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
2021-07-22, RAISE WP2 Monthly Meeting July 2021, Online

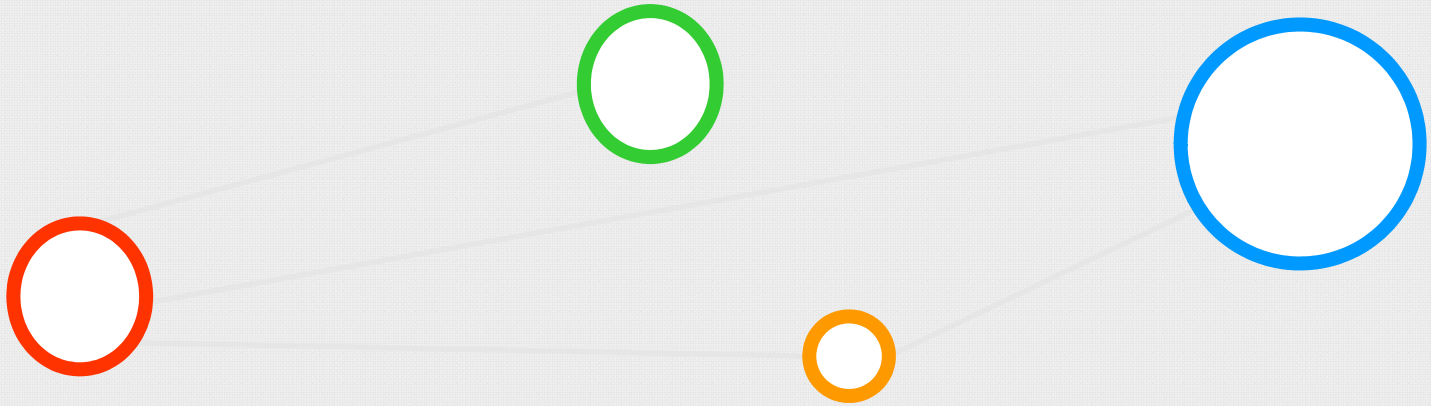
@ProfDrMorrisRiedel @Morris Riedel @MorrisRiedel @MorrisRiedel
https://www.youtube.com/channel/UCWC4VKHmL4NZgFfKoHtANKg morris@hi.is

WP2 July Meeting – Welcome & Agenda

RAISE Center of Excellence

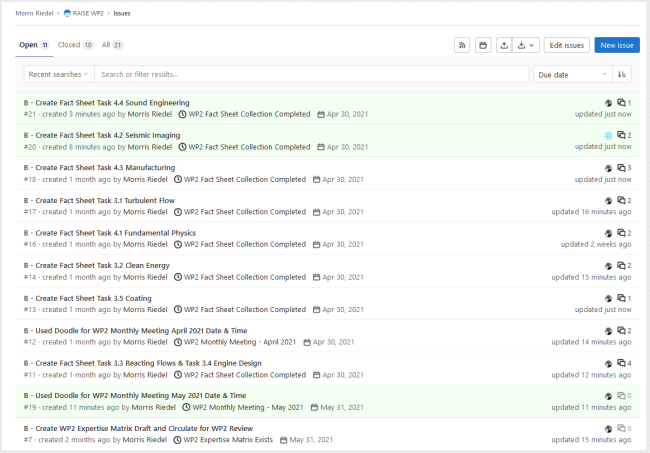
1. Approval of minutes from Monthly Meeting June 2021
   - (All), ~5 Min
2. WP2 Quaterly Report 2 (April-June)
   - (All), ~ 5 Min
3. Review WP2 Status on Interaction Rooms
   - (Morris Riedel, Matthias Book, Helmut Neukirchen), ~5 Min
4. Status RAISE Data Project & Survey Results
   - (Andreas Lintermann), ~5 Min
5. Upcoming Milestone AI/HPC Methods (M7)
   - (Morris Riedel & Andreas Lintermann), ~15 Min
6. Early Plans Deliverable D2.12 Framework (M9)
   - (Morris Riedel & Andreas Lintermann), ~15 Min
7. Compelling Scoreboard Review & Next Steps
   - (All), ~5 Min

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



Minutes Approval – Monthly Meeting June 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!



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Summary of the fitness-check, which has taken place on 22.04.2021			
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T2.2 Support activities	1.2 M	eray	2021-05-28 17:01
by Marcel Aach and Eray Inanc			
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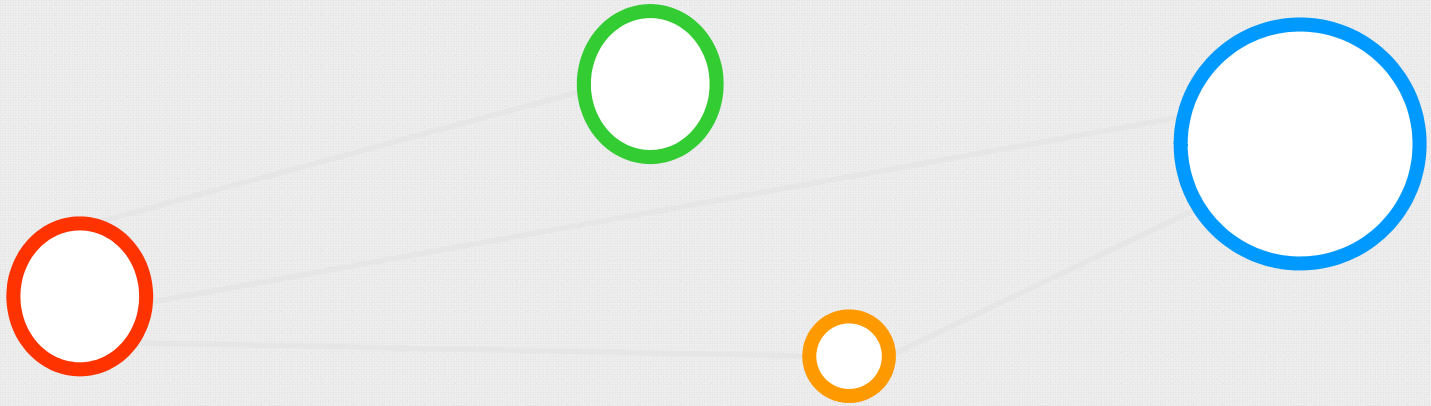
Slides & Materials from meeting 2021-07-22			

