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

Prof. Dr. – Ing. Morris Riedel et al.
School of Engineering & Natural Sciences, University of Iceland

2022-01-31, RAISE WP2 Monthly Meeting January 2022, Online

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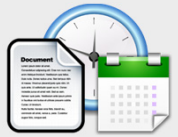
https://www.youtube.com/channel/UCWC4VKHmL4NZgFfKoHtANKg morris@hi.is

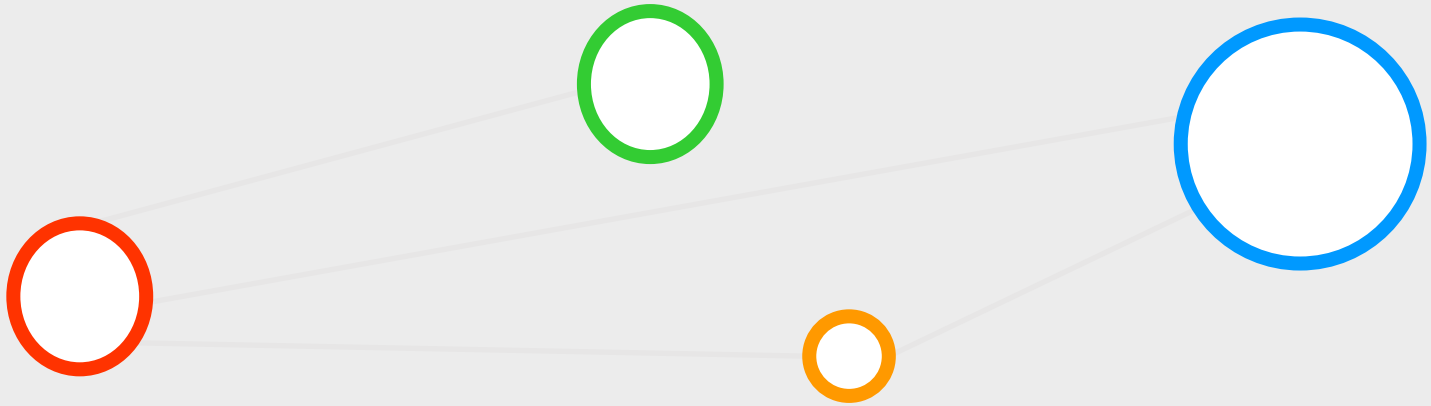
WP2 January Meeting – Welcome & Agenda

RAISE Center of Excellence

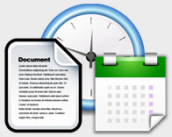
1. Approval of minutes from Monthly Meeting November 2021
   - (All), ~5 Min
2. Review WP2 Status on Interaction Rooms
   - (Morris Riedel, Matthias Book, Helmut Neukirchen), ~15 Min
3. Reflect on M12 Deliverables
   - (Morris, Cristóbal), ~10 Min
4. Status WP2 Seminar Plans
   - (Morris & Andi), ~15 Min
5. Compelling Scoreboard Review & Next Steps
   - (All), ~15 Min



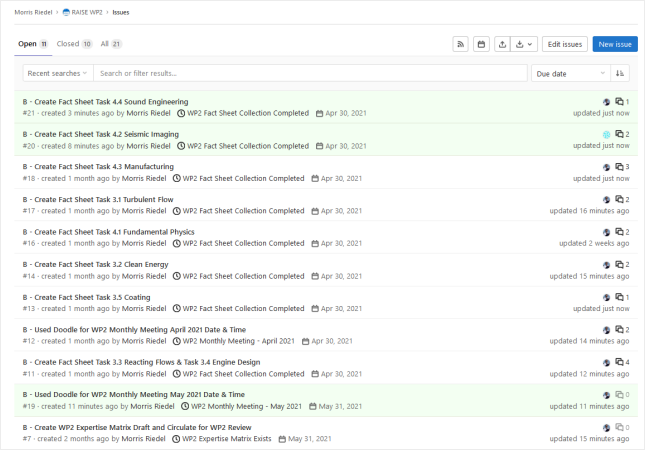
Agenda Item (1) – Minutes Approval – Meeting November 2021

