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

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School of Engineering & Natural Sciences, University of Iceland

2021-10-29, RAISE WP2 Monthly Meeting October 2021, Online

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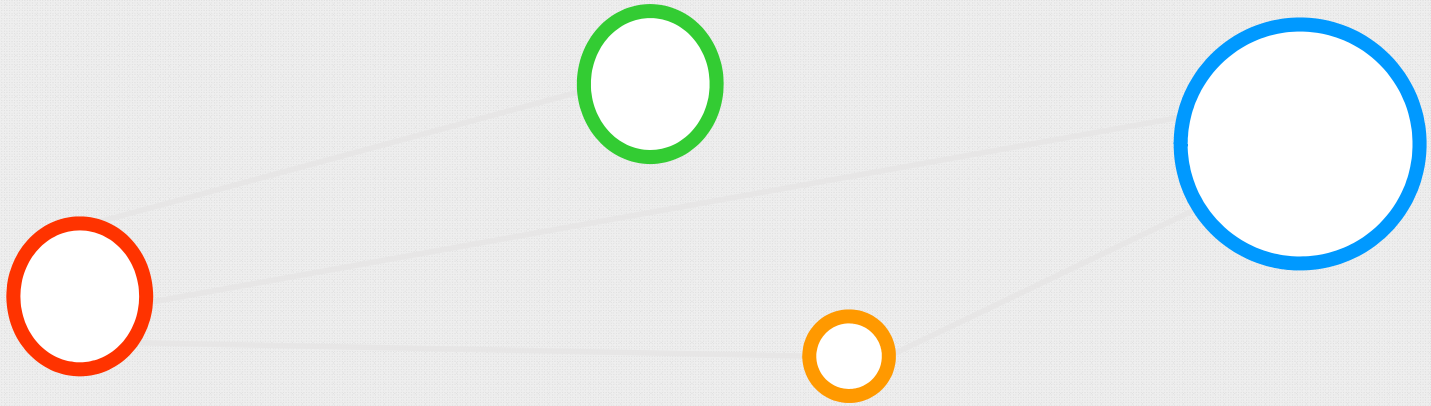
https://www.youtube.com/channel/UCWC4VKHmL4NZgFfKoHtANKg morris@hi.is

WP2 October Meeting – Welcome & Agenda

RAISE Center of Excellence

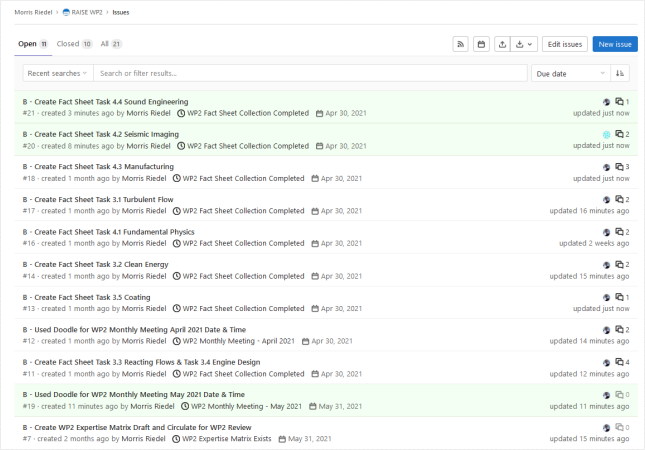
1. Approval of minutes from Monthly Meeting September 2021
   - (All), ~5 Min
2. Review WP2 Status on Interaction Rooms
   - (Morris Riedel, Matthias Book, Helmut Neukirchen), ~5 Min
3. Status D2.2 (M12)
   - (Guillaume, Guillermo, Cristóbal), ~10 Min
4. Status D2.14 (M12)
   - (Morris et al.), ~10 Min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

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



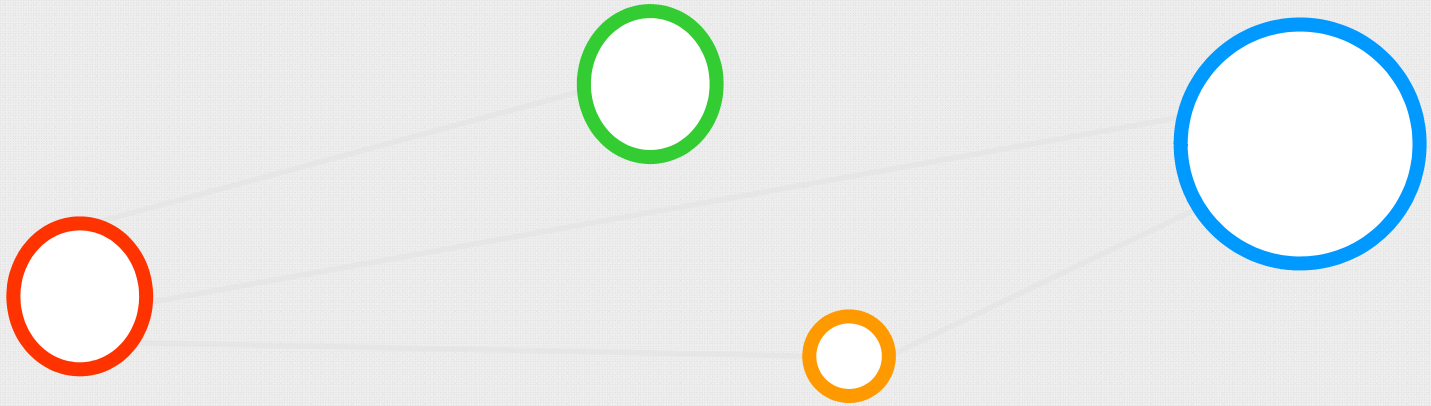
Minutes Approval – Monthly Meeting September 2021

