



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



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

Prof. Dr. – Ing. Morris Riedel et al.

School of Engineering & Natural Sciences, University of Iceland

2021-05-28, RAISE WP2 Monthly Meeting May 2021, Online



@ProfDrMorrisRiedel



@Morris Riedel



@MorrisRiedel



@MorrisRiedel



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

morris@hi.is

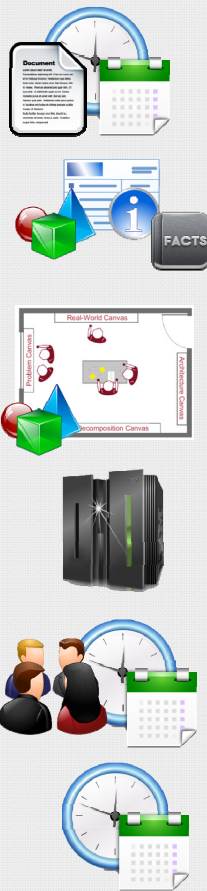


WP2 May Meeting – Welcome & Agenda

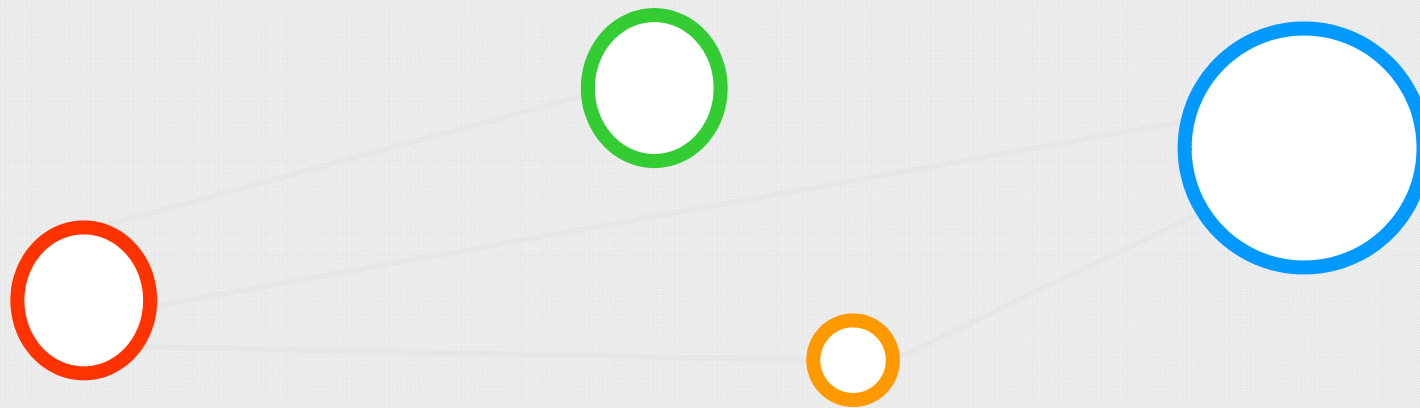


RAISE
Center of Excellence

1. Approval of minutes from Monthly Meeting April 2021
 - (All), ~5 Min
2. Review WP2 Status on Fact Sheets & Interaction Rooms
 - (Morris Riedel, Matthias Book, Helmut Neukirchen), ~15 Min
3. Plan & Start Deliverable D2.6 “Support Report”
 - (Eray Inanc), ~15 Min
4. Clarify Resource Provisioning
 - (Andreas Lintermann, Lauris Cikovskis), ~10 Min
5. Compelling Scoreboard Review & Next Steps
 - (All), ~10 Min
6. Next Monthly Meeting June & AOB
 - Doodle & Discussions, ~5 Min



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



Minutes Approval – Monthly Meeting April 2021



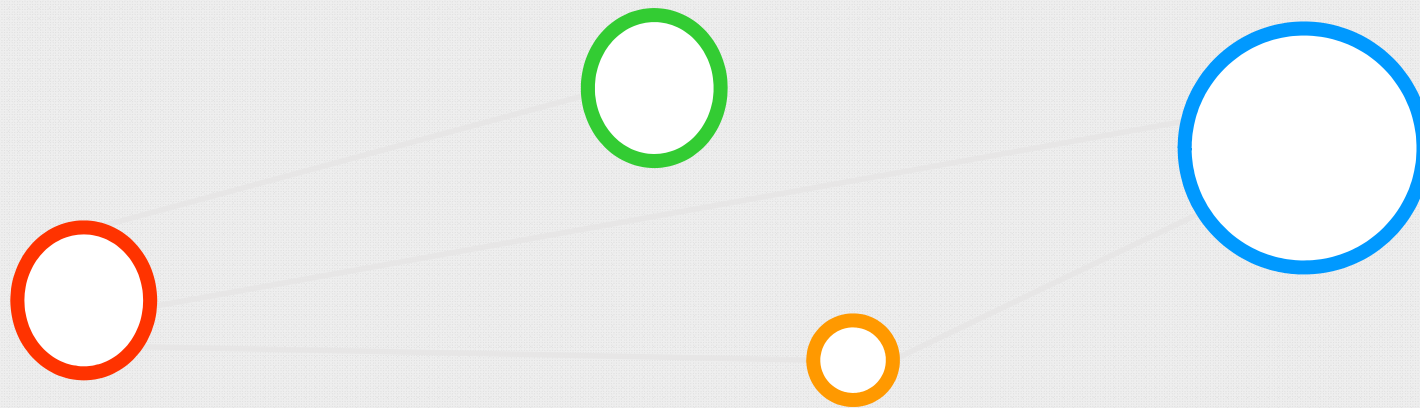
1. Minutes available in BSCW

- <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 action items for Interaction Room meetings

Open	Closed	All
Recent searches		
Search or filter results...		
Due date		
1s		
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 4.2 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 Flow & 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		
#10 - 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		

Monthly Meetings				insgesamt 4 Einträge		
Name	Aktion	Größe	Erzeugt von	Priorität	Letzte Änderung	Neu
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 15:13	
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 15:13	
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 2021-4-30						
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	
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		0	M.Riedel		2021-05-28 13:33	
Slides & Materials from meeting 2021-05-28						

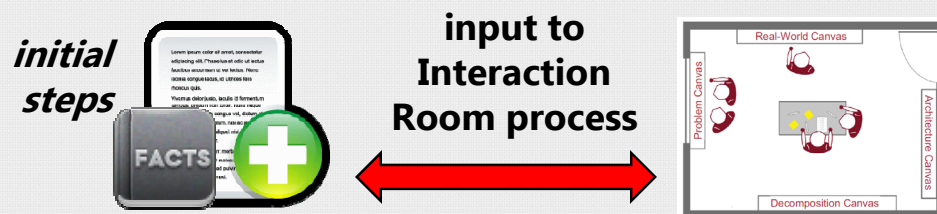
Agenda Item (2) – Review Status on Fact Sheets & Interaction Rooms