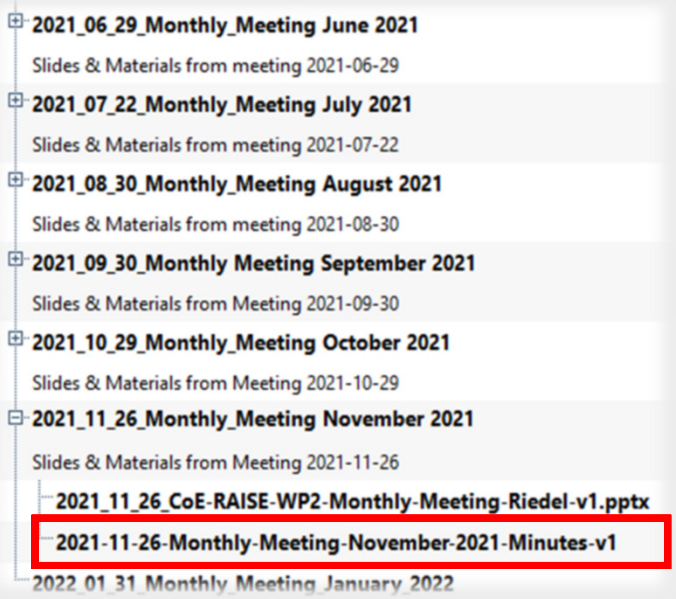


Minutes Approval – Monthly Meeting November 2021

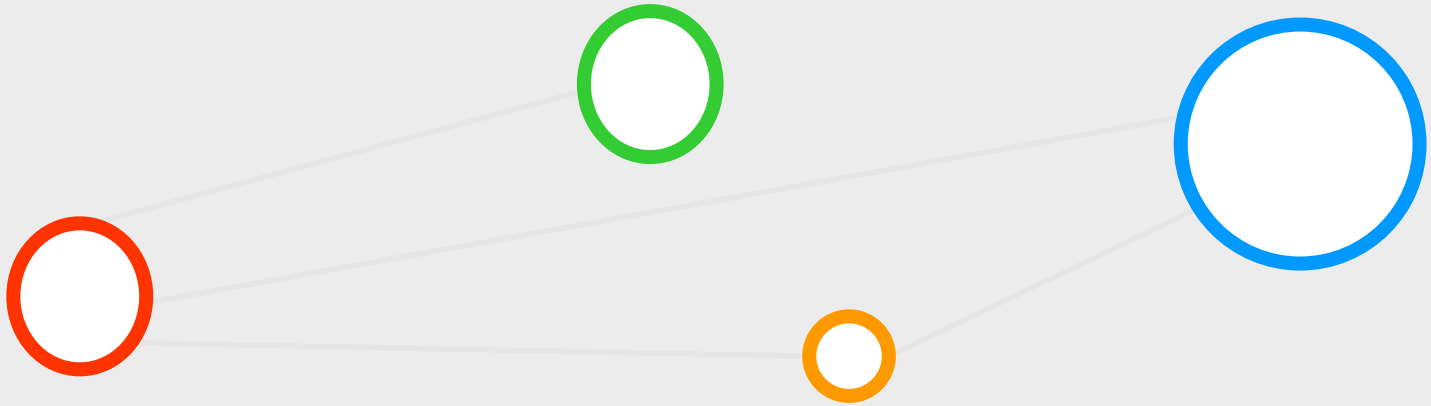


- Minutes available in BSCW
  - https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3704758
  - TBD(all): Any objections or additions/changes?
  - TBD(Guillaume, Cristóbal, Lauris): Upload presentation

