

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

Prof. Dr. – Ing. Morris Riedel et al.

School of Engineering & Natural Sciences, University of Iceland

2022-08-26, RAISE WP2 Monthly Meeting August 2022, Online



@ProfDrMorrisRiedel



@Morris Riedel



@MorrisRiedel



@MorrisRiedel



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



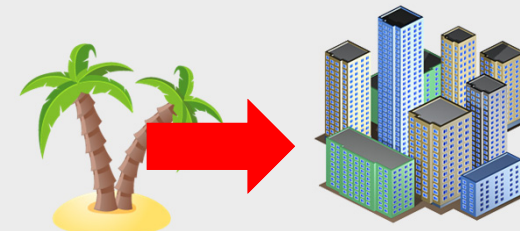
morris@hi.is



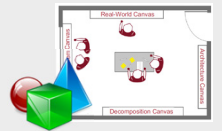
WP2 Meeting August – Welcome & Agenda



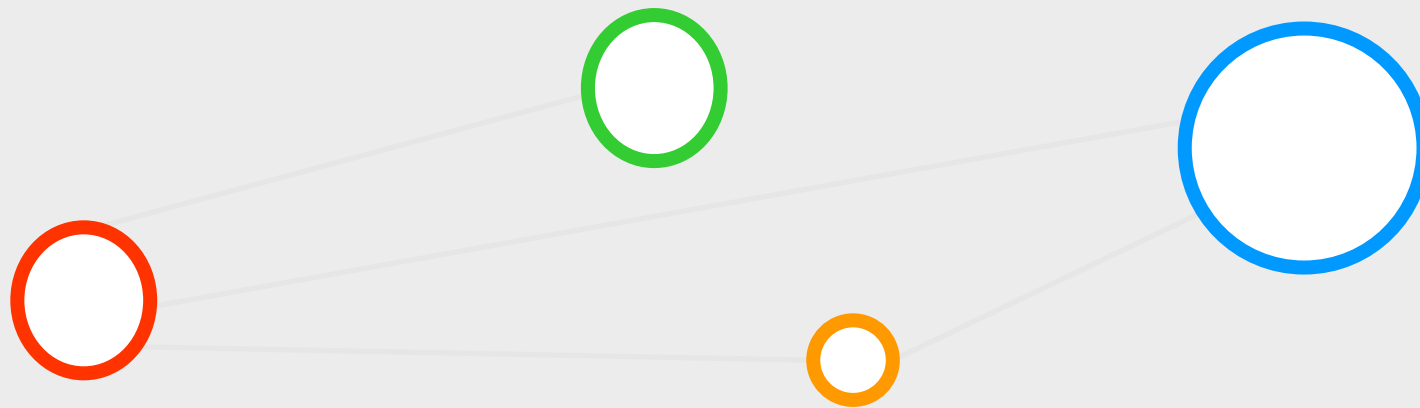
1. Approval of minutes from Monthly Meeting July 2022
 - (All), ~5 Min
2. Review WP2 Status on Interaction Rooms
 - (Morris Riedel, Matthias Book, Helmut Neukirchen), ~5 Min
3. September Review Preparation (M21)
 - (Morris, Andreas, et al.), ~20 Min
4. New Task 2.3 – Quantum Computing
 - (Marcel et al.), ~10 Min
5. Status WP2 Training Plans
 - (Morris et al.), ~5 Min
6. Compelling Scoreboard Review & Next Steps
 - (All), ~10 Min



**Back to action
after vacation – We
face an EC Review!**



Agenda Item (1) – Minutes Approval – July 2022



Minutes Approval – Monthly Meeting July 2022



➤ Minutes available in BSCW

- <https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3340884>
- **TBD(all): Any objections or additions/changes?**

Morris Riedel - RAISE WP2 - Issues

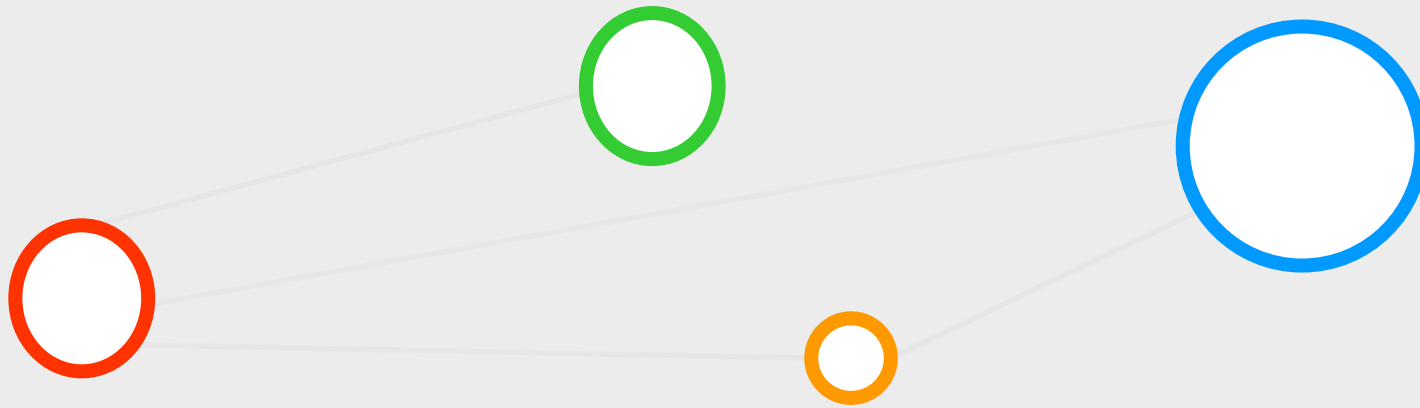
Open	Closed	All
Recent searches - Search or filter results...		
Due date - 1h		
B - Create Fact Sheet Task 4.4 Sound Engineering		
#21 - created 3 minutes ago by Morris Riedel	WP2 Fact Sheet Collection Completed	Apr 30, 2021
updated just now		
B - Create Fact Sheet Task 4.2 Seismic Imaging		
#20 - created 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 Flows & 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		
#19 - 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		

