

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

Prof. Dr. – Ing. Morris Riedel et al.

School of Engineering & Natural Sciences, University of Iceland
2021-11-26, RAISE WP2 Monthly Meeting November 2021, Online



@ProfDrMorrisRiedel



@Morris Riedel



@MorrisRiedel



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



morris@hi.is

WP2 November Meeting – Welcome & Agenda

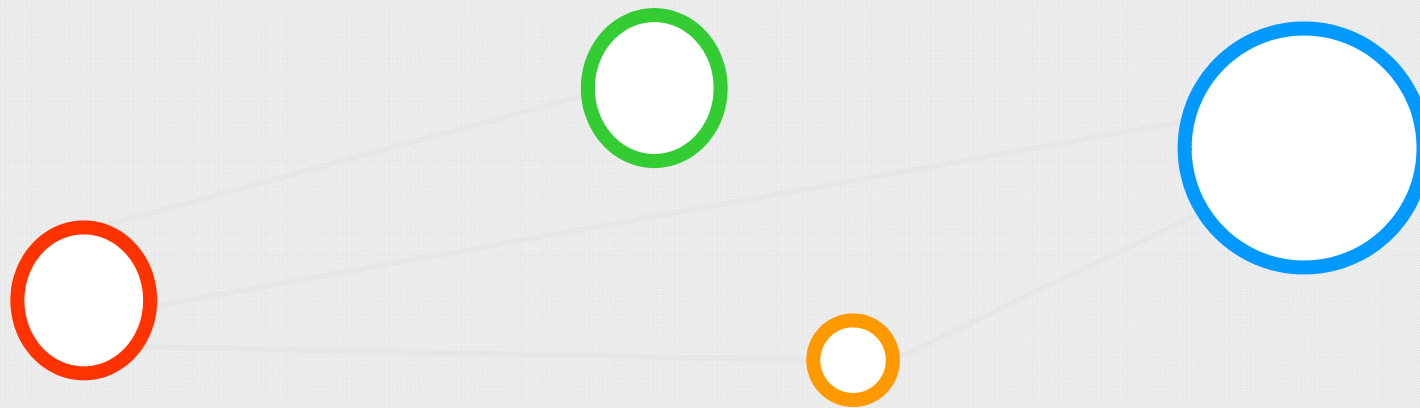


RAISE
Center of Excellence

1. Approval of minutes from Monthly Meeting October 2021
 - (All), ~5 Min
2. Review WP2 Status on Interaction Rooms
 - (Morris Riedel, Matthias Book, Helmut Neukirchen), ~5 Min
3. Status D2.2 (M12)
 - (Guillaume, Guillermo, Cristóbal), ~10 Min
4. Status D2.14 (M12)
 - (Morris et al.), ~20 Min
5. AHM Meeting Action Items Debrief
 - (Morris & Andi), ~5 Min
6. Network Testing RAISE Partners
 - (Lauris), ~5 Min
7. Hands-on Workshop on GPUs & CUDA
 - (Lauris), ~5 Min
8. Compelling Scoreboard Review & Next Steps
 - (All), ~5 Min



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



Minutes Approval – Monthly Meeting October 2021

➤ Minutes available in BSCW

- <https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3704758>
- TBD(all): Any objections or additions/changes?
- TBD(Guillaume, Guillermo, Cristóbal): Upload presentation



Morris Riedel - RAISE WP2 - Issues		
Open	Closed	All
Recent searches - Search or filter results...		
Due date - All		
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 4.3 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

2021_05_28_Monthly_Meeting May 2021

Slides & Materials from meeting 2021-05-28

2021_06_29_Monthly_Meeting June 2021

Slides & Materials from meeting 2021-06-29

2021_07_22_Monthly_Meeting July 2021

Slides & Materials from meeting 2021-07-22

2021_08_30_Monthly_Meeting August 2021

Slides & Materials from meeting 2021-08-30

2021_09_30_Monthly Meeting September 2021

Slides & Materials from Meeting 2021-09-30

2021_10_29_Monthly_Meeting October 2021

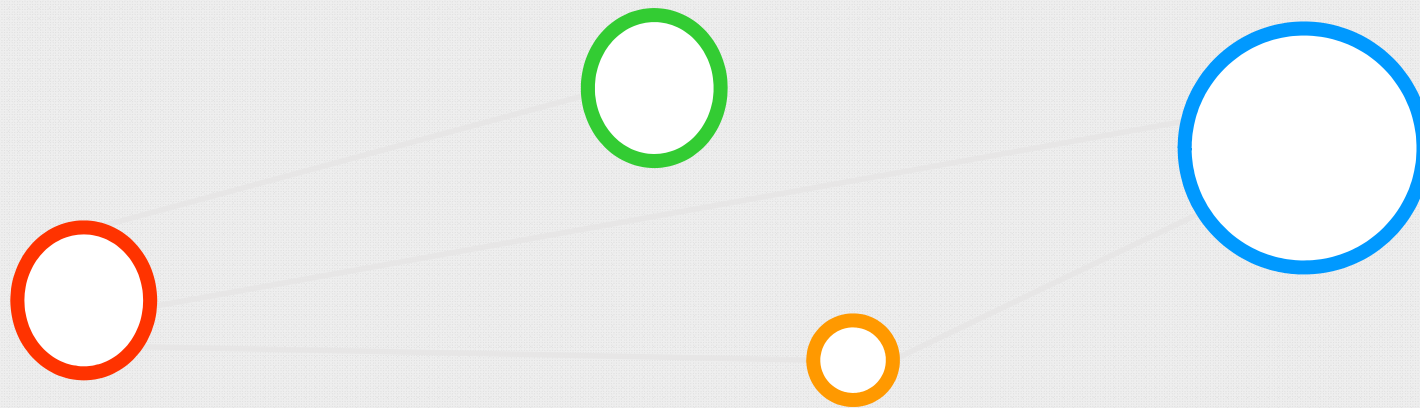
Slides & Materials from Meeting 2021-10-29

