



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

*2021-04-30, RAISE WP2 Monthly Meeting April 2021, Online*



@ProfDrMorrisRiedel



@Morris Riedel



@MorrisRiedel



@MorrisRiedel



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

morris@hi.is



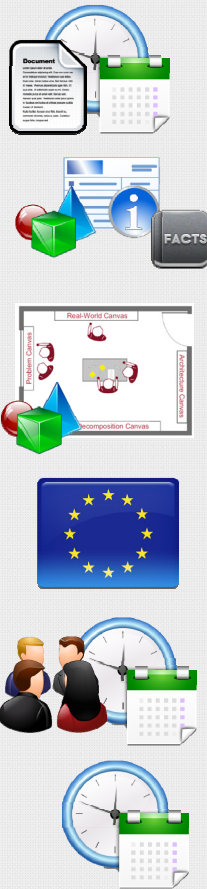


# WP2 April Meeting – Welcome & Agenda



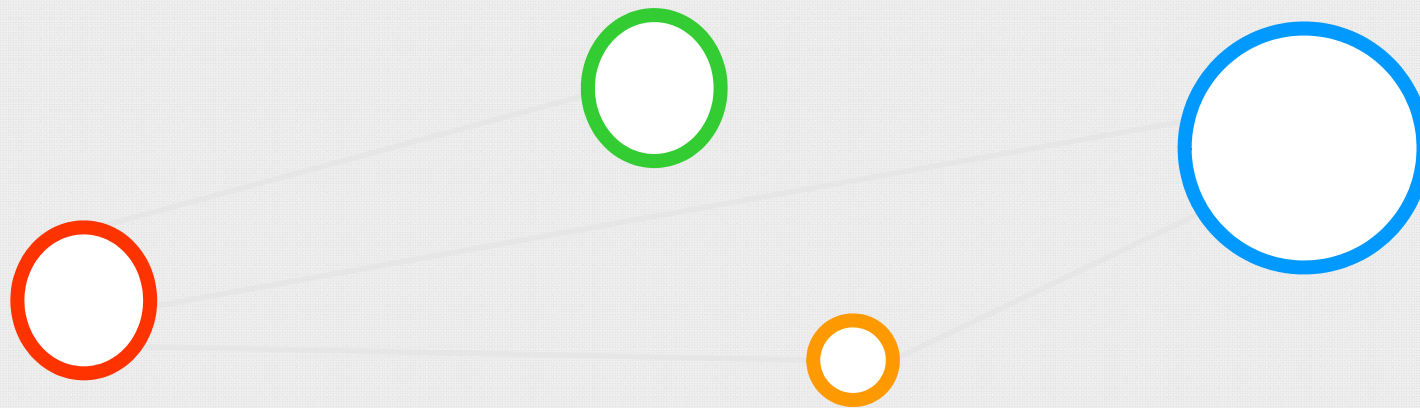
**RAISE**  
Center of Excellence

1. Approval of minutes from Monthly Meeting March 2021
  - (All), ~5 Min
2. Review WP2 Status on Fact Sheets and Quarterly Report 1
  - (Morris Riedel & Use Case Teams), ~15 Min
3. Discuss feedback Interaction Room Seminar & Next Steps
  - (Matthias Book, Helmut Neukirchen, Morris Riedel & All), ~15 Min
4. Discuss feedback from EU Fitness check of CoEs Event (2021-04-22)
  - (Andreas Lintermann, Morris Riedel), ~10 Min
5. Compelling Scoreboard Review & Next Steps
  - (All), ~10 Min
6. Next Monthly Meeting May & AOB
  - Doodle & Discussions, ~5 Min





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



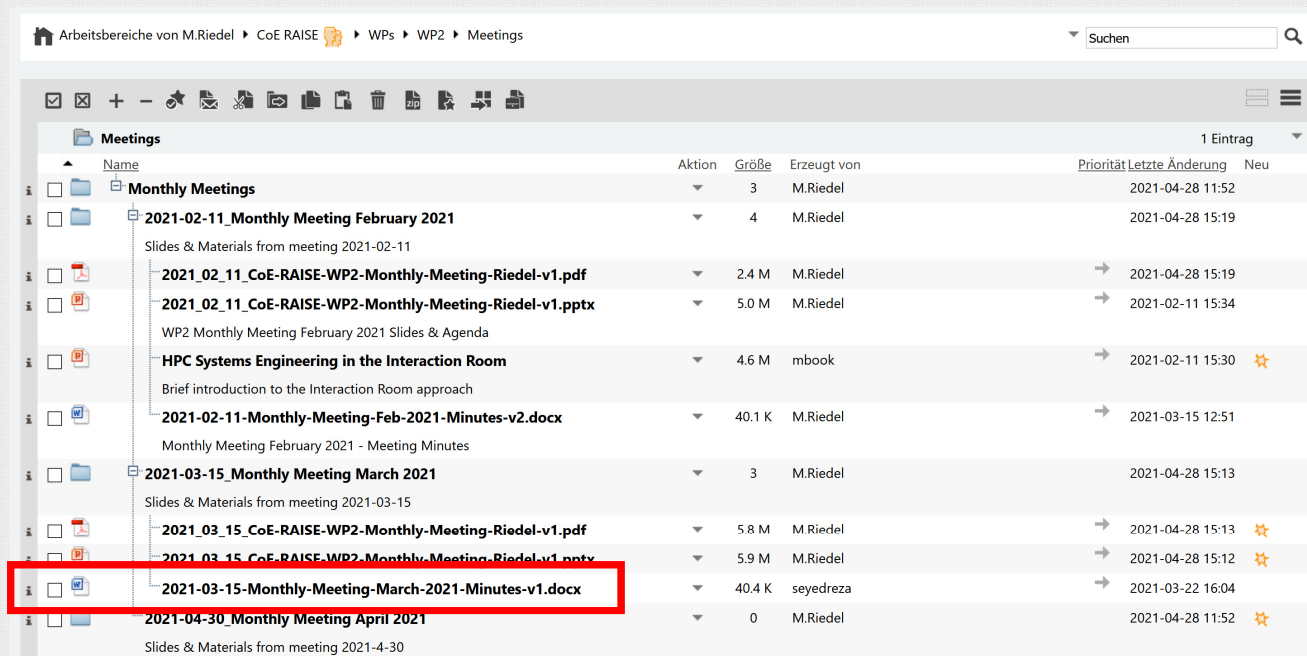
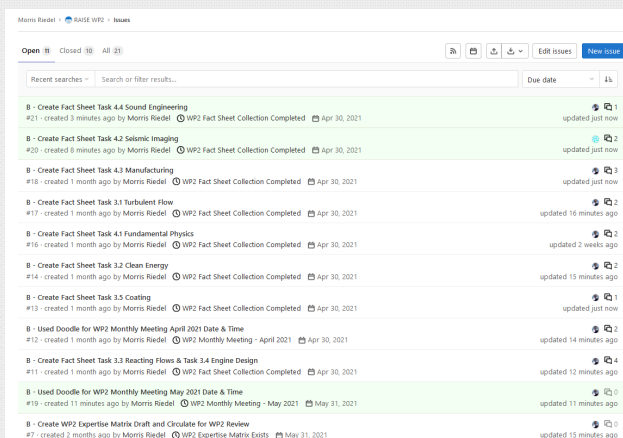


