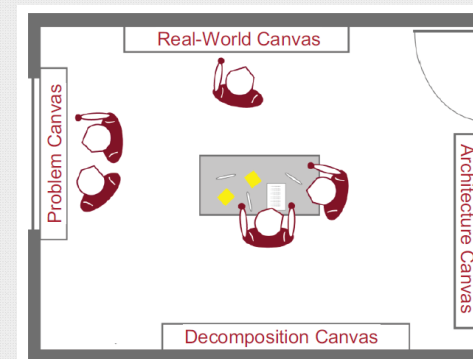
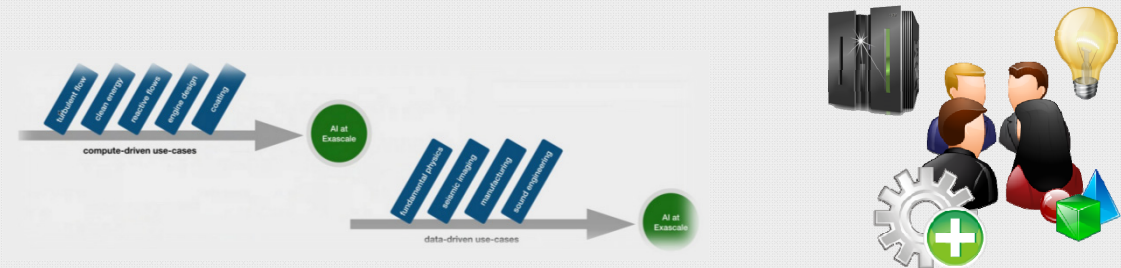


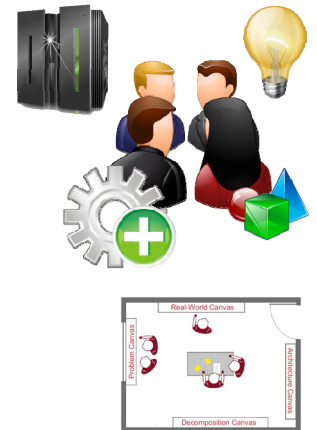
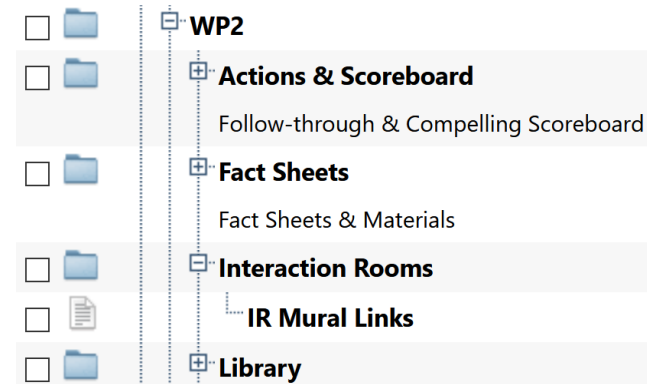
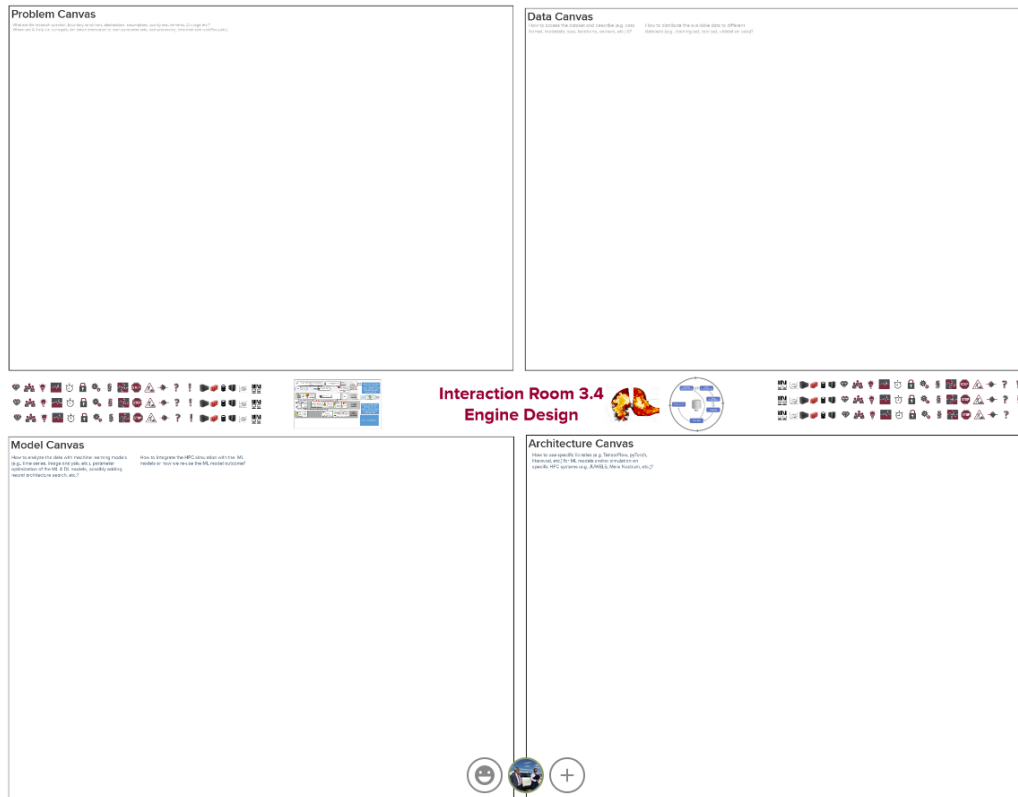
Table 6: Use-case vs. AI-methods matrix.