2021_10_29_CoE-RAISE-WP2-Monthly-Meeting-Riedel-v1.pptx

2021-10-29-Monthly-Meeting-October-2021-Minutes-v1



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



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)

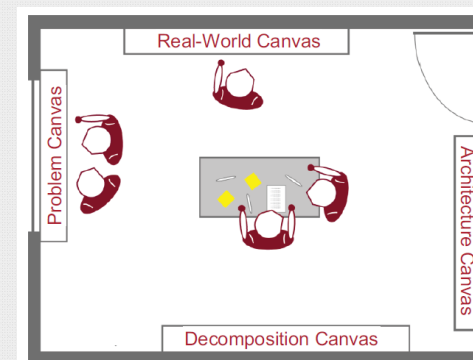
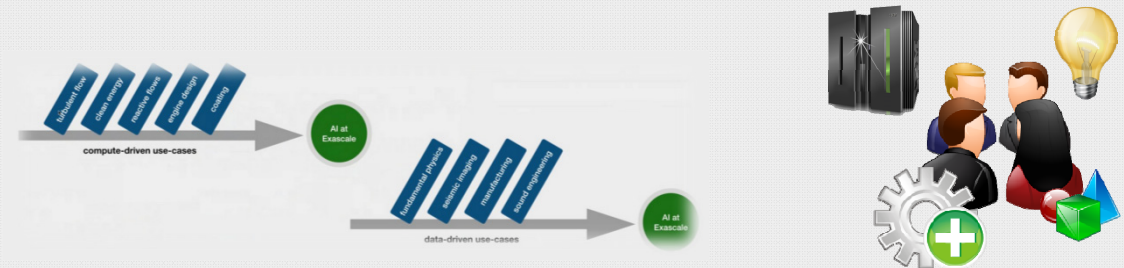


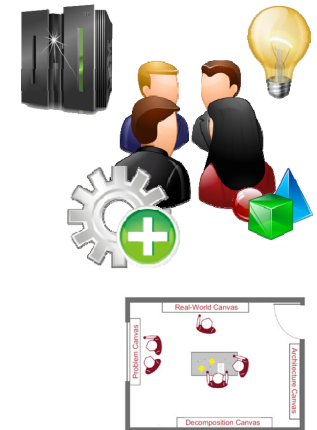
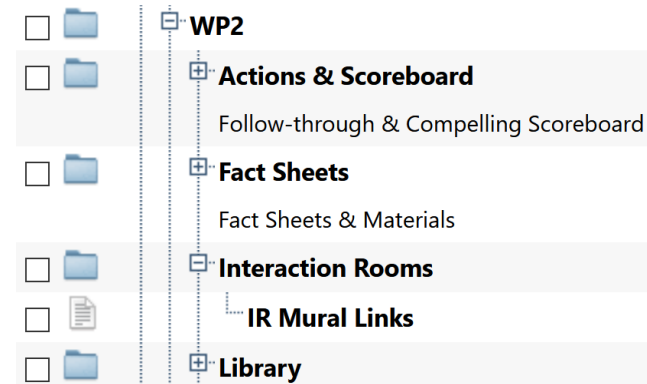
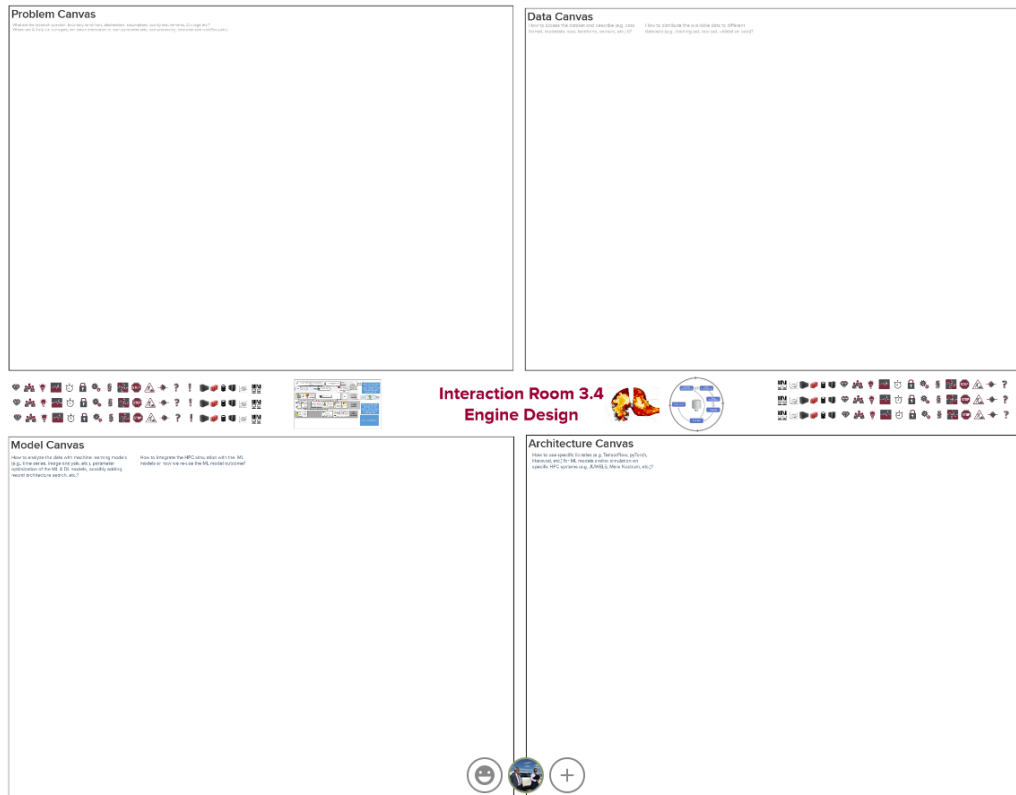
Table 6: Use-case vs. AI-methods matrix.