# Minutes Approval – Monthly Meeting March 2021



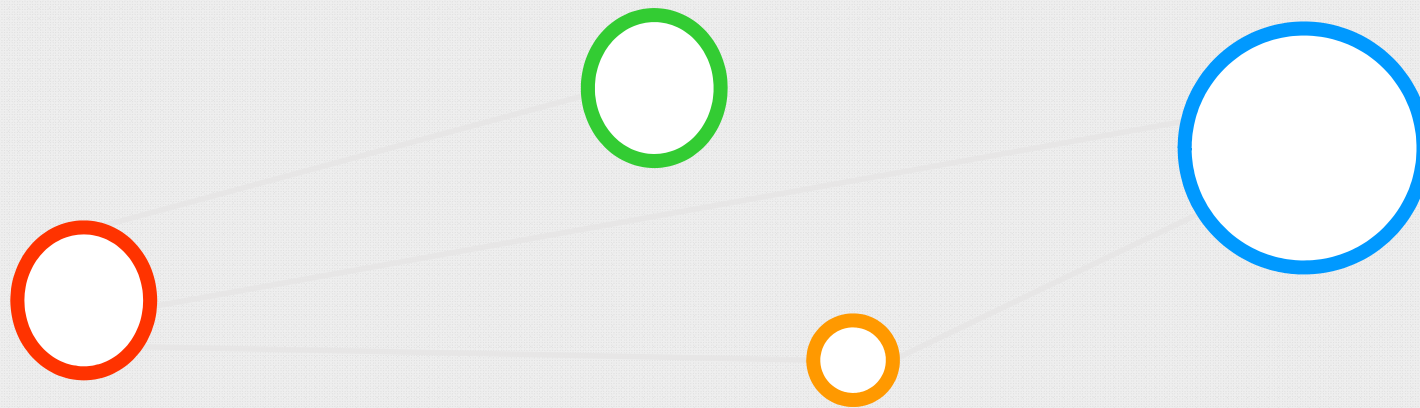
## 1. Minutes available in BSCW

- <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?
- No action items added to Action item tracker





## Agenda Item (2) – Review WP2 Status on Fact Sheets & QR1





# WP2 Updates – Quaterly Report 1 (QR1) in Library

- Thanks for all your contributions
  - QR1 shows already lots of activities and performed actions!
- QR1 Finalized
  - Clarifying one partner issue → done
  - Available in WP2 folder:  
<https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3396813>
- Published to PMO
  - Available also in RAISE project QR1 folder:  
<https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3270531>
- Process
  - Needs improvement for WP2 the next time (earlier call for inputs)
  - TBD(Morris, Reza): Add WP2 QR2, QR3, QR4 in Github Tracker



**RAISE** Center of Excellence

**CoE RAISE Quarterly Work Package Activity Report**

Work Package: AI- and HPC-Cross Methods at Exascale (WP2)  
Reporting Period: 01/2021 - 03/2021  
Author: Morris Riedel, UOI

**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 | not started yet |
| D2.13    | Report on novel AI technologies                                 | UOI              | 31.12.2021 | not started yet |
| D2.2     | Report on porting & performance engineering                     | BSC              | 31.12.2021 | not started yet |
| D2.10    | Monitoring report   | UOI              | 30.06.2022 | not started yet |
| D2.7     | Support report  | FZJ              | 30.06.2022 | not started yet |
| D2.14    | Report on novel AI technologies                                 | UOI              | 31.12.2022 | not started yet |
| D2.3     | Report on porting & performance engineering                     | BSC              | 31.12.2022 | not started yet |
| D2.8     | Benchmarking & support report                                   | FZJ              | 31.12.2022 | not started yet |
| D2.12    | Software framework layout plan                                  | UOI              | 31.10.2023 | not started yet |
| D2.11    | Monitoring report   | UOI              | 31.12.2023 | not started yet |
| D2.15    | Report on novel AI technologies                                 | UOI              | 31.12.2023 | not started yet |
| D2.4     | Report on porting & performance engineering                     | BSC              | 31.12.2023 | not started yet |
| D2.9     | Benchmarking & support report                                   | FZJ              | 31.12.2023 | not started yet |
| 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 |



# WP2 Updates – Library – Reminder & Update

## ➤ Collecting document relevant for WP2

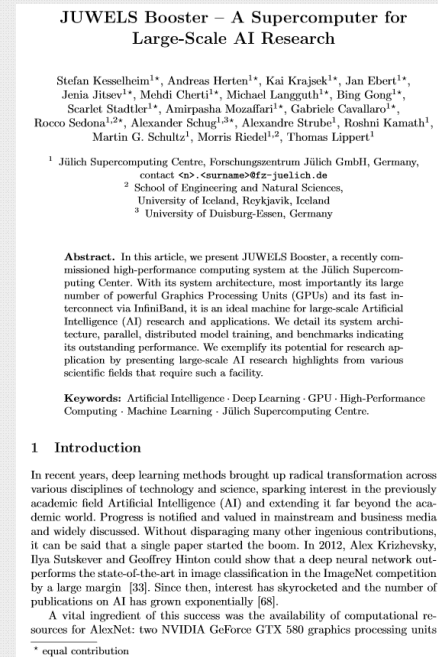
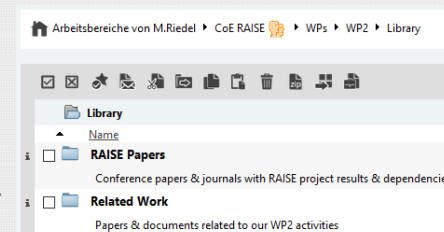
- Two major sections
- <https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3373074>