Use-Case vs. AI-Methods	DA	NAS	AE	TL	PF	PDL	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

➤ Next Steps

- Carve out more details on AI/HPC methods
- Identify concrete detailed algorithms
- Input to Milestone MS2

Interaction Rooms via MURAL Boards & Milestone Inputs

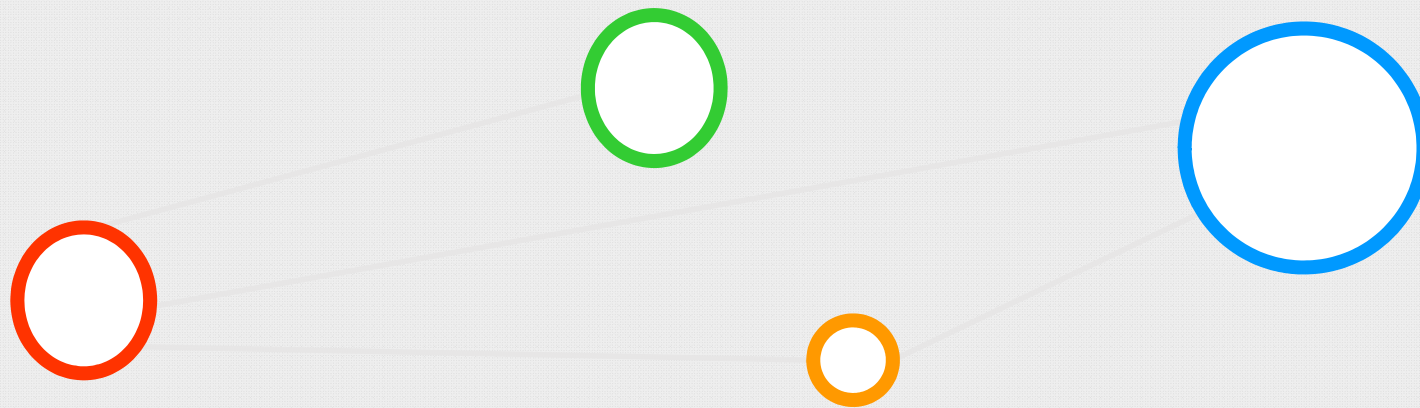


IR Mural Links

- 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/cb44cca3eed3bb9964fbfa36a1f6b1bfce085f?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/matthiasbook8855/1621377991014/7a5d7e1ea230178342d1e1d4a84d656d9055d52?sender=u15c3008bb41d6628a5bb5701>
- IR4.1 Fundamental Physics: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378007335/6f0d5285feaec3eaf515bd6676e84d8b4879d39?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/matthiasbook8855/1621378038069/93df6fa7a41093f4eaae7bc9d72979dc2ba42b9d?sender=u15c3008bb41d6628a5bb5701>
- IR4.4 Sound Engineering: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa12219002404059f90a4bbb0101fa379a8503?sender=u15c3008bb41d6628a5bb5701>