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

➤ 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

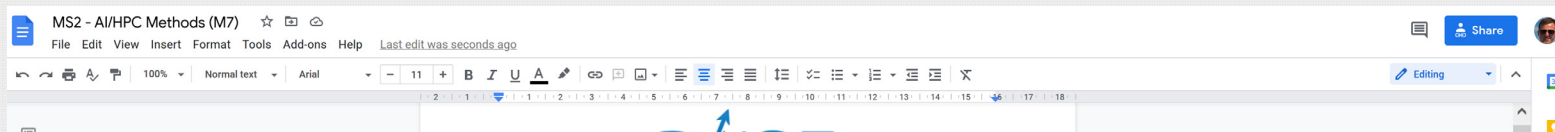


IR Mural Links

- IR3.1 Turbulent Flow: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377866397/8613c384d54f66fb5e78599ff307a4ce8a9090c0?sender=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/matthiasbook8855/1621377991014/7a5d7e1ea230178342d1e1d4a84d656d9055d52?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>

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



Continuously Updating



BEFORE

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

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

Draft



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



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

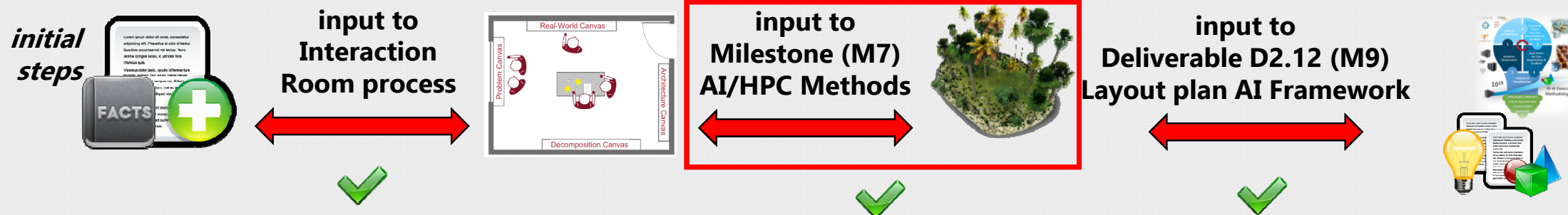
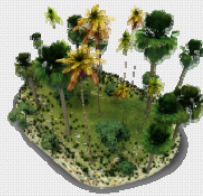
- Google Document to keep it as a living document with important updates from Mural over time



- TBD: Snapshot at end of August for archiving via Word document as MS2 document (optional)

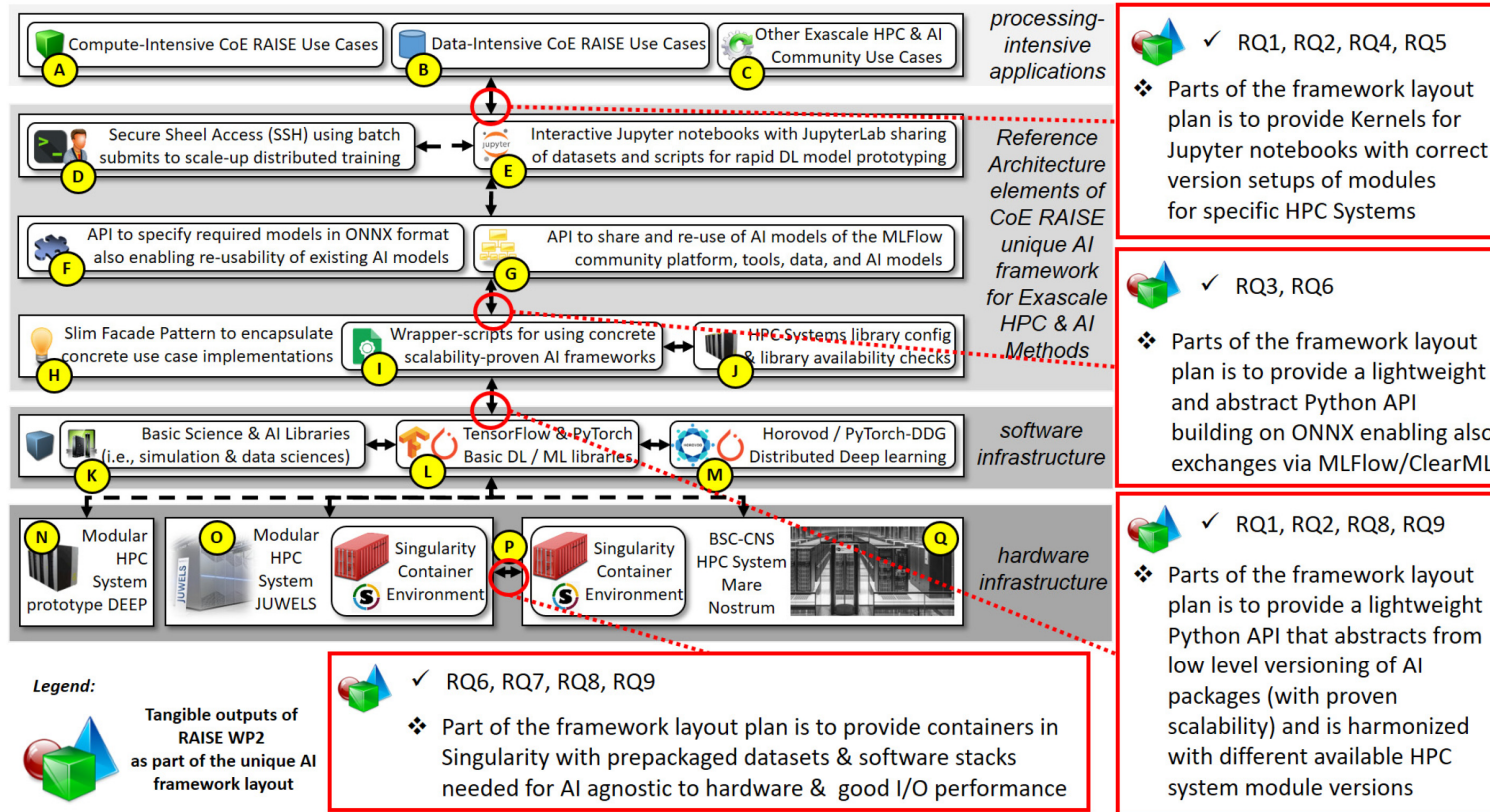
- Location (shared for everyone to edit):

