

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

Prof. Dr. – Ing. Morris Riedel et al.

School of Engineering & Natural Sciences, University of Iceland

2022-09-30, RAISE WP2 Monthly Meeting September 2022, Online



@ProfDrMorrisRiedel



@Morris Riedel



@MorrisRiedel



@MorrisRiedel



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



morris@hi.is



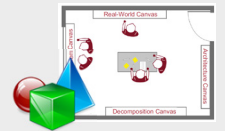
WP2 Meeting September – Welcome & Agenda



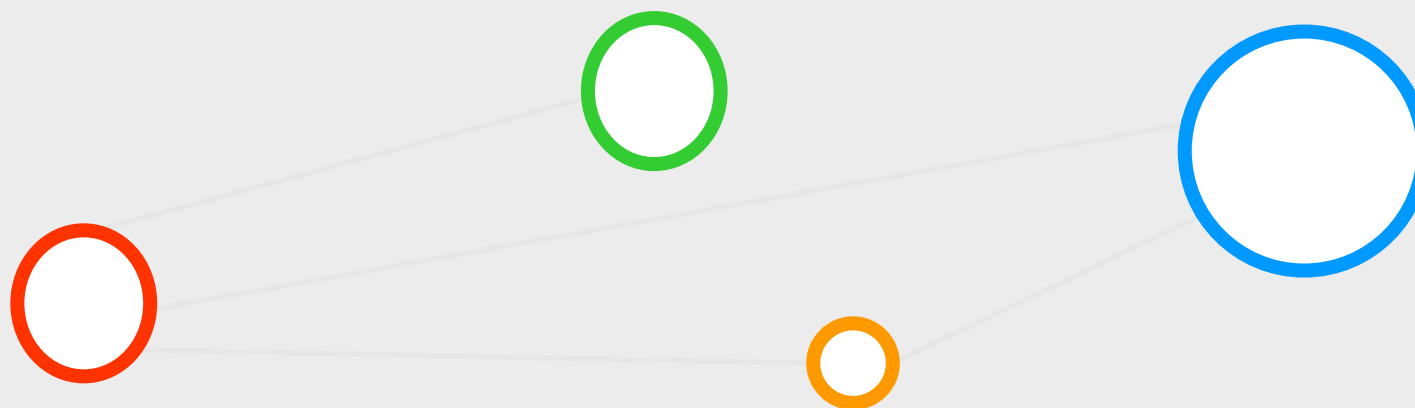
1. Approval of minutes from Monthly Meeting August 2022
 - (All), ~5 Min
2. Review WP2 Status on Interaction Rooms
 - (Morris Riedel, Matthias Book, Helmut Neukirchen), ~5 Min
3. Towards SW Framework Adoptions
 - (Morris, Guillaume, Andreas, et al.), ~20 Min
4. SW Framework Component DALI Data Loader Update
 - (Marcel et al.), ~10 Min
5. Status WP2 Training Plans
 - (Morris et al.), ~5 Min
6. Compelling Scoreboard Review & Next Steps
 - (All), ~10 Min