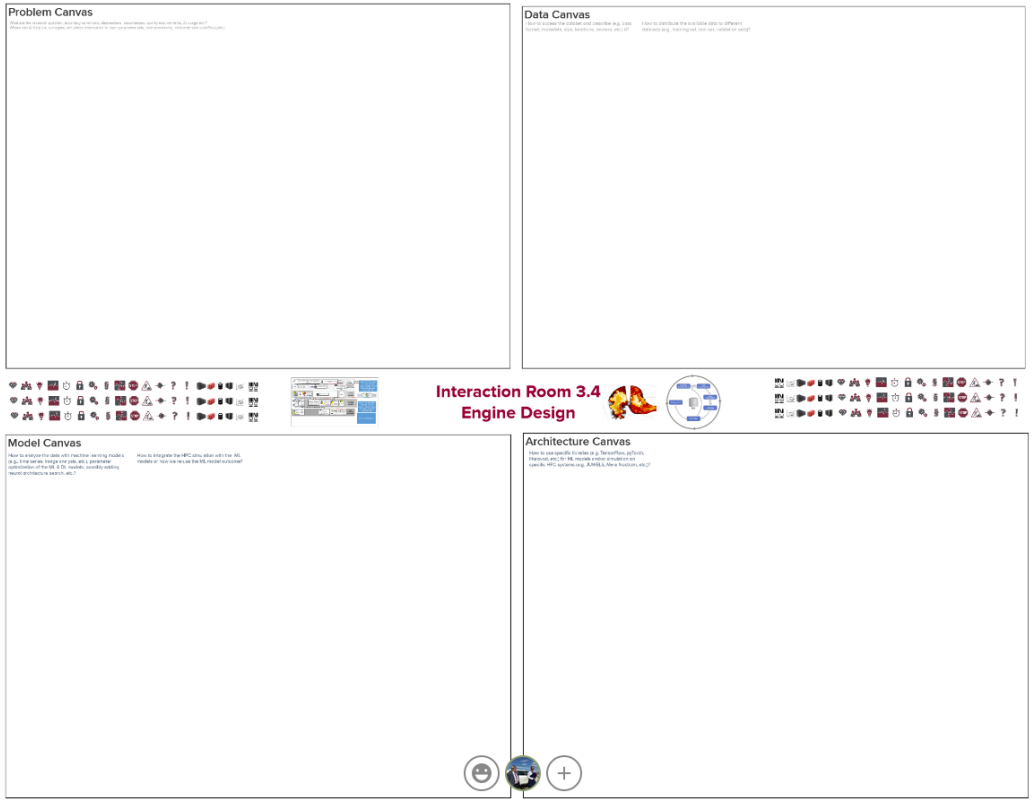


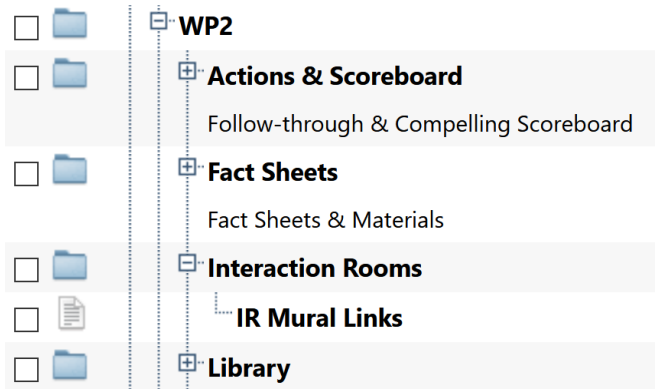


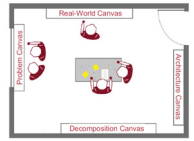
Agenda Item (2) – Review WP2 Status on Interaction Rooms



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

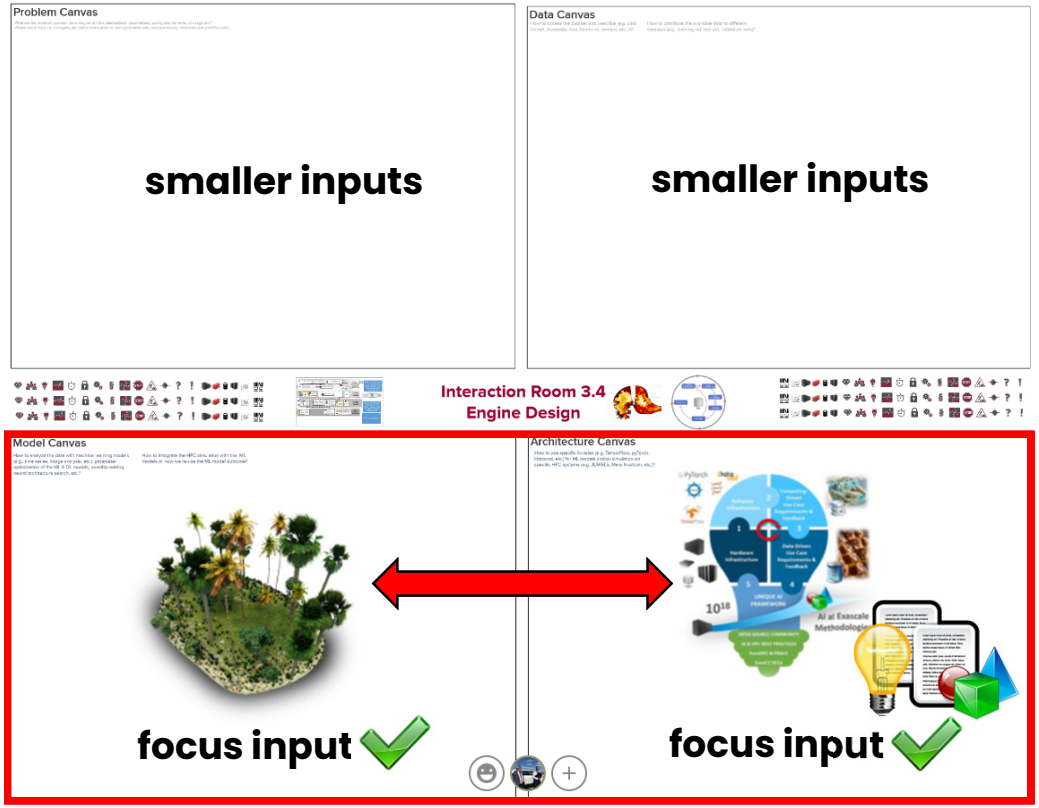
IR4.2 Seismic Imaging: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ae3e28af4bb8d9adbec33874998?sender=u15e3008bb41d6628a5bb5701

