



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



# WP<sub>2</sub> AI- & HPC-Cross Methods at Exascale – Monthly Meeting

Prof. Dr. – Ing. Morris Riedel et al.

School of Engineering & Natural Sciences, University of Iceland

*2021-06-29, RAISE WP2 Monthly Meeting June 2021, Online*



@ProfDrMorrisRiedel



@Morris Riedel



@MorrisRiedel



@MorrisRiedel



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

morris@hi.is



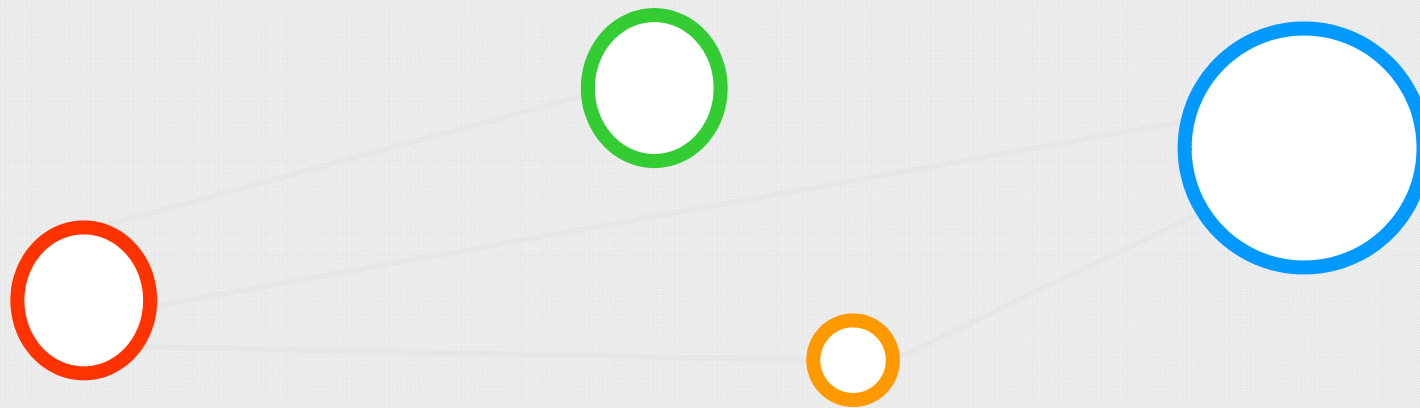
# WP2 June Meeting – Welcome & Agenda



1. Approval of minutes from Monthly Meeting May 2021
  - (All), ~5 Min
2. Review WP2 Status on Interaction Rooms
  - (Morris Riedel, Matthias Book, Helmut Neukirchen), ~15 Min
3. Status Deliverable D2.6 "Support Report"
  - (Eray Inanc & Marcel Aach), ~5 Min
4. Upcoming Milestone AI/HPC Methods (M7)
  - (Morris Riedel & Andreas Lintermann), ~5 Min
5. Status RAISE Data Project
  - (Andreas Lintermann), ~10 Min
6. Compelling Scoreboard Review & Next Steps
  - (All), ~10 Min
7. Summer Vacation Plans & Next Monthly Meeting July & AOB
  - Doodle & Discussions, ~5 Min



# Agenda Item (1) – Minutes Approval – Meeting May 2021



# Minutes Approval – Monthly Meeting May 2021



## 1. Minutes available in BSCW

- <https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/d3380922/2021-03-15-Monthly-Meeting-March-2021-Minutes-v1.docx>
- TBD(all): Any objections or additions/changes?
- Added Data project to the agenda today

