



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

2021-02-11, RAISE WP2 Monthly Meeting February 2021, Online



@ProfDrMorrisRiedel



@Morris Riedel



@MorrisRiedel



@MorrisRiedel



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

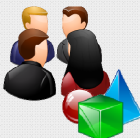
morris@hi.is



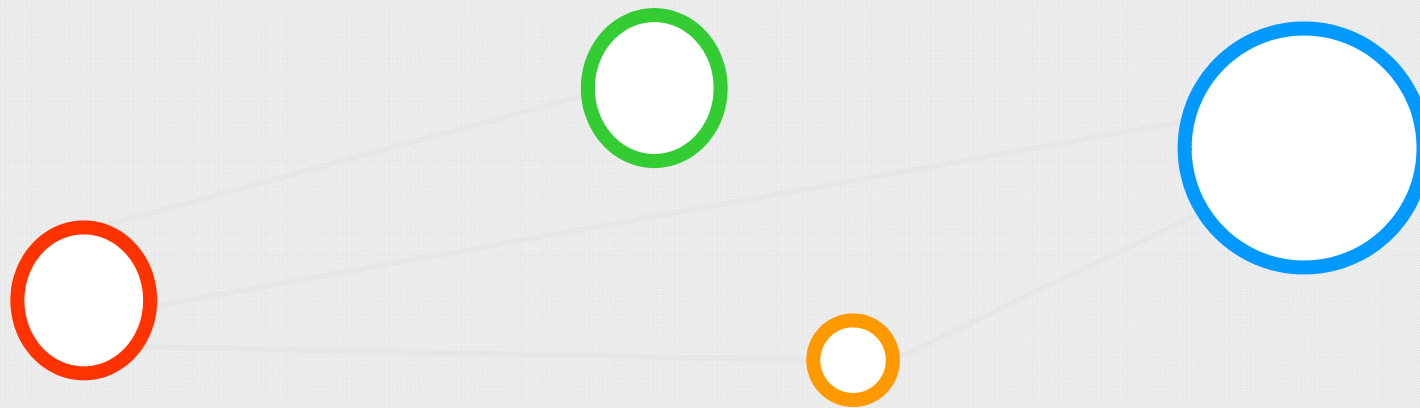
WP2 February Meeting – Welcome & Agenda



1. WP2 Short Overview
 - (Morris Riedel), ~15 Min
2. Get to know WP2 people & Clarify missing contacts of WP2 people
 - (All), ~15 Min
3. Deliverables Month 2, Progress overview & status of documents
 - (Guillaume Houzeaux & Andreas Lintermann), ~10 Min
4. WP2 Next Steps Appetizer: Software layout plan for a unique AI framework
 - Short Introduction to the Interaction Room (Matthias Book), ~10 Min
5. Next Monthly Meeting March & AOB
 - Doodle & Discussions, ~10 Min



Agenda Item (1) - WP2 Short Overview



Agenda Item (1) - WP2 Short Overview

1. Brief Introduction to WP2

- Recap from Kick-Off Objectives & Interworking with WP3 & WP4
- Objectives, Tasks & Deliverables Timeline

2. Organizational Aspects

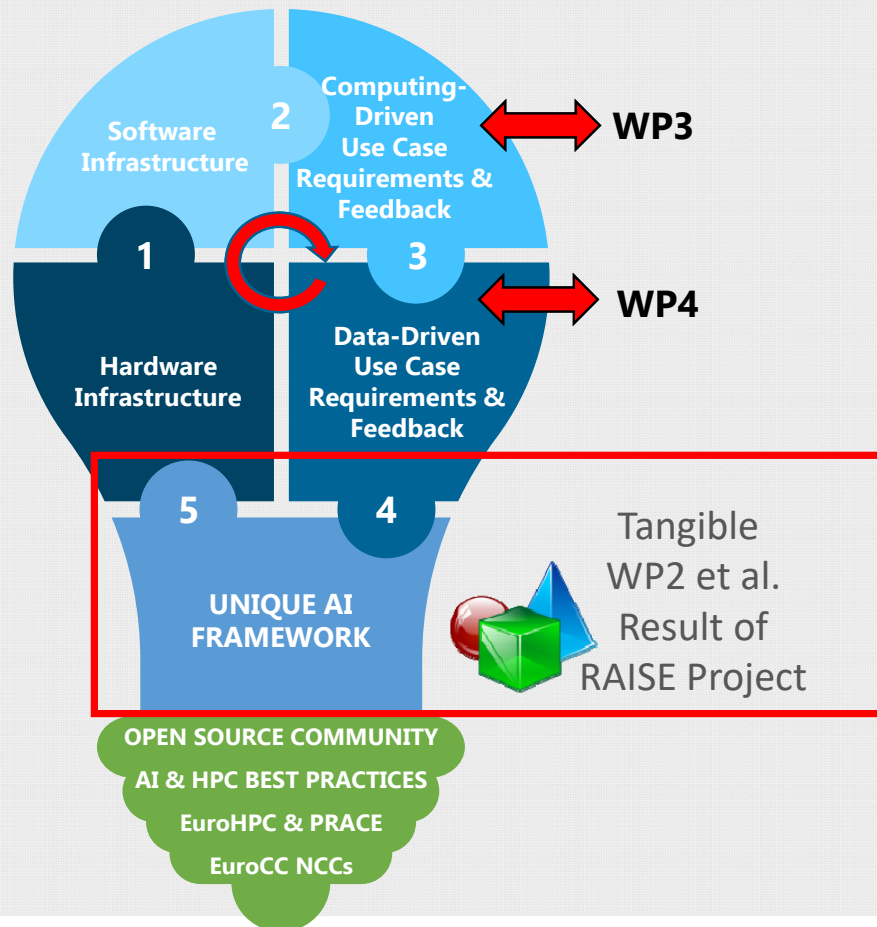
- Monthly Meetings
- Document Store
- Mailing List check
- Role of Fact Sheets
- Role of Interaction Room Meetings, etc.