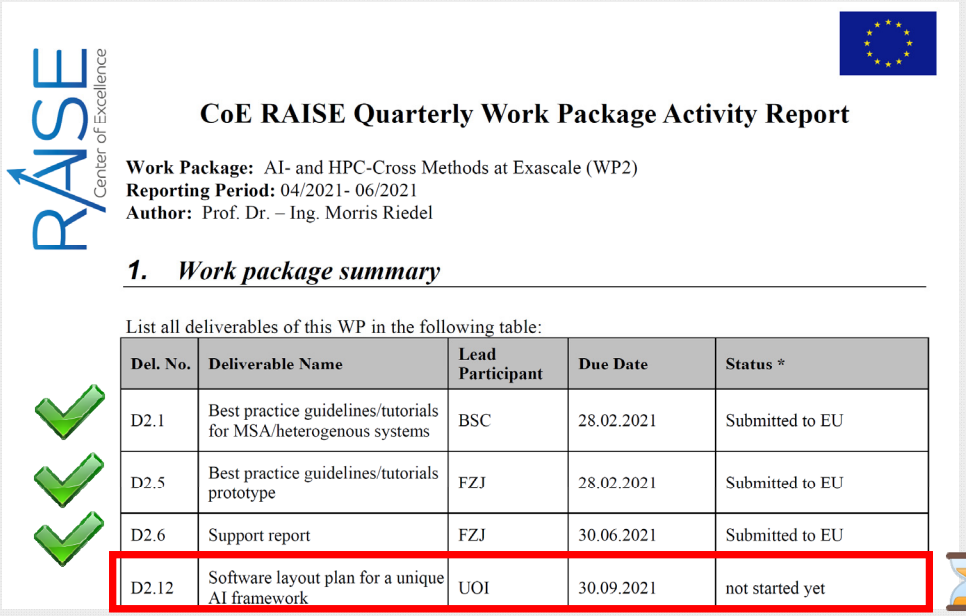
Agenda Item (2) – WP2 Quaterly Report 2 (April – June)



WP2 Quaterly Report 2 (April – June)

- Quaterly Report 2 finished
  - Report available at:
  - https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/d3659739/CoE_RAISE_WP2_Quarterly_Report-2.pdf

- Thanks to all your contributions
  - Keep up the good work!
  - 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

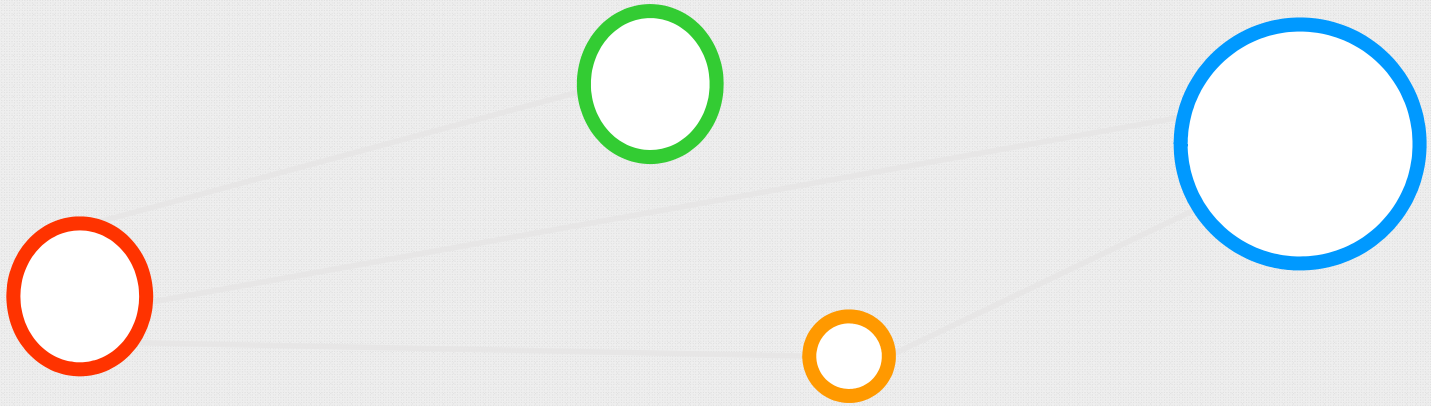
Work Package: AI- and HPC-Cross Methods at Exascale (WP2)
Reporting Period: 04/2021- 06/2021
Author: Prof. Dr. – Ing. Morris Riedel