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 (available on BSCW)

Arbeitsbereiche von M.Riedel > CoE RAISE > WPs > WP2 > Fact Sheets

Suchen

Fact Sheets
Fact Sheets & Materials

insgesamt 12 Einträge

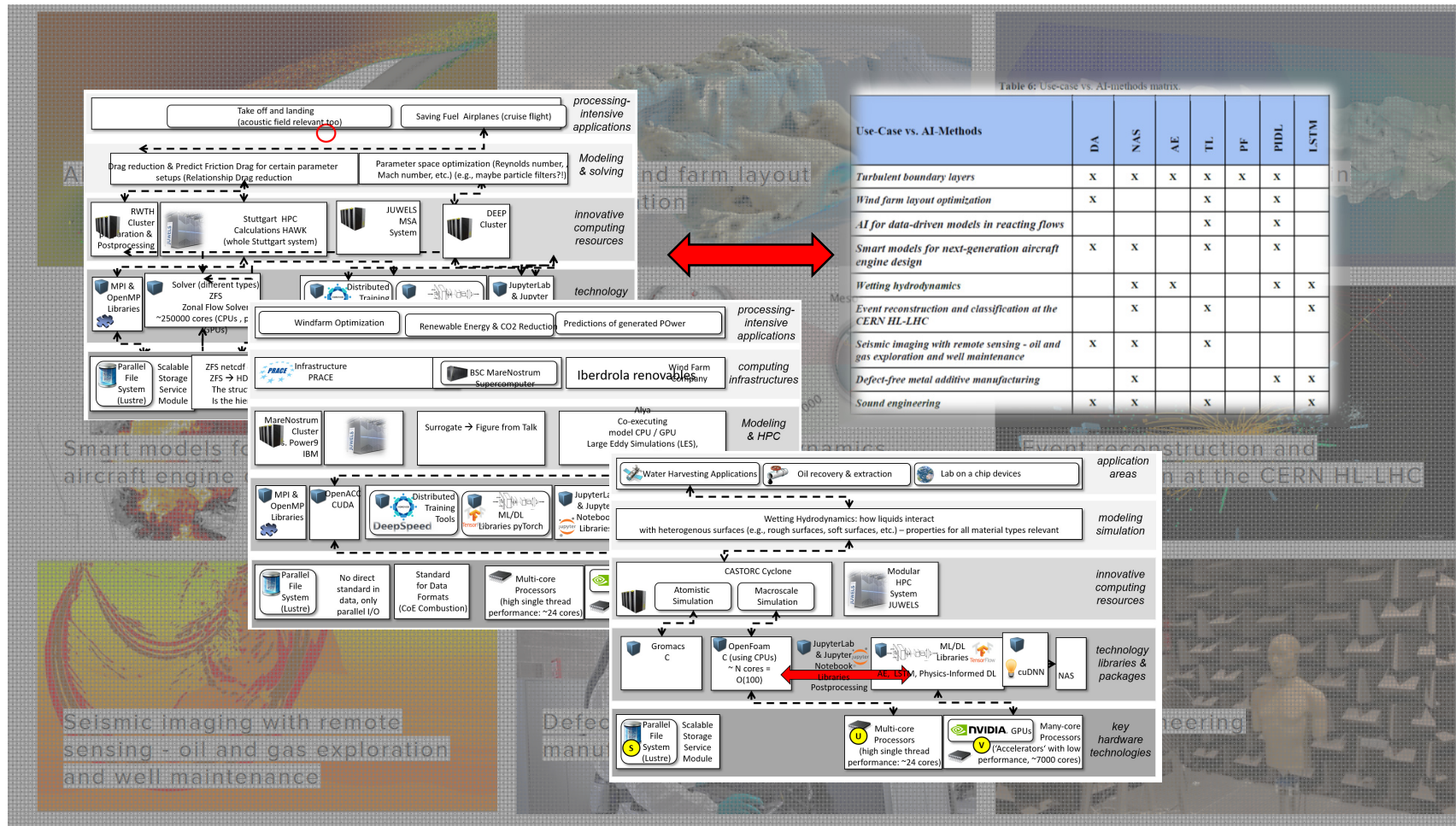
Name	Aktion	Größe	Erzeugt von	Priorität	Letzte Änderung	Neu
Examples from other Projects & Initiatives		4	M.Riedel		2021-04-29 21:42	
A selection of examples of Fact Sheets from previous projects and initiatives.						
T3.1 Turbulent Flow		2	M.Riedel		2021-04-29 22:26	
Task 3.1 AI for turbulent boundary layers <Leader: RWTH> <M1-M36>						
T3.2 Clean Energy		2	M.Riedel		2021-04-29 22:35	
Task 3.2 AI for wind farm layout optimization <Leader: BSC> <M1-M36>						
T3.3 Reactive Flows		2	M.Riedel		2021-04-29 22:46	
Task 3.3 AI for data-driven models in reacting flows <Leader: CERFACS> <M1-M36>						
T3.4 Engine Design		1	M.Riedel		2021-04-29 22:47	
Task 3.4 Smart models for next-generation aircraft engine design <Leader: SAFRAN> <M3-M36>						
T3.5 Coating		2	M.Riedel		2021-04-29 22:54	
Task 3.5 AI for wetting hydrodynamics <Leader: CYI> <M1-M36>						
T4.1 Fundamental Physics		2	M.Riedel		2021-04-30 00:53	
Task 4.1 Event reconstruction and classification at the CERN HL-LHC <Leader: CERN> <M1-M36>						
T4.2 Seismic Imaging		2	M.Riedel		2021-04-30 01:02	
Task 4.2 Seismic imaging with remote sensing - oil and gas exploration and well maintenance <Leader: CYI> <M1-M36>						
T4.3 Manufacturing		2	M.Riedel		2021-04-30 01:10	
Task 4.3 Defect-free metal additive manufacturing <Leader: FM> <M1-M36>						
T4.4 Sound Engineering		2	M.Riedel		2021-04-30 01:19	
Task 4.4 Sound engineering <Leader: UOI> <M1-M36>						
COE-RAISE-Proposal-Short-Names-Use-Cases-Overview.png		599 K	M.Riedel		2021-04-29 21:58	
Overview of short names of Use Cases from WP3 & WP4 (from CoE RAISE proposal)						
COE-RAISE-Proposal-Use-Cases-vs-AI-Methods.png		347 K	M.Riedel		2021-04-29 22:18	
Matrix of initial ideas of Use Cases vs. AI Methods (from CoE RAISE proposal)						