- 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



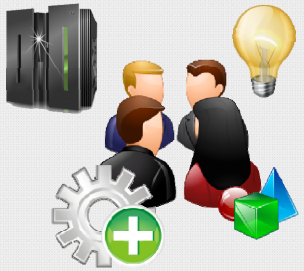
- **2021_07_22_Monthly_Meeting July 2021**
  - Slides & Materials from meeting 2021-07-22
    - **2021_07_22_CoE-RAISE-WP2-Monthly-Meeting-Riedel-v1.pdf**
    - **2021_07_22_CoE-RAISE-WP2-Monthly-Meeting-Riedel-v1.pptx**
    - **2021-07-22-Monthly-Meeting-July-2021-Minutes-v1.docx**
- **2021_08_30_Monthly_Meeting August 2021**
  - Slides & Materials from meeting 2021-08-30
    - **2021_08_30_CoE-RAISE-WP2-Monthly-Meeting-Riedel-v1.pdf**
    - **2021_08_30_CoE-RAISE-WP2-Monthly-Meeting-Riedel-v1.pptx**
    - **2021-08-30-Monthly-Meeting-August-2021-Minutes-v1.docx**
    - 2021-08-30-Monthly-Meeting-August-2021-Minutes-v1
- **2021_09_30_Monthly Meeting September 2021**
  - Slides & Materials from Meeting 2021-09-30
    - **2021_09_30_CoE-RAISE-WP2-Monthly-Meeting-Riedel-v1.pptx**
    - **2021-09-30-Monthly-Meeting-September-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)



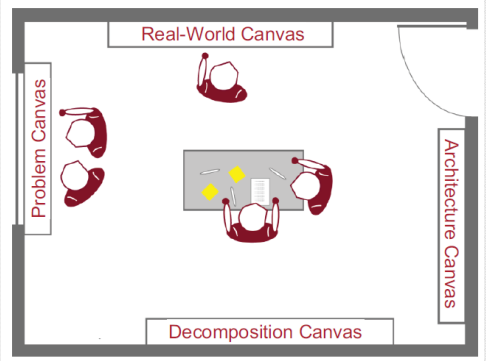
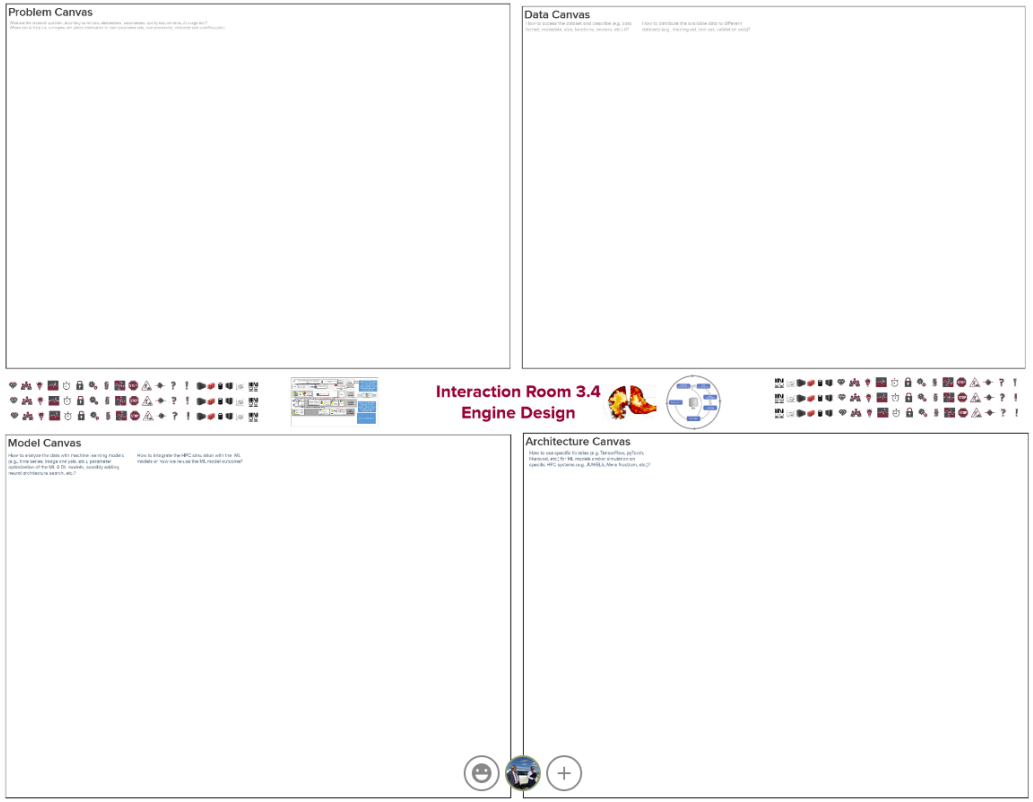