https://docs.google.com/document/d/1Az88KP9Z4USFA5hPMnqRhCE_8I9IzxnvsYlhE2UXzc/edit?usp=sharing



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

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



Continuously 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](https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/d3287337/CoE%20RAISE%20Deliverables%20Status.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.



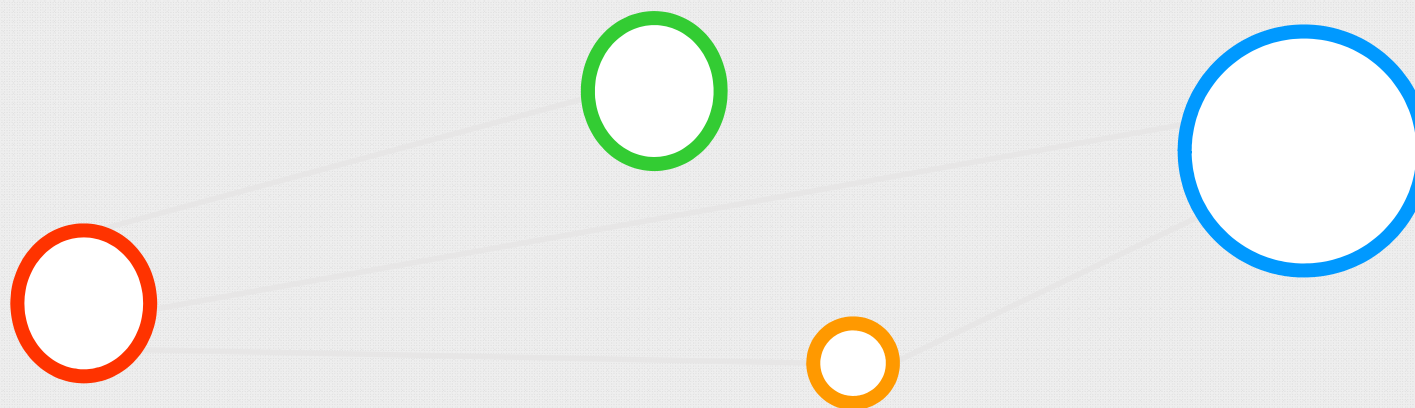
Changed Time Schedule for M12/December Deliverables (2)

- 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 (3) – Status D2.2 (M12)

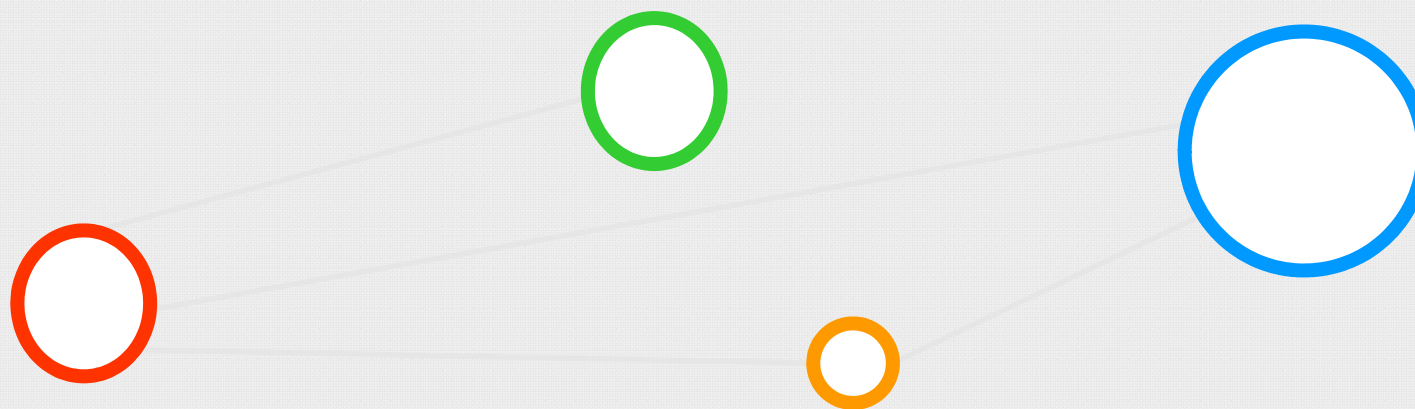


Agenda Item (3) – Status D2.2 (M12)