## ➤ RAISE Papers

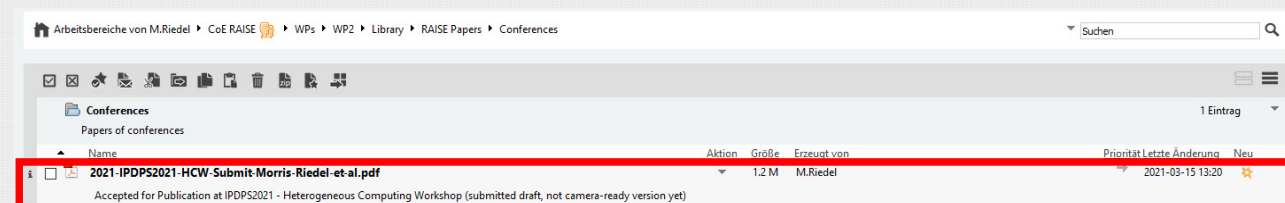
- Publications from us in RAISE!
- Project outcome descriptions
- Direct relevance for RAISE, e.g., RAISE acknowledgements in paper

## ➤ Related Work

- Papers & Technical Reports
- Policy documents
- ...



**availability  
pending  
main  
author**

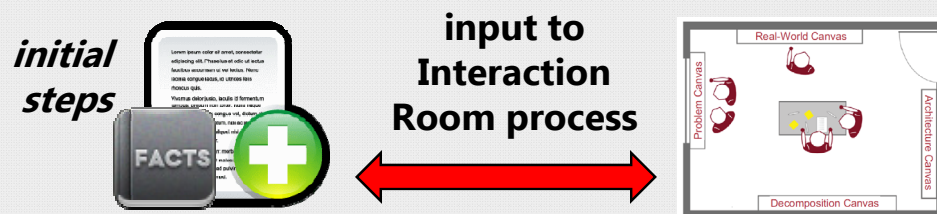




# WP2 Updates – Action Items Tracker

## ➤ 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



- TBD(Morris): Matrix of Experts (upload to BSCW)

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

Morris Riedel > RAISE WP2 > Issues

Open 11 Closed 10 All 21

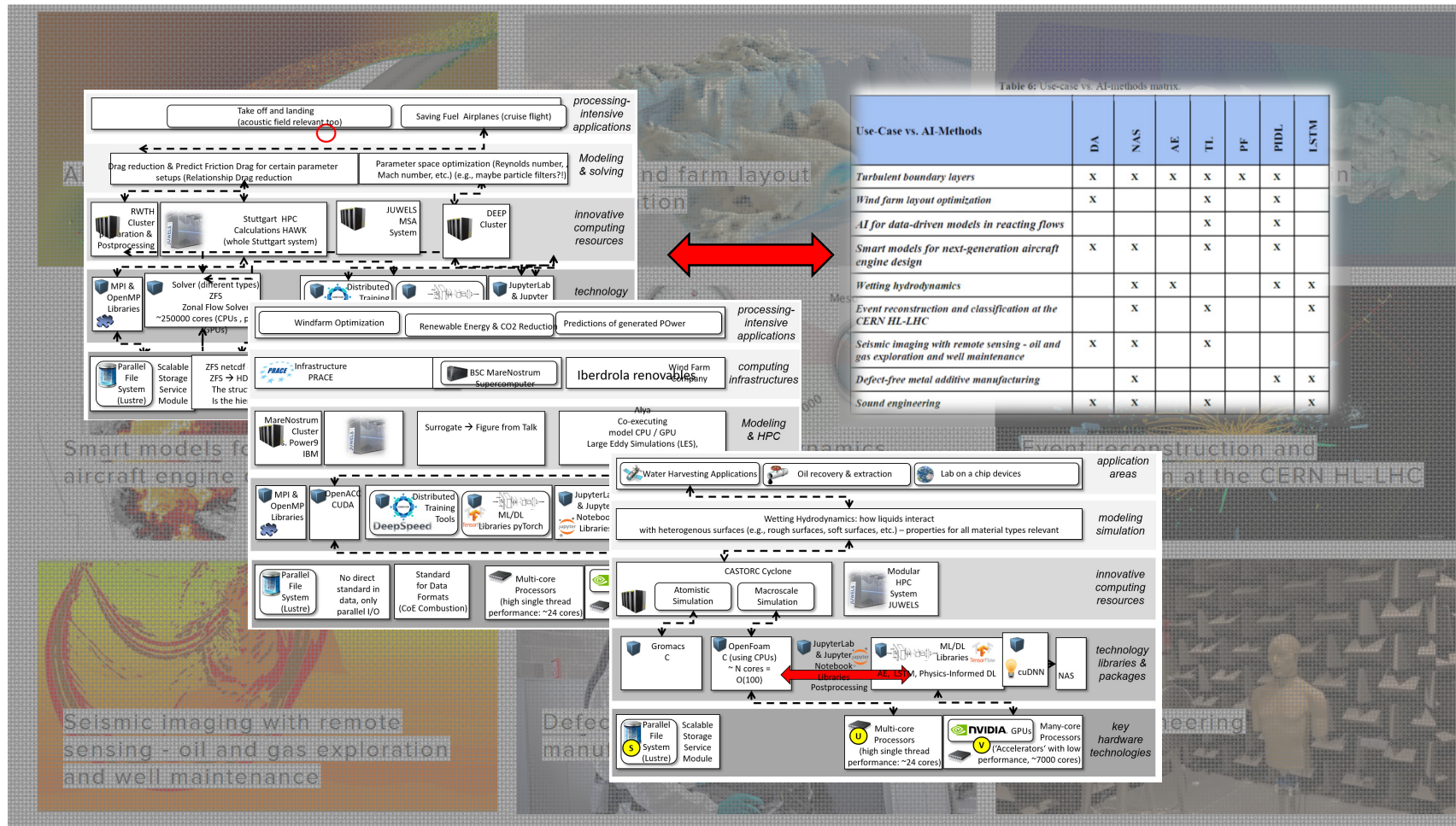
Recent searches Search or filter results... Due date