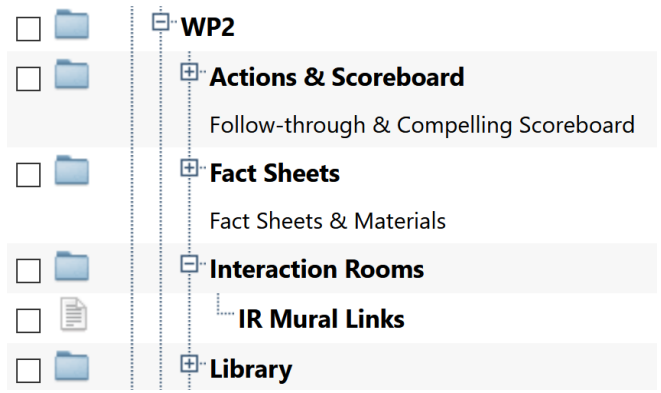
IR4.3 Manufacturing: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378038069/93df6fa7a41093f4eaae7be9d72979dc2ba42b9d?sender=u15e3008bb41d6628a5bb5701

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

- TBD(all): Do people use the MURAL boards (e.g., Task 3.4 is pretty empty but with Task 3.3)?
- https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3591551

MURAL Board contents for Deliverables & Milestones





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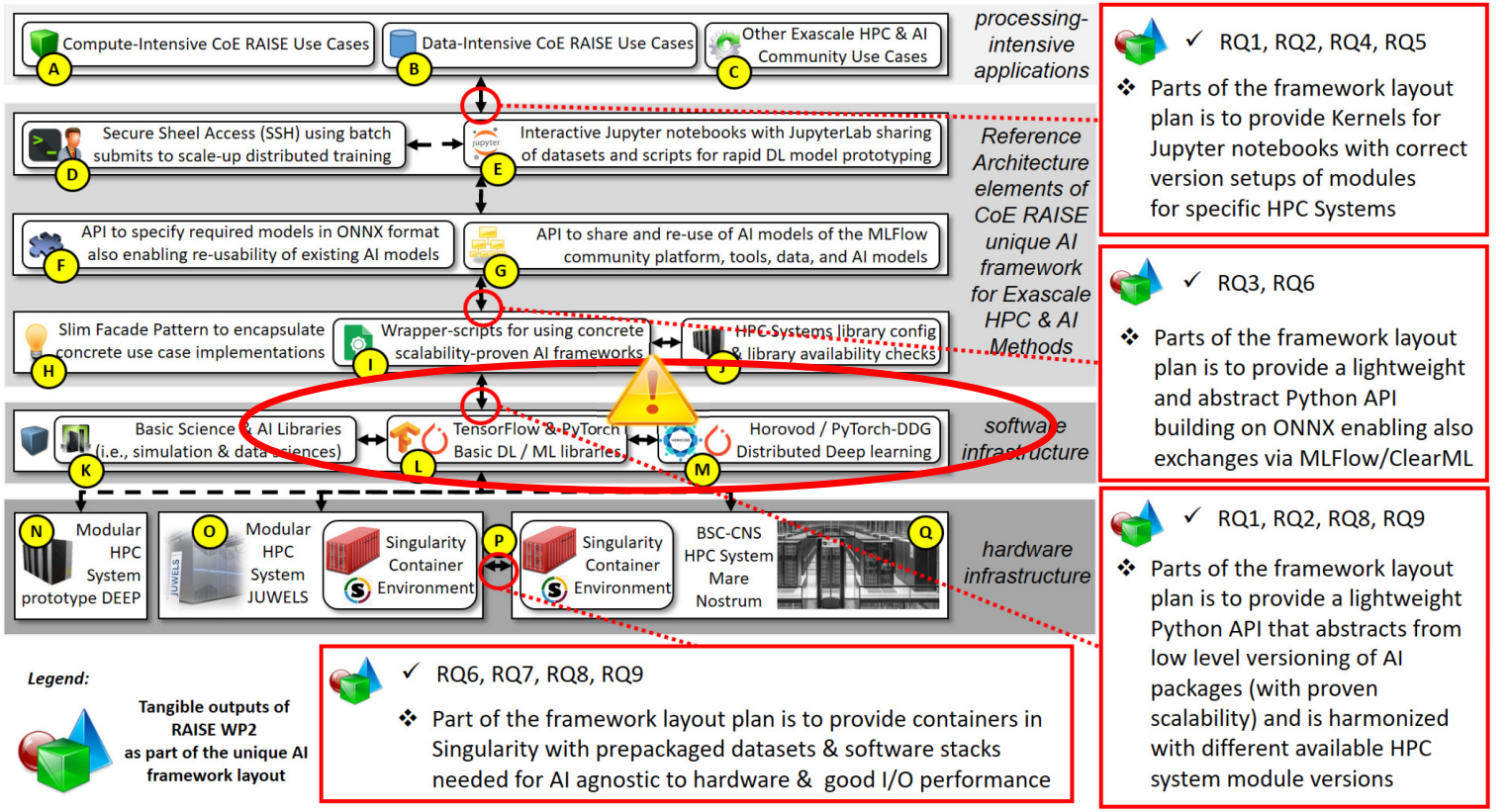
IR4.3 Manufacturing: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378038069/93df6fa7a41093f4eaae7be9d72979dc2ba42b9d?sender=u15e3008bb41d6628a5bb5701