3. Q&A Session

- Questions from the participants



WP2 Objectives – 'AI & HPC at Exascale backbone'



Hardware Infrastructure

Prepare & Document available production systems at partners' HPC centers

Examples: JUWELS (JUELICH), LUMI (UoICELAND), DEEP Modular Prototypes, JUNIQ (JUELICH), etc.

Software Infrastructure

Prepare & Document available open source tools & libraries for HPC & AI useful for implementing use cases

Examples: DeepSpeed and/or Horovod for interconnecting N GPUs for a scalable deep learning jobs

Computing-driven Use Cases Requirements & Feedback (→ WP3)

Use cases with emphasize on computing bring in co-design information about AI framework & hardware

Examples: Use feedback that TensorFlow does not work nicely, so WP2 works with use cases on pyTorch

Data-driven Use Cases Requirements & Feedback (→ WP4)


Use cases with emphasize on data bring in co-design information about AI framework & hardware

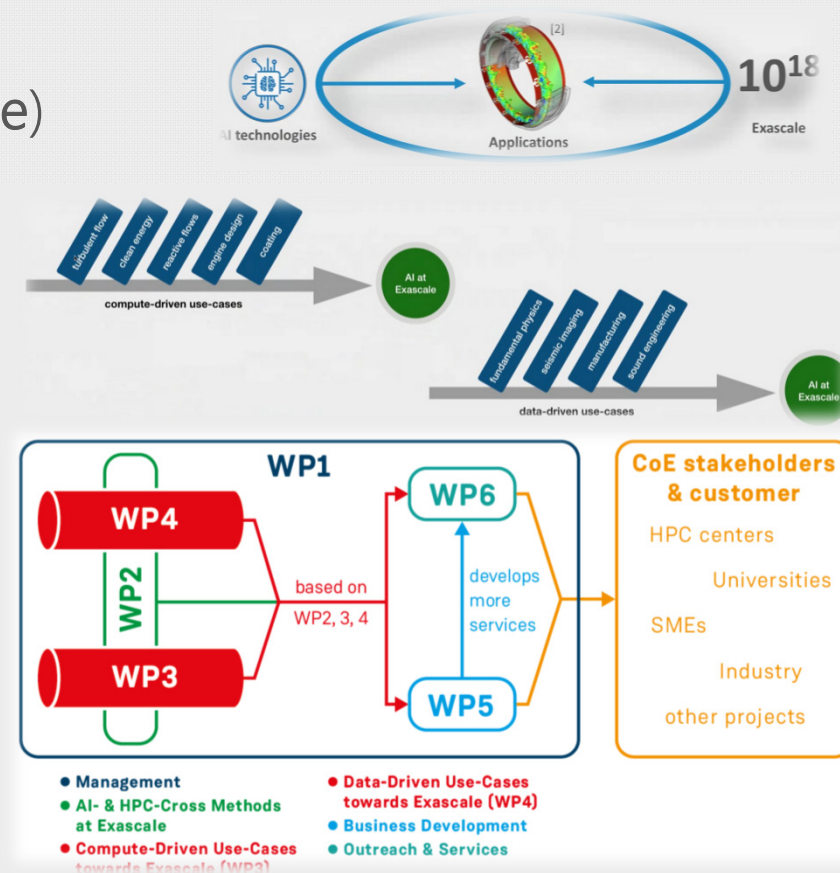
Examples: Deployment blueprint by using AI training on cluster module & inference/testing on booster

UNIQUE AI FRAMEWORK

Living design document & software framework blueprint for using HPC & AI offering also pretrained AI models

WP2 & Connections to other WPs – 'WP2 in a nutshell'

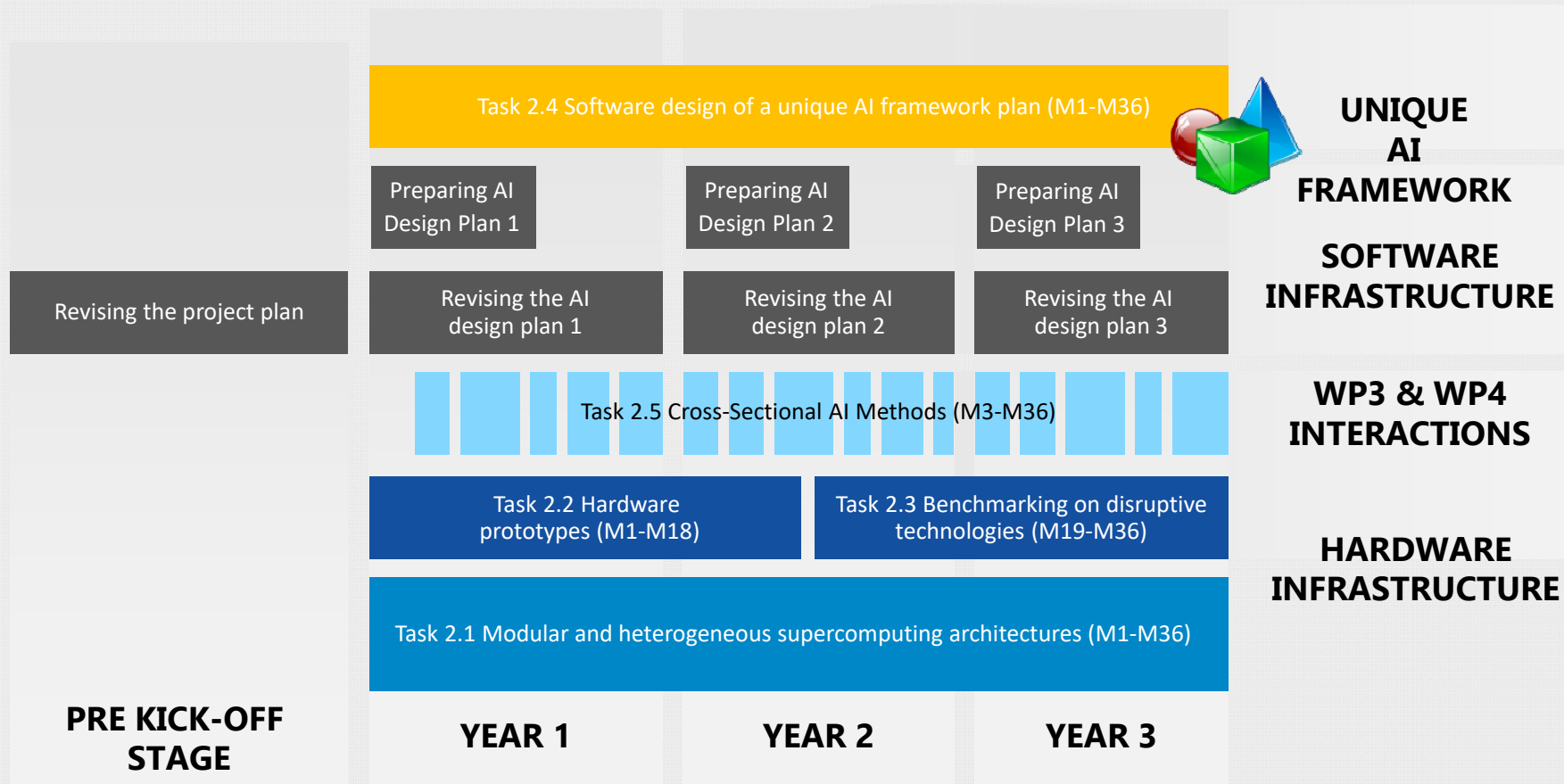
- WP3 (Compute-Driven Use-Cases towards Exascale)
 - WP4 (Data-Driven Use-Cases towards Exascale)
 - Developments in these WPs will be supported by the cross-linking activities of WP2
 - E.g. scaling machine & deep learning codes with frameworks like Horovod/Deepspeed
 - E.g. introduction to new AI methods such as Long-Short Term Memory (Time series)
 - E.g. data augmentation approaches
 - E.g. benchmarking HPC machines and offer also pre-trained AI algorithms (i.e., transfer learning)
 - E.g. offer neural architecture search methods for hyperparameter – tuning in semi-automatic way
- 