|  |   |                                     |              |   |                        |
|--|---|-------------------------------------|--------------|---|------------------------|
| 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 | 1 | 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 | 2 | 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 | 3 | 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 | 2 | 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 | 2 | 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 | 2 | 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 | 1 | 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 | 2 | updated 14 minutes ago |
| B - Create Fact Sheet Task 3.3 Reacting Flows & Task 3.4 Engine Design | #11 · created 1 month ago by Morris Riedel    | WP2 Fact Sheet Collection Completed | Apr 30, 2021 | 4 | updated 12 minutes ago |
| B - Used Doodle for WP2 Monthly Meeting May 2021 Date & Time           | #19 · created 11 minutes ago by Morris Riedel | WP2 Monthly Meeting - May 2021      | May 31, 2021 | 0 | 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 | 0 | updated 15 minutes ago |





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



**WORK  
IN  
PROGRESS**



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



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PROGRESS**

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



# Lessons Learned from CoE RAISE Draft Factsheets

## ➤ Fact Sheet process

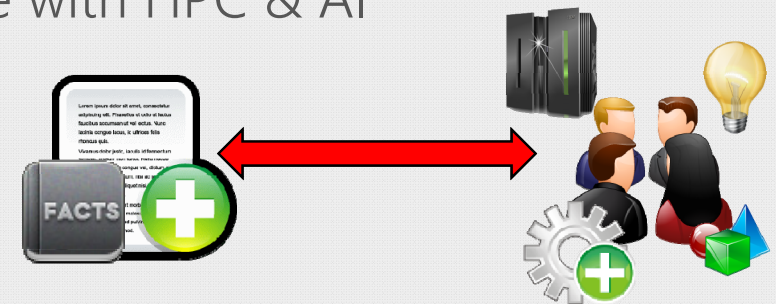
- Participants have been very positive understanding use cases & each other much better
- Enables really to understand where what components of use cases are running & why needed
- Fosters understanding what is confidential, e.g., what could be goals to for industry for a patent

## ➤ 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**

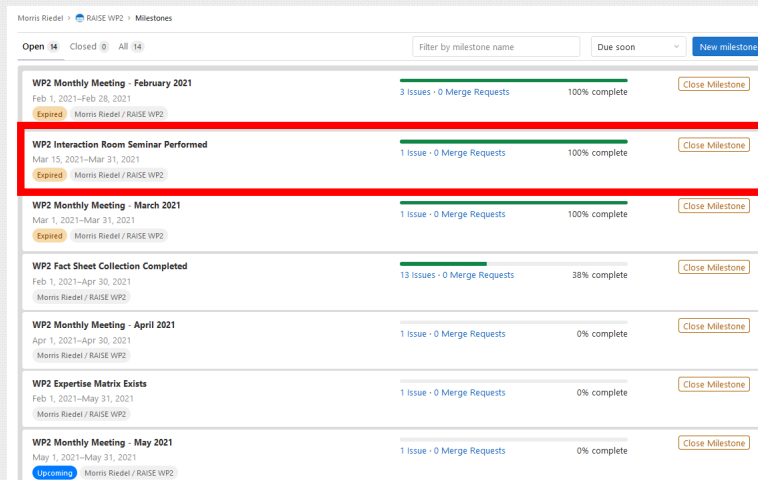
- Essential and lots of expertise area-specific terminology and misunderstandings
- Need for a systematic method to succeed in the nine use cases of CoE RAISE & external use cases



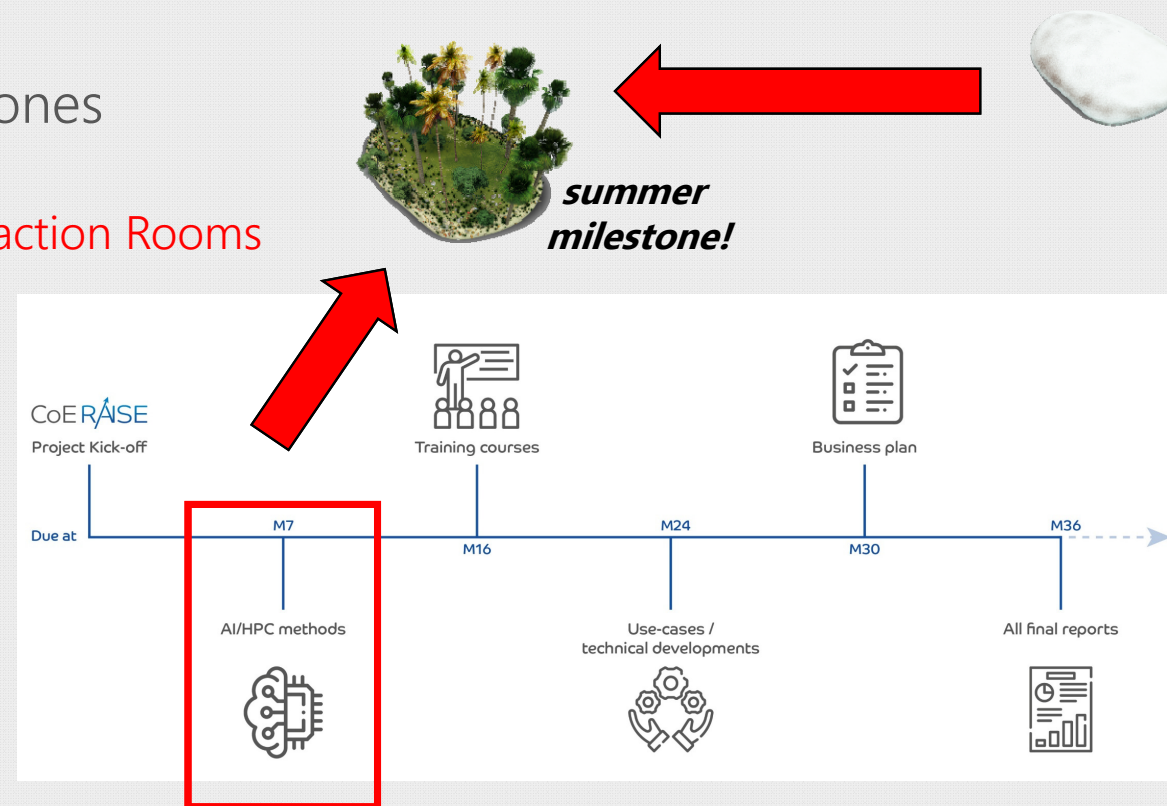


# WP2 Updates – Milestones Review → Summer Milestone!

- WP Milestones & Project-Wide Milestones
  - WP2 Milestones in GitHub ok so far
  - TBD(Morris, Helmut, Matthias): Add Interaction Rooms