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

Round Two IRs to Discuss our Unique AI/HPC Framework

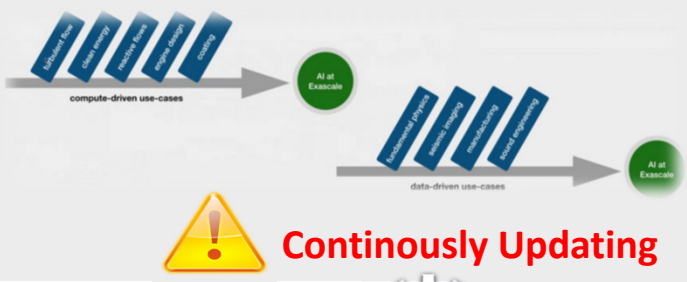
- Available in BSCW: https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3694045



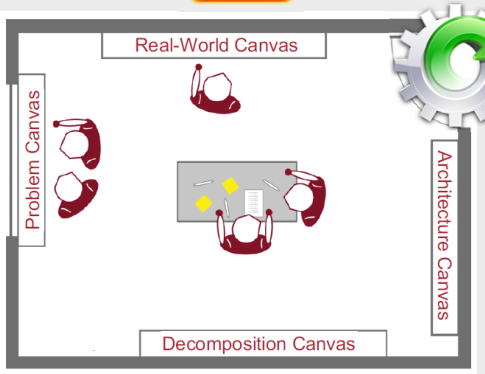
Continously Updating: e.g., add hyper-parameter optimization tools?!

Interaction Room Status & Discussions – WP3/WP4 Overview

- WP3 (second round IRs)
  - T3.1: Turbulent Flow (not started)
  - T3.2: Clean Energy (not started)
  - T3.3: Reactive Flows (not started)
  - T3.4: Engine design (not started)
  - T3.5: Coating (not started)
- WP4 (second round IRs)
  - T4.1: Fundamental physics (not started)
  - T4.2: Seismic imaging (not started)
  - T4.3: Manufacturing (not started)
  - T4.4: Sound engineering (not started)



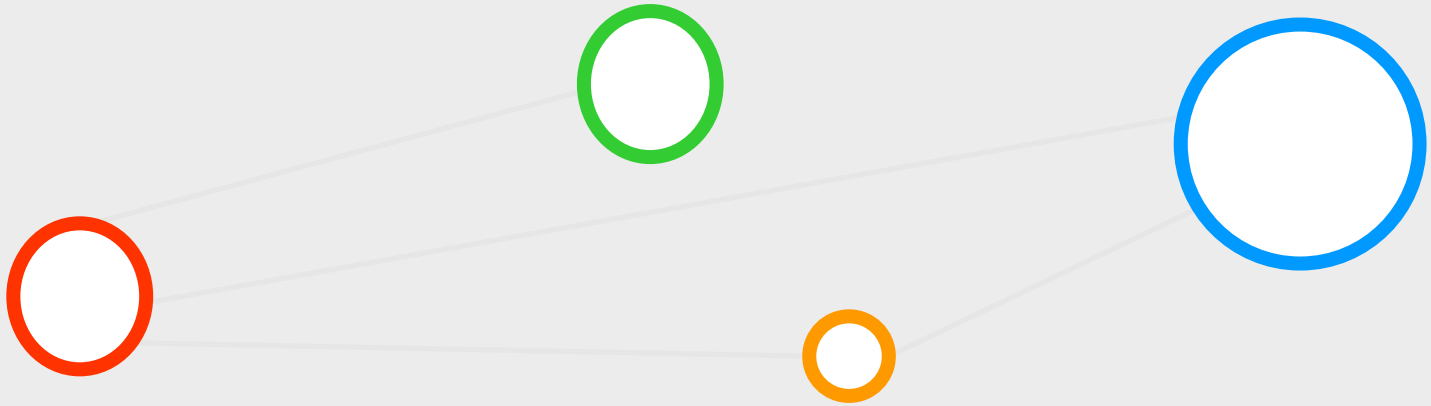
Continously Updating



Use Case	AE	PIML	ANNs	CNN		NO	SMs			GNN	IN	LSTM	GRU
Details	*CAE*		*RBF-ANN*	*U-Net*	*RESNET*	*FNO*	*AR*	*ARMA*	*ARIMA*		*JEDI-net*		
AI for turbulent boundary layers	X	X											
AI for 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			
AI for wetting hydrodynamics						X							
Event reconstruction and classification at the CERN HL-LHC use case										X	X		
Seismic imaging with remote sensing for energy applications	X				X								
Detect-free metal additive manufacturing	X				X								
Sound Engineering												X	X