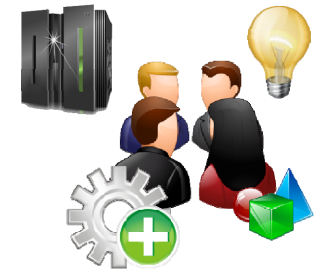
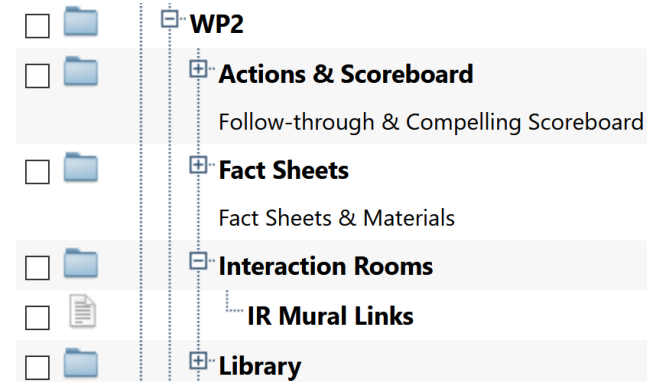
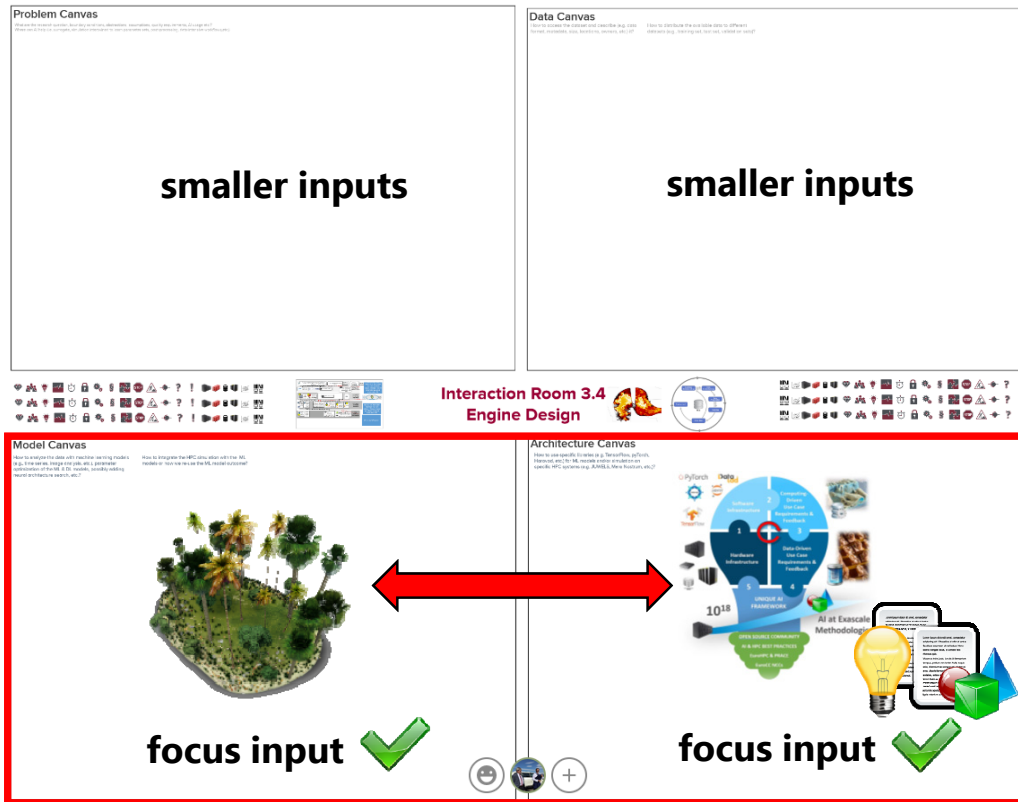
- (Guillaume, Guillermo, Cristóbal), ~5 Min



Agenda Item (4) – Status D2.14 (M12)



Interaction Rooms via MURAL Boards & Refinements for D2.14



IR Mural Links

- IR3.1 Turbulent Flow: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377866397/8613c384d54f66fb5e78599ff307a4ce8a9090c0?sender=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/matthiasbook8855/16213779590220c363886f24833eeb19b025d87324b57fd50e2db?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/matthiasbook8855/1621378007335/6f0d5285feaec3eaf515bd6676e84d8b4879d39?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>