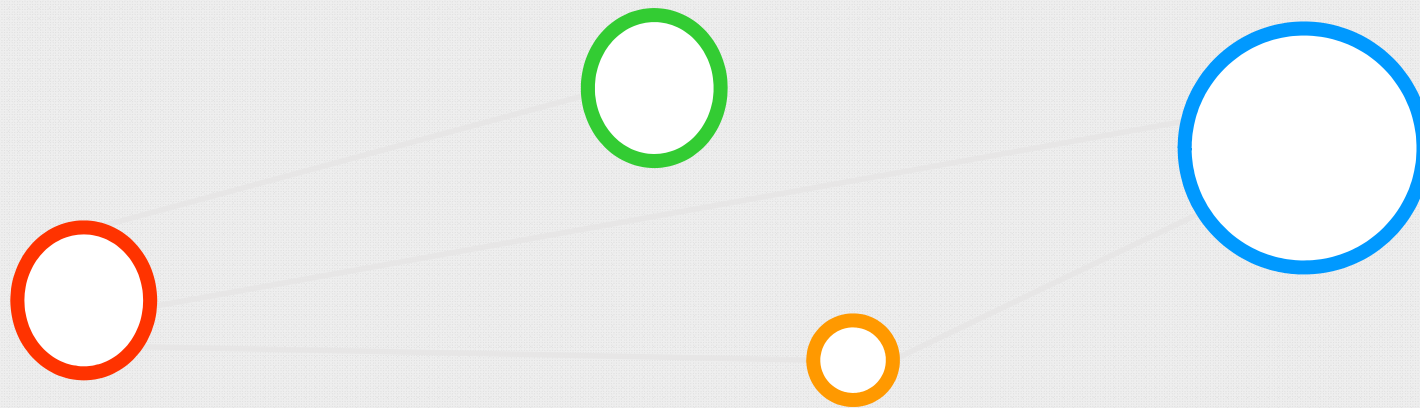
Monthly Meetings

Name	Aktion	Größe	Erreicht von	insgesamt 5 Einträge
2021-02-11 Monthly Meeting February 2021		4	M.Riedel	2021-04-28 15:19
Slides & Materials from meeting 2021-02-11				
2021_02_11 CoE RAISE WP2 Monthly Meeting Riedel v1.pdf		2.4 M	M.Riedel	2021-04-28 15:19
2021_02_11 CoE RAISE WP2 Monthly Meeting Riedel v1.pptx		5.0 M	M.Riedel	2021-02-11 15:34
WP2 Monthly Meeting February 2021 Slides & Agenda				
HPC Systems Engineering in the Interaction Room		4.6 M	mbook	2021-02-11 15:30
Brief introduction to the Interaction Room approach				
2021-02-11 Monthly Meeting Feb-2021-Minutes-v2.docx		40.1 K	M.Riedel	2021-03-15 12:51
Monthly Meeting February 2021 - Meeting Minutes				
2021-03-15 Monthly Meeting March 2021		3	M.Riedel	2021-04-28 15:19
Slides & Materials from meeting 2021-03-15				
2021_03_15 CoE RAISE WP2 Monthly Meeting Riedel v1.pdf		5.8 M	M.Riedel	2021-04-28 15:19
2021_03_15 CoE RAISE WP2 Monthly Meeting Riedel v1.pptx		5.9 M	M.Riedel	2021-04-28 15:12
2021-03-15 Monthly Meeting March-2021-Minutes-v1.docx		40.4 K	seyedreza	2021-03-22 16:04
2021-04-30 Monthly Meeting April 2021		4	M.Riedel	2021-05-05 17:19
Slides & Materials from meeting 2021-04-30				
2021_04_30 CoE RAISE WP2 Monthly Meeting Riedel v1.pdf		8.5 M	M.Riedel	2021-04-30 21:11
WP2 Monthly Meeting April 2021 Slides & Agenda				
2021-CoE-RAISE-Fitness Check WP2_30.04.2021.pptx [0.2]		1.1 M	andlin	2021-04-30 21:11
Summary of the fitness-check, which has taken place on 22.04.2021				
2021_04_30 CoE RAISE WP2 Monthly Meeting Riedel v1.pptx		9.8 M	M.Riedel	2021-04-30 21:12
WP2 Monthly Meeting April 2021 Slides & Agenda				
2021-04-30 Monthly Meeting April-2021-Minutes-v1		40.6 K	seyedreza	2021-05-05 17:19
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 15:31
2021_05_28 CoE RAISE WP2 Monthly Meeting Riedel v1.pptx		14.6 M	M.Riedel	2021-05-28 17:01
T2.2 Support activities		1.2 M	eray	2021-05-28 17:01
by M.Riedel, A. Zsch and E. Zsch				
2021-05-28 Monthly Meeting Minutes		40.6 K	seyedreza	2021-06-07 15:36
2021-06-29 Monthly Meeting June 2021		2	andlin	2021-06-29 09:22
Slides & Materials from meeting 2021-06-29				





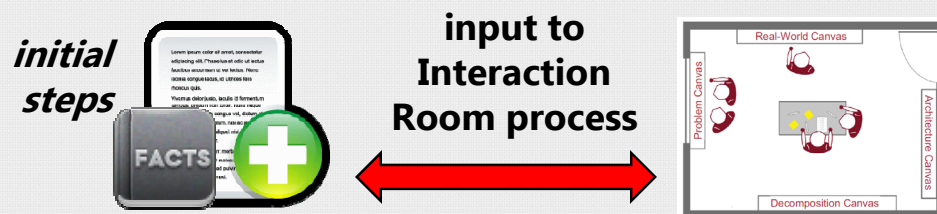
## Agenda Item (2) – Review WP2 Status on Interaction Rooms



# WP2 Updates – Action Items Tracker

## ➤ Follow-Through

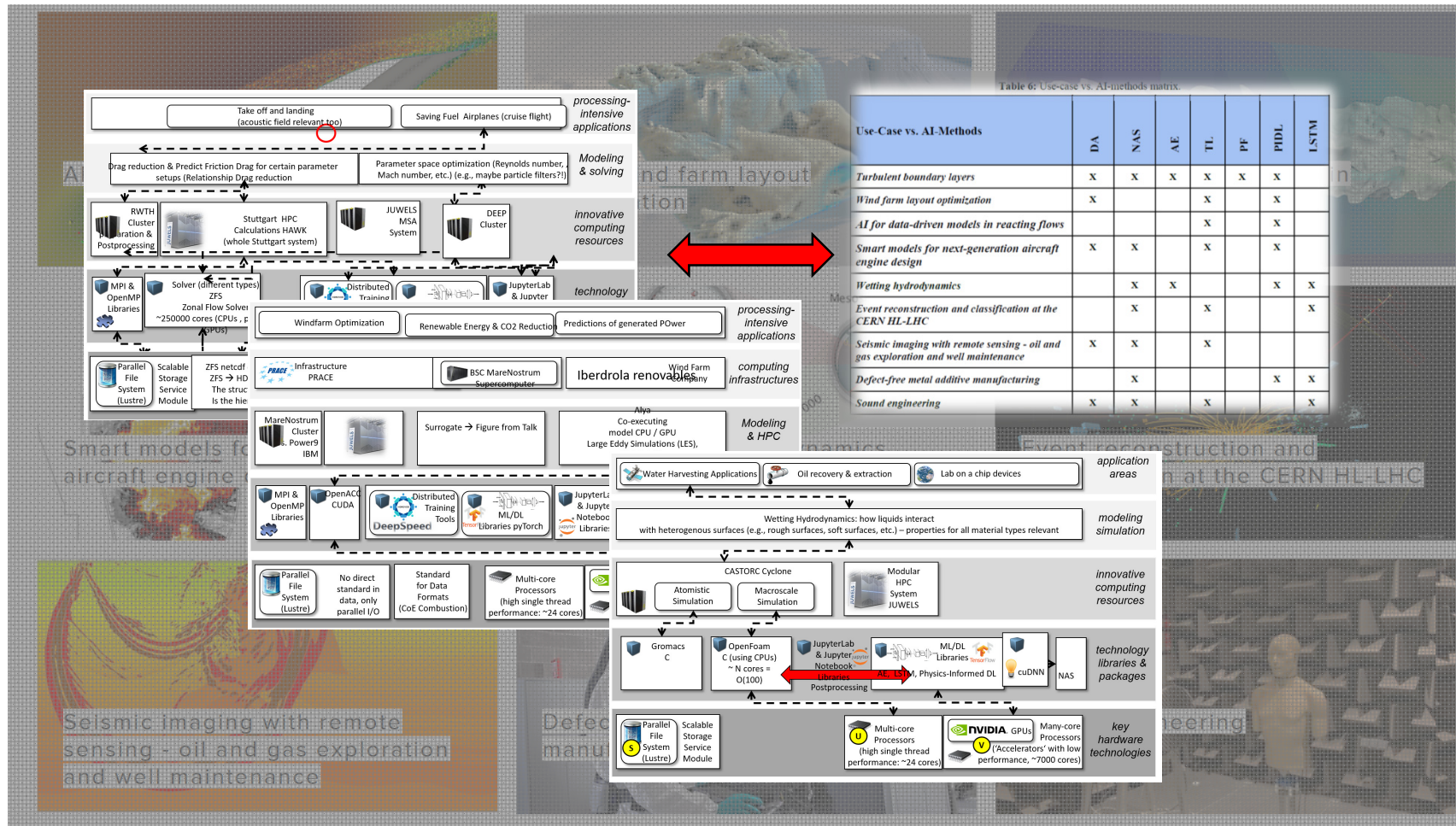
- Fact Sheet Actions done → Closing
- Meeting with each use case teams done
- Fact Sheet Draft existing for use cases
- Refinement via Interaction Rooms started