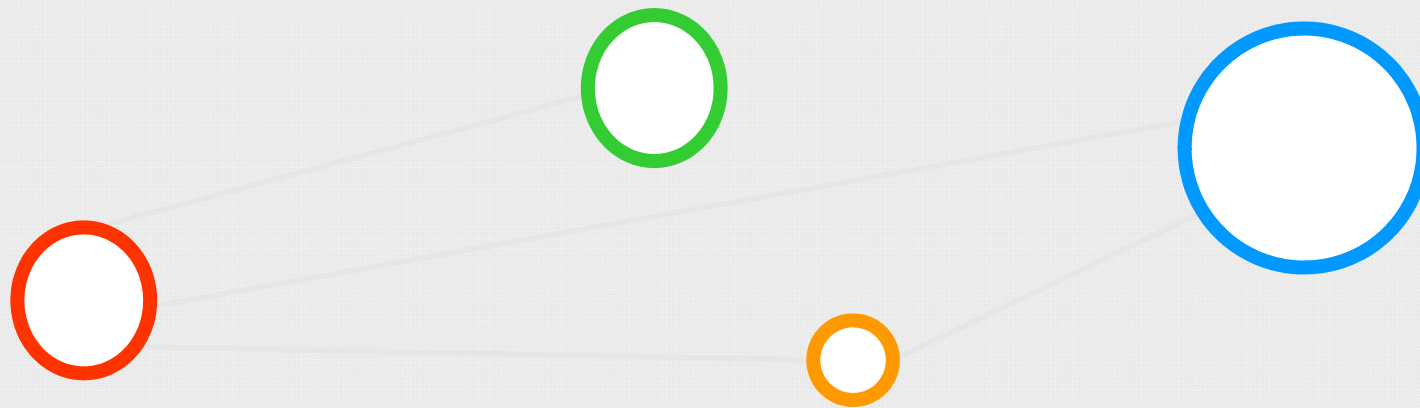
| Milestone                              | Status   | Issues | Merge Requests | Completion    | Action          |
|--|----------|--------|----------------|---------------|-----------------|
| WP2 Monthly Meeting - February 2021    | Expired  | 3      | 0              | 100% complete | Close Milestone |
| WP2 Interaction Room Seminar Performed | Expired  | 1      | 0              | 100% complete | Close Milestone |
| WP2 Monthly Meeting - March 2021       | Expired  | 1      | 0              | 100% complete | Close Milestone |
| WP2 Fact Sheet Collection Completed    | Expired  | 13     | 0              | 38% complete  | Close Milestone |
| WP2 Monthly Meeting - April 2021       | Expired  | 1      | 0              | 0% complete   | Close Milestone |
| WP2 Expertise Matrix Exists            | Expired  | 1      | 0              | 0% complete   | Close Milestone |
| WP2 Monthly Meeting - May 2021         | Upcoming | 1      | 0              | 0% complete   | Close Milestone |



- TBD(Morris): Clarify with PMO expectations on M7 milestone (format) & add to Action Item Tracker



## Agenda Item (3) – Feedback Interaction Room Seminar & Next Steps





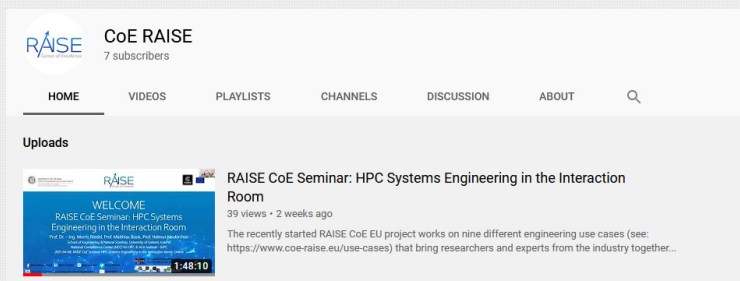
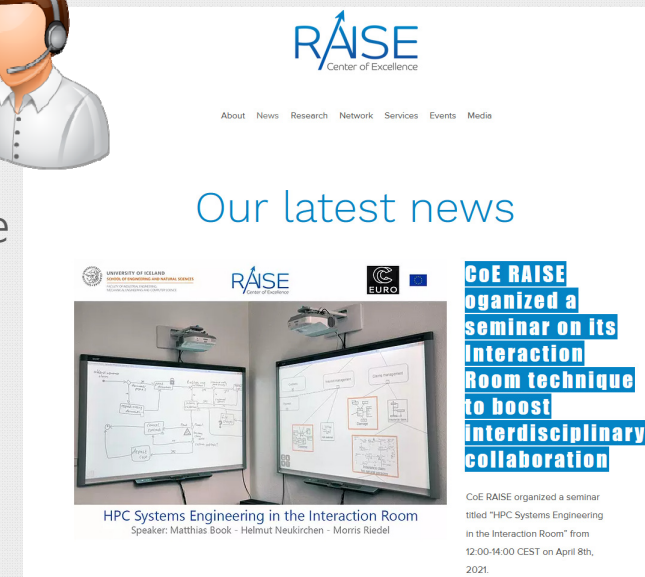
# WP2 Seminar April – Interaction Room Performed on 8<sup>th</sup> April

## ➤ Discuss shortly Feedback

- Open to all communities (beyond RAISE)
- Registration (input from WP6): enables user statistics & avoid trouble
- **TBD(all): Any other comments and/or suggestions?**