D2.14 – Agreement with WP3/WP4

➤ WP leaders meeting WP2/WP3/WP4

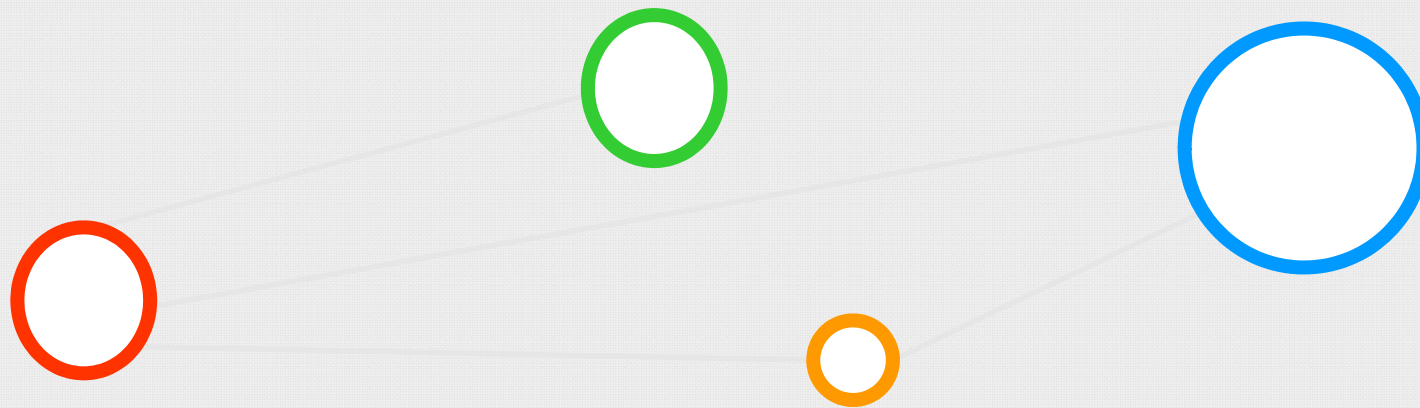
- Use Case authors (from WP3/WP4 and partly WP2) focus on WP3/WP4 deliverables first
- WP2 content on will be partly taken out/copied from WP3/WP4 deliverables (not as planned by WP2, but agreement)
- WP2 deliverable will be later ready then WP3/WP4 (we started, also vacation Morris, Kurt, and others)

➤ Status

- UOI started call for comments (some inputs)
- FZJ already provided excellent content input
- RTU & UOI does as much as we can to push for internal review
- Google Doc: https://docs.google.com/document/d/1JH_q6PLhTWZznKby6VULf6Nc0ozmVxui/edit



Agenda Item (5) –AHM Meeting Action Items Debrief

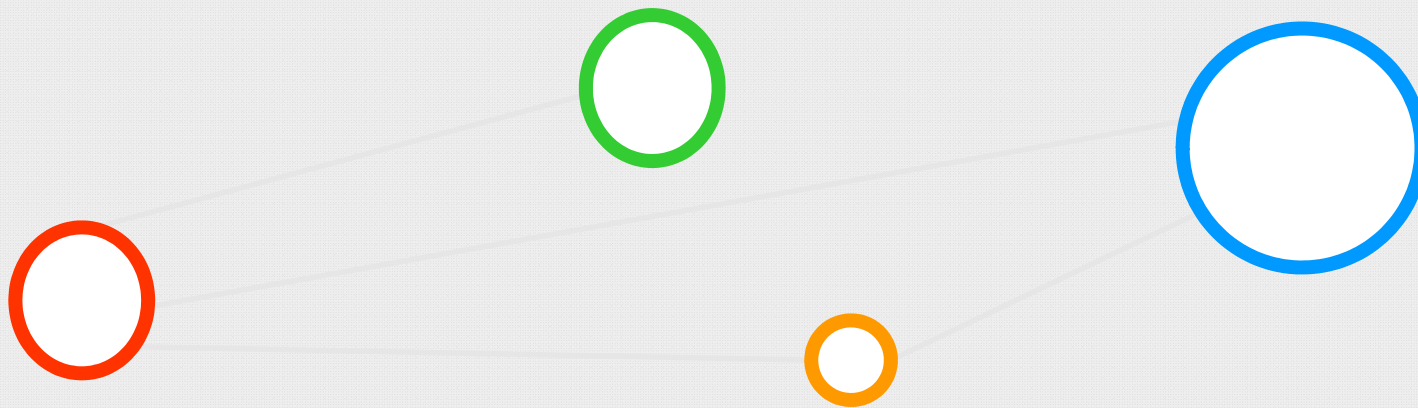


Agenda Item (5) –AHM Meeting Action Items Debrief

- Presentations from WP2
 - Generally ok
 - Not much feedback from participants about Framework AI (Task 2.4) or Methods Matrix (Task 2.5)
- Action Items
 - TBD(Morris): Contact advisory board members for topics on WP2 Seminars
 - TBD(Morris): Planing in advance seminars so that they can be better advertised on social media (WP6)
 - TBD(Morris): WP6 News Item of WP2: AI framework & updated AI Matrix
 - TBD(All): More interactions with WP3/WP4 to encourage exchange/identification of AI methods and transfer to other problems, across WPs → TCB