- 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) – Achieved Milestone AI/HPC Methods (M7)



Achieved Milestone MS2 AI/HPC Methods (M7)



Number	Name	Lead Beneficiary	Delivery Date (Annex I)	Achieved	Delivery Date (actual)	Comments
1	Project kick-off	FZJ	31 Jan 2021	<input checked="" type="checkbox"/>	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	<input checked="" type="checkbox"/>	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 followed by the development of the software engineering process
3	Training courses	BSC	30 Apr 2022	<input type="checkbox"/>		
4	Use-cases / technical developments	UOI	31 Dec 2022	<input type="checkbox"/>		
5	Business plan	FLANDERS MAKE	30 Jun 2023	<input type="checkbox"/>		
6	All final reports	FZJ	31 Dec 2023	<input type="checkbox"/>		

➤ 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'

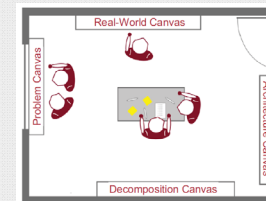
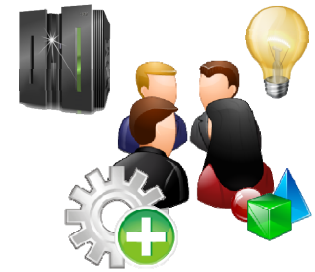
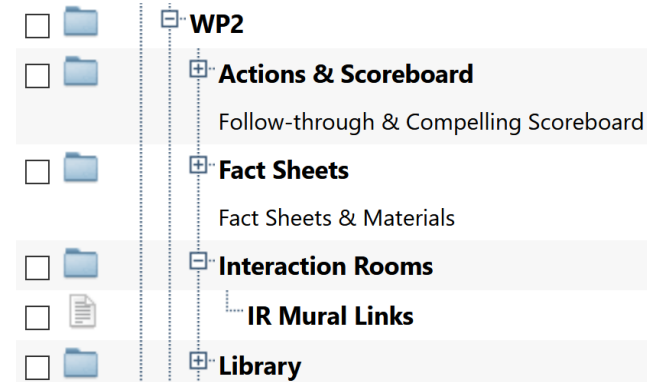
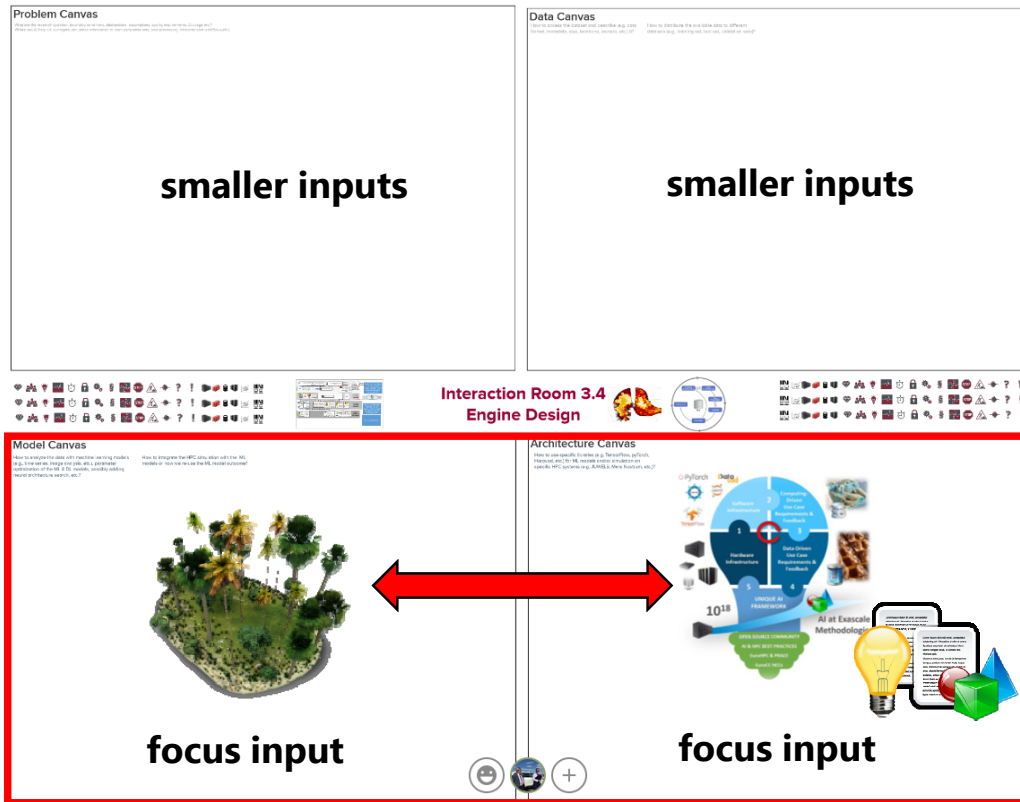