## ➤ 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>



## ➤ Follow-Up

- **TBD(Morris, Rose): Statistics of Interaction Room**
- **TBD(Morris): Add GitLab Seminar to Action Item Tracker**

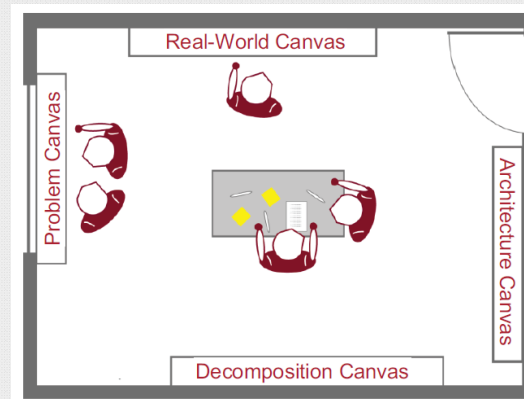


# Next Steps: Interaction Rooms / Use Case in May & June

## ➤ 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

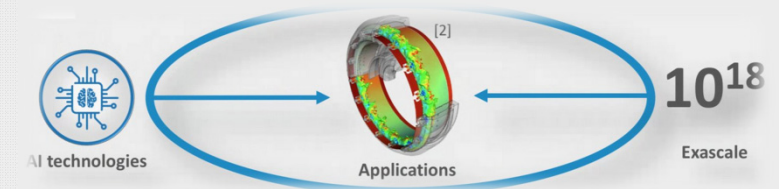
- **Methology as one CoE RAISE outcome**
- **TBD(Matthias, Helmut, Morris): Setup & Review of White Boards**



## HPC Systems Engineering in the Interaction Room

Matthias Book

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

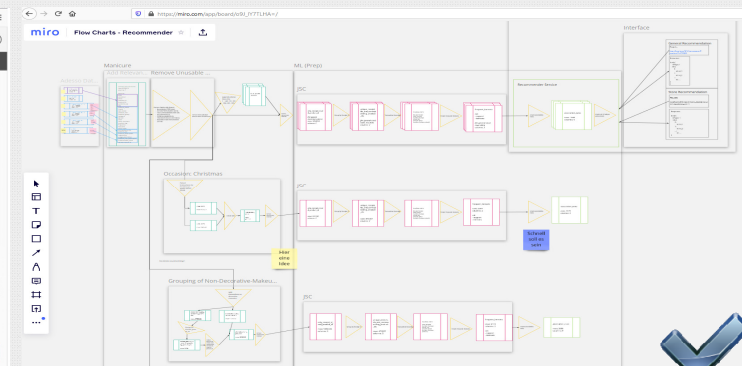
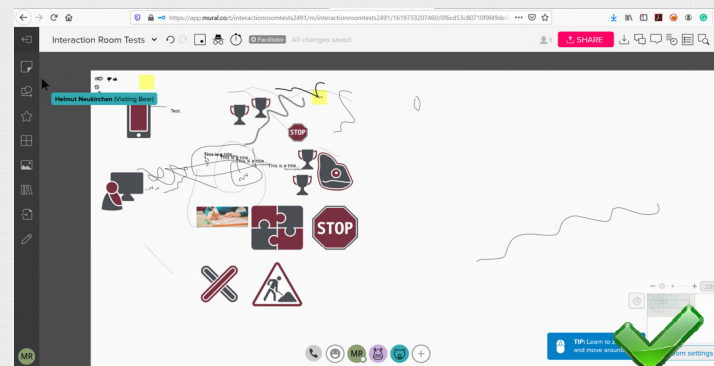
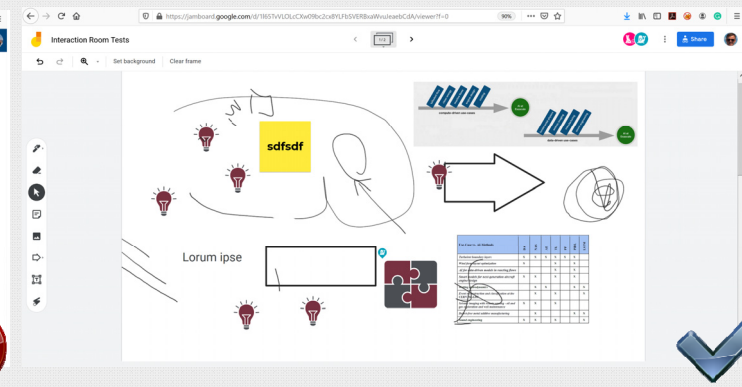
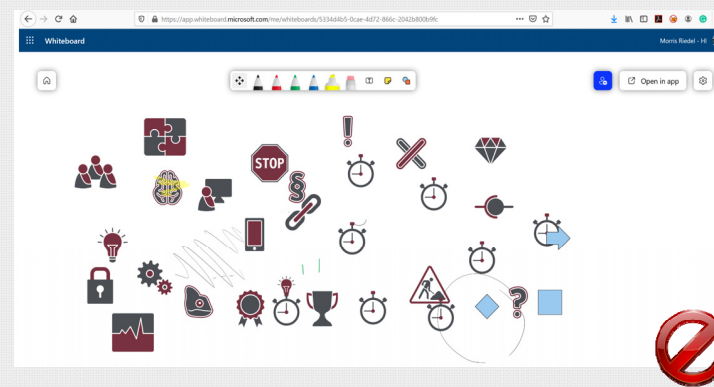


Book, M., Riedel, M., Neukirchen, H., Goetz, M.: [Facilitating Collaboration in High-Performance Computing Projects with an Interaction Room](#), in conference proceedings of the 4th ACM SIGPLAN International Workshop on Software Engineering for Parallel Systems (SEPS 2017), October 22-27, 2017, Vancouver,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