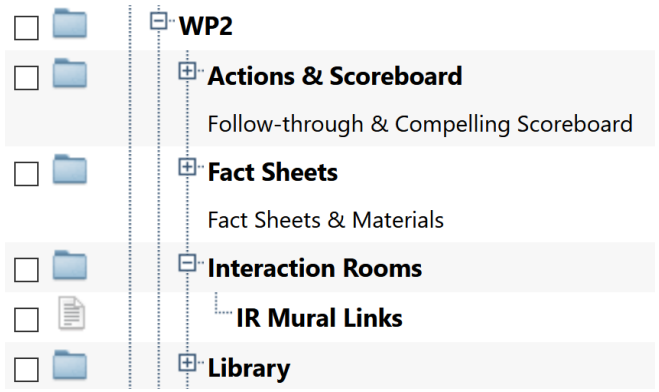
Table 6: Use-case vs. AI-methods matrix.

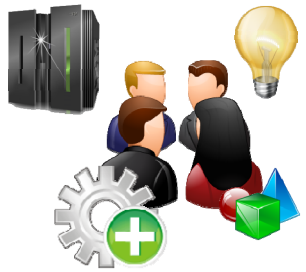
Use-Case vs. AI-Methods	DA	NAS	AE	TL	PF	PIDL	LSTM
Turbulent boundary layers	x	x	x	x	x	x	
Wind farm layout optimization	x			x		x	
AI for data-driven models in reacting flows				x		x	
Smart models for next-generation aircraft engine design	x	x		x		x	
Wetting hydrodynamics		x	x			x	x
Event reconstruction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

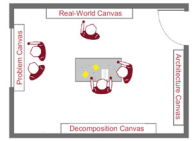
- Continuing Steps
  - Carve out more details on AI/HPC methods
  - Identify concrete detailed algorithms
  - Evaluate and benchmark scalability of methods

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

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

MS2 - AI/HPC Methods (M7)

File Edit View Insert Format Tools Add-ons Help Last edit was seconds ago

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Editing

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

Draft

Continously Updating

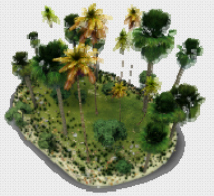
BEFORE

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

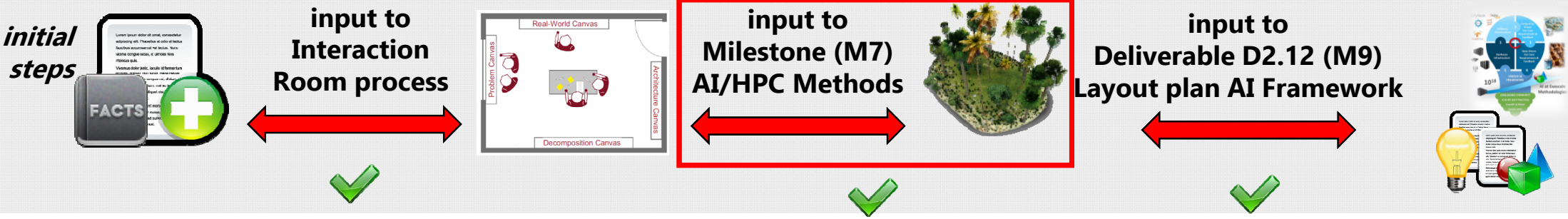
Use-Case vs. AI-Methods	DA	NAS	AE	TL	PF	PIDL	LSTM
Turbulent boundary layers	X	X	X	X	X	X	
Wind farm layout optimization	X			X		X	
AI for data-driven models in reacting flows				X		X	
Smart models for next-generation aircraft engine design	X	X		X		X	
Wetting hydrodynamics		X	X			X	X
Event reconstruction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

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)