Agenda Item (6) – Network Testing RAISE Partners

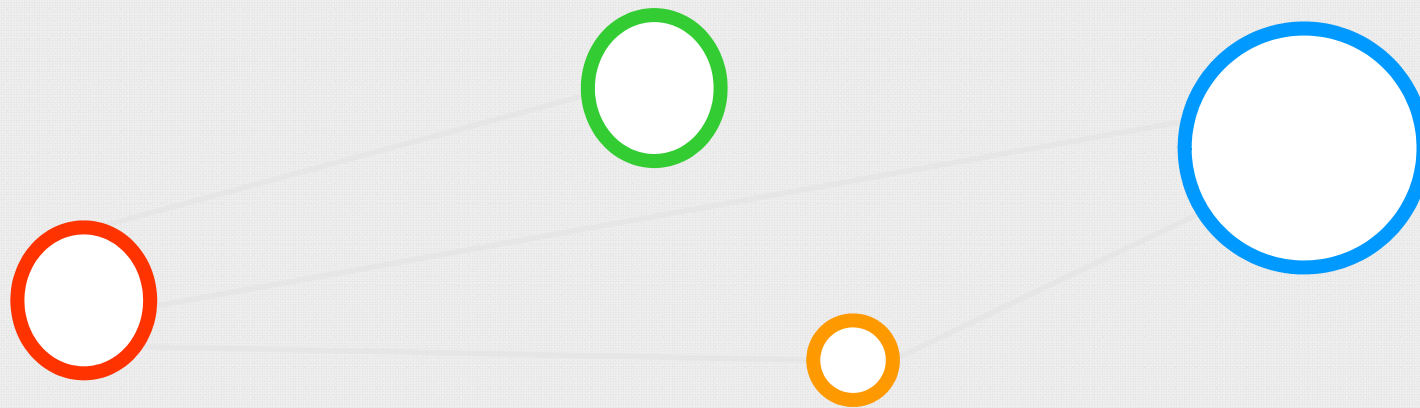


Agenda Item (6) – Network Testing RAISE Partners

➤ (Lauris), ~5 Min

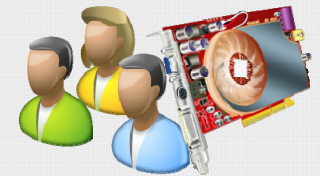


Agenda Item (7) – Hands-on Workshop on GPUs & CUDA



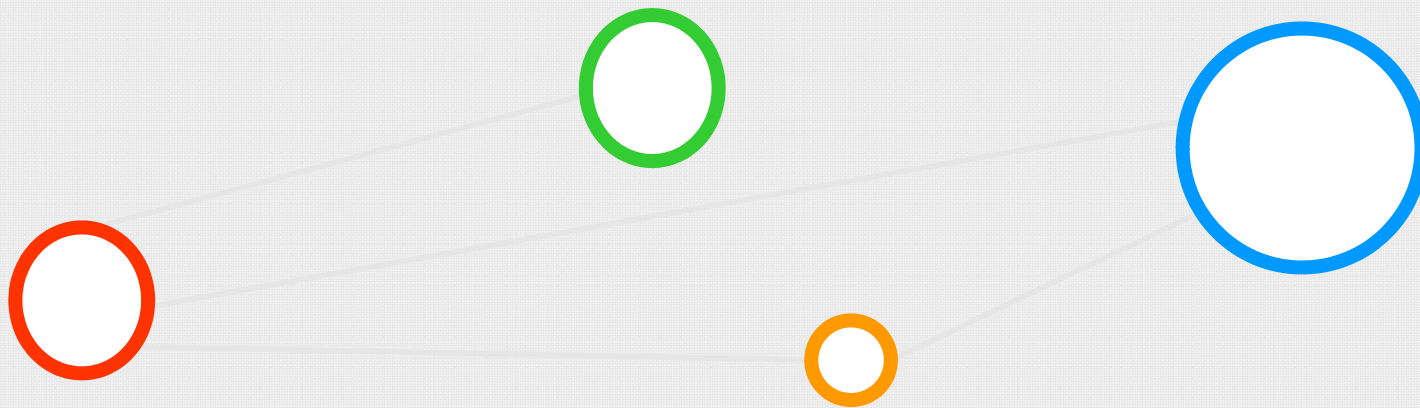
Agenda Item (7) – Hands-on Workshop on GPUs & CUDA

- (Lauris), ~5 Min
- TBD(Lauris et al.): Exact Date and Time of Seminar, Training or WP2 Seminar?
- TBD(Arnis): Organize Event, practical tasks, low-level neural networks, cp. pyTorch, maybe mid-January → WP2 mailing list, early WP6 announcements
- Training from RAISE, maybe first internal, then external?
- 2 days workshop (4 hours per day)
- WP6 educational group?
- WP2: Who is delivering what training when (milestone)?