- Next round of Interaction Rooms with WP2
  - Carve out more details on AI/HPC methods
  - Contribute to the Unique AI Framework
  - Update our HPC/AI Methods Matrix

Agenda Item (3) – Reflect on M12 Deliverables

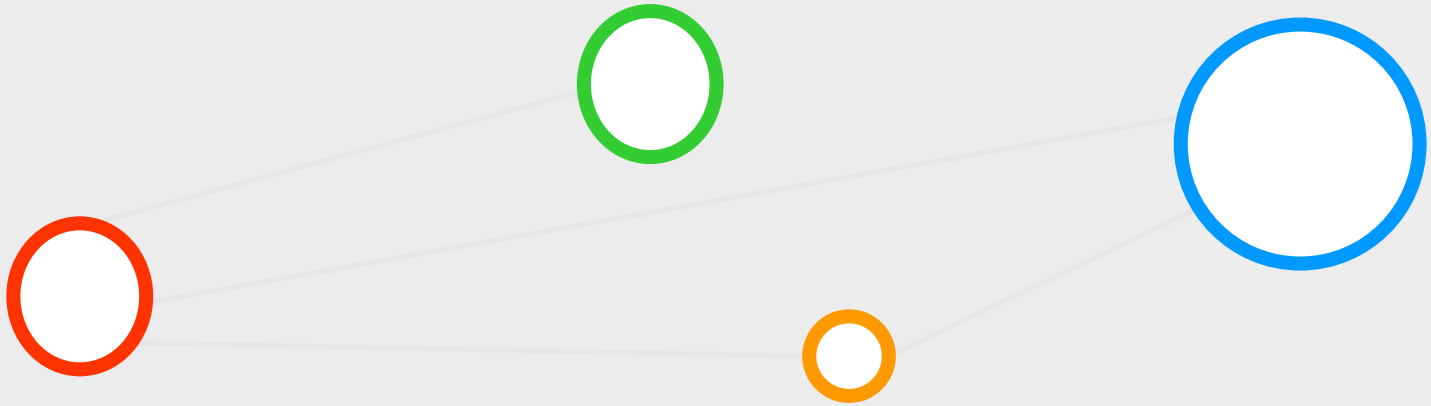


Reflect on M12 Deliverables – Makes sense for WP2 to look at them!

- All deliverables can be found on BSCW (please have a look!): https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3270543

D2.2	Report on porting & performance engineering	BSC	R	PU	12	M. Riedel/ UOI	G. Houzeaux/ BSC	M. Meinke/ RWTH	A. Lintermann/ FZJ	29.11.2021	31.12.2021
D2.14	Report on novel AI technologies	UOI	R	CO	12	M. Riedel/ UOI	M. Riedel/ UOI	S. Kesselheim/ FZJ	J.Lopez/ ParTec	29.11.2021	31.12.2021
D3.1	Report on outcomes of WP3 use-cases	RWTH	R	CO	12	W. Schröder/ RWTH	M. Meinke/ RWTH	S. Schlimpert/ FM	J.Lopez/ ParTec	29.11.2021	31.12.2021
D4.1	Report on outcomes of WP4 use-cases	CERN	R	CO	12	M.Girone/ CERN	V. Khristenko/ CERN	H. Neukirchen/ UOI	I. Schmitz/ ParTec	29.11.2021	31.12.2021
D5.4	IP document and services	FZJ	R	CO	12	K. De Grave/ FM	M. Himmelsbach/ ParTec	I. Slaidins/ RTU	A. Lintermann/ FZJ	29.11.2021	31.12.2021
D6.2	Educational portfolio document	RTU	R	PU	12	R. Gregorio/ BSC	I. Slaidins/ RTU	V. Harmandaris/ CYI	K. Pausch/ FZJ	29.11.2021	31.12.2021
D6.9	Visual identity	FZJ	DEC	PU	12	R. Gregorio/ BSC	M. Bresser/ FZJ	G. Exilard/ SAFRAN	I. Schmitz/ ParTec	29.11.2021	31.12.2021
D6.10	Communication and dissemination plan	FZJ	R	PU	12	R. Gregorio/ BSC	M. Bresser/ FZJ	D. Southwick/ CERN	J. Lopez/ ParTec	29.11.2021	31.12.2021

Agenda Item (4) – Status WP2 Seminar Plans



WP2 Monthly Seminars – Review & Plan

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December:
No Seminar

January:
RTU CUDA Seminar
(THANKS!)

February:
UNets
(Atos, FZJ, ???)