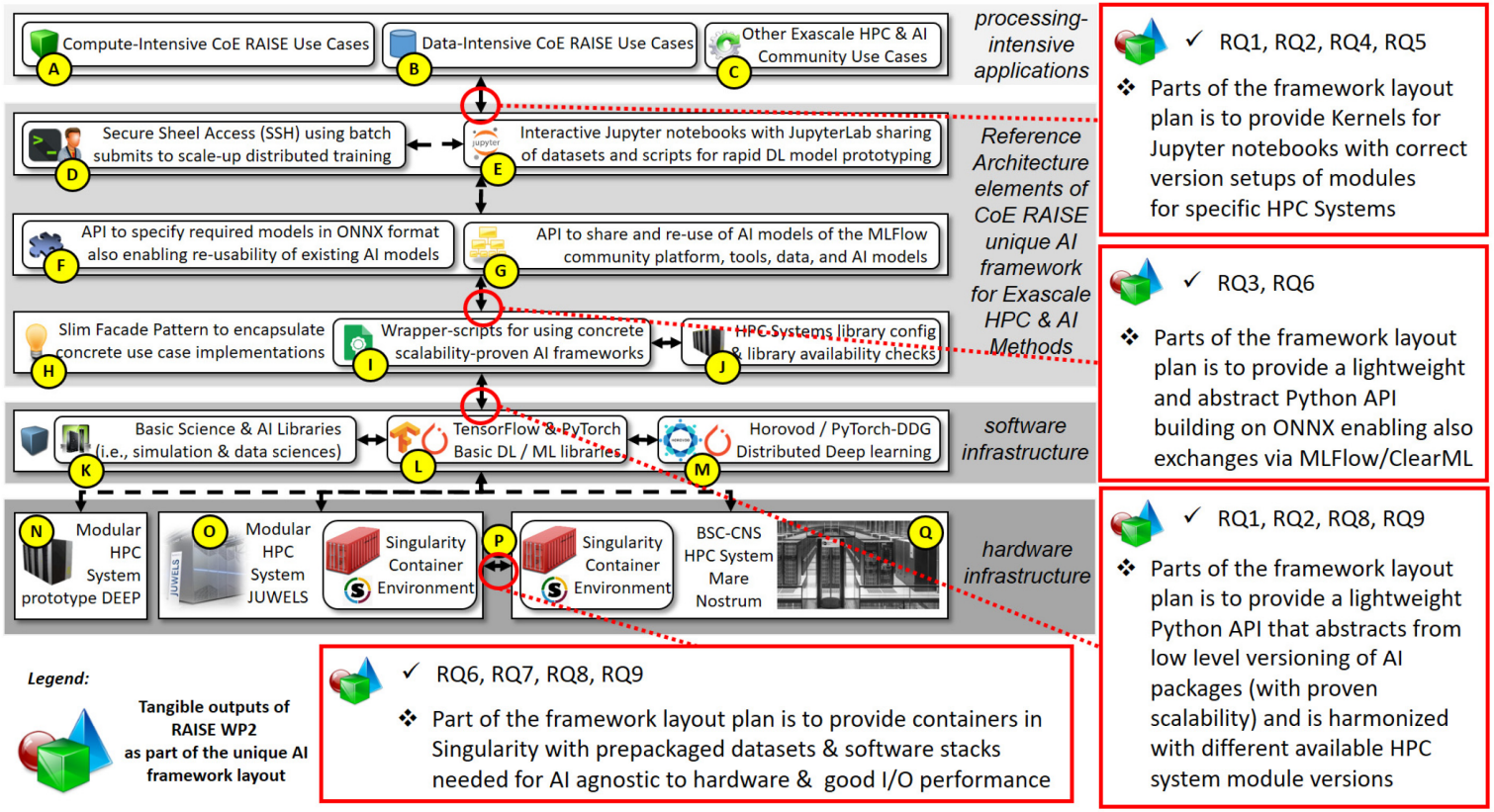


- Milestone MS2 – AI/HPC Methods (M7)
  - Format and Template clarified with PMO: https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/d3657643/CoE%20RAISE_MS_Template.docx
  - Not an official document, maybe only useful in the review;
  - Summary (1/4 page) provided as comment in EU portal by clicking the 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_8I9IzxnnvsYIhE2UXzc/edit?usp=sharing



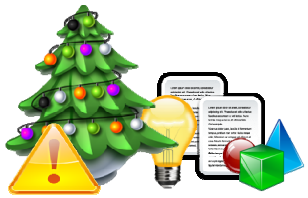
Debrief Deliverable D2.12 Framework (M9) – Initial Blueprint

- 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.

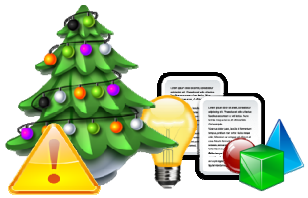
- 14.12.2021 - 21.12.2021:
Continuous exchange between the author(s), the reviewer, and the author(s). At the end, all corrections requested by the PMT have been included and the document is uploaded to the BSCW server. The file name includes the term “Final”.

- 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.