Table 6: Use-case vs. AI-methods matrix.

Use-Case vs. AI-Methods	DA	NAS	AE	TL	PF	PDL	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

Interaction Rooms via MURAL Boards & Milestone / Deliverable



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/matthiasbook8855/1621377991014/7a5d7e1ea230178342d1e1d4a84d656d9055d52?sender=u15c3008bb41d6628a5bb5701>
- IR4.1 Fundamental Physics: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378007335/6f0d5285f6aec3eaf515bd6676e84d8b4879d39?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>

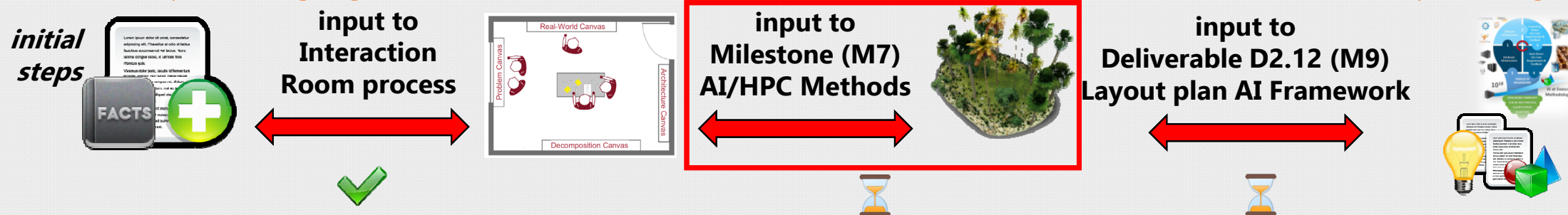
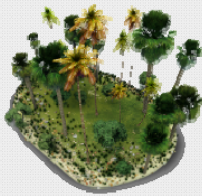
➤ <https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3591551>



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
- Snapshot at end of August for archiving via official Word document as official MS2 document
- Location (shared for everyone to edit):
https://docs.google.com/document/d/1Az88KP9Z4USFA5hPMnqRhCE_8l9IzxnvsYlhE2UXzc/edit?usp=sharing