Slides & Materials from Meeting 2021-11-26

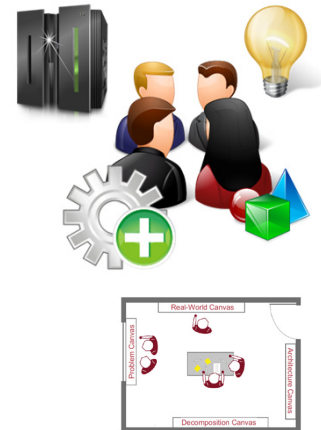
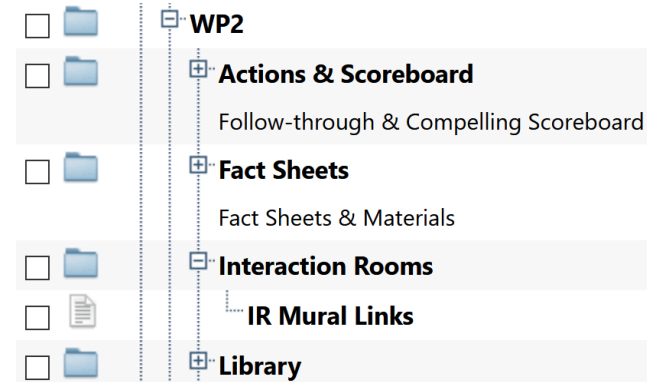
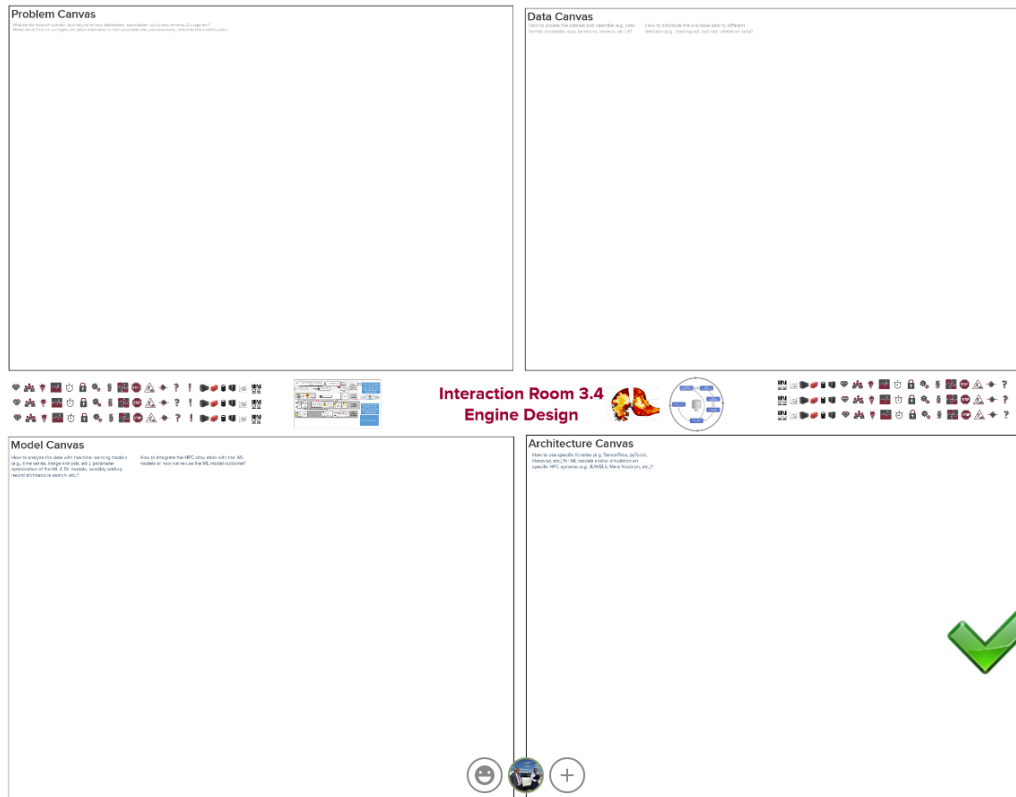
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Slides & Materials from Meeting 2022-01-31			
2022_02_28_Monthly_Meeting_February_2022	2	M.Riedel	2022-03-30 09:41
Slides & Materials from Meeting 2022-02-28			
2022_03_30_Monthly_Meeting_March_2022	2	Katrine	2022-04-29 10:23
Slides & Materials from Meeting 2022-03-30			
2022_04_29_Monthly-Meeting_April_2022	2	M.Riedel	2022-05-31 11:23
Slides & Materials from Meeting 2022-04-29			
2022_05_31_Monthly_Meeting_May_2022	2	Katrine	2022-06-27 13:03
Slides & Materials from 2022_05_31_Monthly_Meeting_May_2022			
2022_06_28_Monthly_Meeting_June_2022	2	M.Riedel	2022-07-28 14:51
Slides & Materials from Meeting 2022-06-28			
2022_07_29_Monthly_Meeting_July_2022	2	M.Riedel	2022-08-03 09:49
Slides & Materials from Meeting 2022-07-29			
2022-07-29-WP2-Monthly-Meeting-Minutes.pdf	439 K	M.Riedel	2022-08-03 09:49
2022_07_29_CoE-RAISE-WP2-Monthly-Meeting-Riedel-v1.pptx	31.3 M	M.Riedel	2022-08-03 09:49



Agenda Item (2) – Review WP2 Status on Interaction Rooms RAISE Center of Excellence