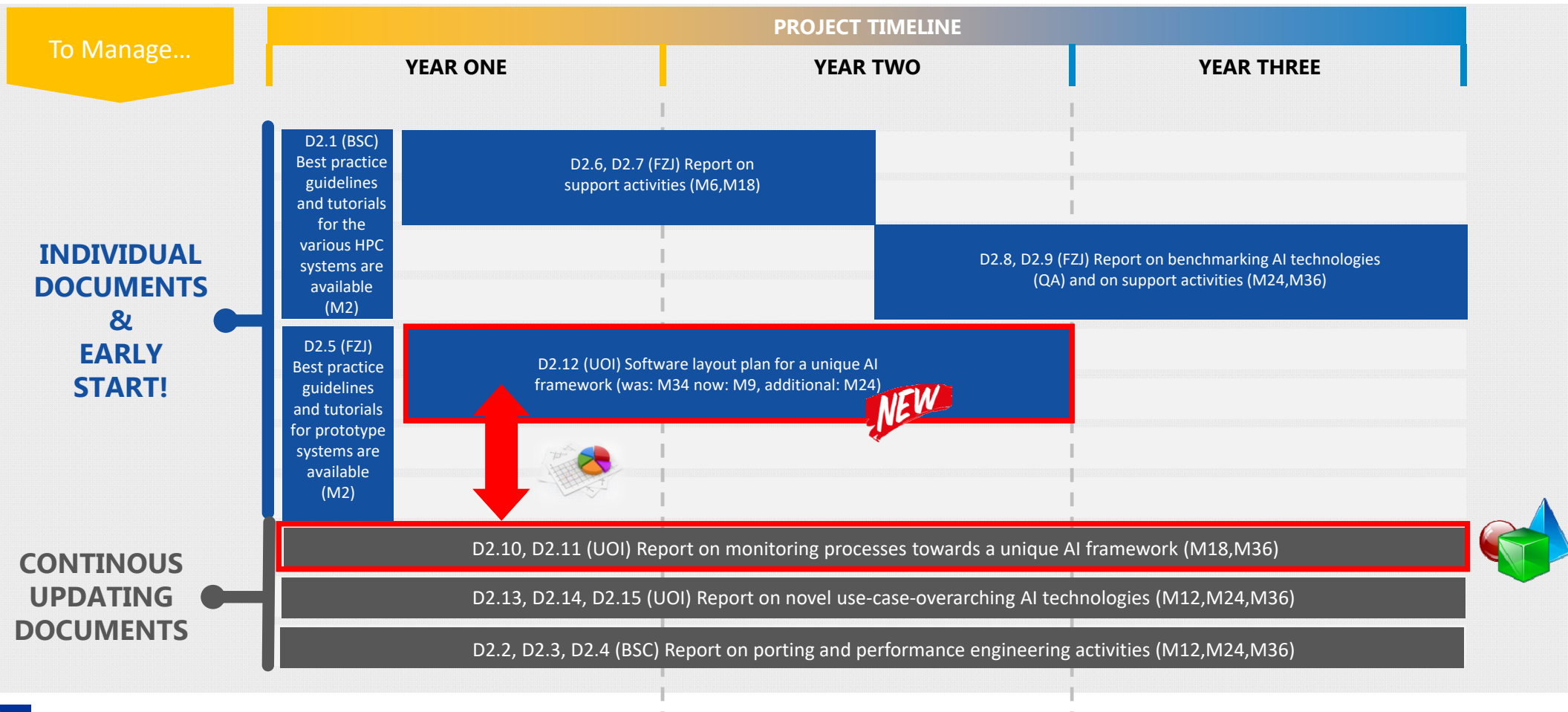
WP2 Tasks



TIME →



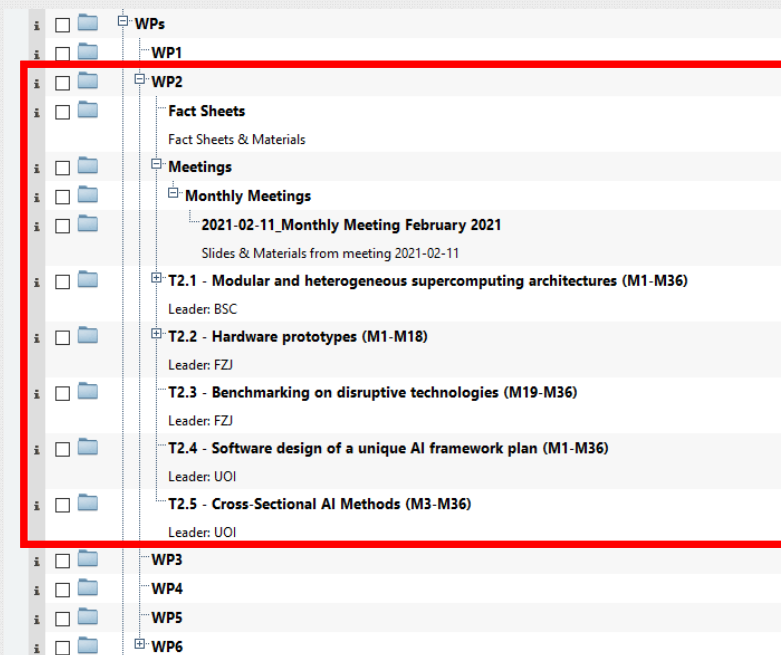
WP2 Work on Deliverables & Milestones



WP2 Document Store BSCW & Monthly Meetings

➤ BSCW Store:

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



- To share documents, reports, etc.
 - Access given by PMT

➤ Monthly Meetings:

- From March: Short Status Update of Task Leaders
- Update on Fact Sheets & Interaction Room Process
- Tracking Deliverable Progress



WP2 & More Information RAISE & WPx → Kick-off Slides

➤ BSCW Folder:

<https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3321793>

The screenshot shows the BSCW web interface. The browser address bar displays the URL: <https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3321793>. The BSCW logo is in the top left, and a 'Logout' button is in the top right. Below the logo is a navigation bar with links: Datei, Bearbeiten, Ansicht, Optionen, Anzeigen, Hilfe. A toolbar with various icons is below the navigation bar. The main content area shows the breadcrumb path: Arbeitsbereiche von M.Riedel > CoE RAISE > Meetings > 2021_01_22_Kick-Off > talks. A search bar with the text 'Suchen' is on the right. Below the breadcrumb path is a table of files in the 'talks' folder. The table has columns: Name, Aktion, Größe, Erzeugt von, Priorität, Letzte Änderung, and Neu. There are 9 entries in the table.

Name	Aktion	Größe	Erzeugt von	Priorität	Letzte Änderung	Neu
2021_01_22_CoE-RAISE-Kickoff-06-WP4.pdf	▼	1.9 M	andlin	→	2021-01-22 19:32	