Google Doc Milestone AI/HPC Methods (M7) – Current Draft



UPDATED

BEFORE

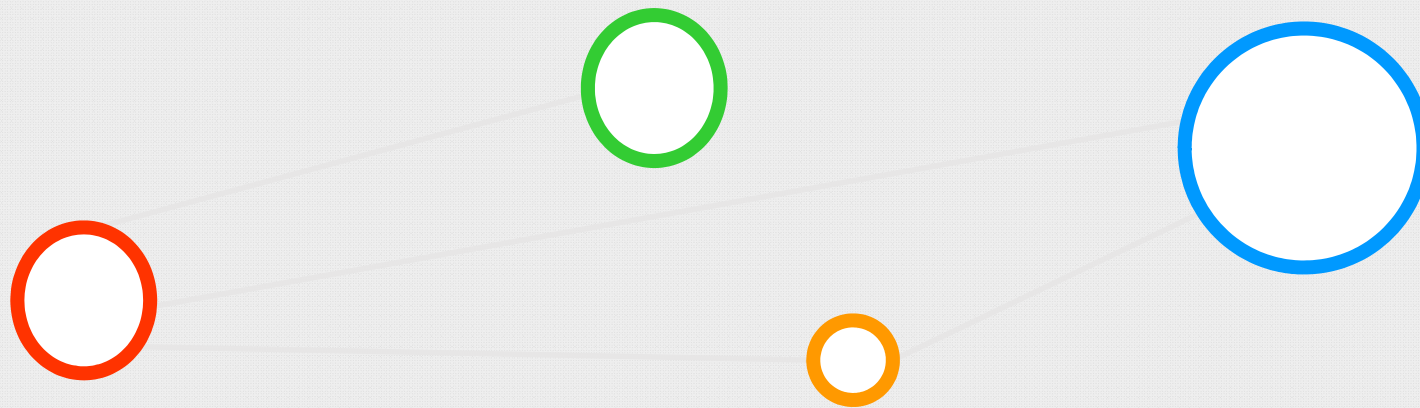
Table 6: Use-case vs. AI-methods matrix.

Use-Case vs. AI-Methods	DA	NAS	AE	TL	PF	PDDL	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

Use Case	AE	PIML	ANNs	CNN		NO	SMs			GNN	IN
<i>Details</i>	<i>CAE</i>		<i>RBF-ANN</i>	<i>U-Net</i>	<i>RESNET</i>	<i>FNO</i>	<i>AR</i>	<i>ARMA</i>	<i>ARIMA</i>	<i>MLPF</i>	<i>JED-net</i>
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							
Smart models for next generation aircraft				X							





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



Plans Deliverable D2.12 (M9)

➤ Next steps in looking at software frameworks

- Keep up the good work!
- Initial approaches of many AI/HPC methods are clear, to be revised during the project
- Report shows good project activity (monthly seminars, interaction rooms, individual meetings, etc.)
- All deliverables submitted in time
- **Next deliverable work started already with Interaction Rooms & Canvas content**




CoE RAISE Quarterly Work Package Activity Report

Work Package: AI- and HPC-Cross Methods at Exascale (WP2)
Reporting Period: 04/2021- 06/2021
Author: Prof. Dr. – Ing. Morris Riedel

1. Work package summary

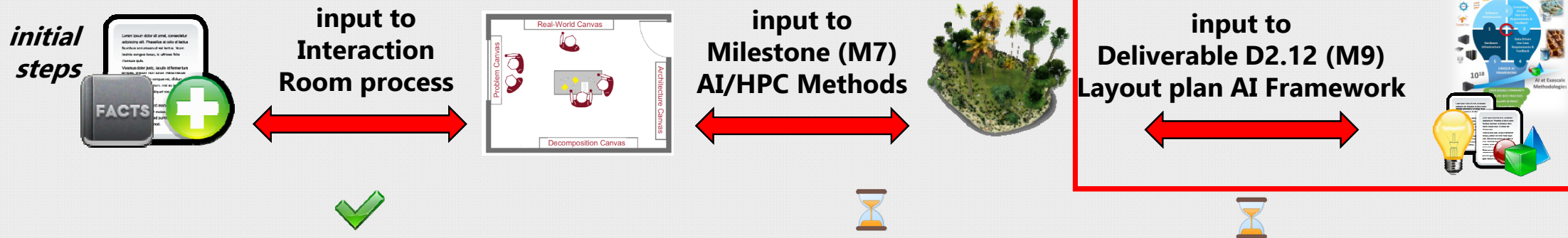
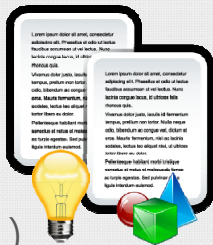
List all deliverables of this WP in the following table:

Del. No.	Deliverable Name	Lead Participant	Due Date	Status *
D2.1	Best practice guidelines/tutorials for MSA/heterogenous systems	BSC	28.02.2021	Submitted to EU
D2.5	Best practice guidelines/tutorials prototype	FZJ	28.02.2021	Submitted to EU
D2.6	Support report	FZJ	30.06.2021	Submitted to EU
D2.12	Software layout plan for a unique AI framework	UOI	30.09.2021	not started yet



Plans Deliverable D2.12 Framework (M9)

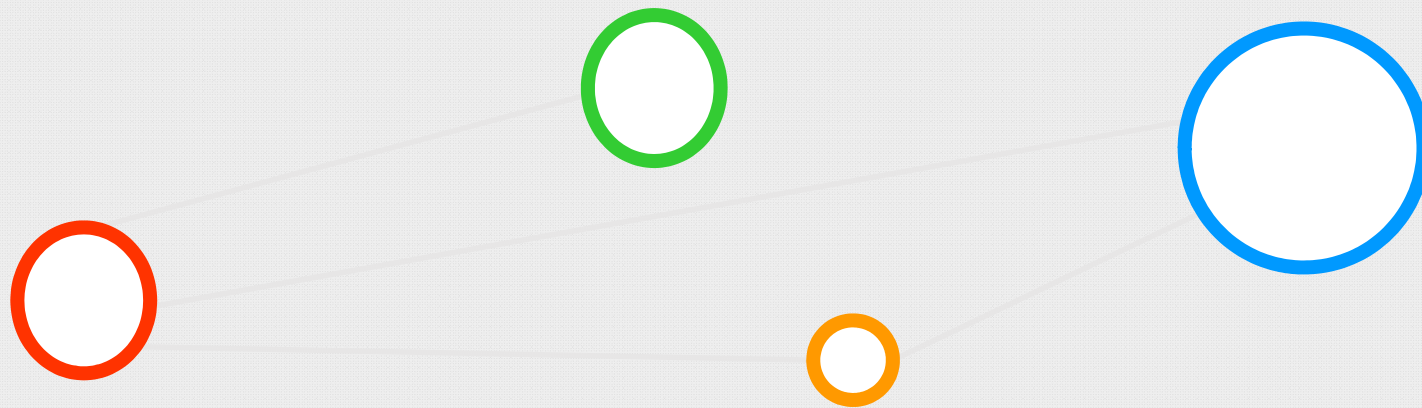
- Deliverable D2.12 - Software layout plan for a unique AI framework
 - Initial ideas around a comprehensive set of tools, also consider OpenML.org work
 - Challenge: massive toolsets available (e.g., distributed training tools via GPUs are ~10, etc.)
 - No need to re-invent the wheel, consider ONNX 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)



Plans Deliverable D2.12 Framework (Mg) – Discussions Telco

1. TBD(Morris, Gael): Discuss architecture approach and consider Atos AI4Sim library experience & license aspects
2. Software layout top-down and discussions with AI4Sim library setup example
3. Similiar goals with similiar models, decisions and guidelines for use cases, architectures
4. Choosing metrics: scalability proven, GPU types, etc?
5. One version of AI4SIM library as open source and fork with new developments and share
6. Knowledge around common themes, sequence vs. non sequence models, Unets, etc.
7. Data-driven → organize the models around data aspects (e.g., time, data elements, etc.)
 1. Challenge maybe, as use cases are quite heterogenous
8. General recommendations of the framework / reference models
 1. Business experience and academic studies (batch sizes, what framework scales, jupyter notebooks, etc.)
 2. How to structure the library, including benchmark data, initial scripts, e.g. U-Nets, etc.
9. Still a plan status