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

Agenda Item (3) – Review WP2 Status on Interaction Rooms



WP2 Updates – Action Item Fact Sheets (refinement started)

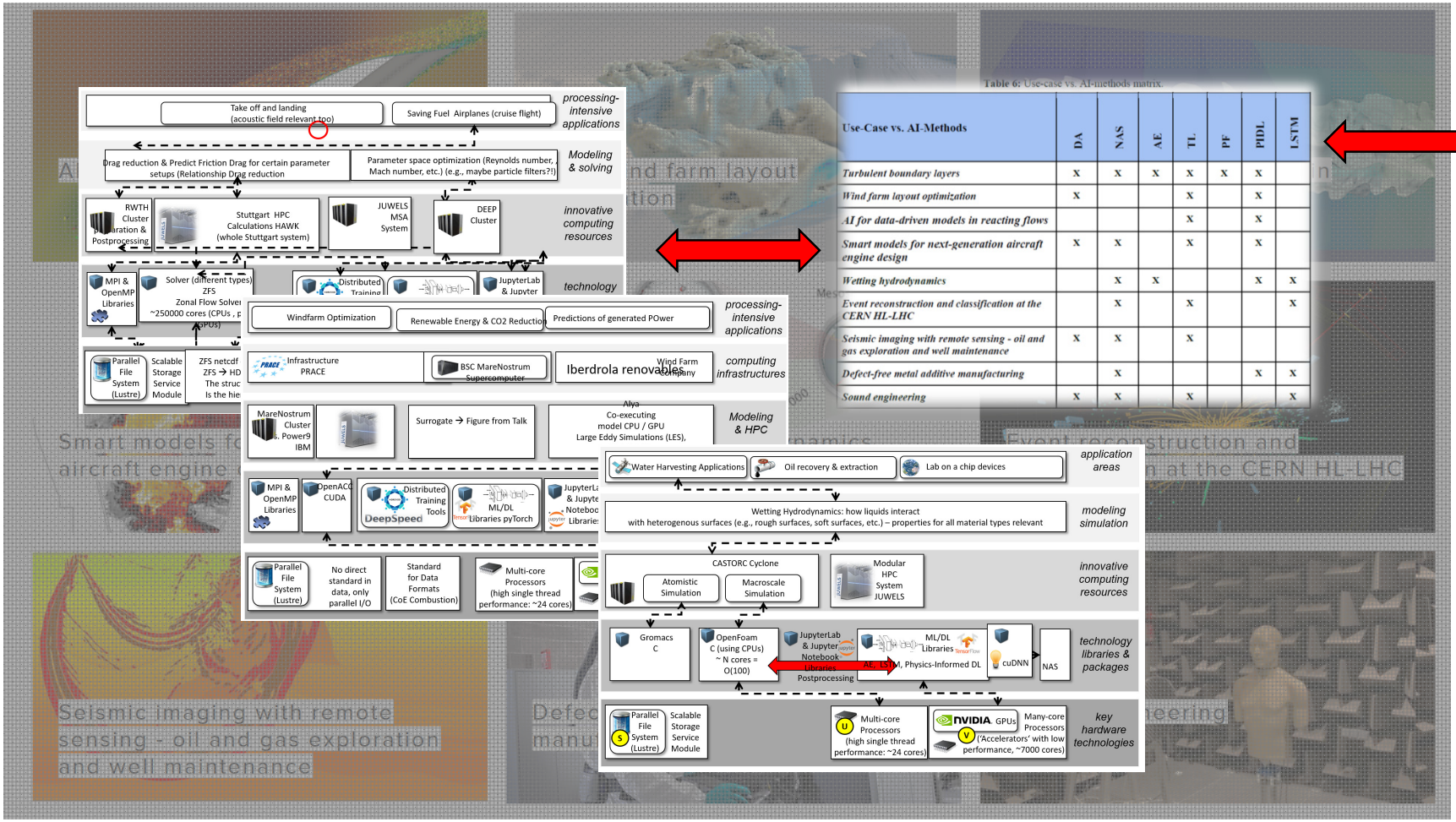
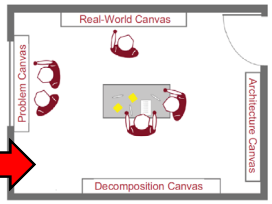