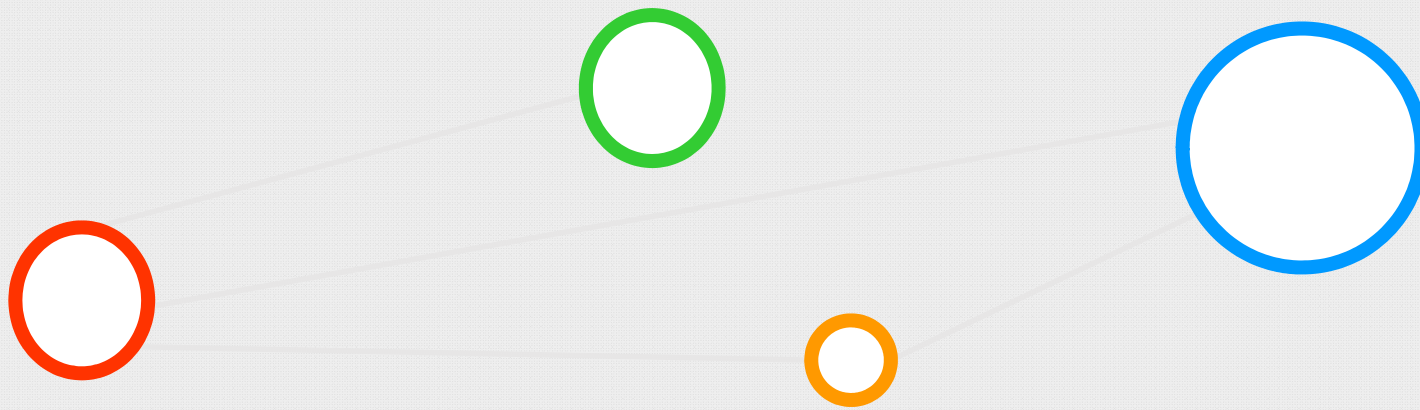
# Interaction Rooms – Reviewed White Boards vs. Planned F2F

- Covid-19 Impact
  - No F2F meetings ('less productive')
  - Alternative: Online White Boards Tools
  - N<sup>infinity</sup> 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?





# Agenda Item (4) – Feedback of EU Fitness check of CoEs Event





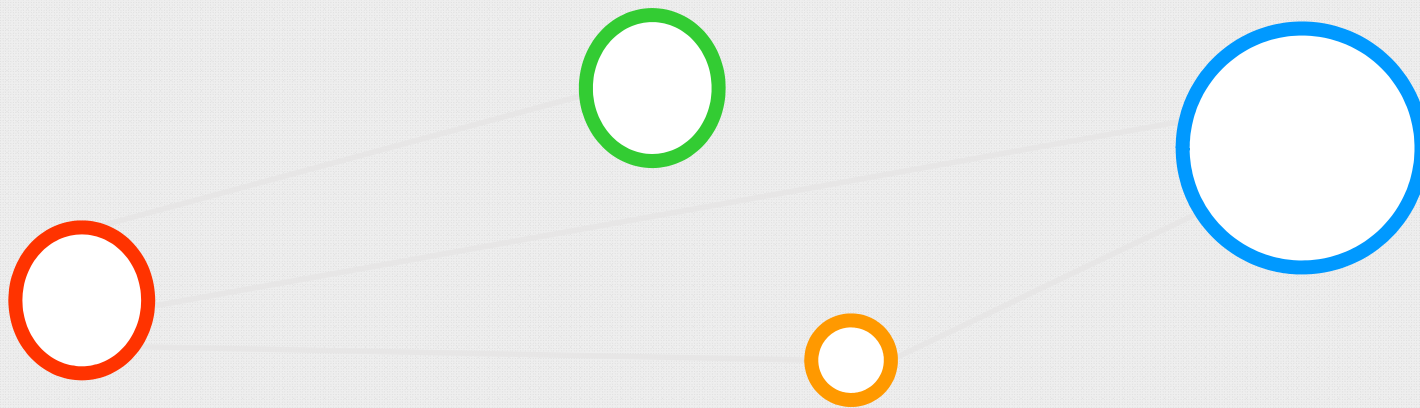
# Feedback of EU Fitness check of CoEs Event

- See slides from Andreas Lintermann





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





# Fact Sheet Status & Discussions – WP<sub>3</sub>/WP<sub>4</sub> 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)

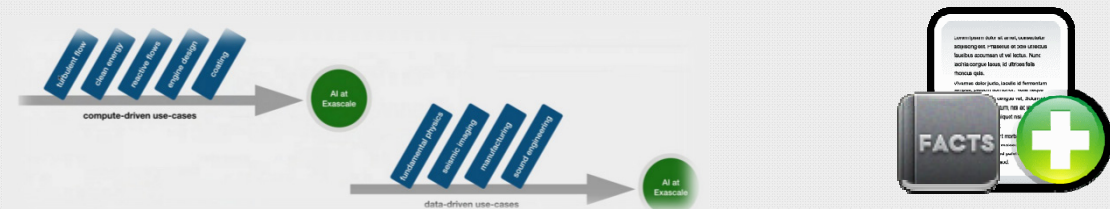


Table 6: Use-case vs. AI-methods matrix.