Interaction Rooms via MURAL Boards & Milestone Inputs

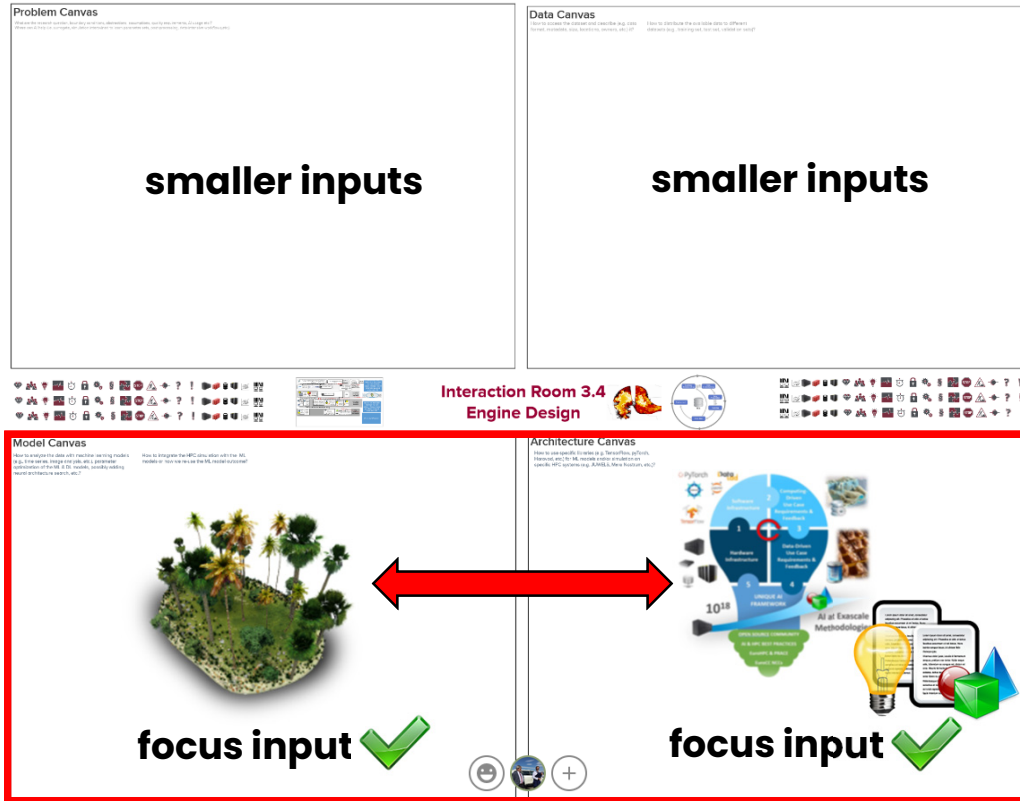


IR Mural Links

- 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/cb44cca3eed3bb9964fbfa36a1f6b1bfce085f?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/matthiasbook8855/1621377976343/8d7aba6be09af3b2fd305d2f709e53661ac889d?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/matthiasbook8855/1621378007335/6f0d5285feaec3eaf515bd6676e84d8b4879d39?sender=u15e3008bb41d6628a5bb5701>
- IR4.2 Seismic Imaging: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ac3e28a4bb8d9adbec33874998?sender=u15e3008bb41d6628a5bb5701>
- IR4.3 Manufacturing: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378038069/93df6fa741093f4eaae7be9d72979dc2ba42b9d?sender=u15e3008bb41d6628a5bb5701>
- IR4.4 Sound Engineering: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa12219002404059f90a4bbb0101fa379a8503?sender=u15e3008bb41d6628a5bb5701>

- 2nd Iteration with all teams completed – Strategy for Task 3.4 has been discussed!
- <https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3591551>

MURAL Board contents for Deliverables & Milestones



- ☐ **WP2**
- ☐ **Actions & Scoreboard**
Follow-through & Compelling Scoreboard
- ☐ **Fact Sheets**
Fact Sheets & Materials
- ☐ **Interaction Rooms**
- ☐ **IR Mural Links**
- ☐ **Library**



IR Mural Links

- IR3.1 Turbulent Flow: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377866397/8613c384d54f66fb5e78599ff307a4ce8a9090c0?sender=u15c3008bb41d6628a5bb5701>
- IR3.2 Clean Energy: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377887905/cb44cca3eed3bb9964fbfa36af16b1bfcc085f?sender=u15c3008bb41d6628a5bb5701>
- IR3.3 Reactive Flows: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377959022/0c363886f24833eeb19b025d87324b57fd50e2db?sender=u15c3008bb41d6628a5bb5701>
- IR3.4 Engine Design: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377976343/8d7aba6be09af3b2fd305d2f709e53661ac889d?sender=u15c3008bb41d6628a5bb5701>
- IR3.5 Coating: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377991014/7a5d7e1eaf230178342d1e1d4a84d656d9055d52?sender=u15c3008bb41d6628a5bb5701>
- IR4.1 Fundamental Physics: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378007335/6f0d3285feac3eaf515bd6676e84d8b4879d39?sender=u15c3008bb41d6628a5bb5701>
- IR4.2 Seismic Imaging: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ac3e28a4fbb8d9adbec33874998?sender=u15c3008bb41d6628a5bb5701>
- IR4.3 Manufacturing: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378038069/93df6fa7a41093f4eaae7be9d72979dc2ba42b9d?sender=u15c3008bb41d6628a5bb5701>
- IR4.4 Sound Engineering: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa12219002404059f90a4bbb0101fa379a8503?sender=u15c3008bb41d6628a5bb5701>

Interaction Room Status & Discussions – WP3/WP4 Overview

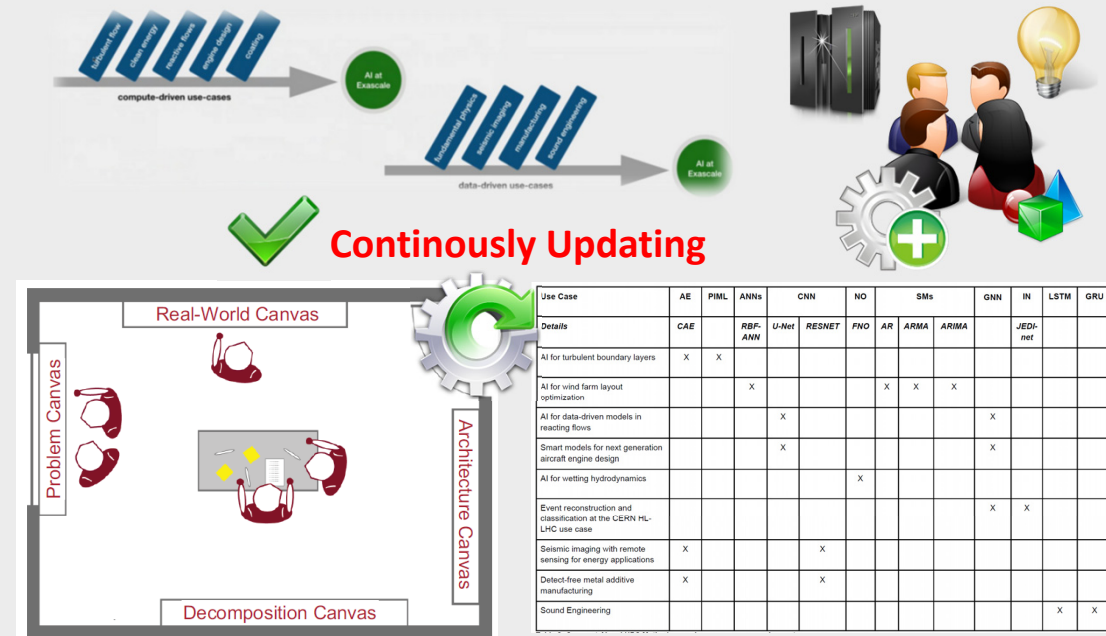
➤ WP3 (third round IRs)

- T3.1: Turbulent Flow → after review
- T3.2: Clean Energy → after review
- T3.3: Reactive Flows → after review
- T3.4: Engine design → after review
- T3.5: Coating → after review