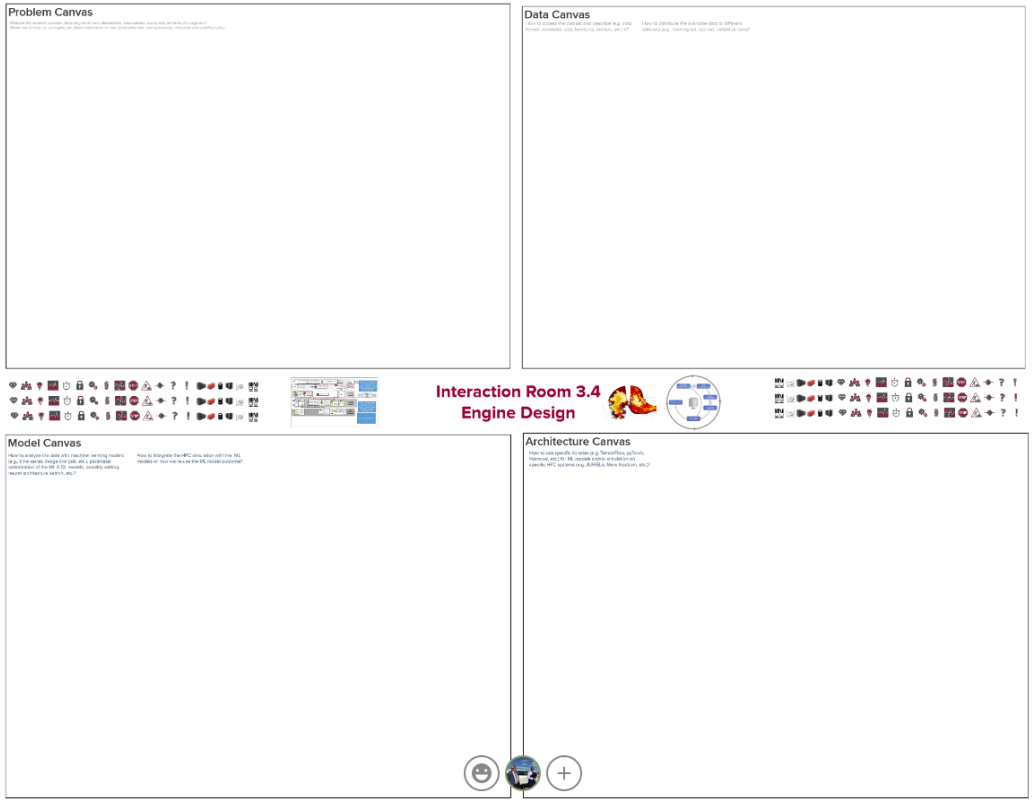
Table 6: Use-case vs. AI-methods matrix.

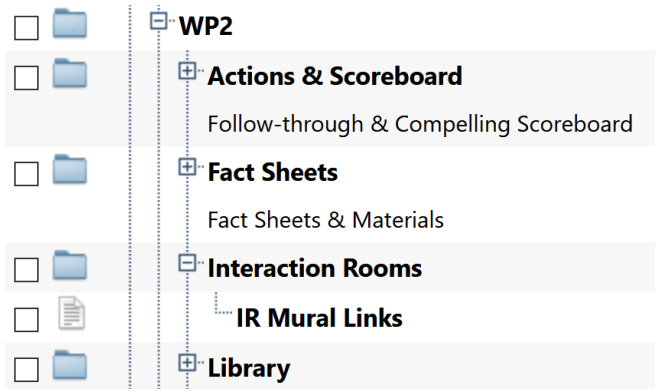
Use-Case vs. AI-Methods	DA	NAS	AE	TL	PF	PIDL	LSTM
Turbulent boundary layers	X	X	X	X	X	X	
Wind farm layout optimization	X			X		X	
AI for data-driven models in reacting flows				X		X	
Smart models for next-generation aircraft engine design	X	X		X		X	
Wetting hydrodynamics		X	X			X	X
Event reconstruction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

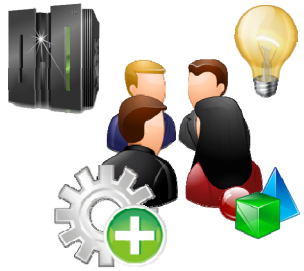


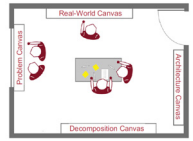
WORK IN PROGRESS

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

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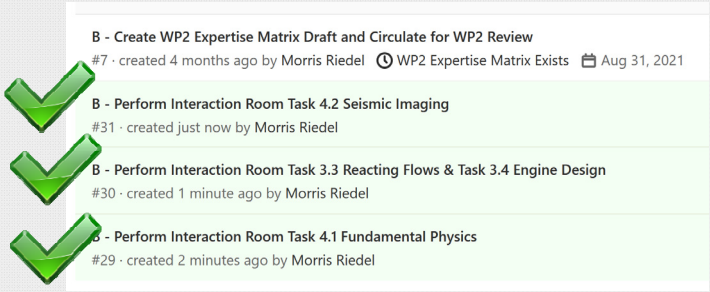
IR4.4 Sound Engineering: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa12219002404059f90a4bbb0101fa379a8503?sender=u15e3008bb41d6628a5bb5701

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

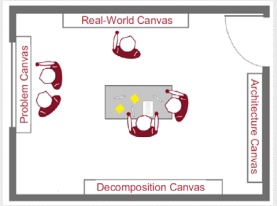
WP2 Updates – Action Items Tracker & Status Updates