**EC Review Success:
Thanks to all WP2 members**



Agenda Item (1) – Minutes Approval – August 2022



Minutes Approval – Monthly Meeting August 2022



➤ Minutes available in BSCW

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

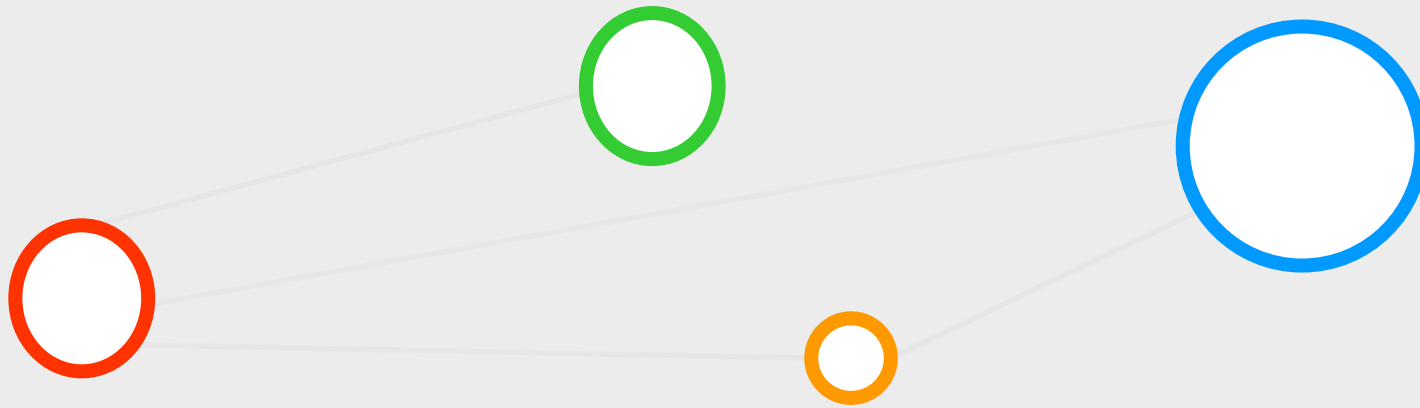
Morris Riedel - RAISE WP2 - Issues

Open	Closed	All	Due date	1s	Edit issues	Item issue
Recent searches - Search or filter results...						
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						

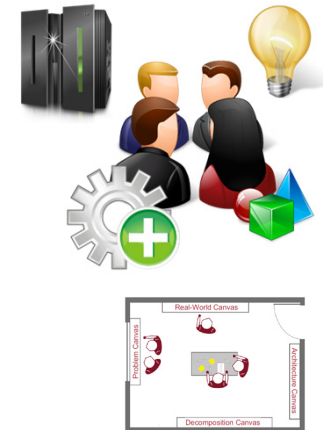
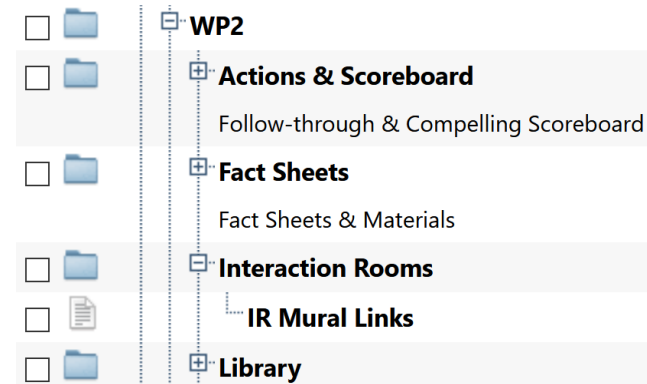
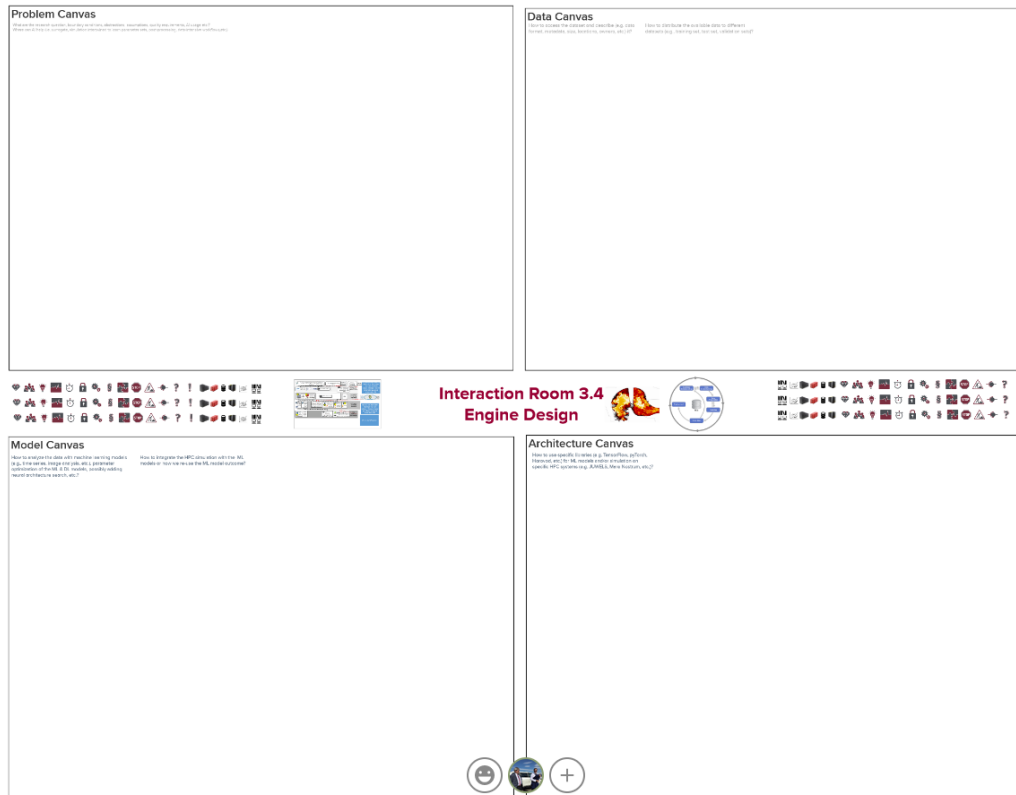
Slides & Materials from Meeting 2021-11-26