➤ WP4 (third round IRs)

- T4.1: Fundamental physics → after review
- T4.2: Seismic imaging → after review
- T4.3: Manufacturing → after review
- T4.4: Sound engineering → after review

➤ 3rd iteration of Interaction Rooms → schedule



➤ Next round Interaction Rooms after Review

- Carve out more details on AI/HPC methods
- Contribute to the Unique AI Framework
- Update our HPC/AI Methods Matrix

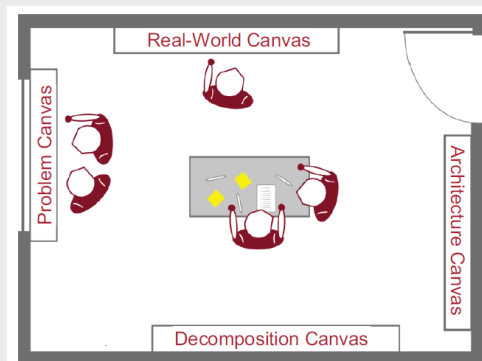
Cross HPC/AI Methods Table – IR Results (D2.10)



Input to Deliverable D2.10

✓ Interaction Rooms

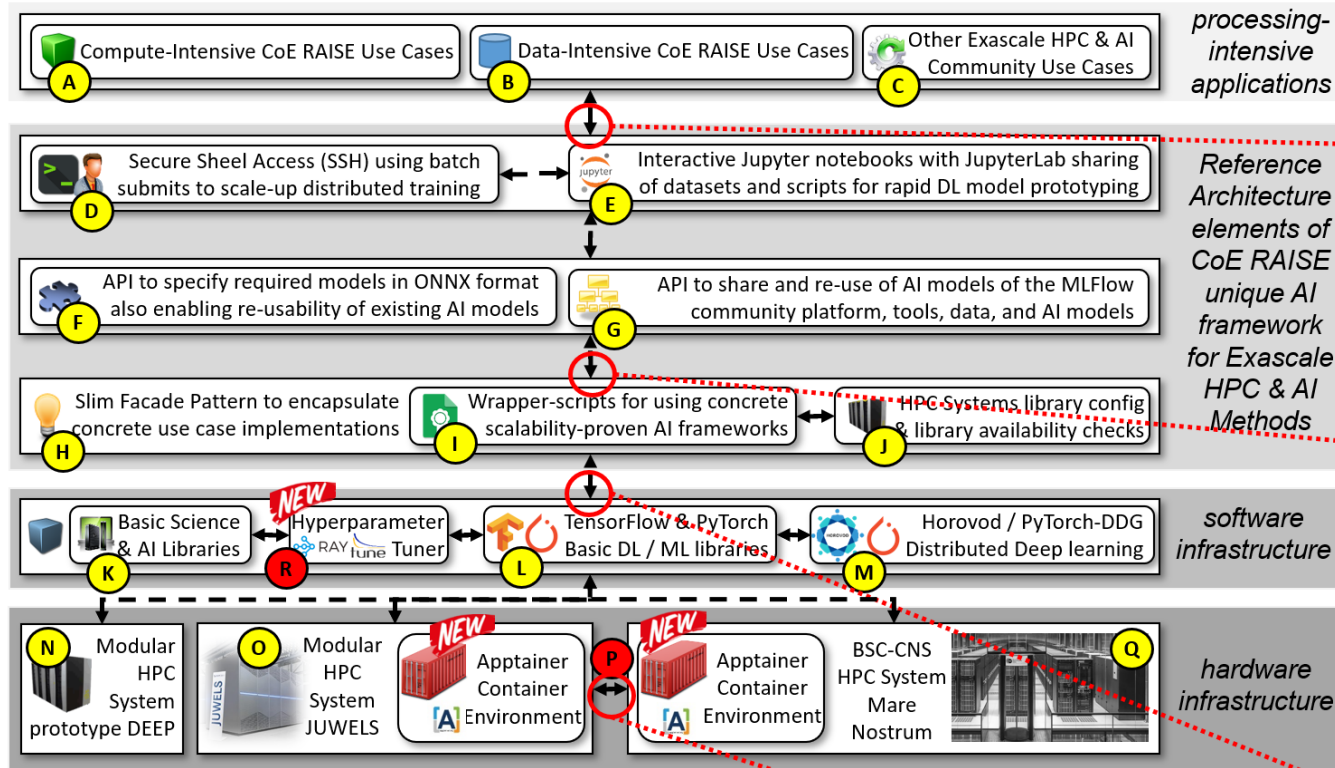
- ✓ Update of Matrix
- ✓ Components relatively constant & common
- ✓ Methods change & new methods added (e.g., Transformers, RFs)



Use Case	AE	PINN	ANNs		CNN		NO	GNN		RNN		GAN	TF				SVM	RF
Details	CAE		ANN	RBF-ANN	U-Net	RES NET	FNO	MLPF	GAT	LSTM	GRU	WGAN	MVIT	VIVIT	Swin			
AI for turbulent boundary layers	X	X	X									X						
AI for wind farm layout optimization				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	X					X			X								
Event reconstruction and classification at the CERN HL-LHC use case								X										
Seismic imaging with remote sensing for energy applications	X	X				X	X			X	X					X	X	X
Detect-free metal additive manufacturing	X		X									X	X	X	X			
Sound Engineering	X		X															



Realization of SW Framework – IR Results (see D2.10)



- ✓ RQ1, RQ2, RQ4, RQ5
- ❖ Parts of the framework layout plan is to provide Kernels for Jupyter notebooks with correct version setups of modules for specific HPC Systems
- ✓ RQ3, RQ6 **NEW**
- ❖ Parts of the framework layout plan is to provide lightweight & abstract Python APIs building on ONNX enabling exchange with MLFlow, **OpenML**, **ClearML**, etc.
- ✓ RQ1, RQ2
- ❖ Parts of the framework layout plan is to provide a lightweight Python API that abstracts from low level versioning of AI packages (with proven scalability) and is harmonized with different available HPC system module versions
- ✓ RQ6, RQ7
- ❖ Part of the framework layout plan is to provide containers in **Apptainer** with prepackaged datasets and required software stacks needed for AI models