March:
Request Project Partners?
ONNX / OpenML
Interoperable formats

TBD (all): Please suggest further training & teaching seminars for YouTube channel on our WP2 mailing list to plan better ahead

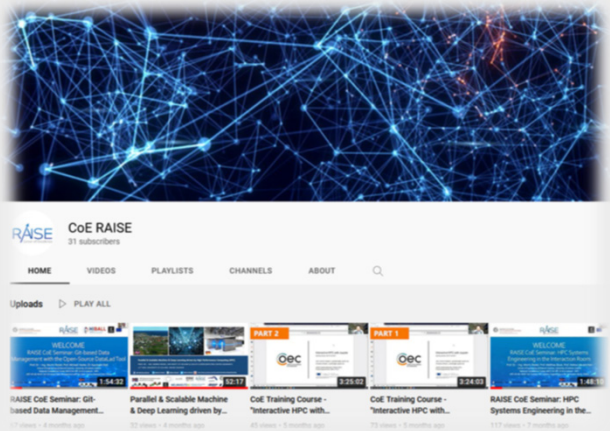
WP2 Monthly Seminars – Review & Plan

April: Quantum Annealing Maybe Gabriele Examles from SVMs, Amer SVR	May: Request Project Partners?	June: Request Project Partners?
July: Request Project Partners?	August: Request Project Partners?	September: Request Project Partners?

TBD (all): Please suggest further training & teaching seminars for YouTube channel on our WP2 mailing list to plan better ahead

WP2 Monthly Seminars – Review & Plan

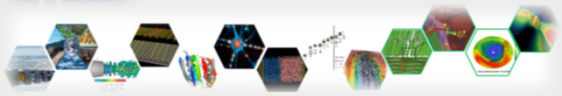
- Monthly WP2 Seminars
  - Co-organized with Icelandic National Competence Center (NCC) funded by the EuroCC project: http://ihpc.is
  - Performed since Quarter 2 of the project (April 2021)
  - Selected dates via agreement of availability of speakers
  - Participated seminar speakers are project external & internal
  - Used as major AI/HPC methods information/training for WP3/WP4
  - Contributed to outreach via YouTube Channel recordings: https://www.youtube.com/channel/UCAdIZ-v6cWwGdapwYxdN7dg



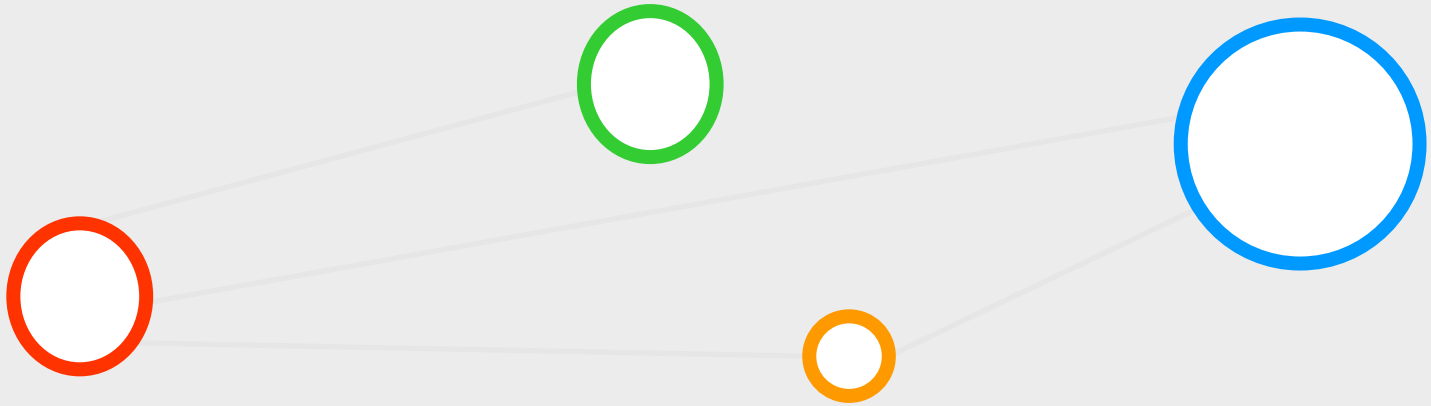
Plan for next 12 Month

- **Carry on with monthly WP2 seminars in the same style, but schedule on 3-4 month horizons**
- **Repeat certain seminars with advanced content and updates of activities (e.g., GraphCore & ATOS)**
- **Work better together with WP6 on releasing seminars on YouTube channel more regularly**
- **Collect slides of speakers and make them available on BSCW and/or on the RAISE Web Page**