2021_01_22_CoE-RAISE-Kickoff-07-WP5.pdf	▼	459 K	andlin	→	2021-01-22 19:33	★
2021_01_22_CoE-RAISE-Kickoff-08-WP6.pdf	▼	645 K	andlin	→	2021-01-22 19:33	★
2021_01_22_CoE-RAISE-Kickoff-01-Welcome.pptx	▼	1.2 M	andlin	→	2021-01-22 19:29	★
2021_01_22_CoE-RAISE-Kickoff-02-Keynote_TL.pptx	▼	9.5 M	andlin	→	2021-01-22 19:30	★
2021_01_22_CoE-RAISE-Kickoff-03-Introduction.pptx	▼	15.6 M	andlin	→	2021-01-22 19:30	
2021_01_22_CoE-RAISE-Kickoff-04-WP2.pptx	▼	4.8 M	M.Riedel	→	2021-02-03 17:36	★
2021_01_22_CoE-RAISE-Kickoff-05-WP3.pptx	▼	1.1 M	andlin	→	2021-01-22 19:31	
2021_01_22_CoE-RAISE-Kickoff-09-WP1.pptx [0.3]	▼	1.5 M	andlin	→	2021-01-22 19:34	

WP2 Mailing List

Email lists and functional emails (to add/remove members, please notify PMT; see also BSCW):

raise_psb@fz-juelich.de

members of the project steering board

raise_finance@fz-juelich.de

all people from the financial departments

raise_pmt@fz-juelich.de

members of the project management team

raise_pc@fz-juelich.de

email address coordinator (Andreas Lintermann)

raise_tcb@fz-juelich.de

members of the technical coordination board

raise_tow@fz-juelich.de

all WP leaders and deputies

raise_pub@fz-juelich.de

all people responsible for publications

[raise_wp\[1-6\]@fz-juelich.de](mailto:raise_wp[1-6]@fz-juelich.de)

participants of the respective WPs

raise_wp2@fz-juelich.de

WP2 mailing list

raise_all@fz-juelich.de

all members

Mailing list raise_leadresearcher@fz-juelich.de will be deleted upon creation of the PSB mailing list!