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



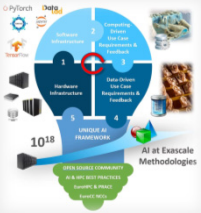
initial steps

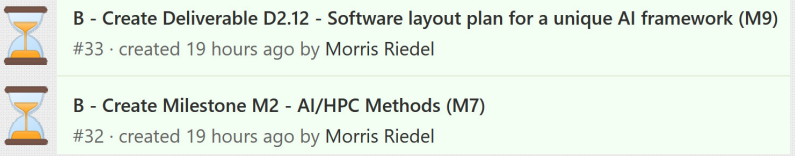
input to Interaction Room process



input to Milestone (M7) AI/HPC Methods

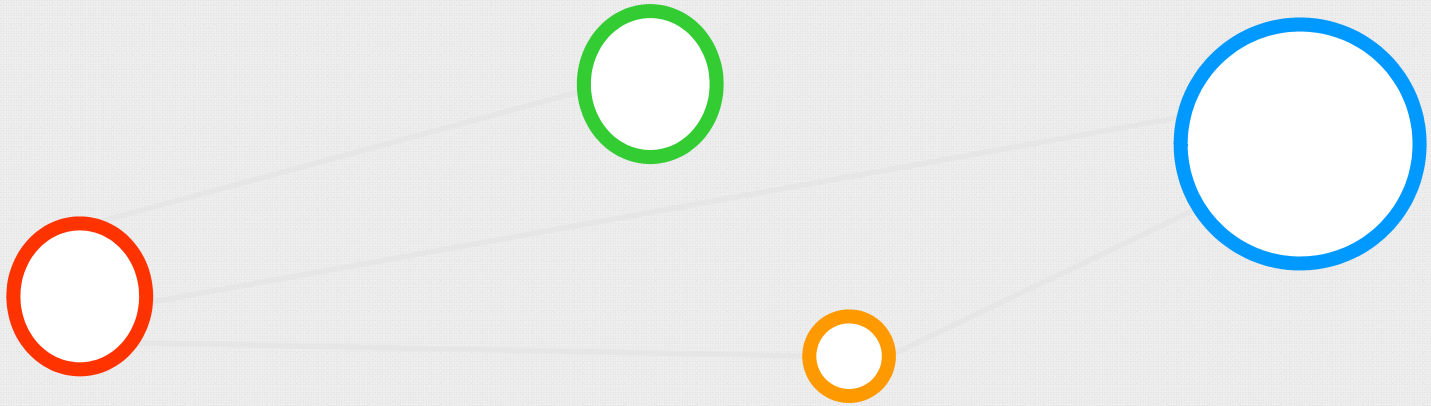
input to Deliverable D2.12 (M9) Layout plan AI Framework





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

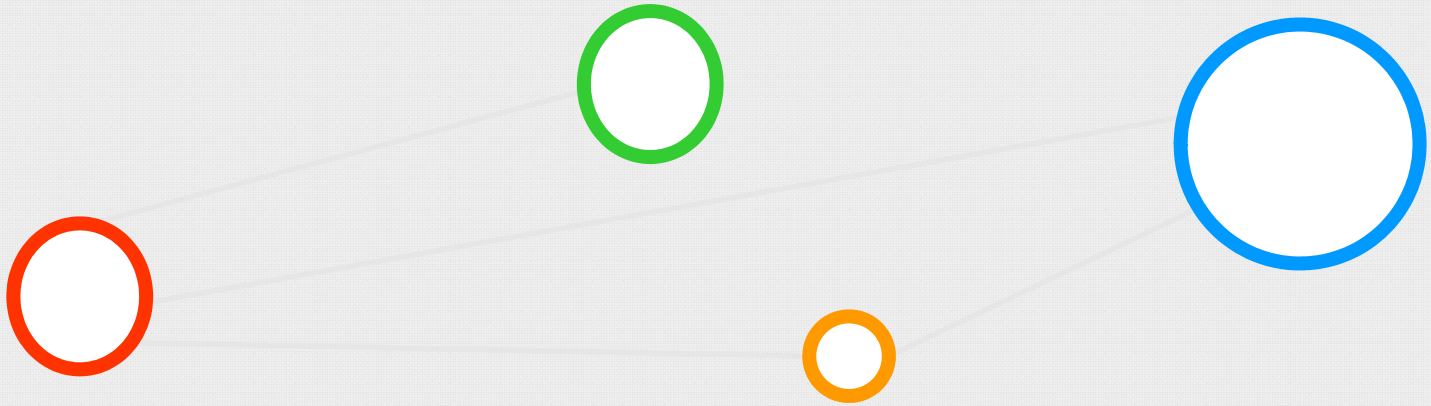
Agenda Item (4) – Status RAISE Data Project & Survey Results



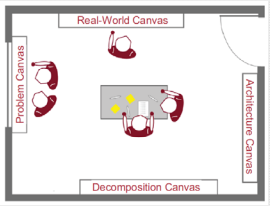
Agenda Item (4) – Status RAISE Data Project & Survey Results

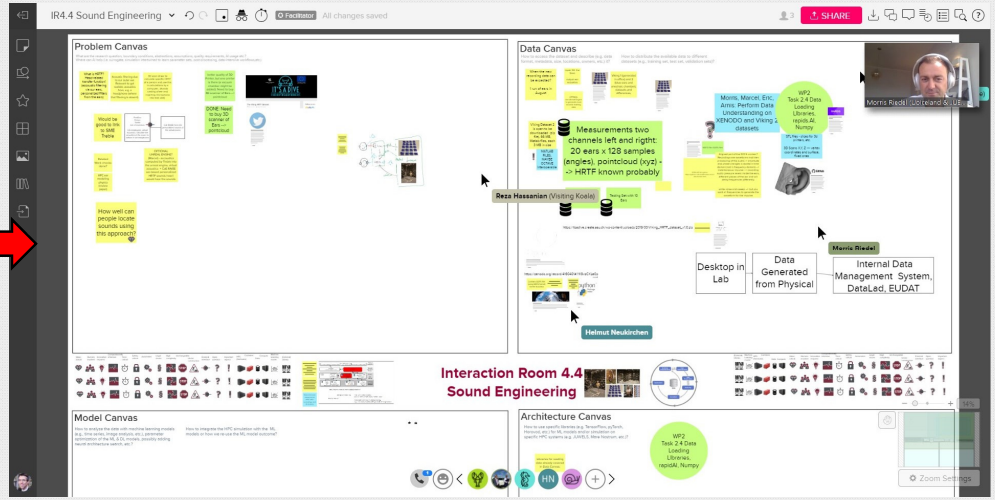
- Update (Andreas Lintermann), ~5min
- Notes:
  - 200 TB Data Project was submitted (pending review)
  - Sharing data in the project and sharing with community
  - Transfer data instead of recreating it
  - $DATA space
- TBD (Lauris, Andreas): Performance Tests of Transfers, RTU/FZJ, FZJ/CERN (e.g. iPerf), FZJ/BSC (maybe via PRACE?)
- TBD (Morris): Seminar (not from COE RAISE) about data transfer tools via email (UFTP, etc.)