**WORK
IN
PROGRESS**

➤ <https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3340953>

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



**WORK
IN
PROGRESS**

Lessons Learned from CoE RAISE Draft Factsheets

➤ Fact Sheet process

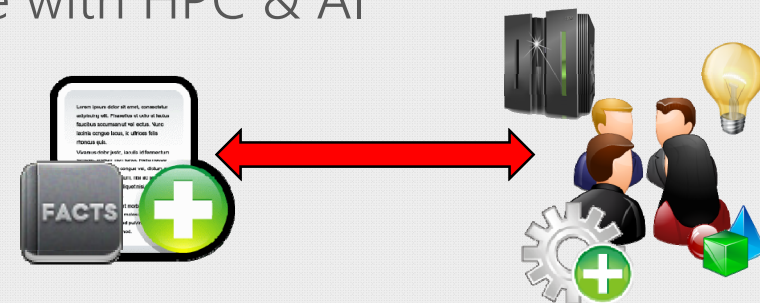
- Participants have been very positive understanding use cases & each other much better
- Enables really to understand where what components of use cases are running & why needed
- Fosters understanding what is confidential, e.g., what could be goals to for industry for a patent

➤ Massive complexity observed moving towards Exascale with HPC & AI

- Software engineering expertise required
- AI expertise required
- HPC expertise required
- Application domain-science know-how required

➤ Understanding & Communication → **Interaction Room Process**

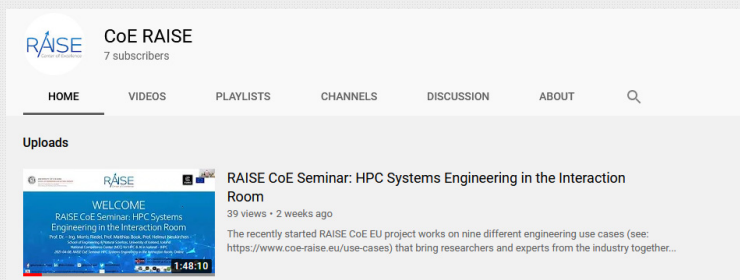
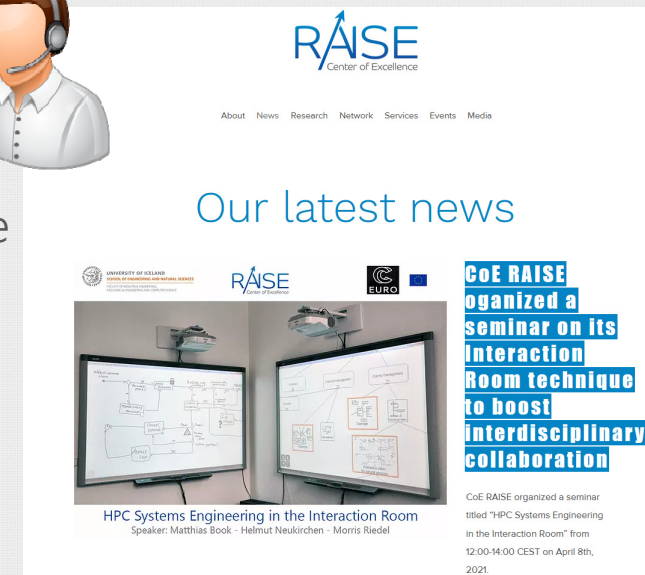
- Essential and lots of expertise area-specific terminology and misunderstandings
- Need for a systematic method to succeed in the nine use cases of CoE RAISE & external use cases



WP2 Seminar April – Interaction Room Performed on 8th April



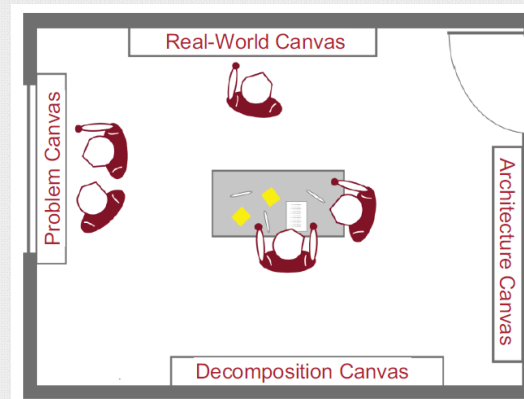
- Discuss shortly Feedback
 - Open to all communities (beyond RAISE)
 - Registration (input from WP6): enables user statistics & avoid trouble
- Material available on BSCW & RAISE@YouTube
 - <https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3396104>
 - @WP2 team: Subscribe to YouTube channel RAISE:
<https://www.youtube.com/channel/UCAdIZ-v6cWwGdapwYxdN7dg>



Started: Interaction Rooms / Use Case in May & June

➤ CoR RAISE Interaction Room Process as Next Step

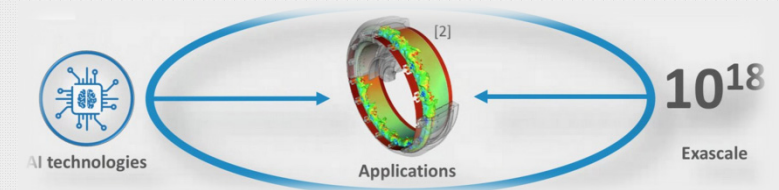
- Supports the proper software engineering design of the unique AI framework blueprint
- Expecting to work with WP3 & WP4 experts in an open minded way
- Process will be guided by Prof. Dr. Matthias Book
- Supported by Software Engineering & testing expert Prof. Dr. Helmut Neukirchen
- **Methology as one CoE RAISE outcome**