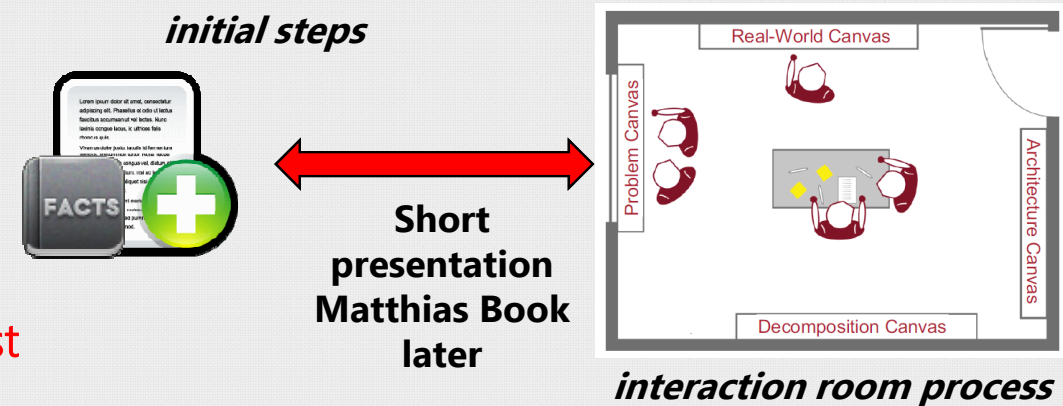
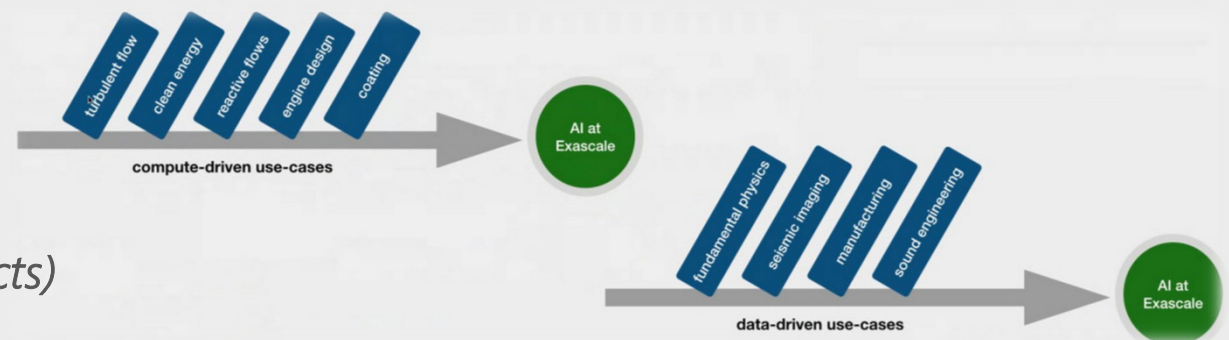
WP2 Process for our Discussion

➤ Fact Sheets

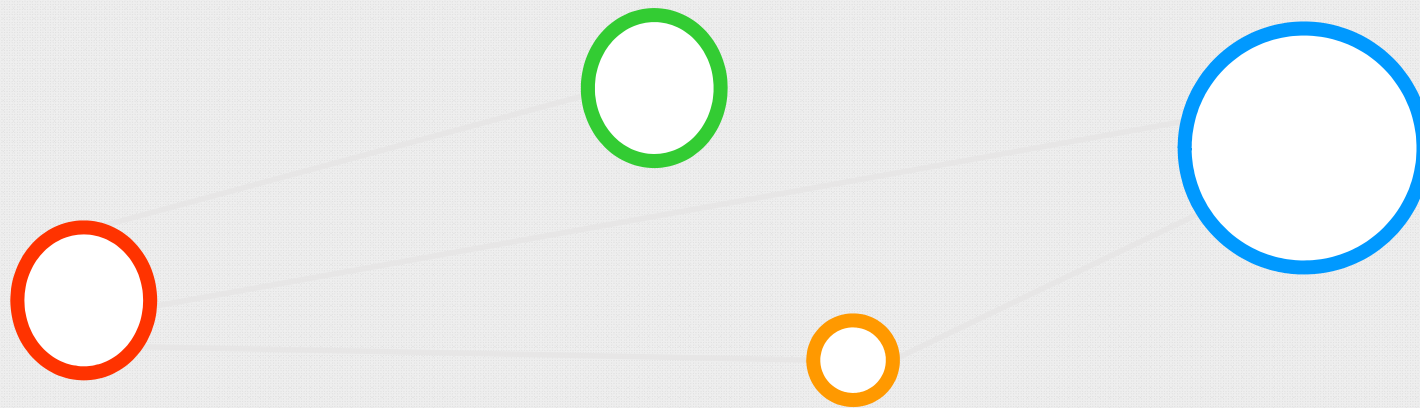
- Foster initial understanding
- Living document & each Fact Sheet per WP3/WP4 Use Case
- *(Experience from many other EU projects)*

➤ Selected Contents

- Short Application Introduction
- Clarify Primary Contacts
- Codes/Libraries/Executables
- HPC System Usage Details
- Specific Platforms & 'where is what data'?
- **Machine/Deep Learning Approaches of Interest**
(WP2 members in turn will then work on this)



Agenda Item (2) - WP2 People



Agenda Item (2) - WP2 People – Goals

1. Short round among call participants
 - E.g. organization, role, expertise
 - Emphasize on WP2 contributions please
 - TBD(Morris): Note partners attending: UOI, ...
2. Missing people per Partner?
 - TBD (all): Please send missing people to the PMT email
 - Do we miss someone not yet in the mailing list?



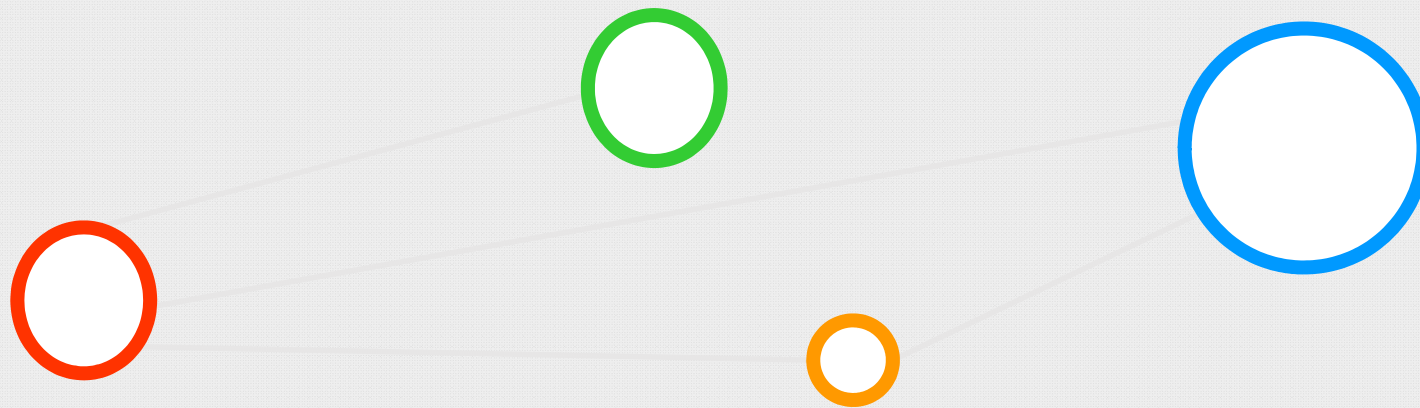
Work package title	AI- and HPC-Cross Methods at Exascale											
Participant No.	1	2	3	4	5	6	7	8	9	10	11	
Short name of participant	FZJ	UOI	CYI	RWTH	BSC	CERN	CERFACS	BULL	RTU	FM	SAFRAN	TOT
PM per partner	43	24	0	10	8	8	0	8	22	12	0	135
Start month	1			End month								36