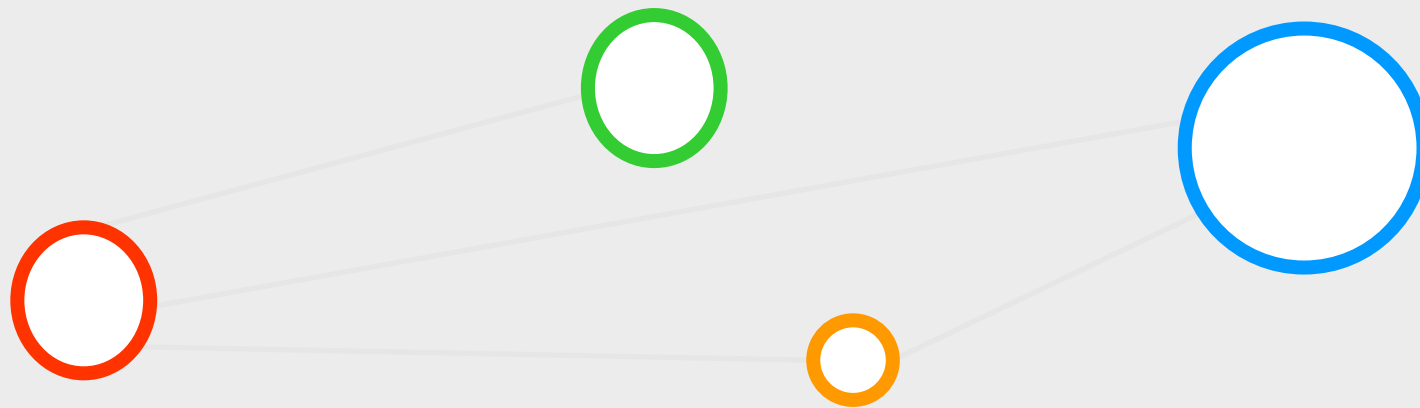


Coupler not from Atos?
Clarify what should be in the framework from ATOS

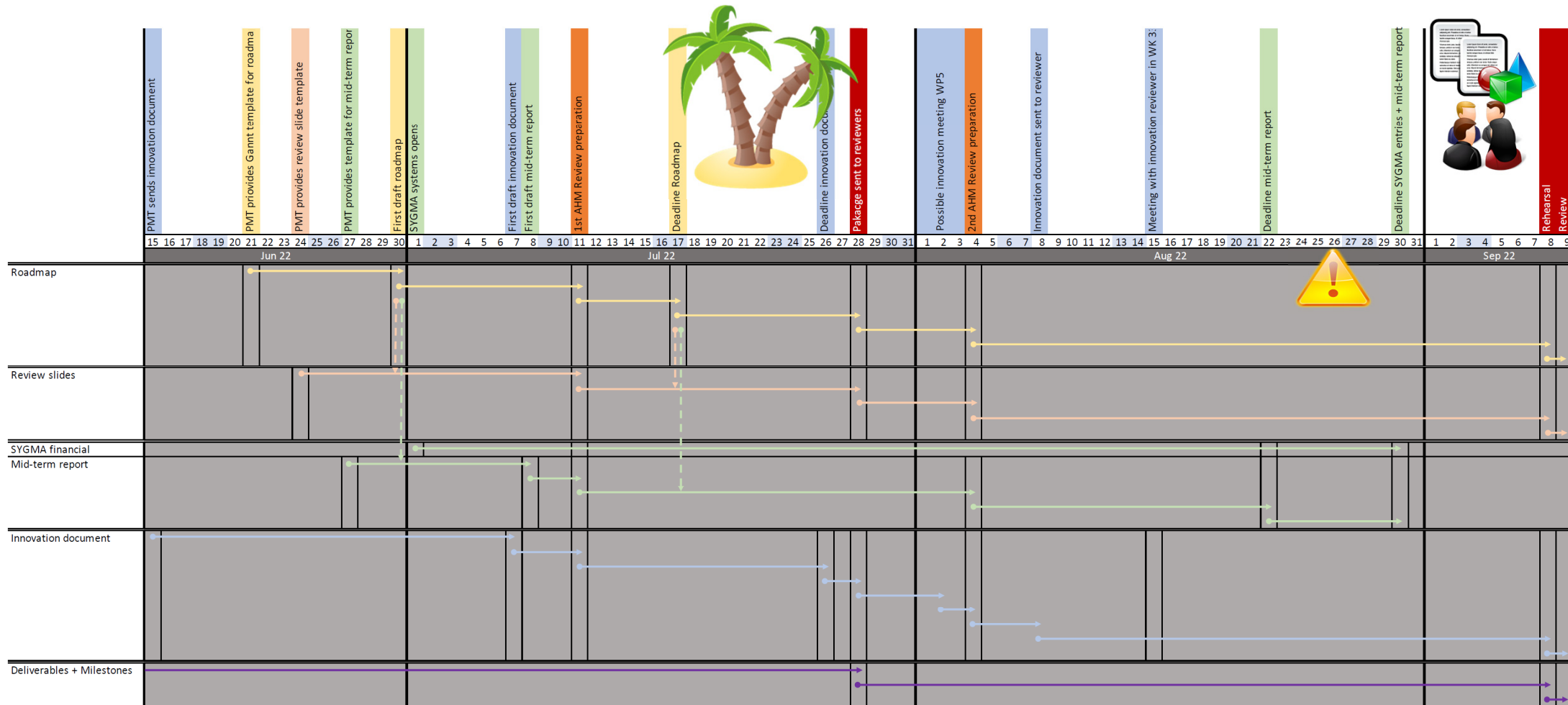


Continuously Updating!

Agenda Item (3) – September Review Preparation (M21)



September Review Preparation: 08.09. + 09.09. (update!)



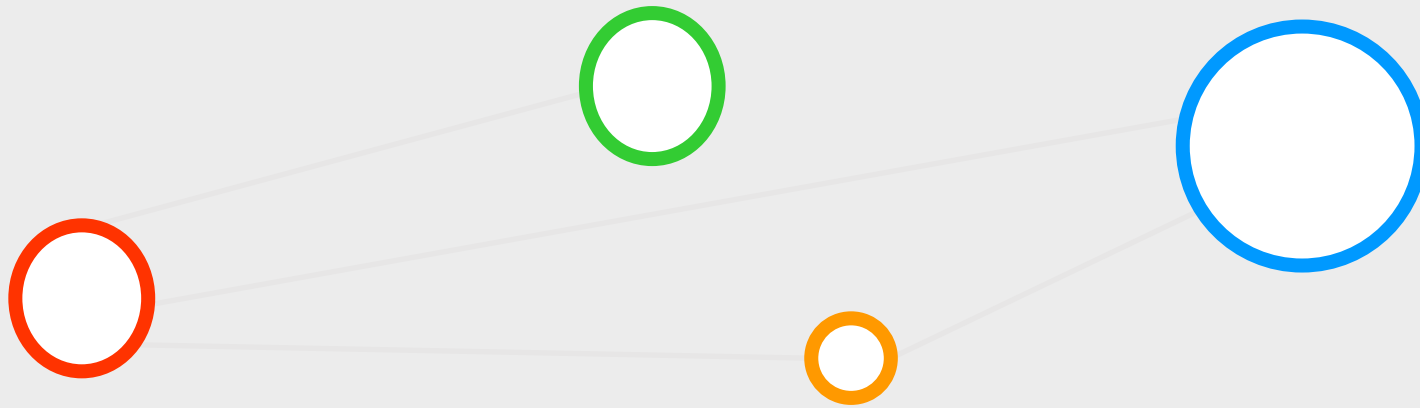
September Review Preparation: WP2 Activities