2022_01_31_Monthly_Meeting_January_2022	2	M.Riedel	2022-02-28 11:10
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



Interaction Rooms via MURAL Boards & Milestone Inputs



IR Mural Links

- IR3.1 Turbulent Flow: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377866397/8613c384d54f66fb5e78599f307a4ce8a9090c0?sender=u15c3008bb41d6628a5bb5701>
- IR3.2 Clean Energy: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377887905/cb44cca3eed3bb9964fbfa36a1f6b1bfcc085f?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/matthiasbook8855/1621377976343/8d7aba6be09af3b2fd305d2f709c53661ac889d?sender=u15c3008bb41d6628a5bb5701>
- IR3.5 Coating: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377991014/7a5d7e1ea230178342d1e1d4a84d656d9055d52?sender=u15c3008bb41d6628a5bb5701>
- IR4.1 Fundamental Physics: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378007335/6f0d5285feac3eaf515bd6676e84d8b4879d39?sender=u15c3008bb41d6628a5bb5701>
- IR4.2 Seismic Imaging: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ac3e28a4bb8d9adbec33874998?sender=u15c3008bb41d6628a5bb5701>
- IR4.3 Manufacturing: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378038069/93df6fa7a41093f4eaae7bc9d72979d2ba42b9d?sender=u15c3008bb41d6628a5bb5701>
- IR4.4 Sound Engineering: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa12219002404059f90a4bbb0101fa379a8503?sender=u15c3008bb41d6628a5bb5701>

- 3rd iteration with a view on EuroHPC Hosting Sites, SMEs/Industry & CoEs will be started
 - Focus on where exactly is code running and what HPC sites might be interesting in the future
 - Update of the SW Framework Components (e.g., scikit-learn for statistics, NumPy, Dali Data Loader, etc.)

Interaction Room Status & Discussions – WP3/WP4 Overview

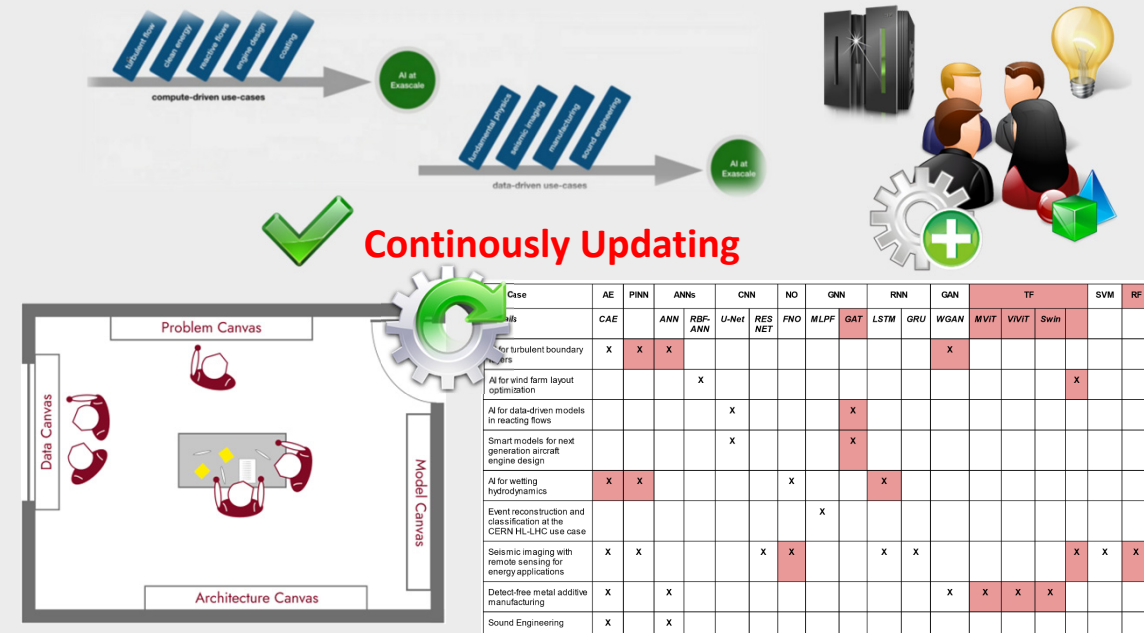
➤ WP3 (third round IRs)