Agenda Item (2) - WP2 People – Initial Expertise List

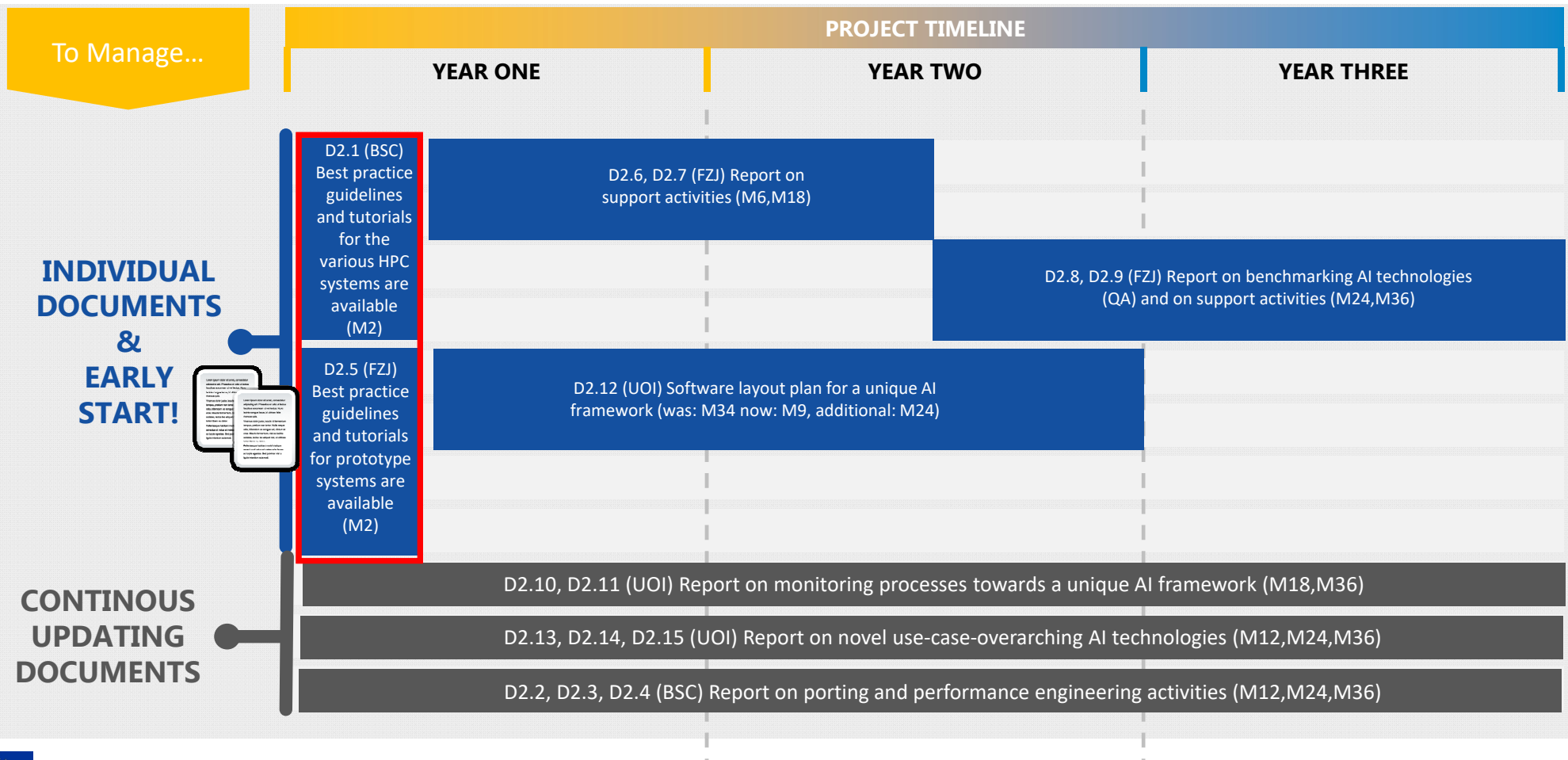
- Andi (FZJ), hardware support to the community (JUWELS, JURECA, DEEP prototypes, quantum annealer, etc.)
- Arnis (RTU): also WP3/4, using AI, some practical background AI solutions, mainly simulation sciences
- Eric (UOI): new PHD in TACTILE engineering,
- Gabriele (FZJ): Remote Sensing, machine learning & HPC experience, contributes to WP2, WP4.2 remote sensing application, drives community remote sensing & HPC
- Guillaume (BSC): hardware support to community, wind turbines, no experience in AI so far
- Guillermo (BSC): GPU computing at BSC, last month AI activities, help in WP3
- Helmut (UOI): sw engineering & distributed systems (HPC, but also others, clouds), DEEP-EST project
- Ilze (RTU): WP2 member, data analysis, ML models, medical/transport data so far, experience in data science/AI/deep learning
- Ina (ParTec): group of project managers (with Jennifer, Andi, Konrad)
- Apologies (Peter Niessen): 2.1 and 2.2 support colleagues, large machines in Juelich, DEEP series of project prototypes
- Jennifer (FZJ): member of PMT
- Julian (RWTH): HPC team, fluid dynamic solvers & GPUs, practical experience , some cluster systems in the project
- Apologies (Christian, RWTH)
- Lauris (RTU): RTU team leader, background HPC, lead of HPC team @ RTU university, not much about AI yet
- Matthias (UOI) SW Engineering & Computer Science, Interaction Room expert, communication between different disciplines (i.e., HPC, AI, Sim)
- Reza (UOI): PHD student in CFD, SimDataLab CFD member at UOI, aircraft engine WP3.4 use case & AI
- Seong (FZJ): CFD background, technical support for user communities, medical imaging,
- Morris (UOI): since 16 years in HPC & FZJ/JSC, now full staff member at UOI and professor for parallel/scalable AI with HPC, Clouds, and Quantum Computing
- **TBD (Morris): WP2 (Name of mailing list will be augmented → add in BSCW WP2: matrix AI vs. HPC & Sim expertise in addition to contact**
- **GDPR consent given for internal BSCW usage in the meeting by everyone (informed consent)**