1. Roadmap Document → Done
 - Interesting Impact part (see WP2 slideset)
2. Innovation Radar → Done
 - Unclear if questions in review or meeting before
3. WP2 Slides → Work in Progress
 1. Input from WP2 Task Leaders (2.1 missing only)
 2. Initial feedback from RAISE WP Leader Meeting (2022-08-25)
 3. Feedback from WP2 folks now



Agenda Item (4) – New Task 2.3 – Quantum Computing

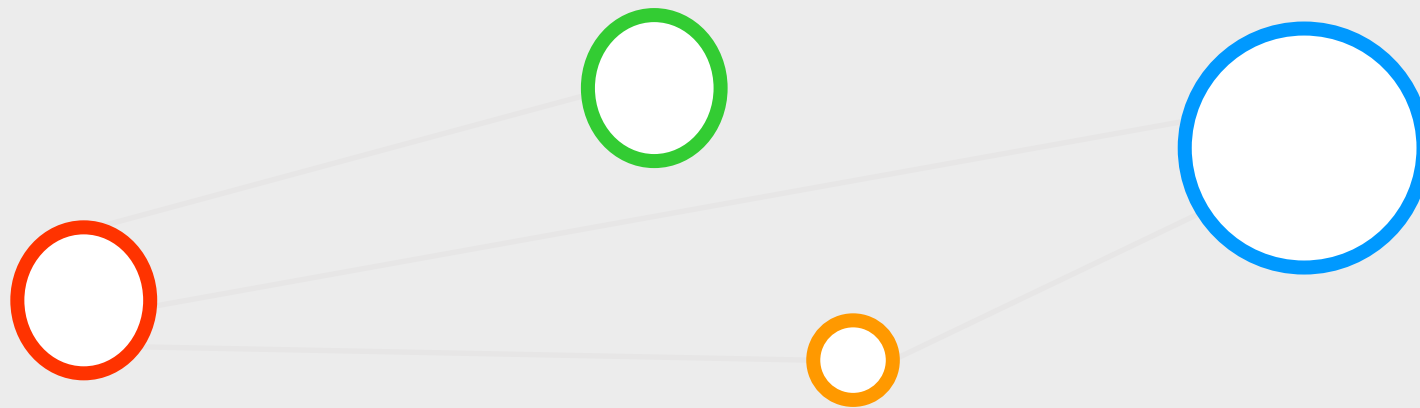


New Task 2.3 – Quantum Computing – Initial Results

➤ Slides Marcel (~10 Min)



Agenda Item (5) – Status WP2 Training Plans



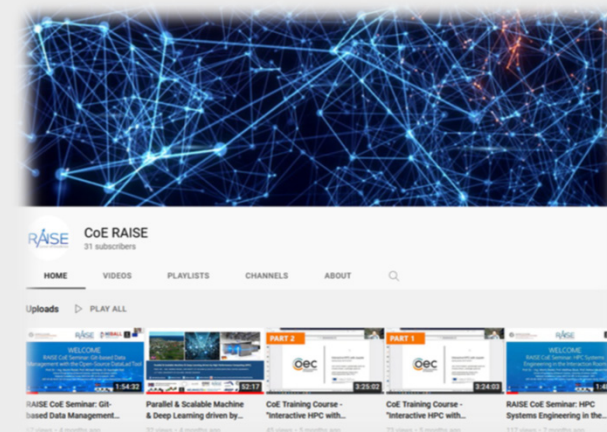
WP2 Monthly Trainings – Review & Plan



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➤ Monthly WP2 Trainings

- 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
- Used as major AI/HPC methods information/training for WP3/WP4
- Contributed to outreach via YouTube Channel recordings: <https://www.youtube.com/channel/UCAdlZ-v6cWwGdapwYxdN7dg>
- TBD(Katrín): Schedule the YouTube Training series with speakers & Update Training Plan

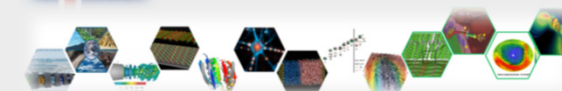


Plan for next months

- Carry on with monthly WP2 trainings in the same style, but schedule on 3-4 month horizons
- Repeat certain trainings with advanced content and updates of activities
- 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



WP2 Monthly Trainings – Review & Plan



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SCHOOL OF ENGINEERING AND NATURAL SCIENCES
RAISE
Center of Excellence

WELCOME
RAISE CoE Seminar: HPC Systems
Engineering in the Interaction Room

Prof. Dr. – Ing. Morris Riedel, Prof. Matthias Book, Prof. Helmut Neukirchen
School of Engineering & Natural Sciences, University of Iceland, Iceland
National Competence Center (NCC) for HPC & AI in Iceland – IHPC
2021-04-08, RAISE CoE Seminar HPC Systems Engineering in the Interaction Room, Online

[f @RuediMorrisRiedel](#) [in @MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#)

<https://www.youtube.com/watch?v=UWCVKXVWkL4g>

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

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Center of Excellence

WELCOME
RAISE CoE Seminar: Git-based Data
Management with the Open-Source DataLad Tool

Prof. Dr. – Ing. Morris Riedel, Prof. Michael Hanke, Dr. Kaustubh Patil
School of Engineering & Natural Sciences, University of Iceland, Iceland
National Competence Center (NCC) for HPC & AI in Iceland – IHPC
2021-05-28, RAISE CoE Seminar Git-based Data Management with the Open-Source DataLad Tool, Online

[f @RuediMorrisRiedel](#) [in @MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#)

<https://www.youtube.com/watch?v=UWCVKXVWkL4g>

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

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Center of Excellence

WELCOME
RAISE CoE Seminar: High Performance Data
Analytics with the Helmholtz Analytics Toolkit (HeAT)