B - Create Fact Sheet Task 4.4 Sound Engineering #21 · created 4 weeks ago by Morris Riedel · WP2 Fact Sheet Collection Completed · Apr 30, 2021	updated 4 weeks ago	
B - Create Fact Sheet Task 4.2 Seismic Imaging #20 · created 4 weeks ago by Morris Riedel · WP2 Fact Sheet Collection Completed · Apr 30, 2021	updated 4 weeks ago	
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 4 weeks ago	
B - Create Fact Sheet Task 3.1 Turbulent Flow #17 · created 2 months ago by Morris Riedel · WP2 Fact Sheet Collection Completed · Apr 30, 2021	updated 4 weeks ago	
B - Create Fact Sheet Task 4.1 Fundamental Physics #16 · created 2 months ago by Morris Riedel · WP2 Fact Sheet Collection Completed · Apr 30, 2021	updated 1 month ago	✓
B - Create Fact Sheet Task 3.2 Clean Energy #14 · created 2 months ago by Morris Riedel · WP2 Fact Sheet Collection Completed · Apr 30, 2021	updated 4 weeks ago	
B - Create Fact Sheet Task 3.5 Coating #13 · created 2 months ago by Morris Riedel · WP2 Fact Sheet Collection Completed · Apr 30, 2021	updated 4 weeks ago	
B - Create Fact Sheet Task 3.3 Reacting Flows & Task 3.4 Engine Design #11 · created 2 months ago by Morris Riedel · WP2 Fact Sheet Collection Completed · Apr 30, 2021	updated 4 weeks ago	
B - Used Doodle for WP2 Monthly Meeting May 2021 Date & Time #22 · created 1 week ago by Morris Riedel · WP2 Monthly Meeting - May 2021 · May 31, 2021	updated 1 week ago	
B - Create WP2 Expertise Matrix Draft and Circulate for WP2 Review #7 · created 3 months ago by Morris Riedel · WP2 Expertise Matrix Exists · May 31, 2021	updated 4 weeks ago	
B - Perform Interaction Room Task 4.4 Sound Engineering #24 · created 3 days ago by Morris Riedel · WP2 Interaction Rooms Performed · Jun 15, 2021	updated 3 days ago	✓
B - Perform Interaction Room Task 3.5 Coating #23 · created 3 days ago by Morris Riedel · WP2 Interaction Rooms Performed · Jun 15, 2021	updated 3 days ago	

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

# WP2 Updates – Action Item Fact Sheets (all use cases done)



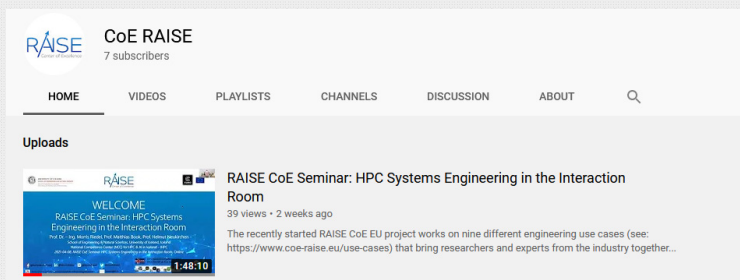
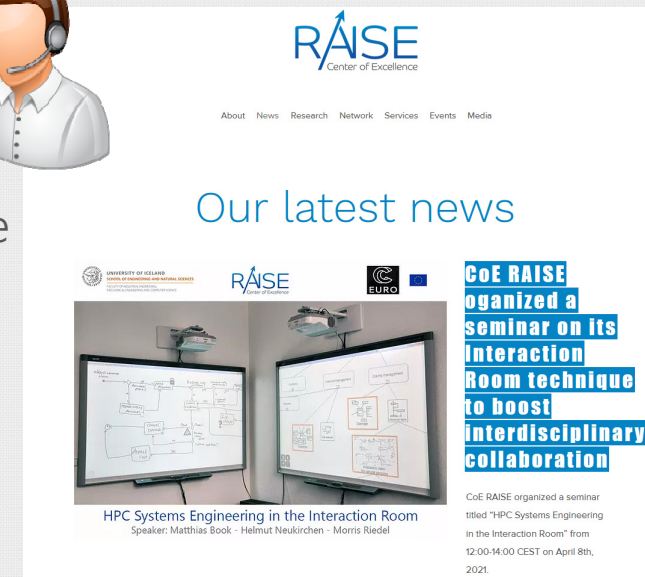
**WORK  
IN  
PROGRESS**



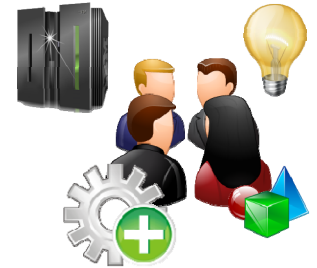
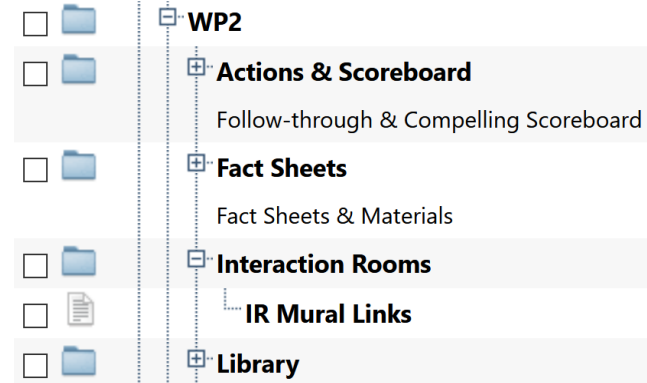
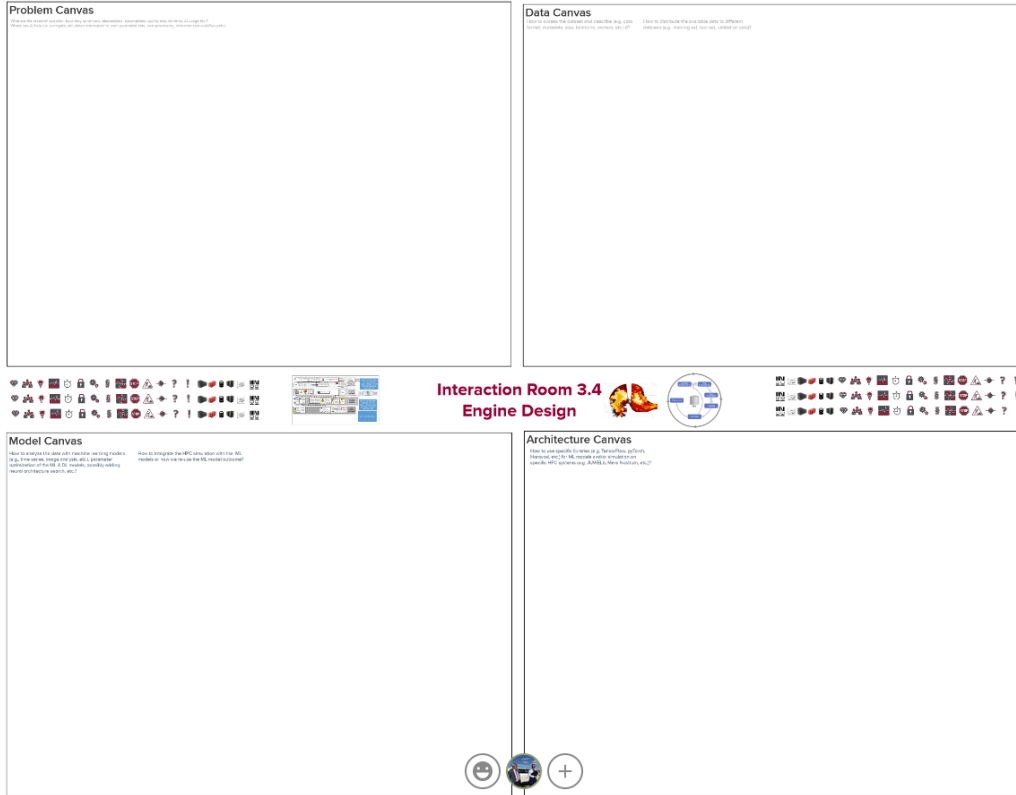
# WP2 Seminar April – Interaction Room Performed on 8<sup>th</sup> April