HPC Systems Engineering in the Interaction Room

Matthias Book

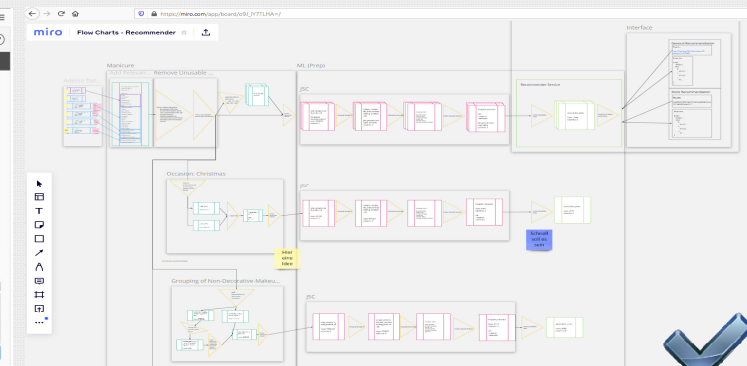
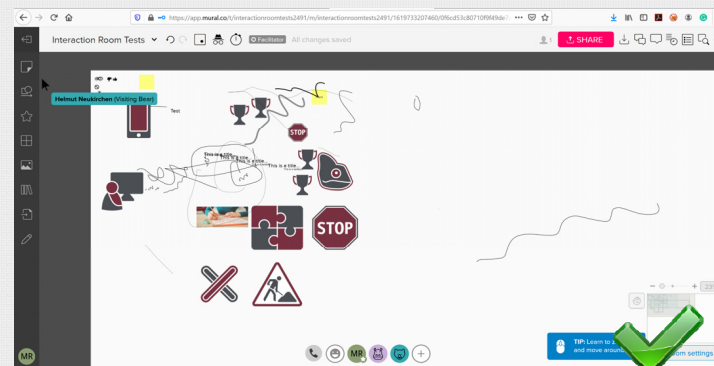
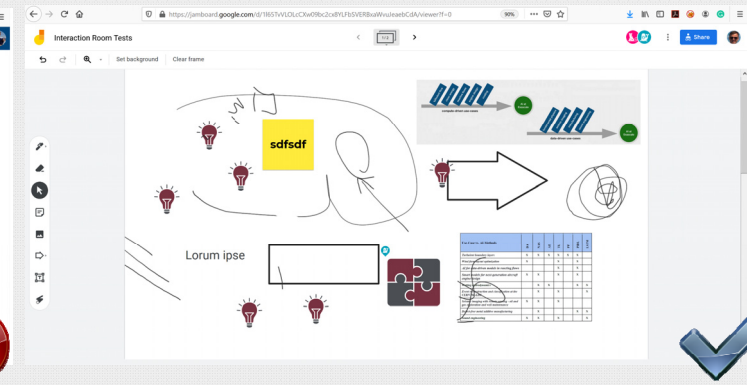
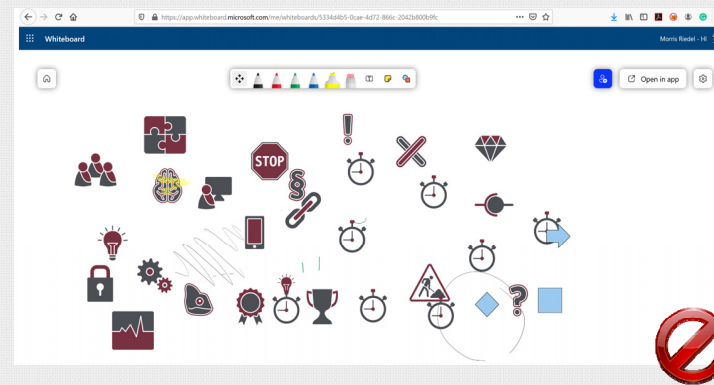
with Morris Riedel, Jülich Supercomputing Centre / UoI and Helmut Neukirchen, University of Iceland



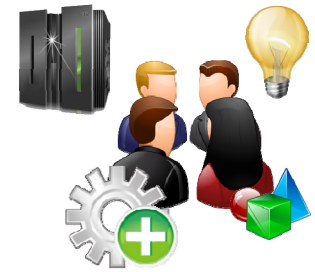
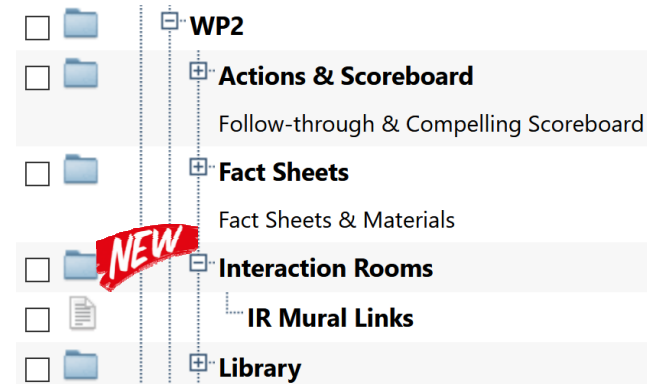
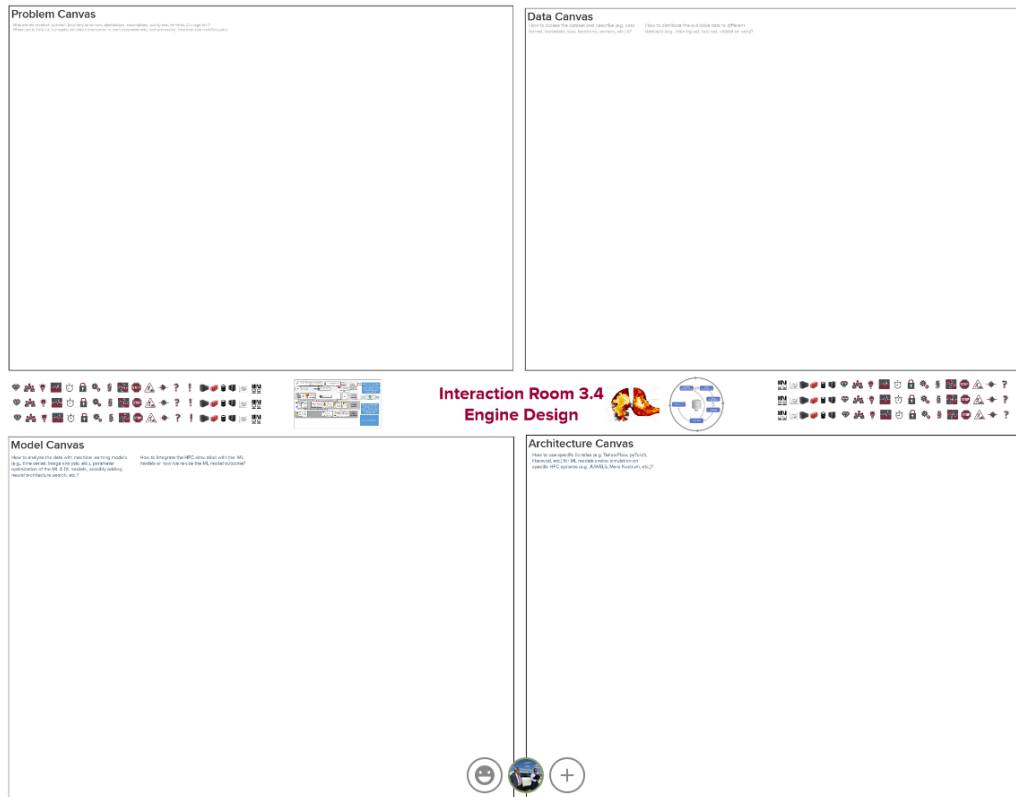
Book, M., Riedel, M., Neukirchen, H., Goetz, M.: [Facilitating Collaboration in High-Performance Computing Projects with an Interaction Room](#), in conference proceedings of the 4th ACM SIGPLAN International Workshop on Software Engineering for Parallel Systems (SEPS 2017), October 22-27, 2017, Vancouver, Canada

Interaction Rooms – Reviewed White Boards vs. Planned F2F

- Covid-19 Impact
 - No F2F meetings ('less productive')
 - Alternative: Online White Boards Tools
 - N^{infinity} of tools available
- Review of White Boards
 - Microsoft White Boards
 - Google Jam Boards
 - Miro Boards
 - Mural Boards seems ok
 - TBD(all): better ideas?
 - 'spatial.io' (Kurt), HW?