Agenda Item (3) - WP2 Deliverable Status D2.1 & D2.5



WP2 Work on Deliverables & Milestones



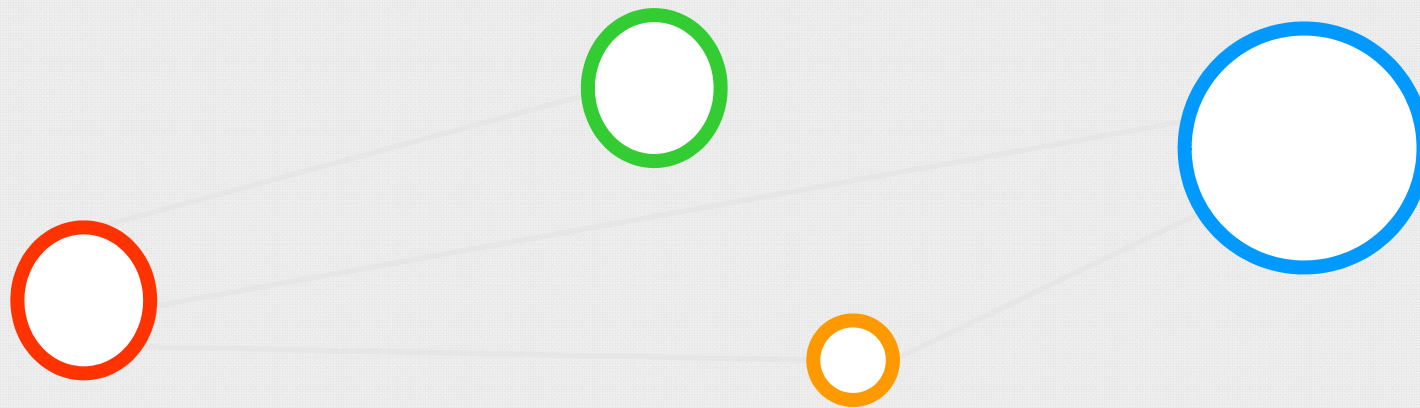
Agenda Item (3) - WP2 Deliverable Status D2.1 & D2.5

1. WP Deliverable (M2) D2.1 Status
 - In Internal Review
 - Andreas Lintermann
2. WP Deliverable (M2) D2.5 Status
 - In Internal Review
 - Guillaume Houzeaux
3. TBD(WP2 Members):
Take a look on the deliverables
& understand systems



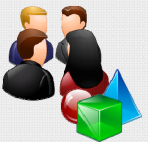
<input type="checkbox"/>		Reports and Deliverables
<input type="checkbox"/>		EC approved
<input type="checkbox"/>		EC submitted
<input type="checkbox"/>		For internal review
<input type="checkbox"/>		Additional reviews
<input type="checkbox"/>		CoE RAISE_Deliverable_D2.1_int_review-MRi-WP2-Lead.docx
		Review by WP2 Lead Morris - mostly only language elements and minor suggestions
<input type="checkbox"/>		CoE RAISE_Deliverable_D2.5_int_review-MRi-WP2-Lead.docx
		Review by WP2 Lead Morris - mostly only language elements and minor suggestions
<input type="checkbox"/>		CoE RAISE_Deliverable_D2.1_int_review.docx
<input type="checkbox"/>		CoE RAISE_Deliverable_D2.5_int_review.docx

Agenda Item (4) - WP2 Next Steps: Interaction Room



Agenda Item (4) - WP2 Next Steps: Interaction Room

- WP2 Next Steps Appetizer: Software layout plan for a unique AI framework
 - Short Introduction to the Interaction Room
 - Given by Prof. Dr. Matthias Book
- WP2 Workshop Interaction Room
 - Dedicated introductory event
 - Timeframe: February/March
- WP2 Usage
 - WP2 Fact Sheet process as input ('initial understanding')
 - Supports the proper software engineering design of the unique AI framework blueprint
 - Understand & Extract requirements & demands from WP3 & WP4 use cases



**HPC Systems Engineering
in the Interaction Room**

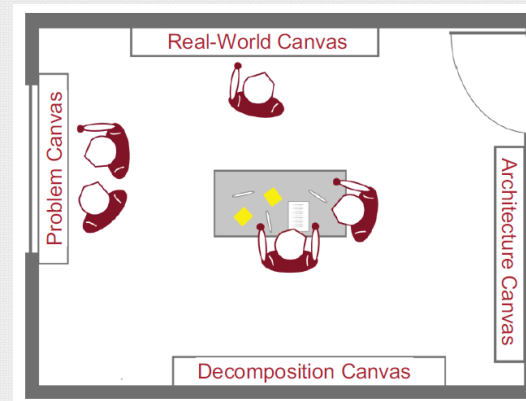
Matthias Book
Morris Riedel
Helmut Neukirchen



WP2 will Start Meetings with WP3 & WP4 for Online Sessions

➤ Start: Interaction Room Process

- 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 (Software Engineering, University of Iceland)
- Supported by Software Engineering & testing expert Prof. Dr. Helmut Neukirchen (University of Iceland)