- Discuss shortly Feedback
  - Open to all communities (beyond RAISE)
  - Registration (input from WP6): enables user statistics & avoid trouble
- Material available on BSCW & RAISE@YouTube
  - <https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3396104>
  - @WP2 team: Subscribe to YouTube channel RAISE:  
<https://www.youtube.com/channel/UCAdIZ-v6cWwGdapwYxdN7dg>



## Interaction Rooms via MURAL Boards



## 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/cb44cca3eedd3bb9964fbfa36af16b1bfccce085f?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=u15c3008bb41d6628a5bb5701>

**IR3.5 Coating:** <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377991014/7a5d7e1caf230178342d1e1d4a84d656d9055d52?sender=u15e3008bb41d6628a5bb5701>

**IR4.1 Fundamental Physics:** <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378007555/6f0d5285fcaec5eafa515bd6676e84d8b4879d39?sender=u15c3008bb41d6628a5bb57>

**IR4.2 Seismic Imaging:** <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ac3e28af4bb8d9adbcc33874998?sender=u15e3008bb41d6628a5bb5701>

**IR4.3 Manufacturing:** <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378038069/93df6fa7a41093f4eaa7be9d72979de2ba42b9d?sender=u15c3008bb41d6628a5bb5701>

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

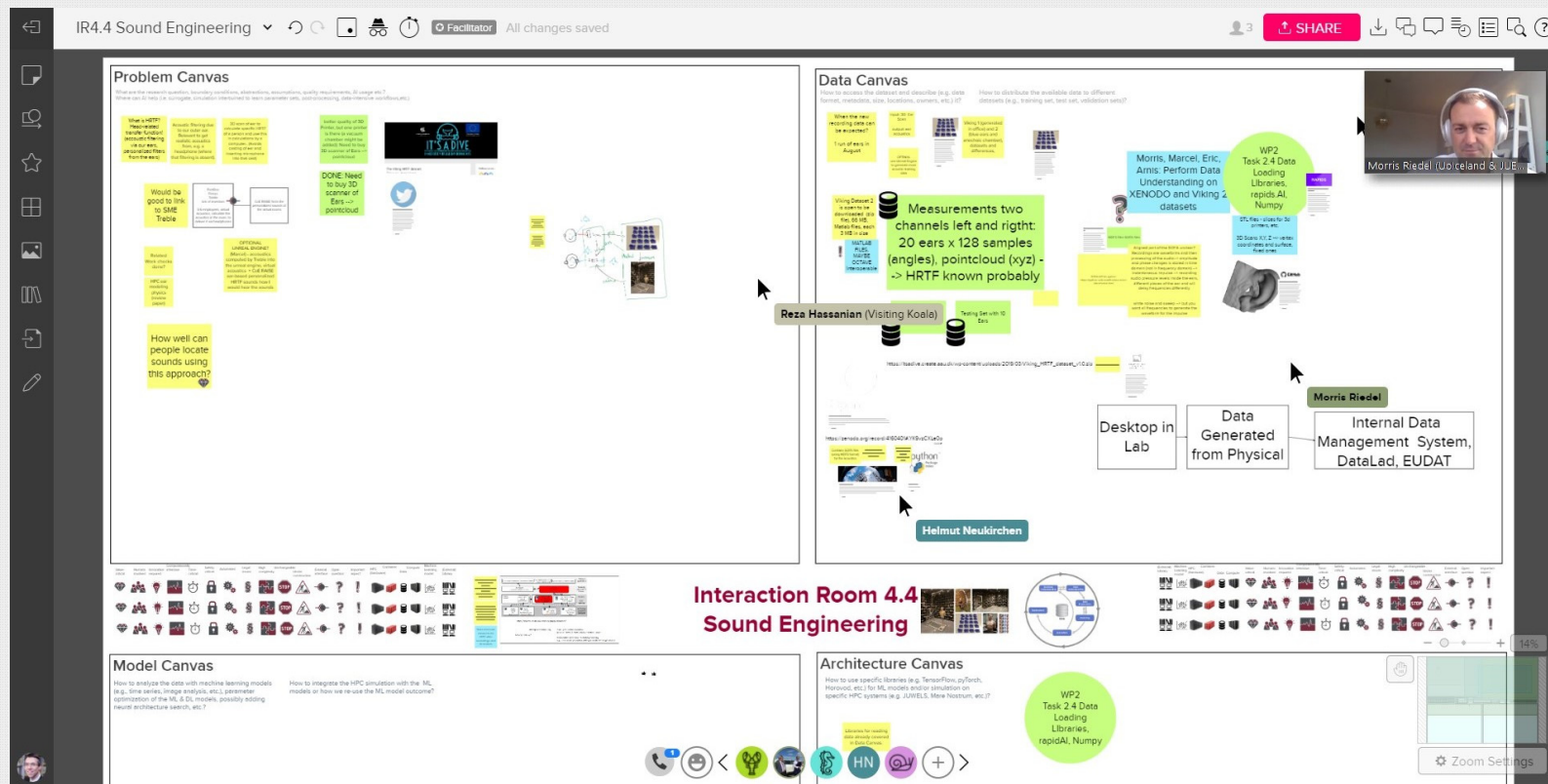
➤ <https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3591551>



# Interaction Rooms via MURAL Boards – Example (T4.4)



→ WP6 Input:  
News Item about  
Fact Sheet &  
Interaction Room  
Process  
Done (Morris,  
Helmut,  
Matthas)



# FactSheet & Interaction Room Webpage & WP2 News Items

## Our latest news



**Summer School on High-Performance and Disruptive Computing in Remote Sensing**

The virtual Summer school of the IEEE GRSS HCRS working group on High-Performance and Disruptive Computing in Remote Sensing

In collaboration with the University of Iceland (UO) and Forschungszentrum Jülich (FZJ), CoE-RAISE co-organized the virtual event in the capacity of partner from May 31 to June 3, 2021.