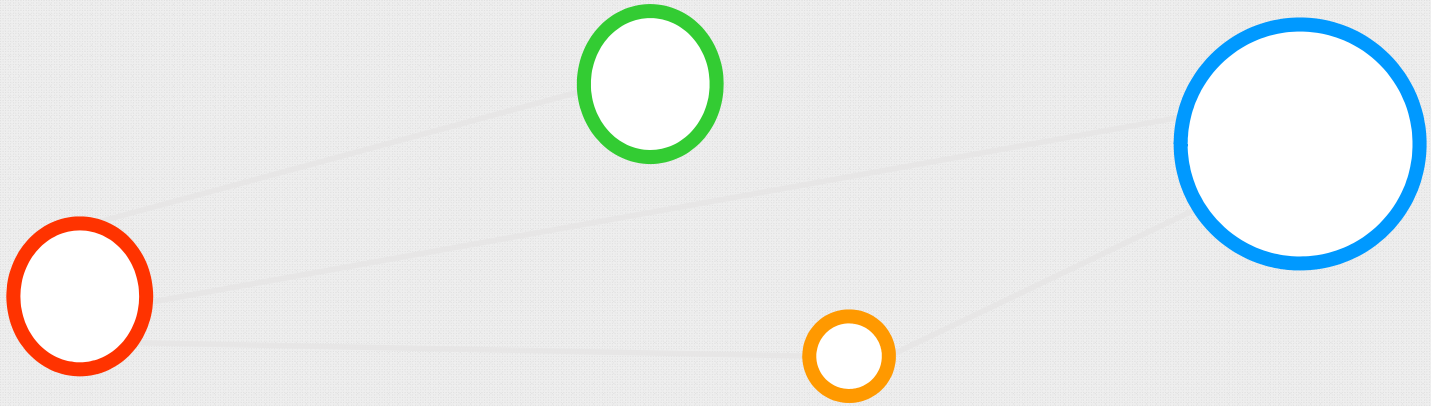
Changed Time Schedule for M12/December Deliverables (2)

- 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



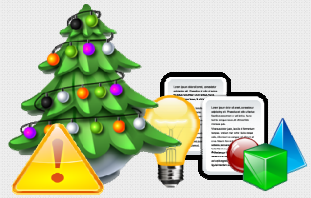
D2.2	Report on porting & performance engineering	BSC	R	PU	12	M. Riedel/ UOI	G. Houzeaux/ BSC	M. Meinke/ RWTH	A. Lintermann/ FZJ	29.11.2021	31.12.2021
D2.14	Report on novel AI technologies	UOI	R	CO	12	M. Riedel/ UOI	M. Riedel/ UOI	S. Kesselheim/ FZJ	J.Lopez/ ParTec	29.11.2021	31.12.2021
D3.1	Report on 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 (3) – Status D2.2 (M12)

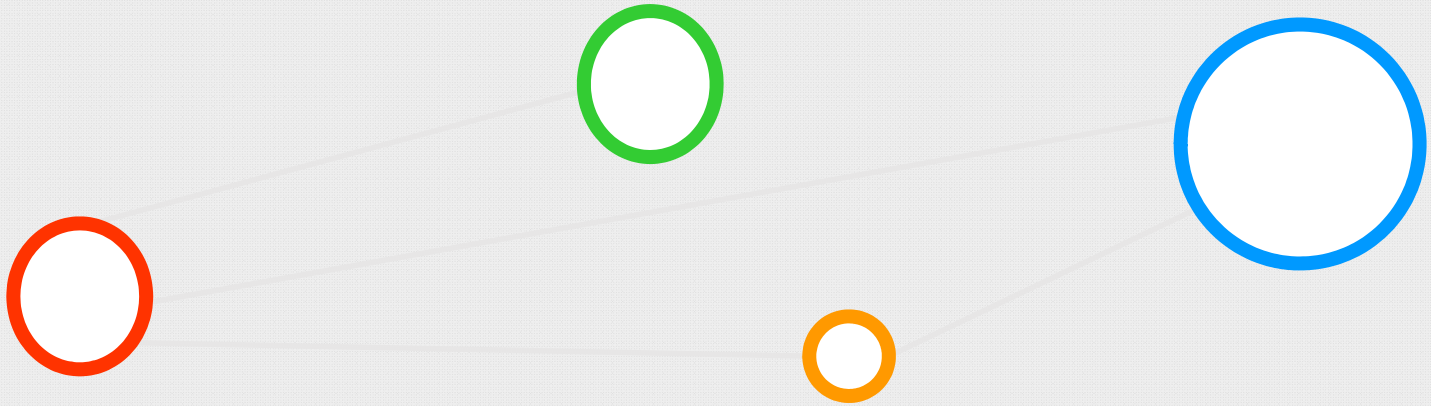


Agenda Item (3) – Status D2.2 (M12)