Agenda Item (5) – Upcoming Milestone AI/HPC Methods (M7)



Upcoming Milestone MS2 AI/HPC Methods (M7)



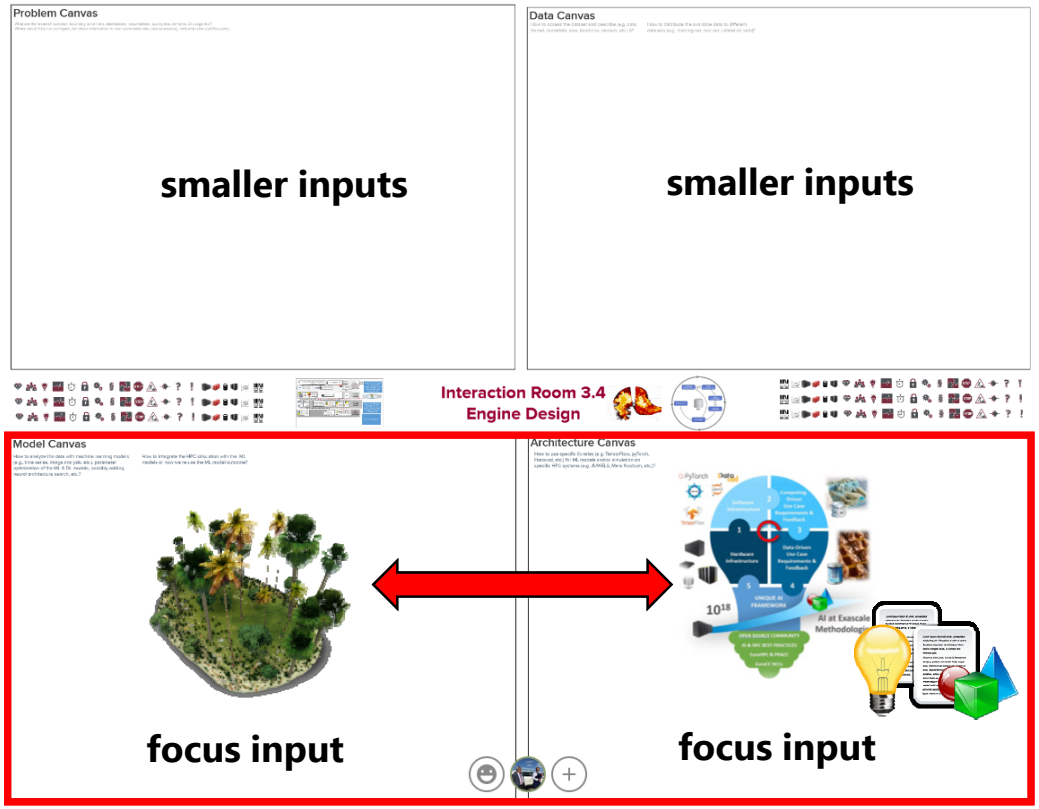


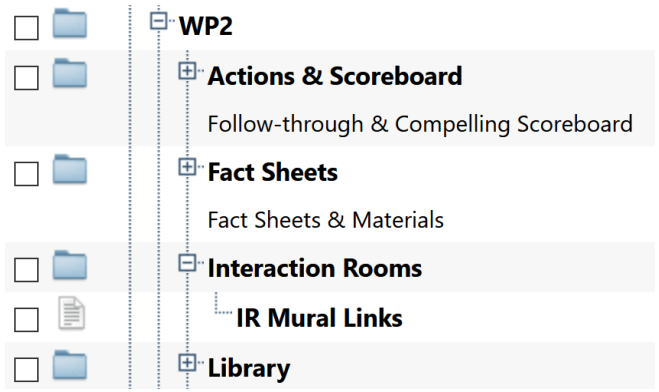
- Discussions with PMO
  - Should be a formal report (not too long, not too short)
  - Links to MURAL Boards included
  - Summarizes findings of MURAL Board discussions (w.r.t. Model/Data/Architecture Canvas)
  - TBD: Refining our initial Matrix of Methods & identify common methods
  - Means of Verification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

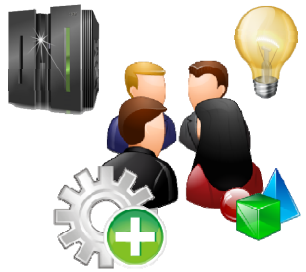
Table 6: Use-case vs. AI-methods matrix.