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/cb44cca3eed3bb9964fbfa36a1f6b1bfcc085f?sender=u15e3008bb41d6628a5bb5701>
- IR3.3 Reactive Flows: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377959022/0c363886f24833eeb19b025d87324b57fd50e2db?sender=u15e3008bb41d6628a5bb5701>
- IR3.4 Engine Design: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377976343/8d7aba6be09af3b2fd305d2f709c53661ac889d?sender=u15e3008bb41d6628a5bb5701>
- IR3.5 Coating: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377991014/7a5d7e1ea7230178342d1e1d4a84d656d9055d52?sender=u15e3008bb41d6628a5bb5701>
- IR4.1 Fundamental Physics: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378007335/6f0d5285f6ee3eaf515bd6676e84d8b4879d39?sender=u15e3008bb41d6628a5bb5701>
- IR4.2 Seismic Imaging: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ac3e28a4fbb8d9adbec33874998?sender=u15e3008bb41d6628a5bb5701>
- IR4.3 Manufacturing: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378038069/93df6fa7a41093f4eaae7bc9d727979dc2ba42b9d?sender=u15e3008bb41d6628a5bb5701>
- IR4.4 Sound Engineering: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa12219002404059f90a4bbb0101fa379a8503?sender=u15e3008bb41d6628a5bb5701>

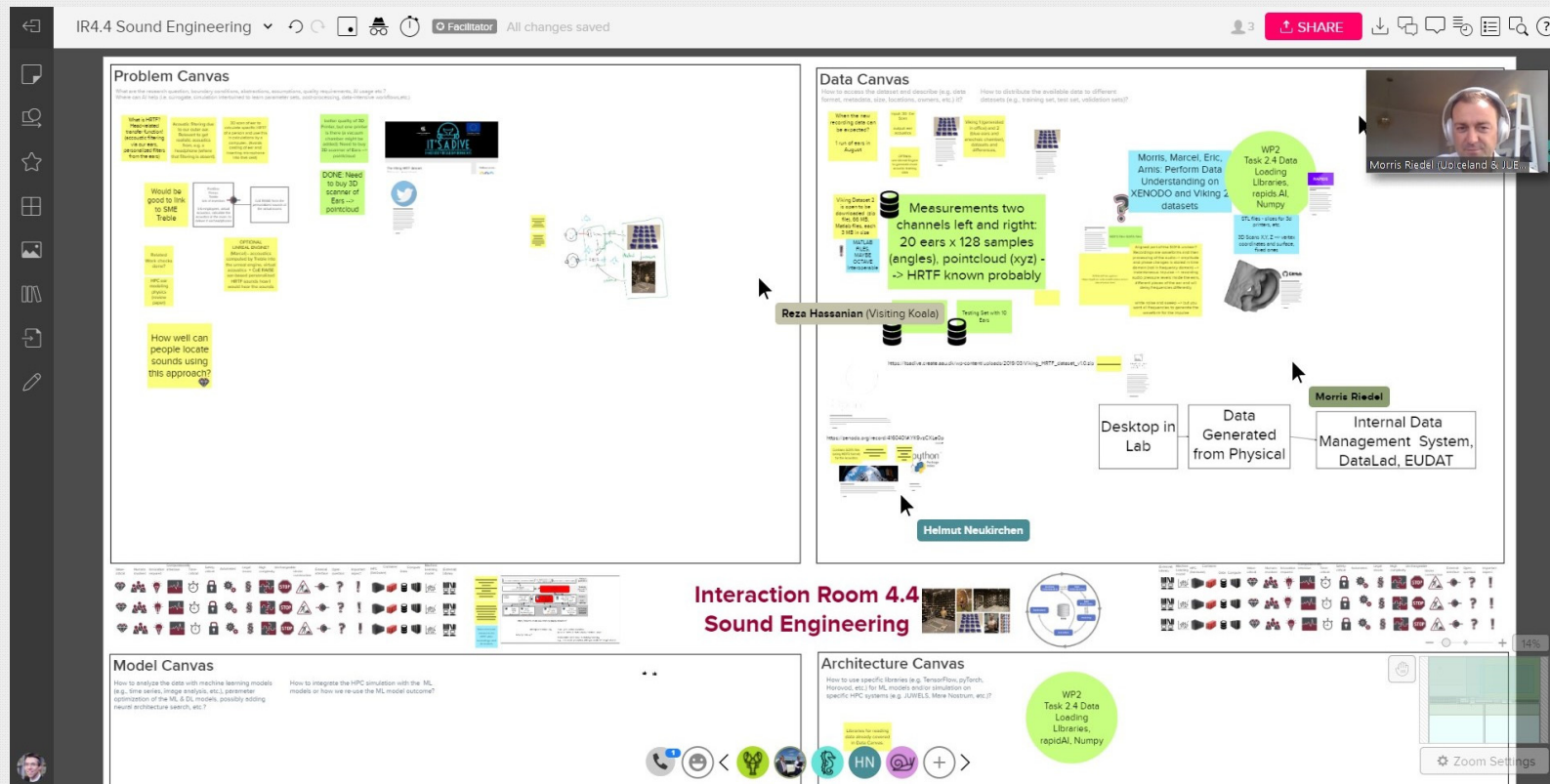
➤ <https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3591551>