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

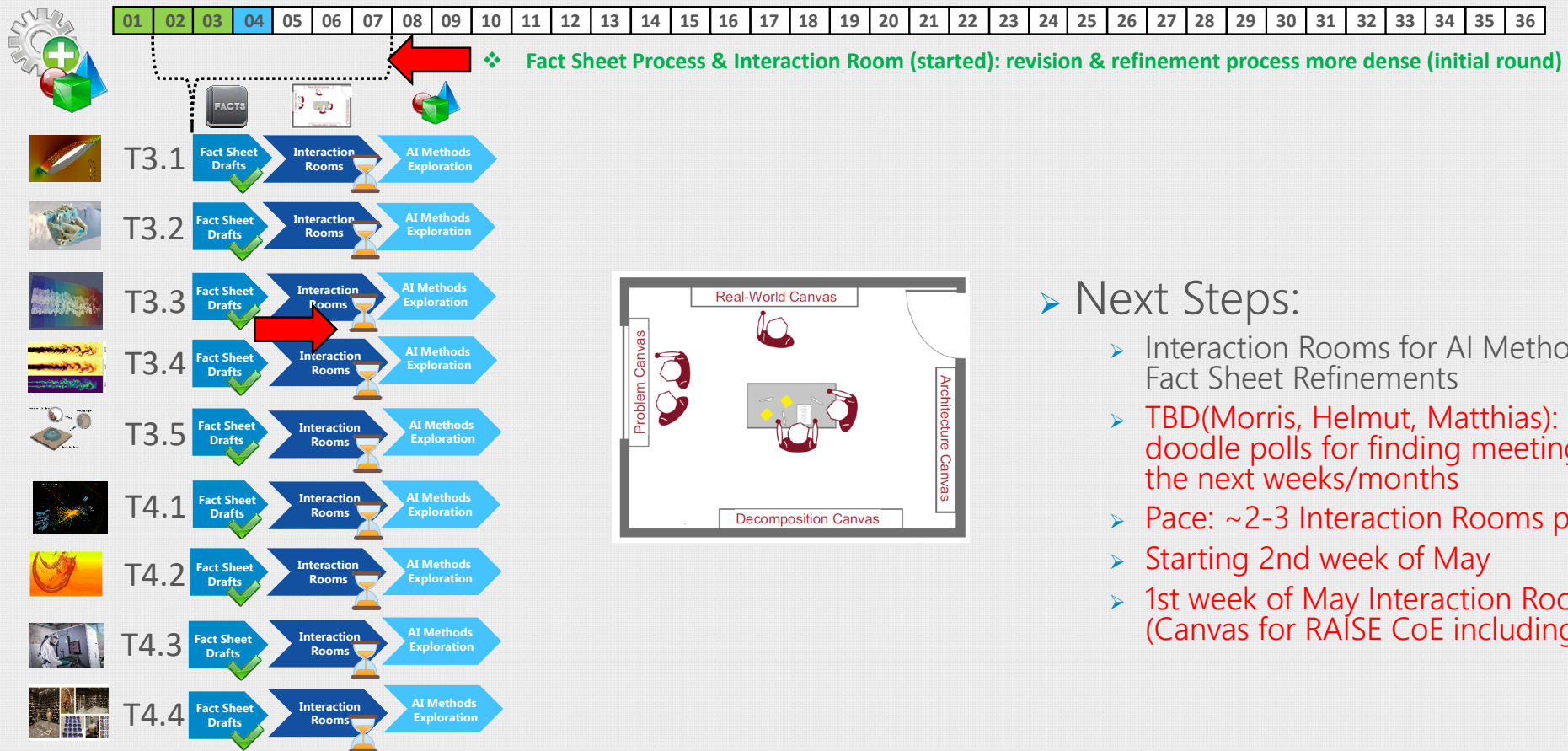
- Interaction Room
- Carve out more details on AI/HPC methods
- Identify concrete detailed algorithms



# Compelling Scoreboard Review – Use Case Progress



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# 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

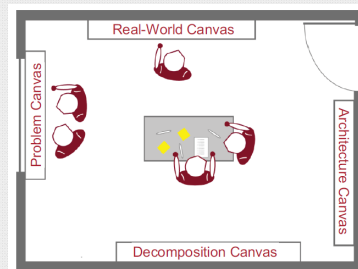
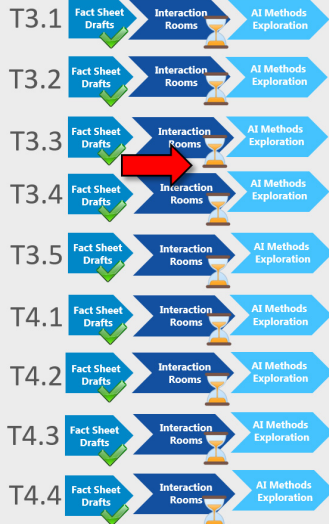
✓ IR Seminar  
2021-04-08

✓ Planing of DataLad Seminar

■ AI/HPC Methods (M7)

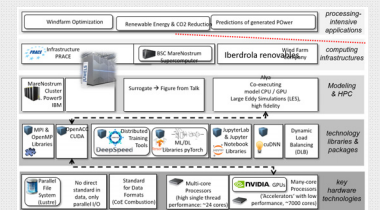
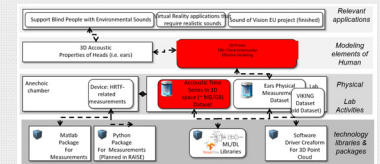
■ D2.12 Software layout plan for a unique AI framework (M10)

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



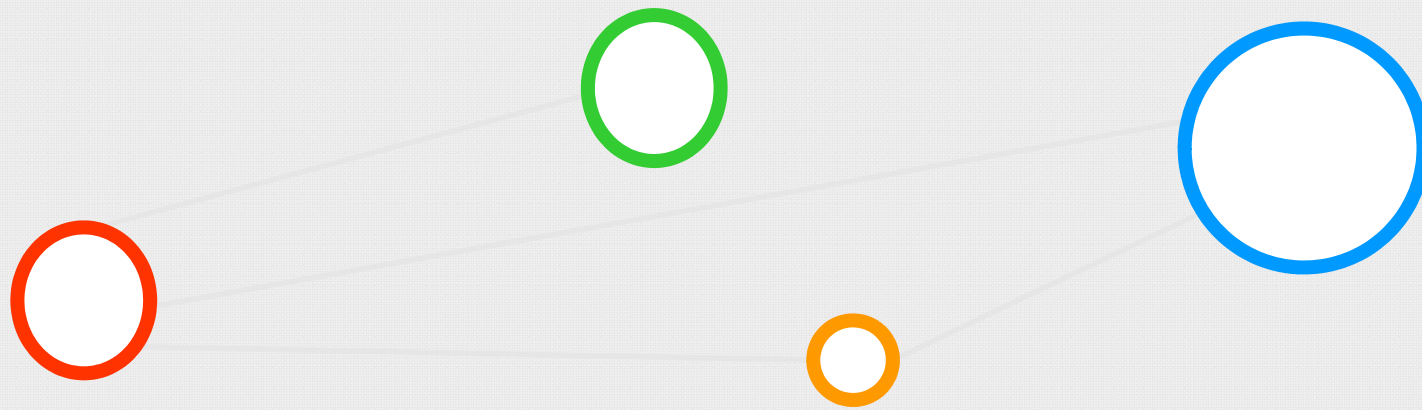
## Next Steps:

- Interaction Rooms for AI Methods & Fact Sheet Refinements





## 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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