[Read more](#)



**Application Co-Design for an AI Framework for Exascale**

One of the CoE RAISE goals is to design, implement, and evaluate an AI framework that is ready for future Exascale HPC systems (see 'AI at Exascale'). This framework is an enabler for highly scalable applications accelerating scientific discovery and advancing engineering in a wide variety of domains. It is co-designed by the RAISE Use Cases from natural sciences and engineering.

[Read more](#)

## Application Co-Design for an AI Framework for Exascale

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Fact Sheets foster the initial understanding of which components in different Use Cases are relevant on different levels. Figure 1 shows that those components include various software aspects required by the applications, such as necessary libraries, software codes, datasets, or container technologies. The hardware infrastructure aspects complement the overview with components such as specific HPC systems, GPU/CPU setups, innovative memory hierarchies, or data storages. As the Fact Sheets evolve, they act as living documents in CoE RAISE. They support the software engineering process driven by multi-disciplinary teams towards designing and implementing the AI framework. In some cases, Fact Sheets are part of scientific publications [1,2] and clarify the used software and hardware aspects. Additionally, they are helpful to explain the application Use Cases in CoE RAISE presentations to an audience outside the RAISE consortium.

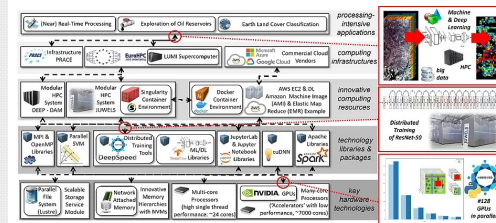


Figure 1: Fact Sheet example of a co-design Use Case in the application area of remote sensing [1].

Another goal of CoE RAISE is knowledge and technology transfer to the industry with many commercial consortium members (see 'Partners'). As shown in Figure 1, the Fact Sheets also demonstrate the bigger picture of Use Cases in delivering interoperability with cloud computing vendors and critical commercial technologies such as containers. The first iteration of Fact Sheets is almost finished. They will be available on the CoE RAISE web page and will include initial results from the Interaction Room process recently started in CoE RAISE.

The Fact Sheet process was received very positively by all members of the Use Case teams in CoE RAISE. It significantly enhanced the understanding of the Use Cases across the multi-disciplinary teams. The groups also noticed the massive complexity of designing an AI framework for Exascale, with the framework requiring a skillset from many domains, including software engineering, AI and HPC expertise, and application domain know-how. CoE RAISE and its Use Case teams have to overcome various understanding and communication challenges due to many different area-specific terminologies and possible misunderstandings. Hence, CoE RAISE requires a systematic interaction methodology to succeed in the co-design process with the nine Use Cases and potentially other future external Use Cases that will adopt the same methods for moving towards 'AI at Exascale'.

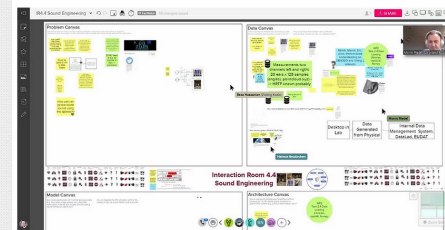


Figure 2: Interaction Room process example of using MURAL-based whiteboards in Zoom meetings.

The approach taken in CoE RAISE to address the challenges mentioned above is the Interaction Room methodology used to design enterprise management systems in the industry. It was adopted by Book et al. for HPC environments [3] and will be advanced in AI within the CoE RAISE project. The Interaction Room technique facilitates interdisciplinary collaboration in complex software projects and aims to improve the cooperation and communication between the Use Case experts from different disciplines.

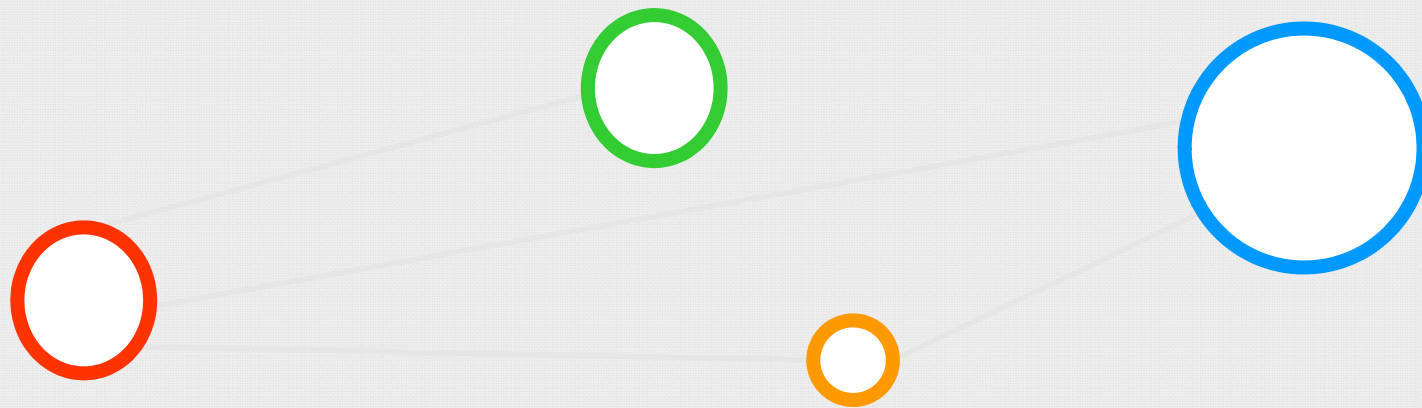
Figure 2 shows an example of the Interaction Room process in the CoE RAISE Use Case Sound Engineering. It is driven by a collaboration between the Icelandic *Acoustic and Tactile Engineering (ACUTE)* lab, the Icelandic start-up company *Treite* and *Forschungszentrum Jülich*. The Problem Canvas supports the understanding of the larger research question of the Use Case, including boundary conditions, abstractions, assumptions, quality requirements, and the goal of using AI. The use of AI varies between Use Cases may include surrogate models, simulation intertwined with AI to learn parameter sets, post-processing, or data-intensive workflows. The Data Canvas is used to clarify available datasets for AI methods such as datasets for training, testing, and validation, including approaches for feature engineering or data format conversions. The Model Canvas is used to identify relevant AI models in the Use Cases. This includes image-based models such as Convolutional Neural Networks (CNNs) or sequence-based models, e.g., Gated Recurrent Units (GRUs) or Long Short-Term Memory (LSTM) for time-series datasets. Finally, the Architecture Canvas maps the Model Canvas and Data Canvas items to corresponding specific HPC machines providing the necessary libraries and software. CoE RAISE just started the Interaction Room process with all the Use Case teams and will offer another news item on its results.