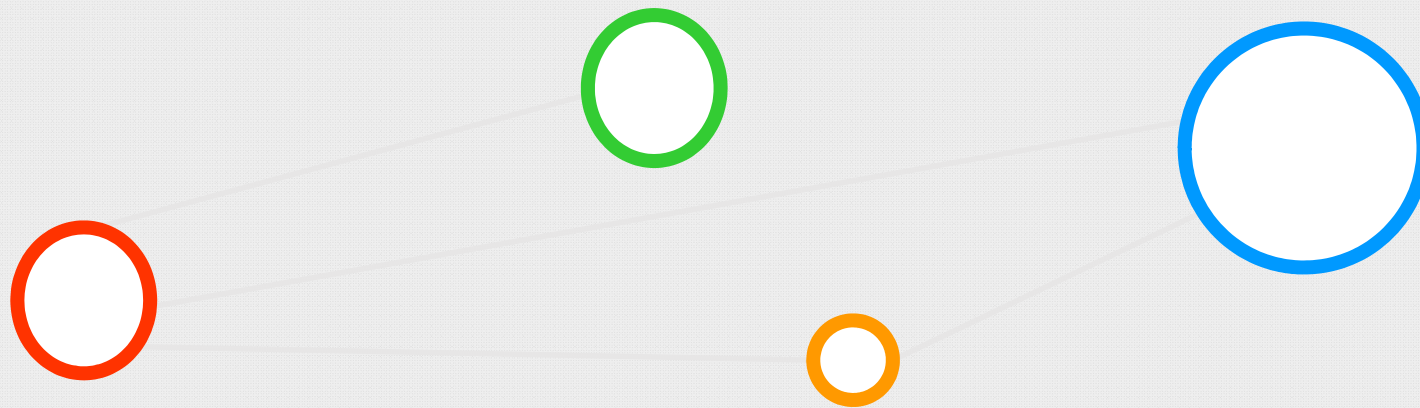
Interaction Rooms via MURAL Boards – Example (T4.4)



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



Agenda Item (3) – Plan & Start D2.6 “Support Report (M6)”

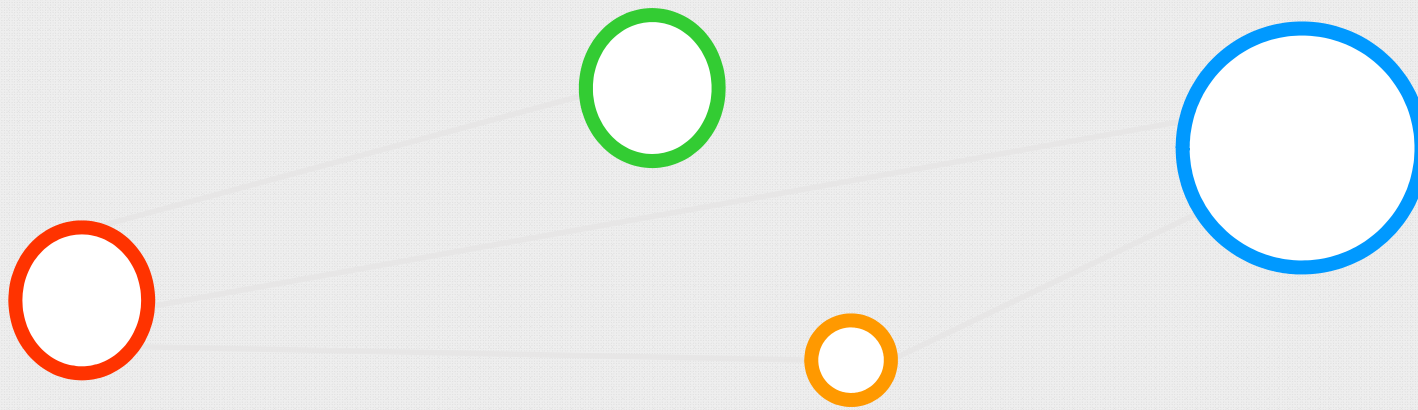


Agenda Item (3) – Plan & Start D2.6 “Support Report (M6)”

➤ Eray Inanc



Agenda Item (4) – Clarify Resource Provisioning

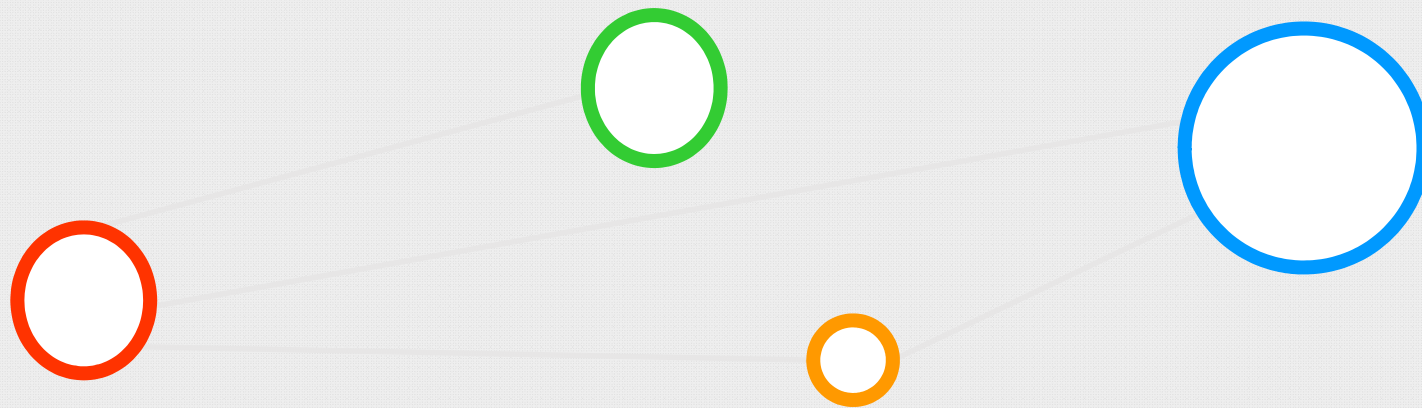


Agenda Item (4) – Clarify Resource Provisioning

➤ Andreas Lintermann, Lauris Cikovskis



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



Fact Sheet Status & Discussions – WP₃/WP₄ Tasks 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 (started)
- T4.2: Seismic imaging (started)
- T4.3: Manufacturing (started)
- T4.4: Sound engineering (started)

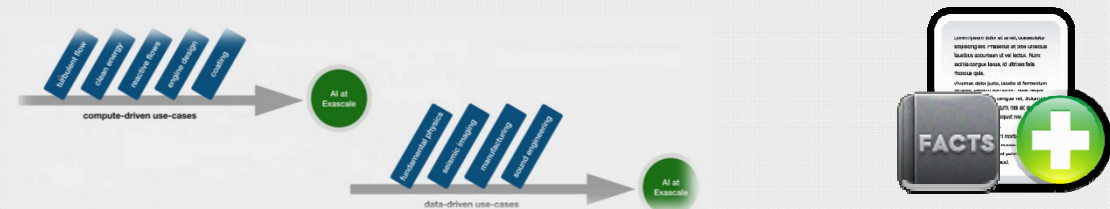


Table 6: Use-case vs. AI-methods matrix.