➤

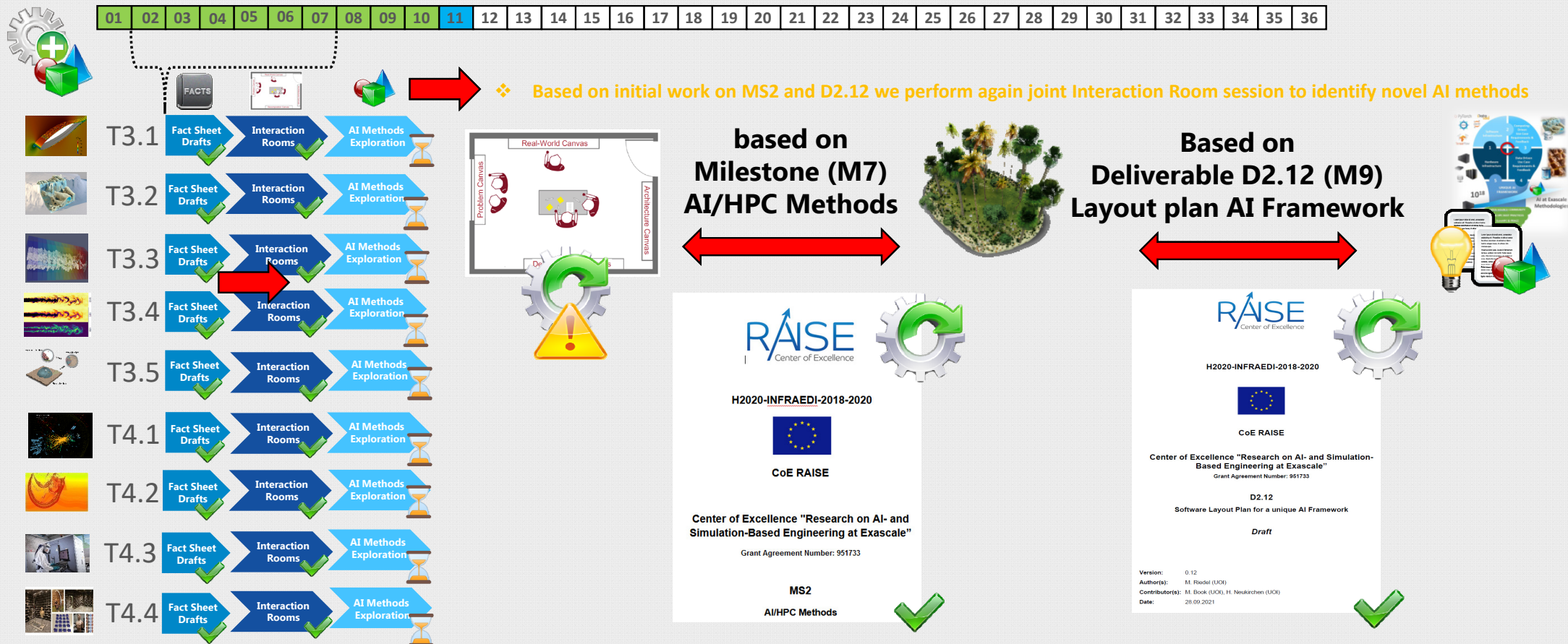
Agenda Item (8) – Compelling Scoreboard Review & Next Steps



Compelling Scoreboard Review – Use Case Progress



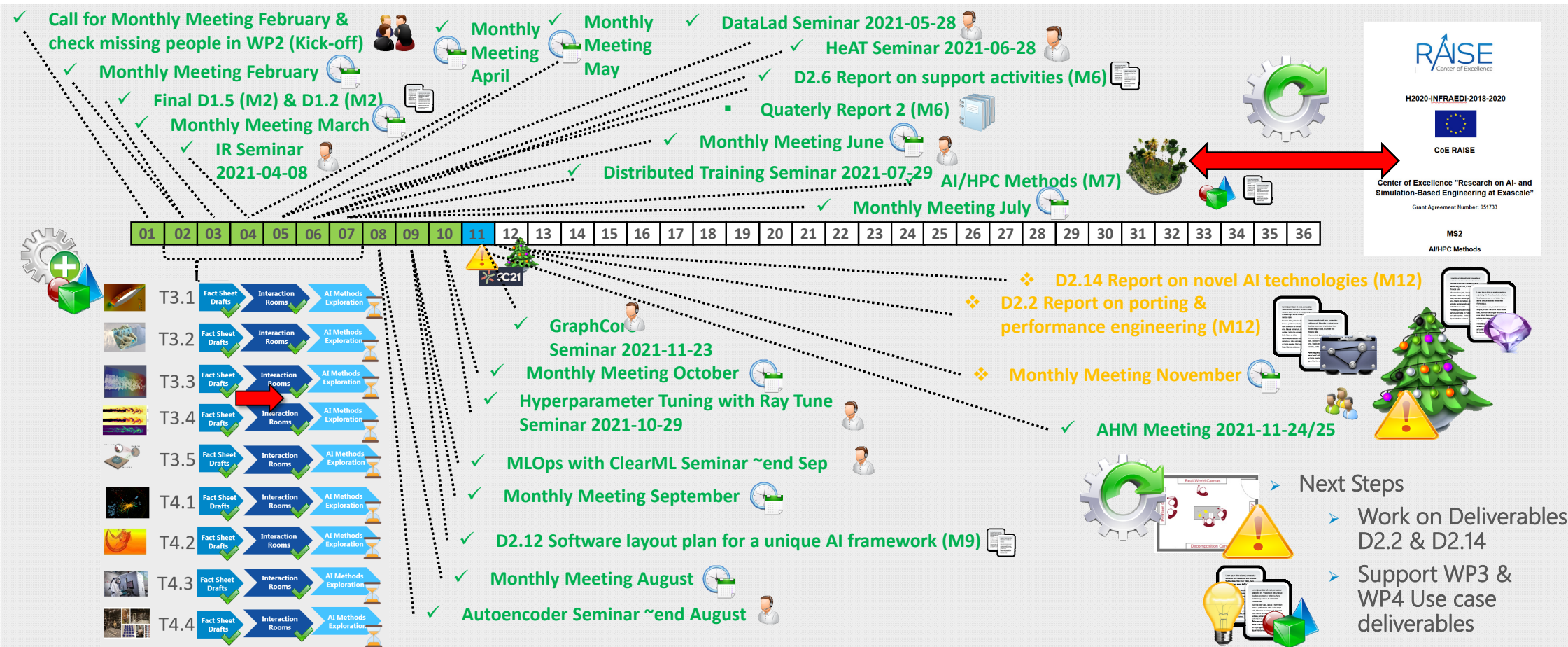
RAISE
Center of Excellence



Compelling Scoreboard Review & Next Steps



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Agenda Item (8) – Next Steps & Follow-Through

1. 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
2. AOB: ADMIRE adopted the Fact sheet and Interaction Room process
 1. Success on the web page, more visible?



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