→ WP6 Input:  
News Item about  
Fact Sheet &  
Interaction Room  
Process  
Done (Morris,  
Helmut,  
Matthias)

<https://www.coe-raise.eu/news-2021-05>

## Agenda Item (3) – Status D2.6 “Support Report (M6)”

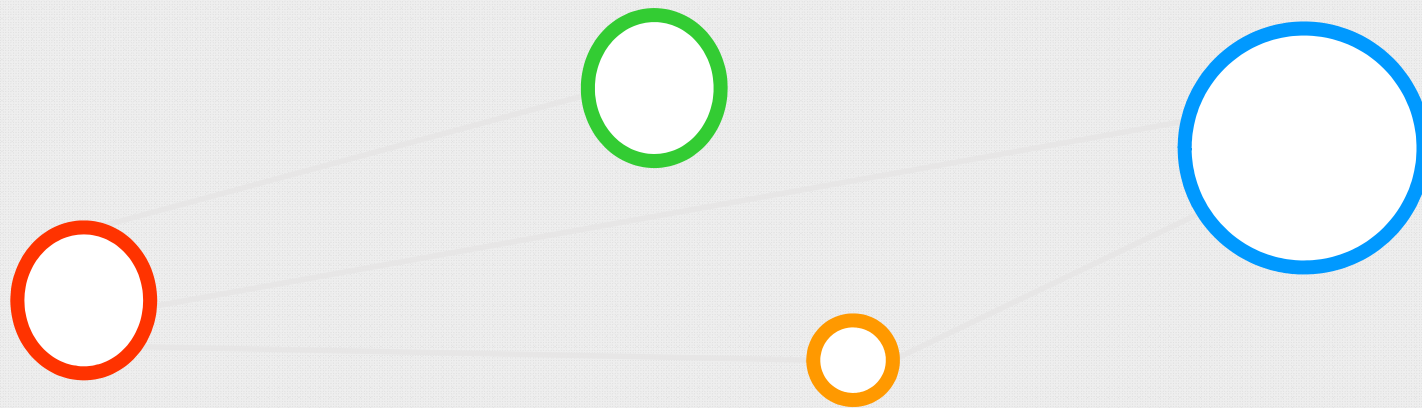


## Agenda Item (3) – Status D2.6 “Support Report (M6)”

➤ Eray Inanc / Marcel Aach



## Agenda Item (4) – Upcoming Milestone AI/HPC Methods (M7)





# Upcoming Milestone 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)
  - Refining our initial Matrix of Methods
  - **Start writing from next week**  
(TBD: Andreas Template? Morris first draft with others)

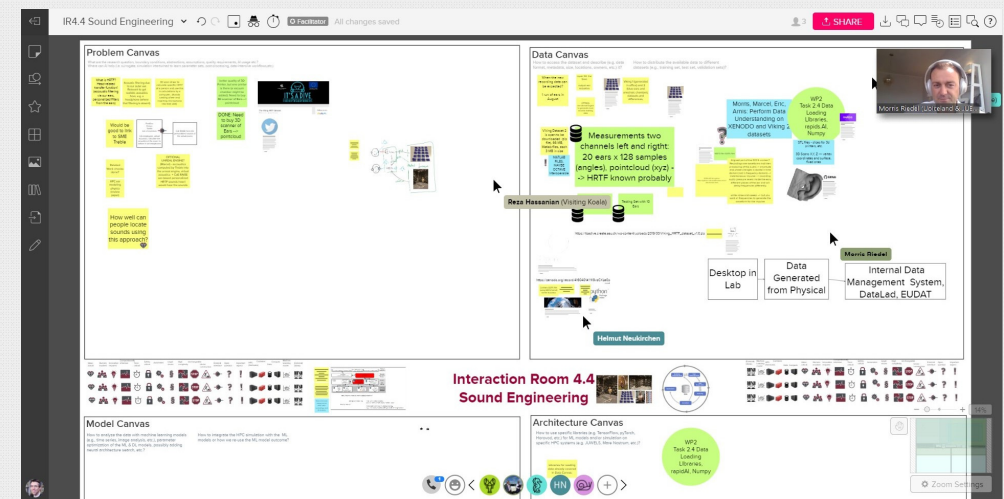
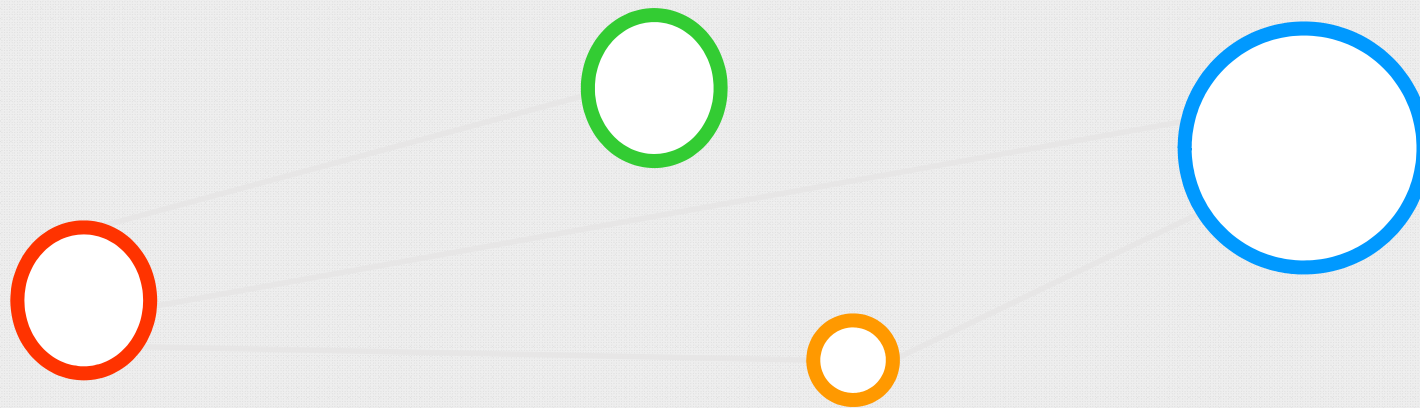


Table 6: Use-case vs. AI-methods matrix.