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

Interaction Rooms via MURAL Boards & Milestone / Deliverable







IR Mural Links

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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

IR3.4 Engine Design: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377976343/8d7aba6be09af3b2ffd305d2f709c53661ac889d?sender=u15e3008bb41d6628a5bb5701

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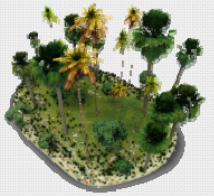
IR4.2 Seismic Imaging: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ae3e28af4bb8d9adbec33874998?sender=u15e3008bb41d6628a5bb5701

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

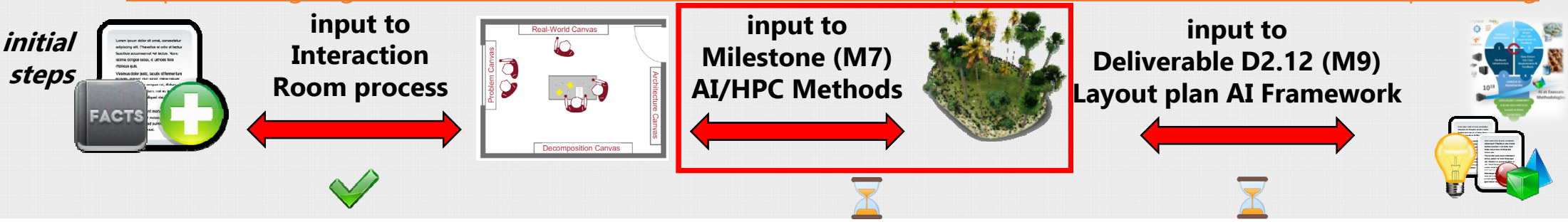
IR4.4 Sound Engineering: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa122190024040 59f90a4bbb0101fa379a8503?sender=u15e3008bb41d6628a5bb5701

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

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

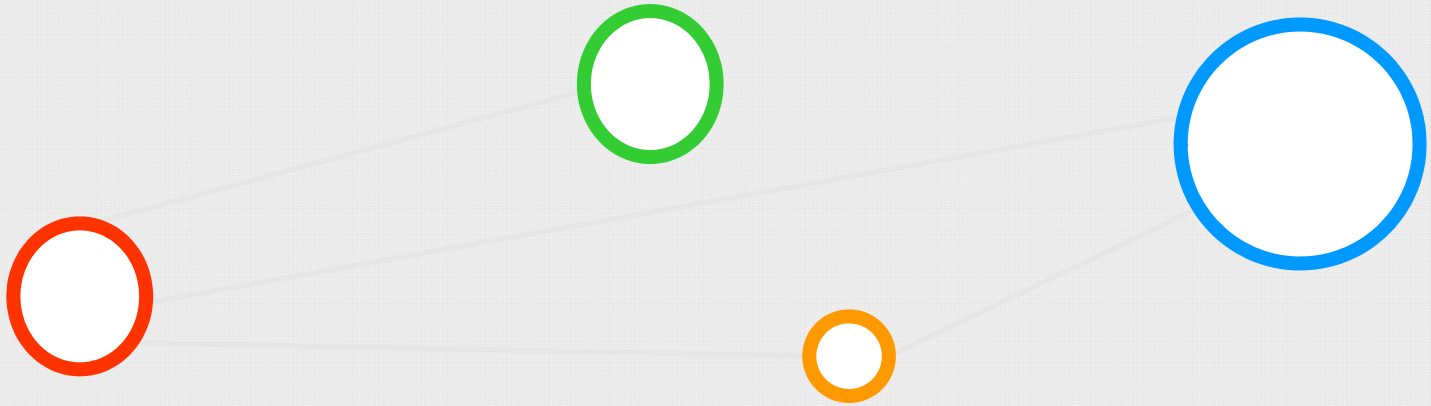


- Milestone MS2 – AI/HPC Methods (M7)
  - Format and Template clarified with PMO: https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/d3657643/CoE%20RAISE_MS_Template.docx
  - Not an official document, maybe only useful in the review;
  - TBD(Morris, Andi): Summary (1/4 page) as comment in EU portal by clicking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



WP2 Updates – Google Doc Milestone AI/HPC Methods (M7)

Agenda Item (6) – Early Plans Deliverable D2.12 (M9)

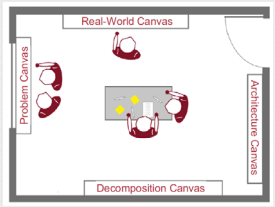


WP2 Updates – Early Plans Deliverable D2.12 Framework (M9)

- 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): How we should design the software layout plan exactly?