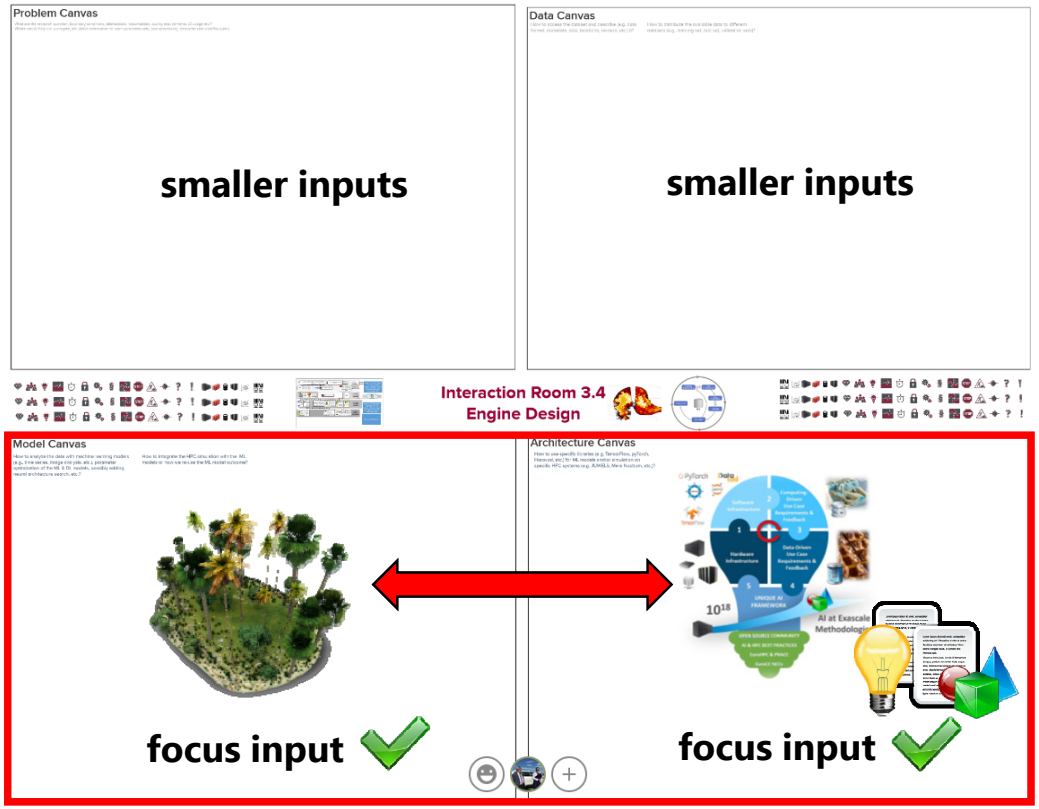
- (Guillaume, Guillermo, Cristóbal), ~5 Min

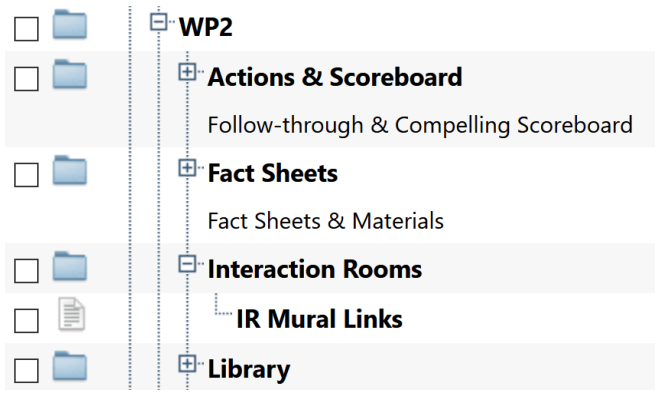


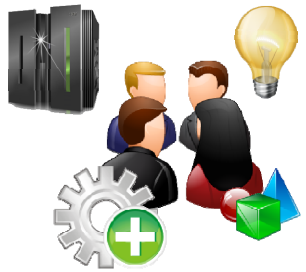
Agenda Item (4) – Status D2.14 (M12)



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=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

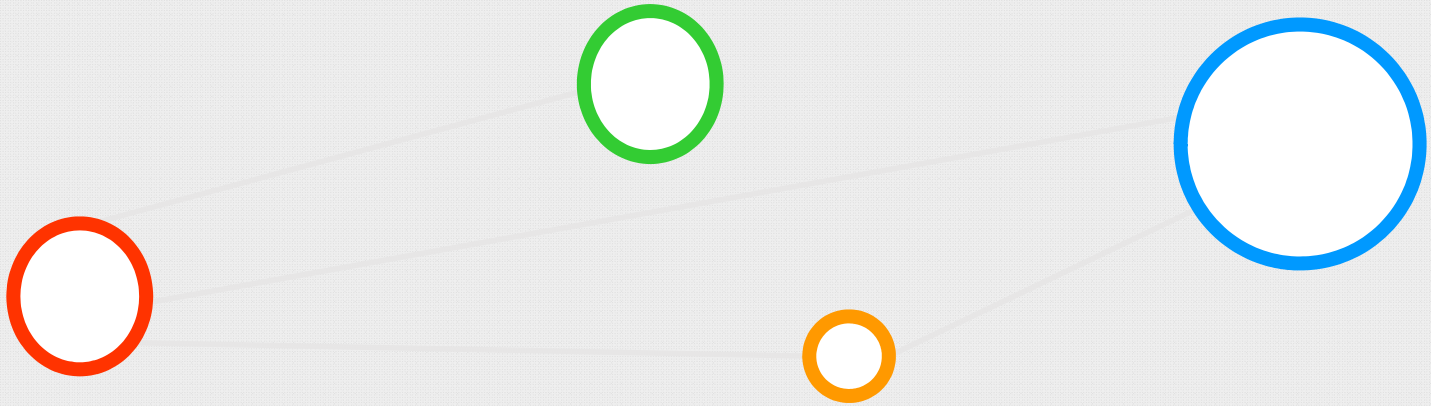
IR4.2 Seismic Imaging: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ae3e28af4bb8d9adbec33874998?sender=u15e3008bb41d6628a5bb5701