Use-Case vs. AI-Methods	DA	NAS	AE	TL	PF	PDL	LSTM
Turbulent boundary layers	x	x	x	x	x	x	
Wind farm layout optimization	x			x		x	
AI for data-driven models in reacting flows				x		x	
Smart models for next-generation aircraft engine design	x	x		x		x	
Wetting hydrodynamics		x	x			x	x
Event reconstruction and classification at the CERN HL-LHC		x		x			x
Seismic imaging with remote sensing - oil and gas exploration and well maintenance	x	x		x			
Defect-free metal additive manufacturing		x				x	x
Sound engineering	x	x		x			x

➤ Next Steps

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

Interaction Room Status & Discussions – WP3/WP4 Overview

➤ WP3

- T3.1: Turbulent Flow (pending)
- T3.2: Clean Energy (pending)
- T3.3: Reactive Flows (pending)
- 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 (pending)
- T4.4: Sound engineering (started)

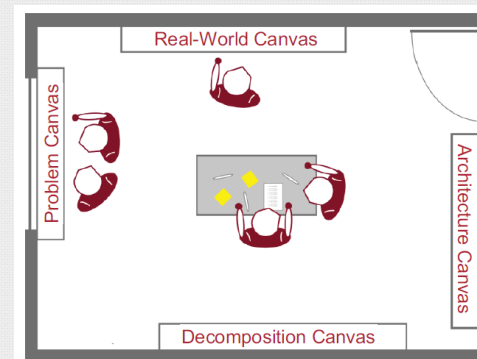
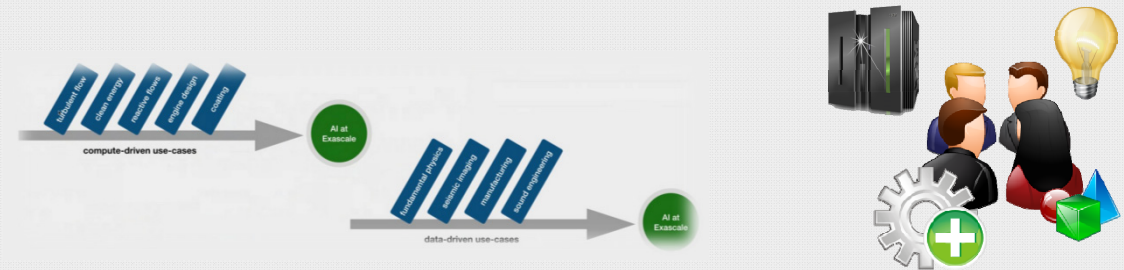


Table 6: Use-case vs. AI-methods matrix.

Use-Case vs. AI-Methods	DA	NAS	AE	TL	PF	PDL	LSTM
Turbulent boundary layers	x	x	x	x	x	x	
Wind farm layout optimization	x			x	x	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

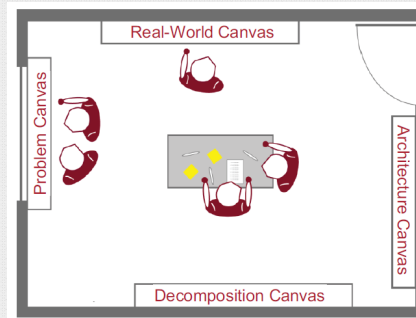
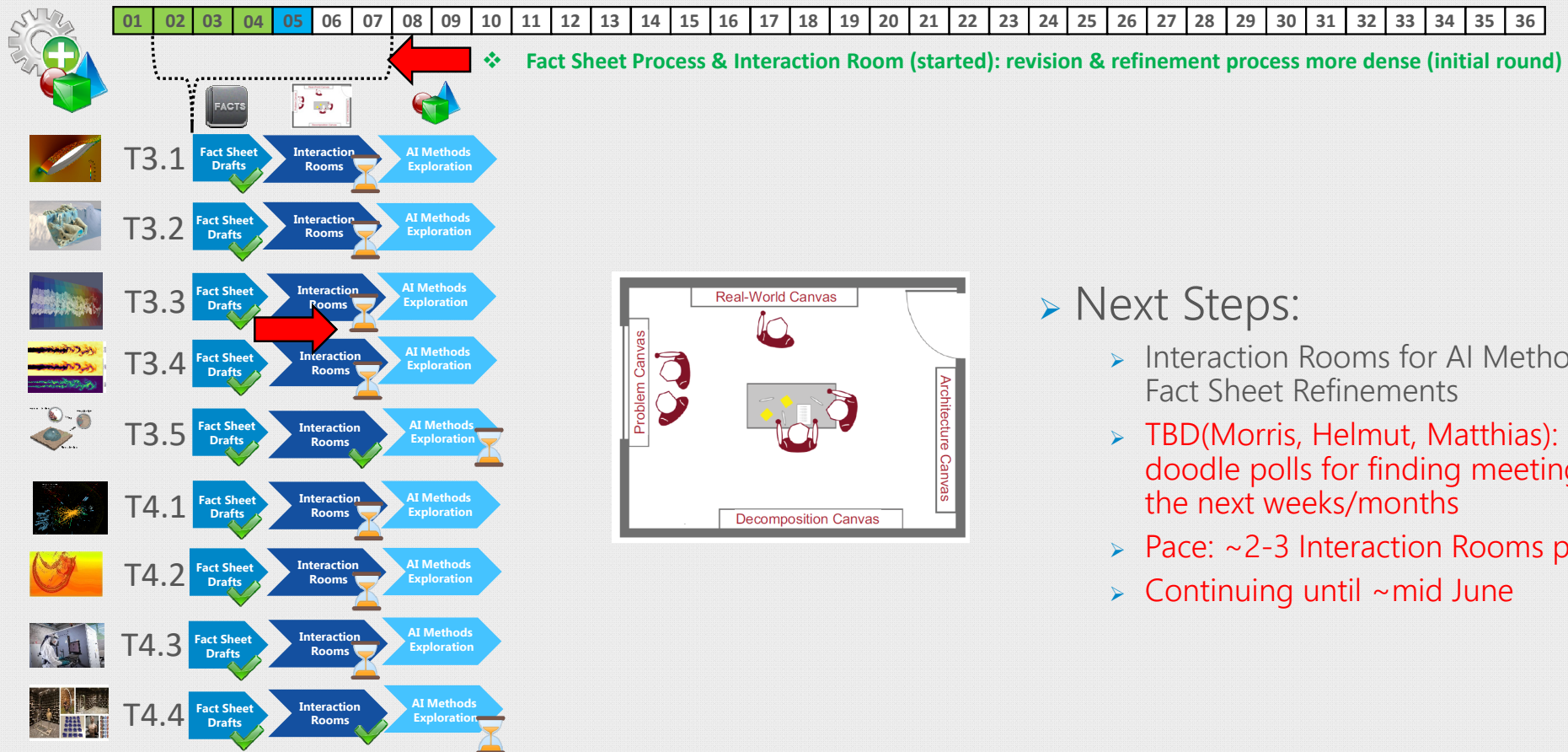
- Interaction Room scheduled with all teams
- Carve out more details on AI/HPC methods
- Identify concrete detailed algorithms