initial steps

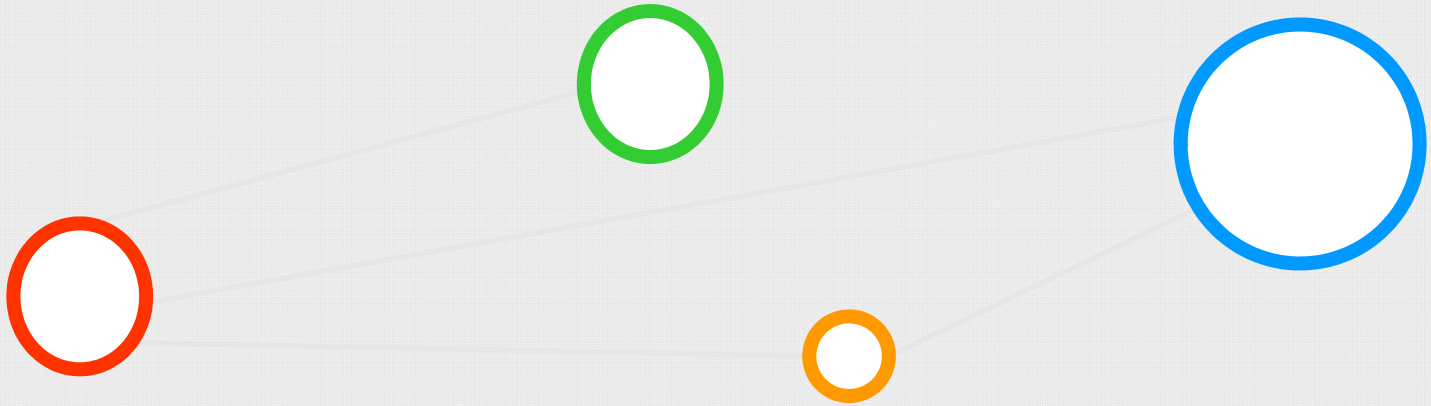
input to Interaction Room process



input to Milestone (M7) AI/HPC Methods

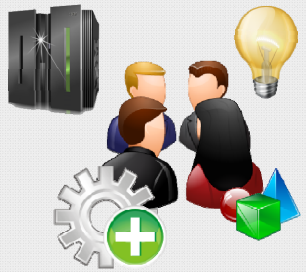
input to Deliverable D2.12 (M9) Layout plan AI Framework

Agenda Item (7) – Compelling Scoreboard Review & Next Steps



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)



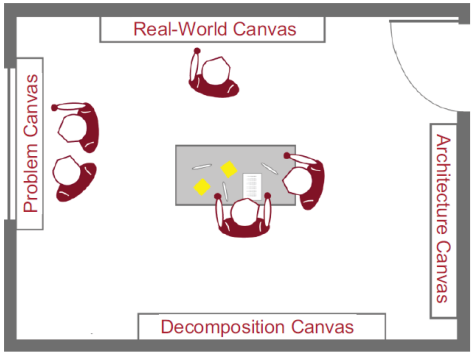


Table 6: Use-case vs. AI-methods matrix.

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

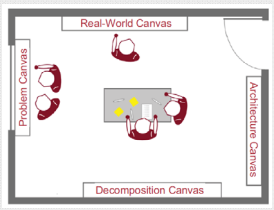
- Next Steps
  - Carve out more details on AI/HPC methods
  - Identify concrete detailed algorithms
  - Input to Milestone MS2

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

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



input to Milestone (M7) AI/HPC Methods

- Next Steps:
  - Interaction Rooms for AI Methods & Fact Sheet Refinements (over time)
  - TBD (Morris): Prefills Milestone document in google
  - TBD (All): review and complement initial milestone version
  - TBD (Morris): Create a final version with word, then Google document remains as living document

Compelling Scoreboard Review & Next Steps

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✓ 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

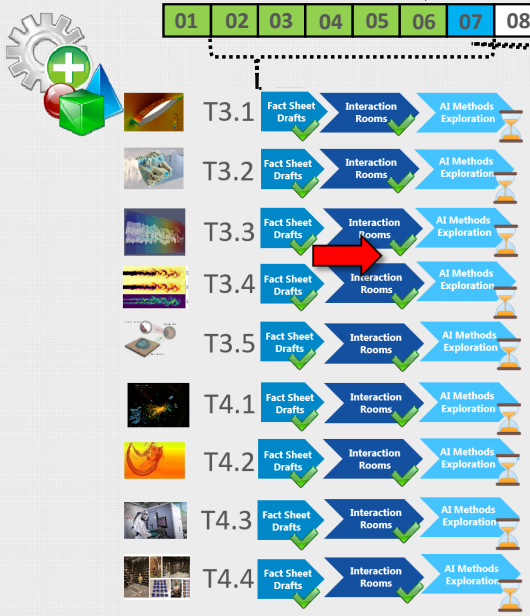
❖ AI/HPC Methods (M7)

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

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

❖ Monthly Meeting July

❖ Distributed Training Seminar ~end July



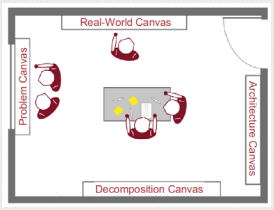
❖ Fact Sheet Process & Interaction Room (started): revision & refinement process ongoing

HOROVOD

PyTorch

➢ Next Steps

➢ Work on milestone MS2 & deliverable D2.12 drafts



input to Milestone (M7) AI/HPC Methods

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

Agenda Item (7) – Vacation WP2 Meeting August & AOB (1)

1. AOB: Distributed Training Seminar (end of July)
    1. Rocco confirmed (video since on vacation)
    2. Marcel confirmed
    3. Gael Atos (confirmed): 20 min, Thursday afternoon
    4. TBD(Morris): Announce date and location via mailng list and inform Michael from WP6
2. AOB: Software layout plan (D2.12) → M9
    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

Agenda Item (7) – Vacation WP2 Meeting August & AOB (2)

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: August Seminar on OpenML & Interopable Formats
    1. TBD (Andi, Morris, Kurt): Advisory board member presentation, and others
3. AOB: September Seminar with Graphcore maybe?
    1. TBD(Gael, Andi): Check benchmarking, etc.
4. AOB: Amendment Process
    1. Signing process performed
    2. Amended version in document: BSCW, COE RAISE
5. AOB: HPC3 meeting
    1. Connect the COEs to connect them to NCCs
    2. Different COEs
    3. Mid-end Septembers
    4. HPC3 will select the NCCs, small workshops CFD

drive. enable. innovate.

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