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

## Agenda Item (5) – Status RAISE Data Project

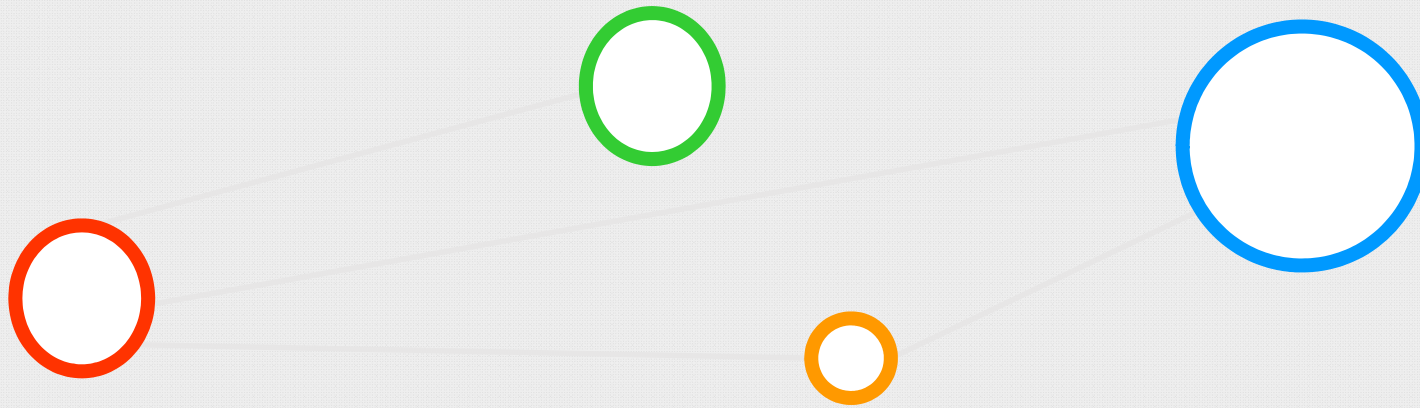


# Agenda Item (5) – Status RAISE Data Project

➤ Andreas Lintermann



# Agenda Item (6) – 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 (partly covered by T3.4)
- T3.5: Coating (started)

## ➤ WP4

- T4.1: Fundamental physics (pending)
- T4.2: Seismic imaging (pending)
- T4.3: Manufacturing (started)
- T4.4: Sound engineering (started)

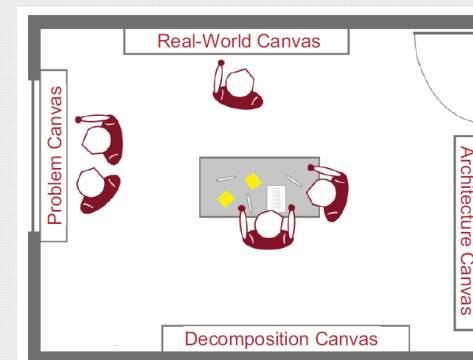
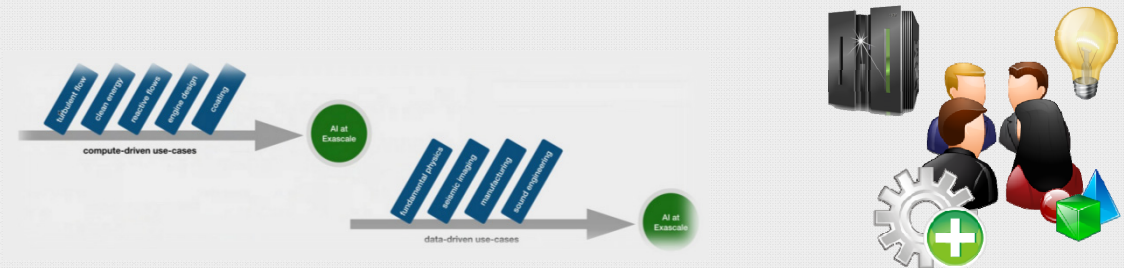


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Use-Case vs. AI-Methods	DA	NAS	AE	TL	PF	PDL	LSTM
Turbulent boundary layers	x	x	x	x	x	x	
Wind farm layout optimization	x			x	x	x	
AI for data-driven models in reacting flows				x		x	
Smart models for next-generation aircraft engine design	x	x		x		x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

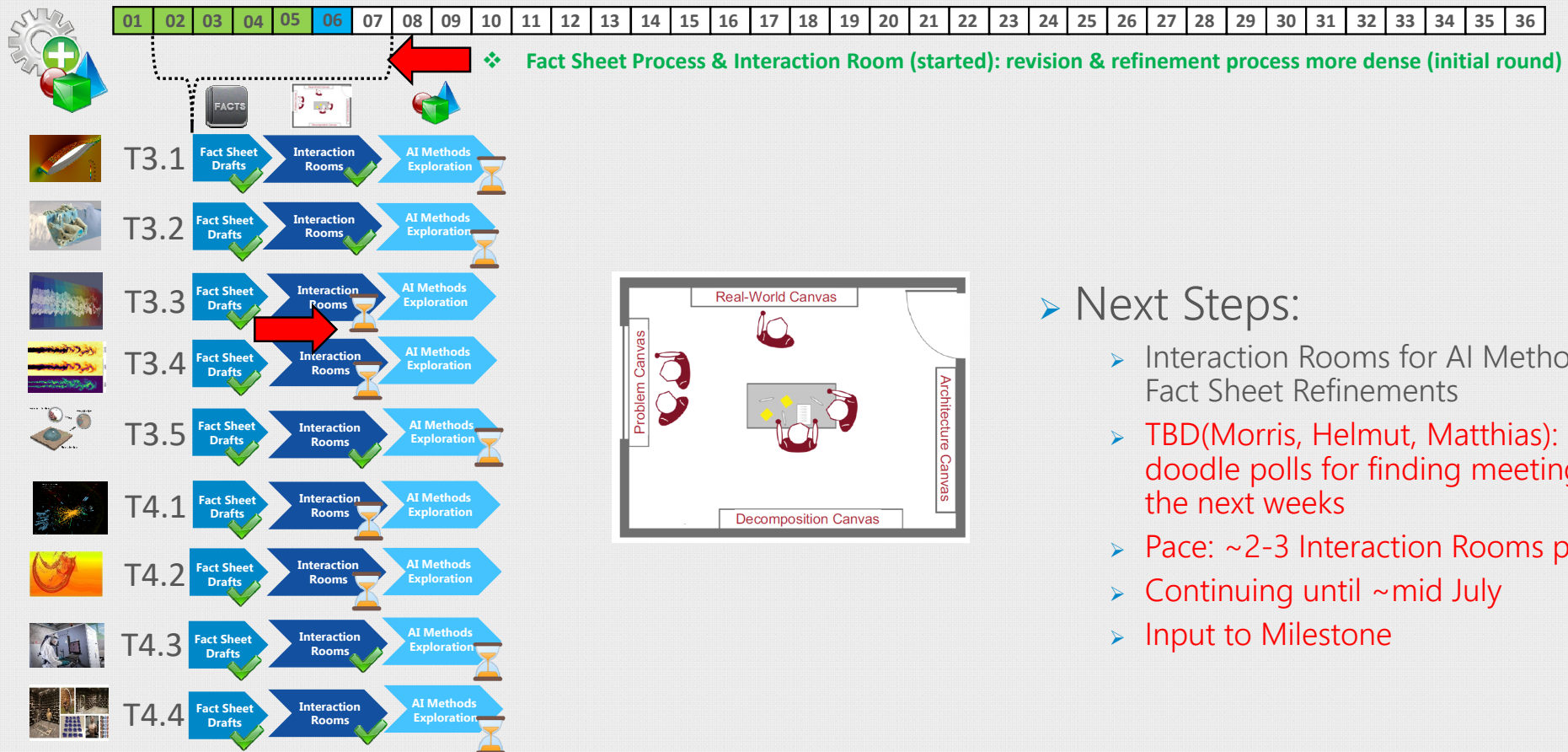
- Interaction Room scheduled with all teams
- Carve out more details on AI/HPC methods
- Identify concrete detailed algorithms