Compelling Scoreboard Review – Use Case Progress



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Next Steps:

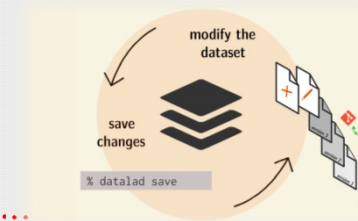
- Interaction Rooms for AI Methods & Fact Sheet Refinements
- TBD(Morris, Helmut, Matthias): invite to doodle polls for finding meeting spots over the next weeks/months
- Pace: ~2-3 Interaction Rooms per week
- Continuing until ~mid June



Seminar May: Git-based Data Management with DataLad

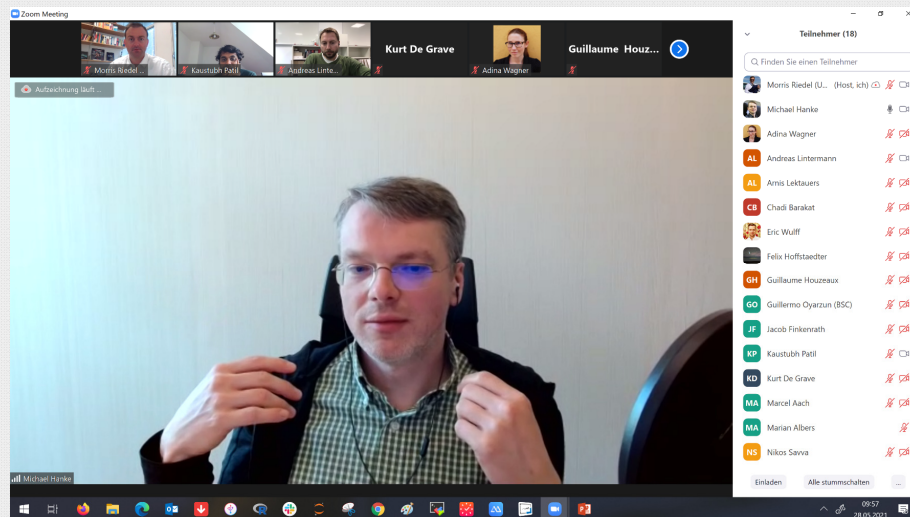
➤ Recorded Event, ~20 Participants

- Soon on our CoE RAISE YouTube Channel
- TBD (Michael, Morris): Needs cut some minutes, emails, sound, ...
- TBD (Morris, Andreas): Data Project in JSC for the project



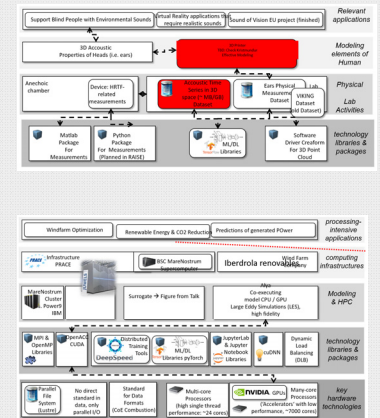
DataLad
DataLad can help
with small or large-scale
data management

<https://www.datalad.org/>

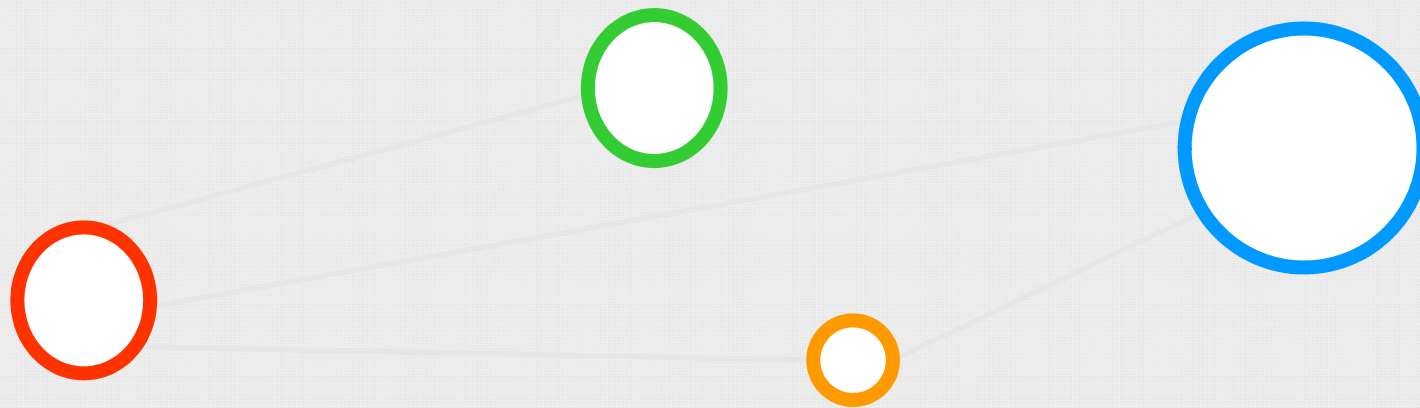




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Agenda Item (6) – WP2 Next Monthly Meeting May & AOB



Agenda Item (6) – WP2 Next Monthly Meeting & AOB



1. Next Monthly Meeting(s)

- May: Doodle will be available soon
- Topics: Selected progress with Factsheets & Interaction Room presentations
- Work towards Frameworks review: e.g. in contact with Helmholtz Analytics Framework (HAF) developers: Similar goals of RAISE CoE and interesting algorithm
 - TBD(Morris, Claudia, Björn): Meeting in May to discuss collaboration
- TBD(All): Discussions & AOB?
 - Lauris: Access to PRACE and partner sites different, (e.g. RTU pay for use)
 - TBD(Morris): Follow-up
 - TBD(Morris, Reza): Call for Interest → e.g., Arnis, etc. join in the interaction rooms
 - TBD(Matthias, Morris, Andreas) → Technical Coordination Board (→Wolfgang), range of expertise good, finding time to meet may be difficult



drive. enable. innovate.



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