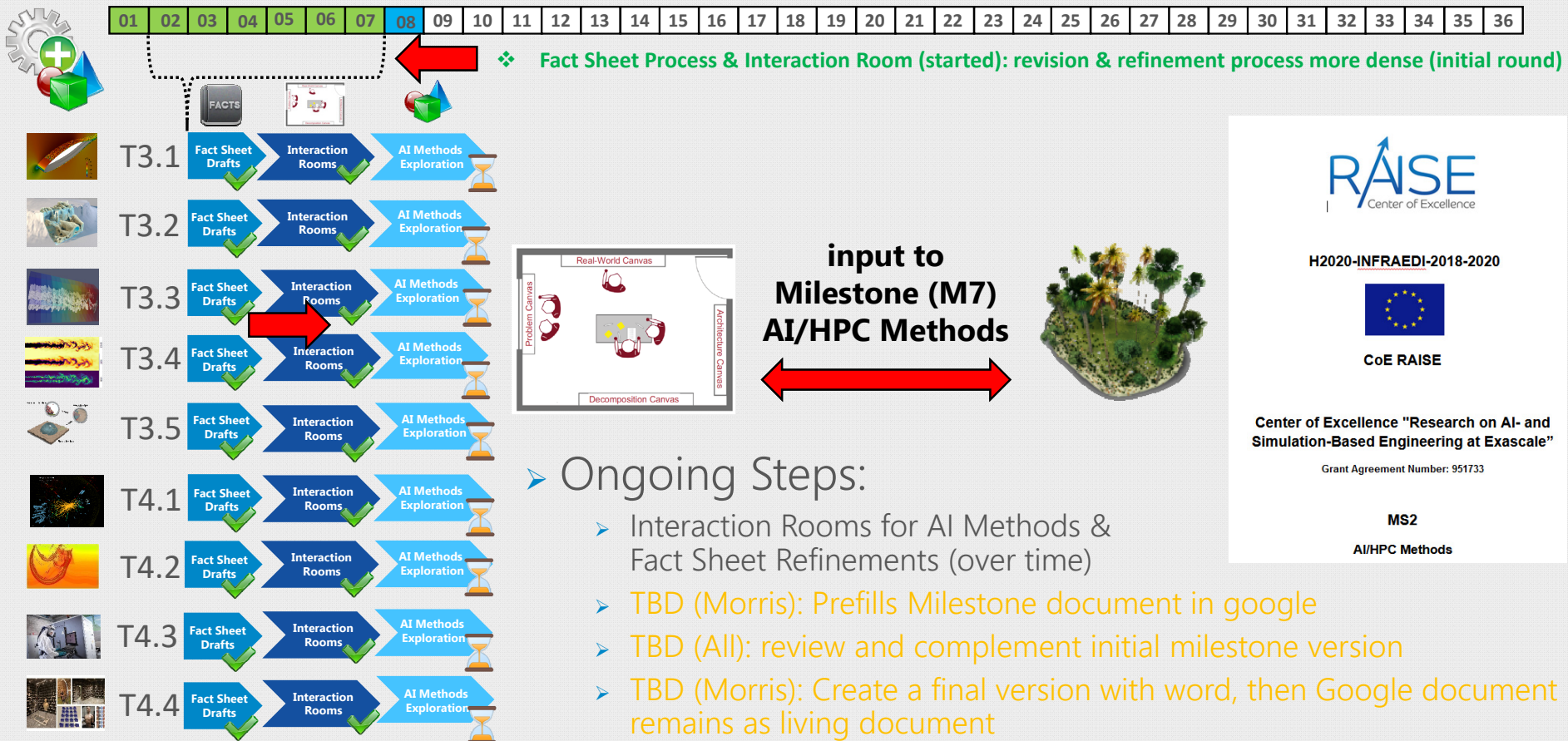
Agenda Item (5) – Compelling Scoreboard Review & Next Steps