IHPC National Competence Center (NCC) for HPC & AI in Iceland

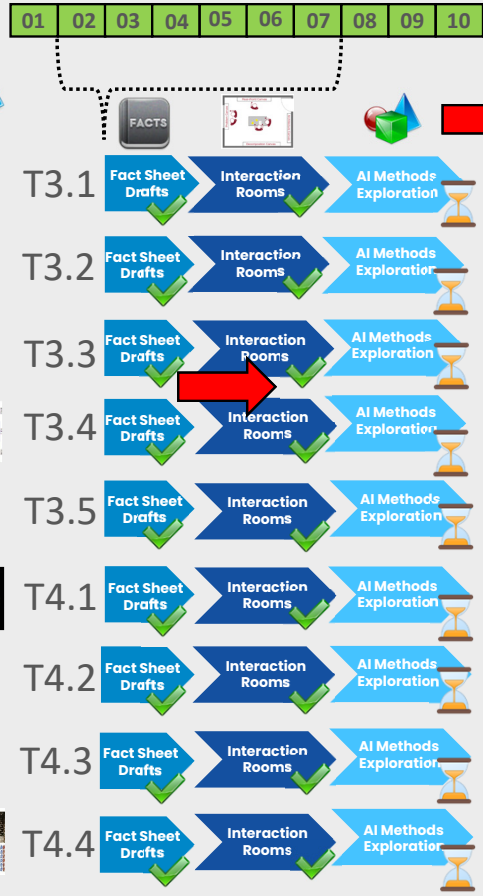


Agenda Item (5) – Compelling Scoreboard Review & Next Steps

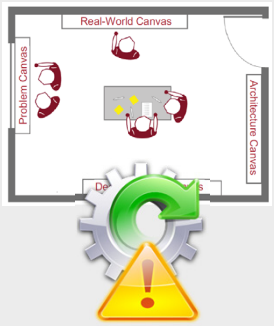


Compelling Scoreboard Review – Use Case Progress

RAISE Center of Excellence



❖ Time to perform again joint Interaction Room session to identify novel AI methods and build unique AI framework parts



based on Milestone (M7) AI/HPC Methods

Based on Deliverable D2.12 (M9) Layout plan AI Framework

RAISE Center of Excellence

H2020-INFRAEDI-2018-2020

CoE RAISE

Center of Excellence "Research on AI- and Simulation-Based Engineering at Exascale"

Grant Agreement Number: 951733

MS2

AI/HPC Methods

RAISE Center of Excellence

H2020-INFRAEDI-2018-2020

CoE RAISE

Center of Excellence "Research on AI- and Simulation-Based Engineering at Exascale"

Grant Agreement Number: 951733

D2.12

Software Layout Plan for a unique AI Framework

Draft

Version: 0.12
Author(s): M. Riedel (UOI)
Contributor(s): M. Book (UOI), H. Neukirchen (UOI)
Date: 28.09.2021

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

✓ 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

✓ Distributed Training Seminar 2021-07-29

✓ AI/HPC Methods (M7)

✓ Monthly Meeting July

YouTube

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
												S:21																									

T3.1 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

T3.2 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

T3.3 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

T3.4 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

T3.5 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

T4.1 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

T4.2 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

T4.3 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

T4.4 Fact Sheet Drafts → Interaction Rooms → AI Methods Exploration

✓ AHM Meeting 2021-11-24/25

✓ GraphCore Seminar 2021-11-23

✓ Monthly Meeting November

✓ Hyperparameter Tuning with Ray Tune Seminar 2021-10-29

✓ Monthly Meeting October

✓ MLOps with ClearML Seminar ~end Sep

✓ Monthly Meeting September

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

✓ Monthly Meeting August

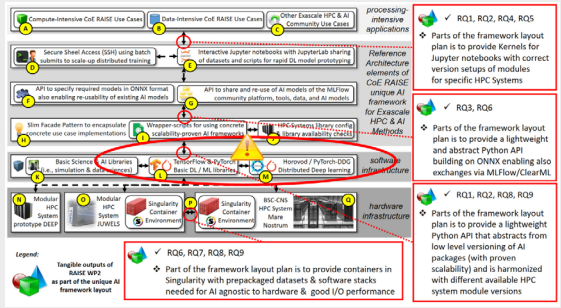
✓ Autoencoder Seminar ~end August

✓ D2.2 Report on porting & performance engineering (M12)

❖ Monthly Meeting January

✓ CUDA Seminar January 2022-01-19/20

✓ D2.14 Report on novel AI technologies (M12)



- Next Steps
  - Interaction Room 2nd Round → Discuss & Implement framework
  - Finish Factsheets → Review
  - YouTube Seminar Plans

Agenda Item (5) – Next Steps & Follow-Through

1. AOB: QR inputs from selected WP2 partners
    1. TBD (Morris et al): PMT waits – urgent!

2. AOB: News Article Last year
    1. Urgent now (Morris), content from deliverables

drive. enable. innovate.

RAISE
Center of Excellence

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

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