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/b5fa122190024040 59f90a4bbb0101fa379a8503?sender=u15e3008bb41d6628a5bb5701

- TBD(Morris & use cases): another round of Mural board sessions

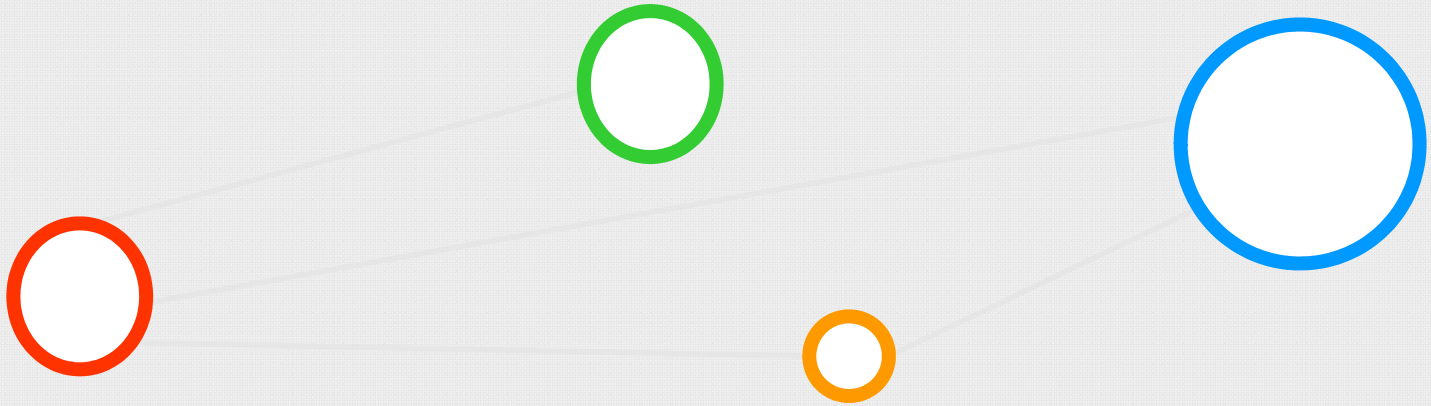
Agenda Item (5) – Upcoming AHM Meeting & Presentations



Agenda Item (5) – Upcoming AHM Meeting & Presentations

- Discussions with WP2 & Project Management
  - How should the agenda look like, focus on topics (framework, AI/HPC methods)
  - TBD(Andi): Send around agenda
    - WP2/3/4 overarching presentation
    - Task Leaders do presentations ~15 Min incl. Discussions
    - WP5&6 next day plus WP1 finance, etc.
  - Perhaps every task leader in WP2 will prepare a presentation (benchmarking, etc.)

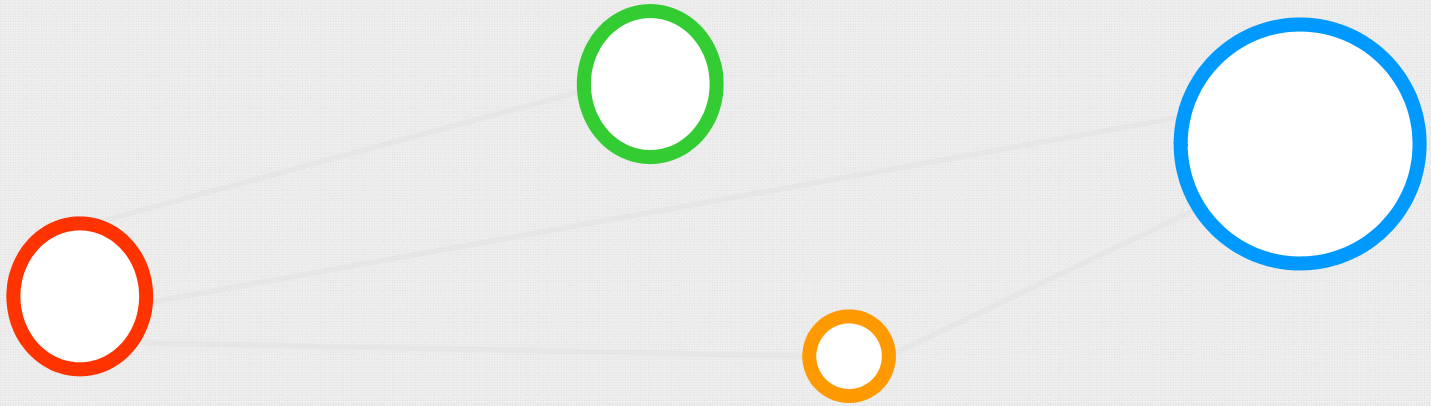
Agenda Item (6) – Network Testing RAISE Partners