Compelling Scoreboard Review – Use Case Progress



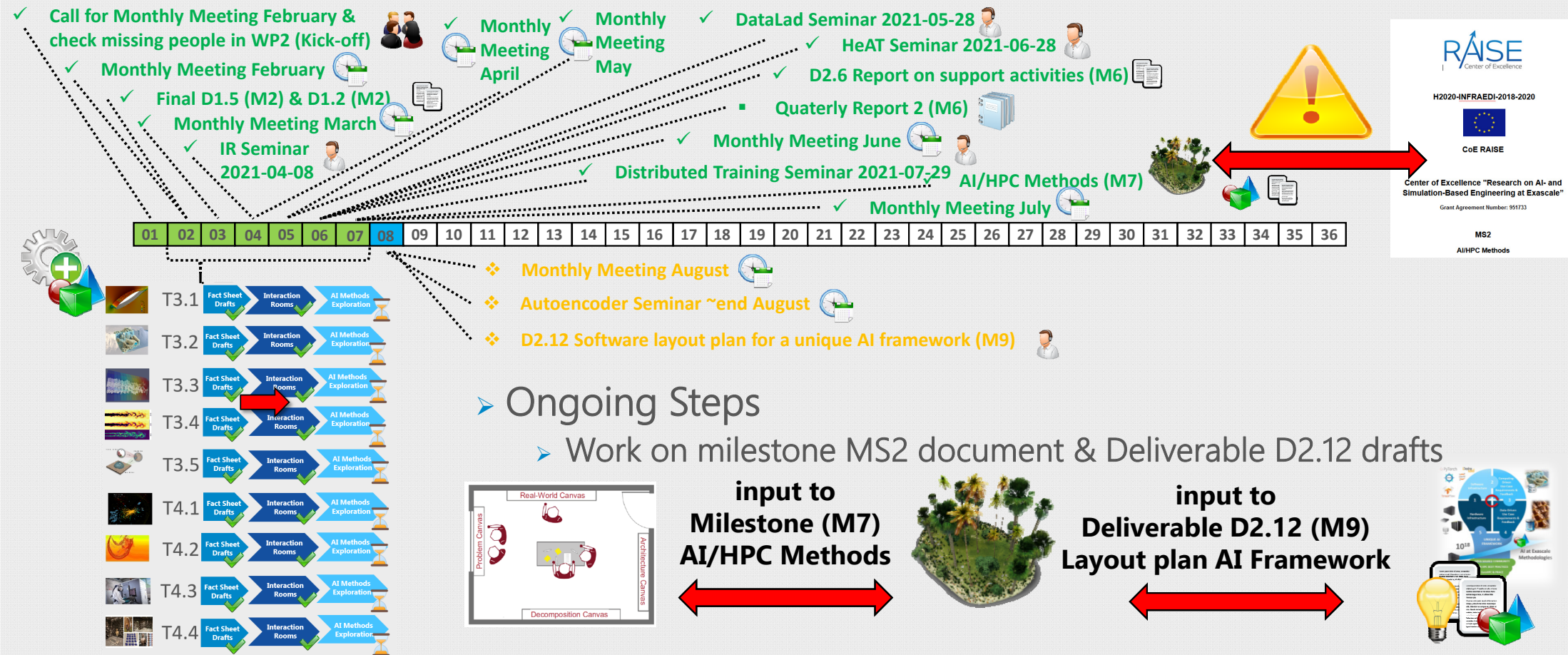
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Compelling Scoreboard Review & Next Steps



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Agenda Item (5) – 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 & Interoperable 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 milestone 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: EPI / EUPEX
 1. Links to RAISE, etc.
 2. PMO/Atos?
 3. Links to Estela (FZJ), sharing EPI information not so easy, hardware access directly not possible, but follow-up good



AOB: Data Transfer & Networking

1. AOB: FZJ – RTU Data transfers
 1. Testing is ongoing
 2. National educational networks
 3. Tests for large data transfers
 4. UFTP service is evaluated
 5. In context with specialists (Olaf Mextorf FZJ, etc.)
2. AOB: CERN – BSC Connection Tests
 1. Any updates on this?
3. AOB: Data Project Proposal
 1. 200 TB to be used available at FZJ now if needed



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