Prof. Dr. – Ing. Morris Riedel, Dr. Claudia Comito, Dr. Charlotte Debus
School of Engineering & Natural Sciences, University of Iceland, Iceland
National Competence Center (NCC) for HPC & AI in Iceland – IHPC
2021-06-28, RAISE CoE Seminar High Performance Data Analytics with the Helmholtz Analytics Toolkit (HeAT), Online

[f @RuediMorrisRiedel](#) [in @MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#)

<https://www.youtube.com/watch?v=UWCVKXVWkL4g>

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Center of Excellence

WELCOME
RAISE CoE Seminar:
Distributed Deep Learning

Prof. Dr. – Ing. Morris Riedel et al.
School of Engineering & Natural Sciences, University of Iceland, Iceland
National Competence Center (NCC) for HPC & AI in Iceland – IHPC
2021-07-29, RAISE CoE Seminar Distributed Deep Learning, Online

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<https://www.youtube.com/watch?v=UWCVKXVWkL4g>

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SCHOOL OF ENGINEERING AND NATURAL SCIENCES
RAISE
Center of Excellence

WELCOME
RAISE CoE Seminar:
Brief Introduction to Autoencoders

Prof. Dr. – Ing. Morris Riedel et al.
School of Engineering & Natural Sciences, University of Iceland, Iceland
National Competence Center (NCC) for HPC & AI in Iceland – IHPC
2021-08-31, RAISE CoE Seminar Brief Introduction to Autoencoders, Online

[f @RuediMorrisRiedel](#) [in @MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#)

<https://www.youtube.com/watch?v=UWCVKXVWkL4g>

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

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WELCOME
RAISE CoE Seminar:
MLOps with ClearML

Prof. Dr. – Ing. Morris Riedel et al.
School of Engineering & Natural Sciences, University of Iceland, Iceland
National Competence Center (NCC) for HPC & AI in Iceland – IHPC
2021-09-30, RAISE CoE Seminar MLOps with ClearML, Online

[f @RuediMorrisRiedel](#) [in @MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#)

<https://www.youtube.com/watch?v=UWCVKXVWkL4g>

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

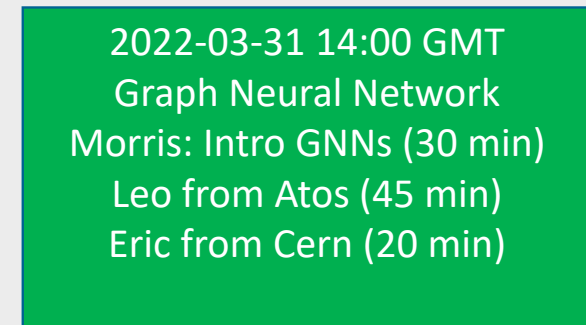
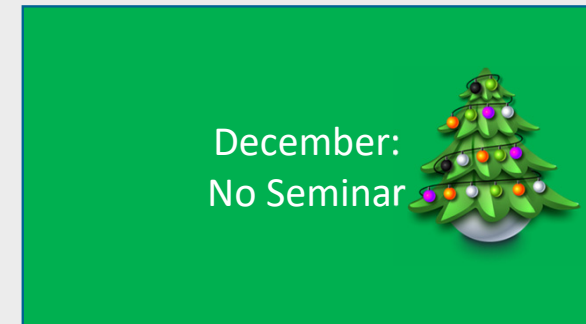


2022-08-26 RAISE WP2 Monthly Meeting August 2022

WP2 Monthly Trainings – Review & Plan



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



WP2 Monthly Trainings – Review & Plan



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April:
Quantum Annealing
Maybe Gabriele Examples from
SVMs, Amer SVR

May:
Using OpenML for sharing
datasets, algorithms, and
experiments

9th of June:
Morris: GPUs in general
Arnis & Cuda @ RTU

July:
none
(vacation period)

JOIN US NEXT WEEK
August: Morris Framework +
Marcel/Rakesh –
implementation on modules
on different HPC Systems

ATOS: affects of
change in persons?

September:
EOSC – NI4OS-Europe or TREX
Project (in scheduling) Request
Project Partners? (continuous
integration ATOS)???
→ Katrin: check and schedule

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



WP2 Monthly Trainings – Review & Plan



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October:
Project Partners?

November:
Project Partners?

December:
Project Partners?



Wait for the feedback from Review:
Otherwise: idea would be to have also trainings on the
adoption of sw framework parts again & AI/HPC Methods

January:
Project Partners?

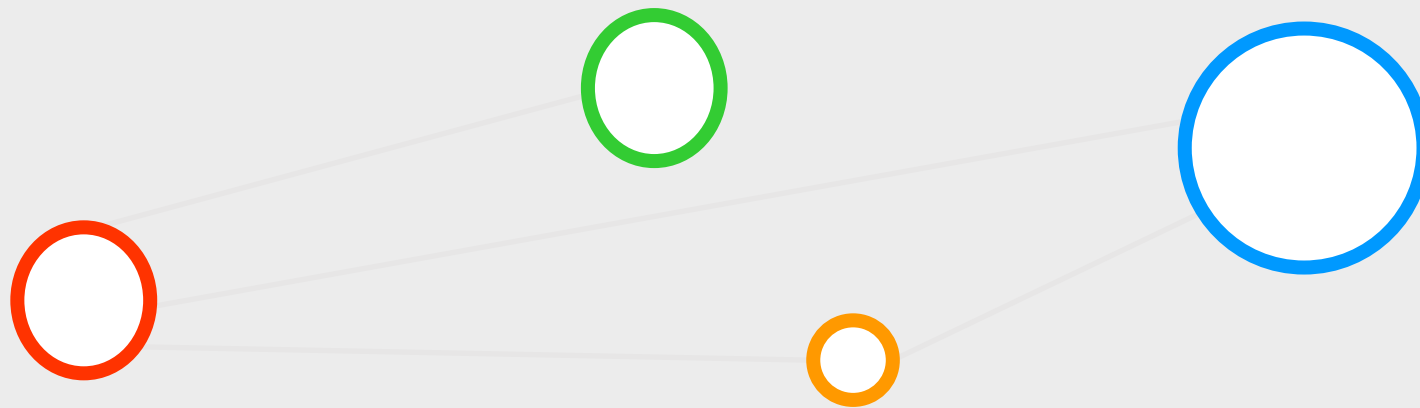
February:
Project Partners?

March
Project Partners?