# Compelling Scoreboard Review – Use Case Progress



RAISE  
Center of Excellence



## Next Steps:

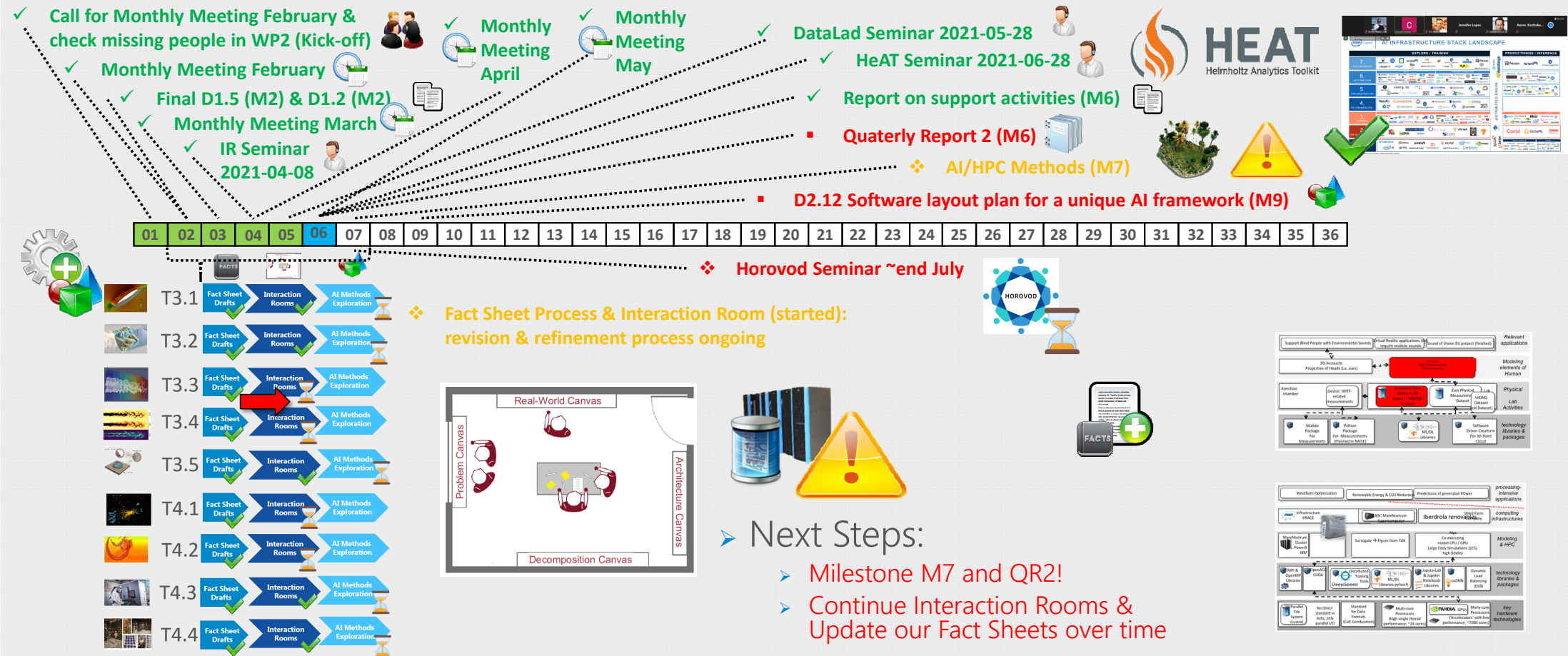
- Interaction Rooms for AI Methods & Fact Sheet Refinements
- TBD(Morris, Helmut, Matthias): invite to doodle polls for finding meeting spots over the next weeks
- Pace: ~2-3 Interaction Rooms per week
- Continuing until ~mid July
- Input to Milestone



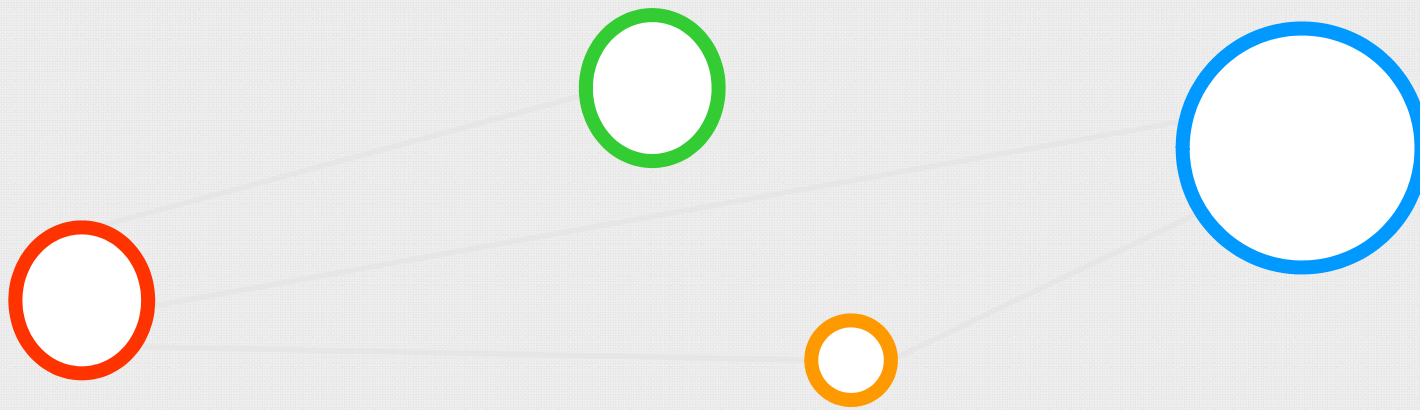
# Compelling Scoreboard Review & Next Steps



**RAISE**  
Center of Excellence



## Agenda Item (7) – Vacation WP2 Meeting July & AOB



# Agenda Item (7) – Vacation WP2 Meeting July & AOB



1. Vacation Period in July?
  1. July meeting feasible (Milestone, deliverable upcoming, etc.)
  2. Doodle poll to find out, maybe before mid July 12-16 July
  3. Seminar in July ok because recorded, but speakers also from us (e.g., Eric, Atos team, etc.)
2. AOB
  1. New slide templates from PMO?
  2. Galaxy to share data?
  3. Schedule in Outlook for Friday Interaction Room! 9:00 GMT / 11:00 CEST



drive. enable. innovate.



The CoE RAISE project have received funding from the European Union's Horizon 2020 – Research and Innovation Framework Programme H2020-INFRAEDI-2019-1 under grant agreement no. 951733