HPC Systems Engineering in the Interaction Room

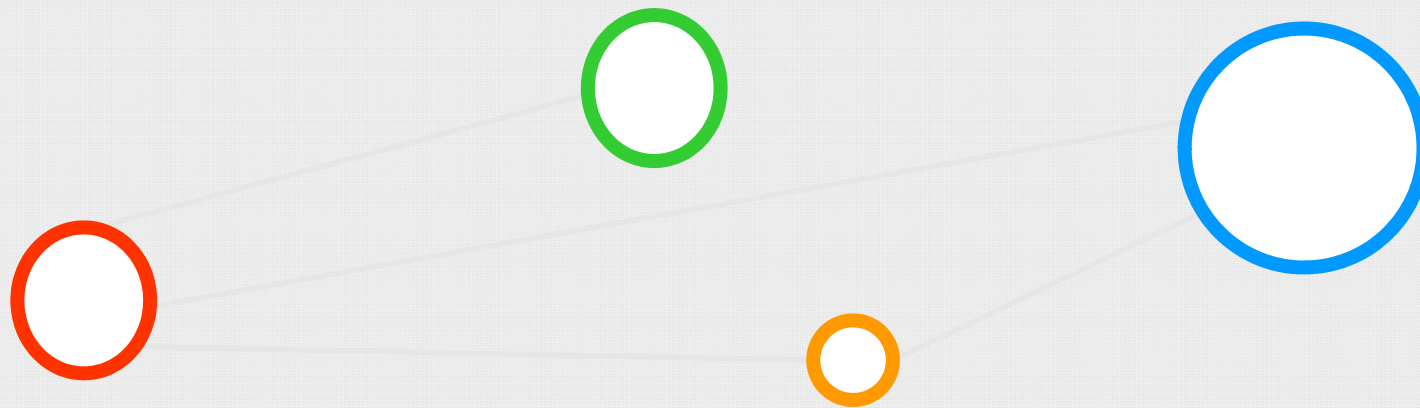
Matthias Book

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

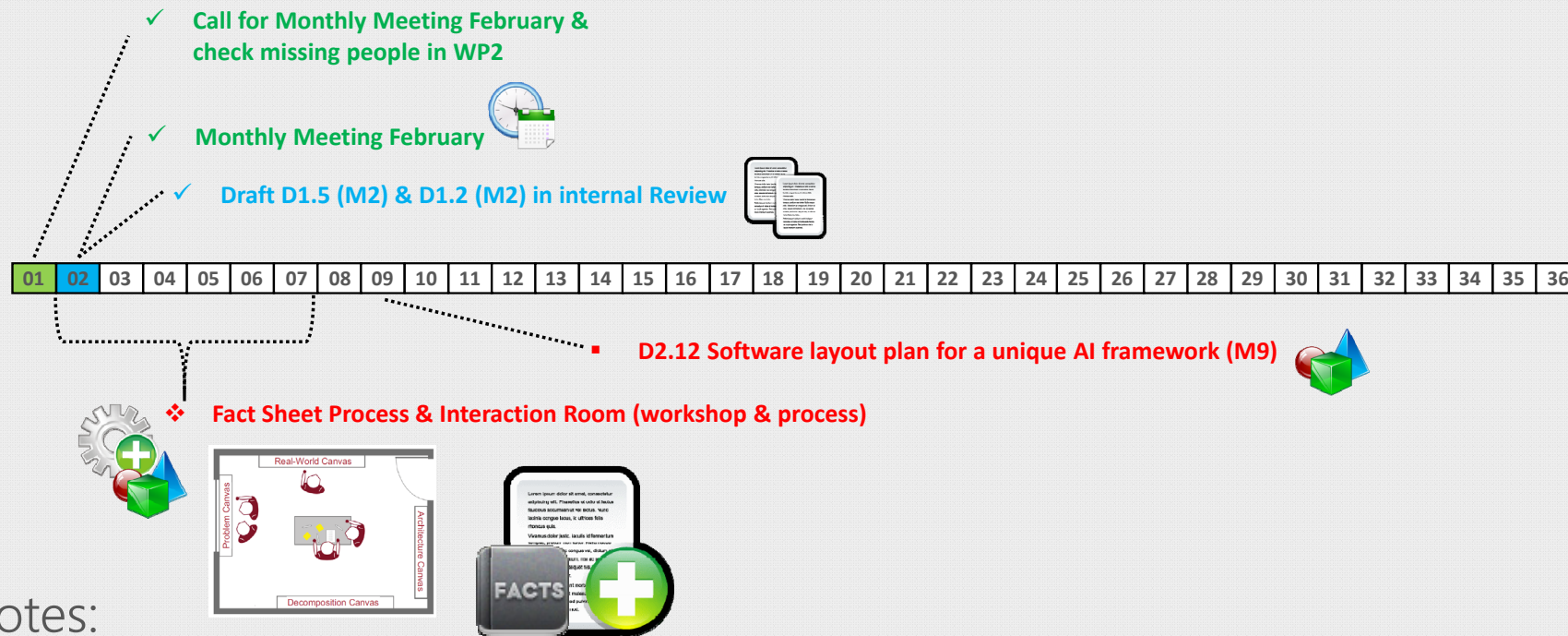


Book, M., Riedel, M., Neukirchen, H., Goetz, M.: [Facilitating Collaboration in High-Performance Computing Projects with an Interaction Room](#), in conference proceedings of the 4th ACM SIGPLAN International Workshop on Software Engineering for Parallel Systems (SEPS 2017), October 22-27, 2017, Vancouver,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

Agenda Item (5) - WP2 Next Monthly Meeting & AOB



Summary & Next Month



➤ Notes:

- Next meeting items: Understanding better the benchmarking activities & plans, resource provisioning (Guillaume)
- TBD(Matthias/Morris): Start process with fact sheets & search for interaction work date&time, monthly meeting doodle
- TBD(Morris): Upload 2-3 examples of fact sheet to the BSCW folder from previous EC projects

Agenda Item (5) – WP2 Next Monthly Meeting & AOB

1. Next Monthly Meeting(s)

- TBD(Morris) Timeframe: March, April, May: Doodle will be available soon
- Topics: Selected progress with Factsheets & Interaction Room presentations
- TBD(All): other topics of relevance, ideas for process, etc.
- TBD(All): Discussions & AOB?



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