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



Agenda Item (6) – Compelling Scoreboard Review



Compelling Scoreboard Review – Use Case Progress



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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



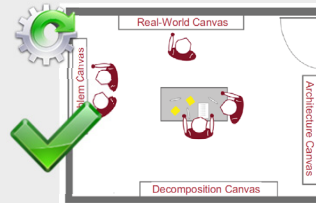
T4.4

Fact Sheet Drafts

Interaction Rooms

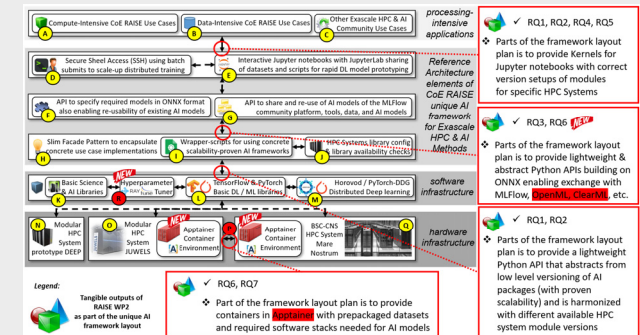
AI Methods Exploration

- ❖ Performing joint Interaction Room sessions: to identify novel AI methods and build unique AI framework parts
- ❖ Realization of SW framework design started → initial collection in WP2 Wiki page RAISE (Jupyter notebooks, etc.)
- ❖ Identified lots of problems → SW framework concept required
- ❖ Collection of software artefacts started for the realization of the framework design bottom-up by use case elements



Lessons Learned from IR Rooms with use cases:
Agreement & common components between use cases realistic → Framework Co-Design ok

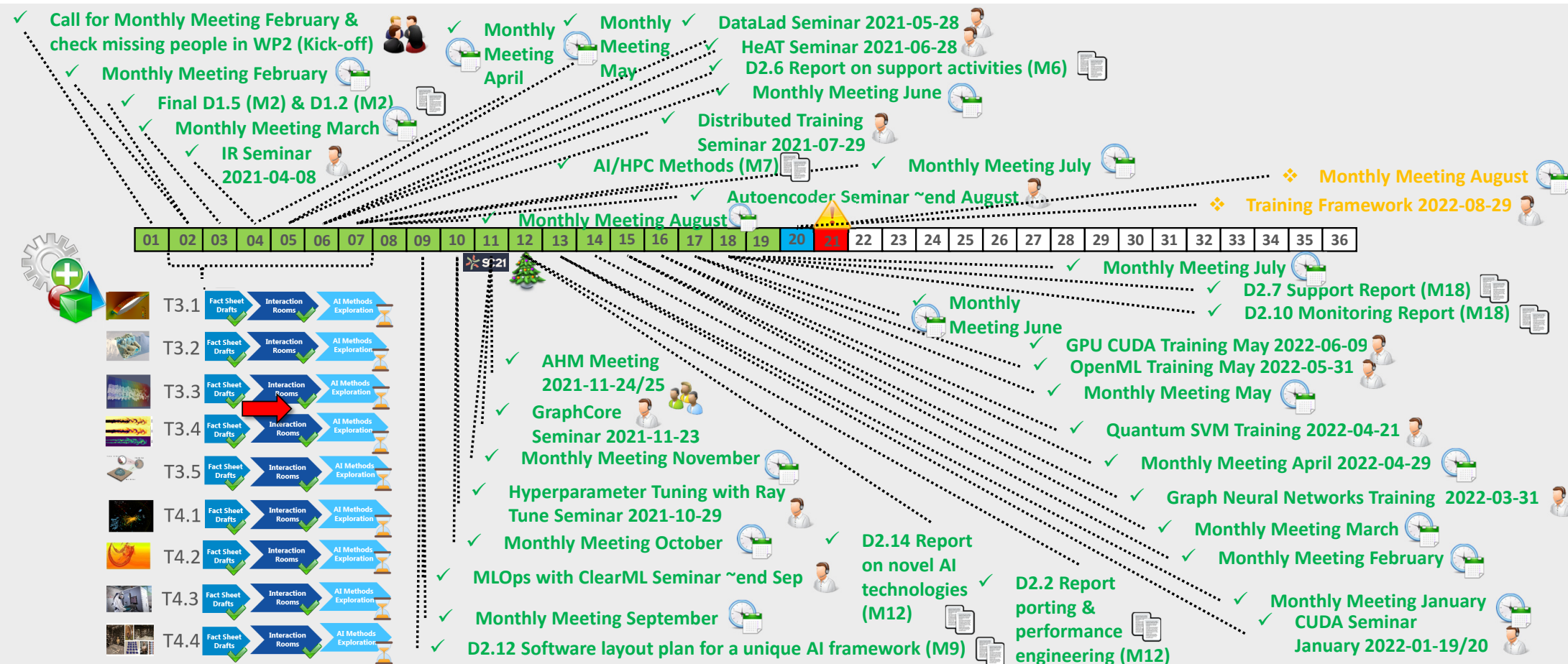
Use Case	AE	PINN	ANNs		CNN		NO	GNN		RNN		GAN	TP				SVM	RF
Details	CAE		ANN	RBF-ANN	U-Net	RES NET	FNO	MLPF	GAT	LSTM	GRU	WGAN	MVIT	VIVIT	Swin			
AI for turbulent boundary layers	X	X	X									X						
AI for wind farm layout optimization				X											X			
AI for data-driven models in reacting flows					X			X										
Smart models for next generation aircraft engine design					X			X										
AI for wetting hydrodynamics	X	X					X			X								
Event reconstruction and classification at the CERN HL-LHC use case								X										
Seismic imaging with remote sensing for energy applications	X	X			X	X				X	X				X	X	X	
Detect-free metal additive manufacturing	X		X									X	X	X	X			
Sound Engineering	X		X															



Compelling Scoreboard Review & Next Steps



RAISE
Center of Excellence



2022-08-26 RAISE WP2 Monthly Meeting August 2022

Agenda Item (6) – Next Steps & Follow-Through

➤ 08.09 - 09.09.2022 (Review Preparations start)

- WP2 Slideset revision in progress

➤ Task 2.1

- LUMI (get access via UICE), Puhuri access
- Mare Nostrum (machine end of the year)
- Contact identified for BSC:
- BSC Backup Contact: Cristóbal Samaniego
- Ahti Saar - Ahti.Saar@ut.ee - was the go-to person to create the access for Iceland LUMI project leaders (i.e. those that can create projects and grant access to users in Iceland etc).
- (Ebba did contact him back in October 2021 to create such an access for Hannes and Henning)
- We need a small justification why access is needed for CoE RAISE
- Q: What exactly will be ported, a short description would be good (3 Lines)



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