Agenda Item (6) – Network Testing RAISE Partners

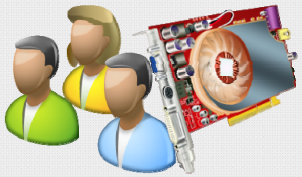
- (Lauris), ~10 Min

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

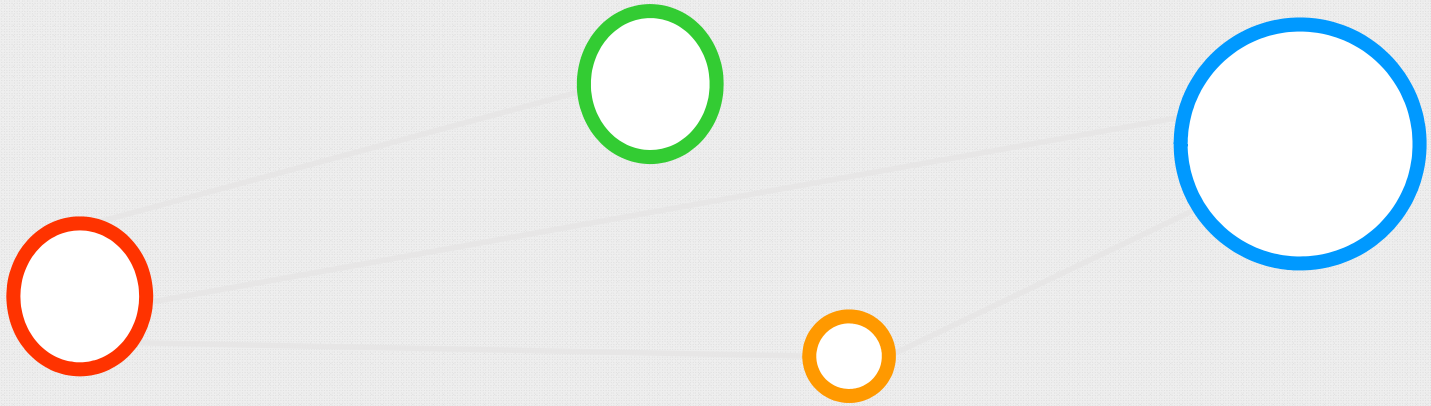


Agenda Item (7) – Hands-on Workshop on GPUs & CUDA

- (Lauris), ~10 Min



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



Compelling Scoreboard Review – Use Case Progress

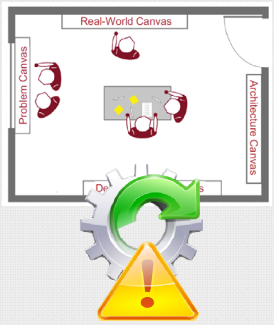
RAISE Center of Excellence

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

FACTS

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

❖ Based on initial work on MS2 and D2.12 we perform again joint Interaction Room session to identify novel AI methods



based on Milestone (M7) AI/HPC Methods

Based on Deliverable D2.12 (M9) Layout plan AI Framework

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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

T3.1 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

T3.2 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

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T3.4 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

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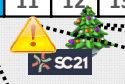
T4.4 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration



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

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

❖ Monthly Meeting October

❖ AHM Meeting 2021-11-24/25

✓ Hyperparameter Tuning with Ray Tune Seminar ~end October

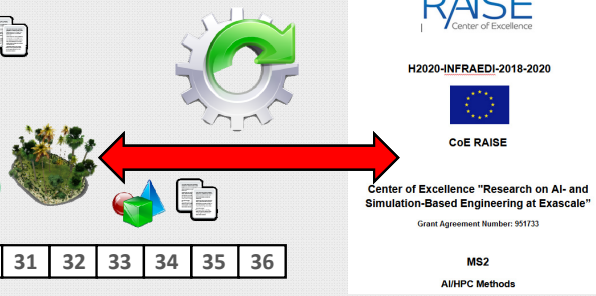
✓ MLOps with ClearML Seminar ~end Sep

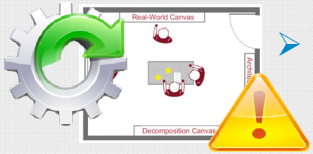
✓ Monthly Meeting September

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

✓ Monthly Meeting August

✓ Autoencoder Seminar ~end August





Next Steps

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

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

drive. enable. innovate.

RAISE Center of Excellence

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