- 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

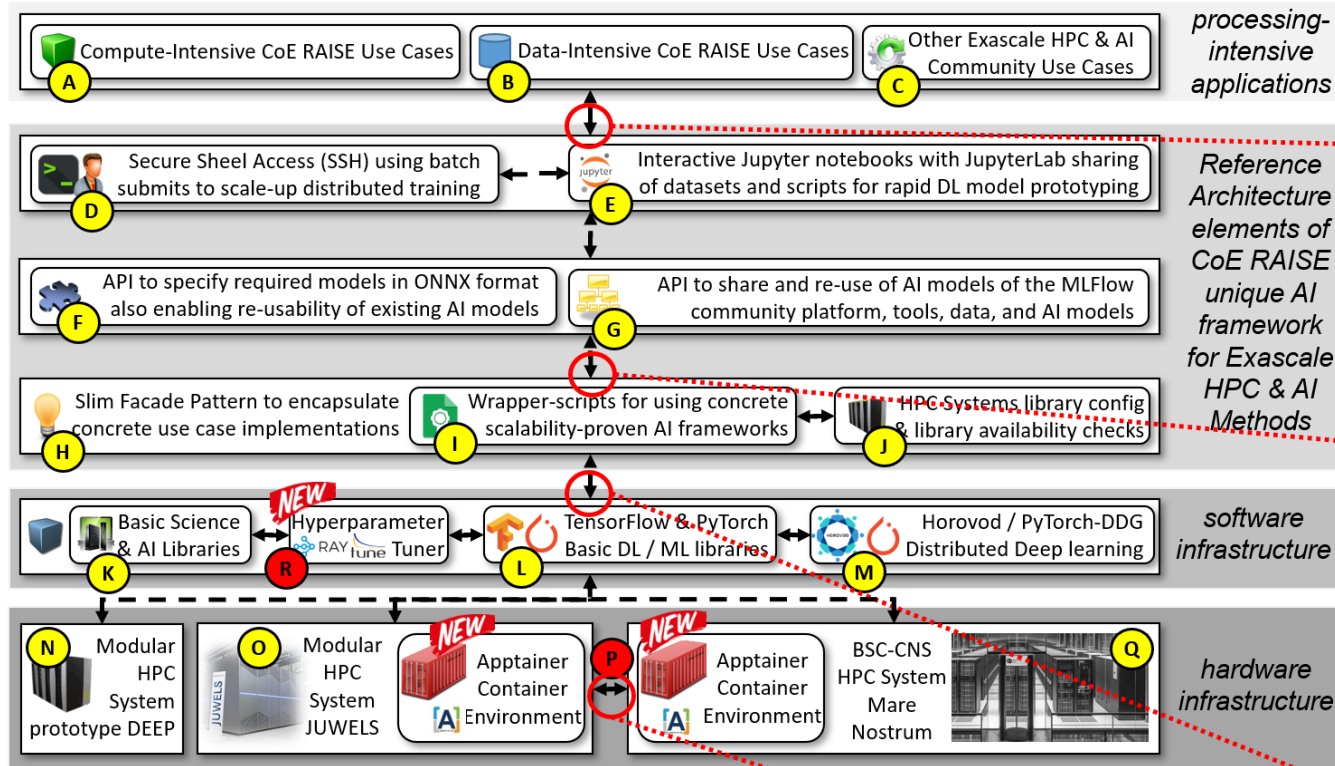
➤ 3rd iteration of Interaction Rooms → schedule



➤ 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

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



Legend:



Tangible outputs of
RAISE WP2
as part of the unique AI
framework layout



✓ 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

processing-intensive applications

Reference Architecture elements of CoE RAISE unique AI framework for Exascale HPC & AI Methods

software infrastructure

hardware infrastructure

- ✓ 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

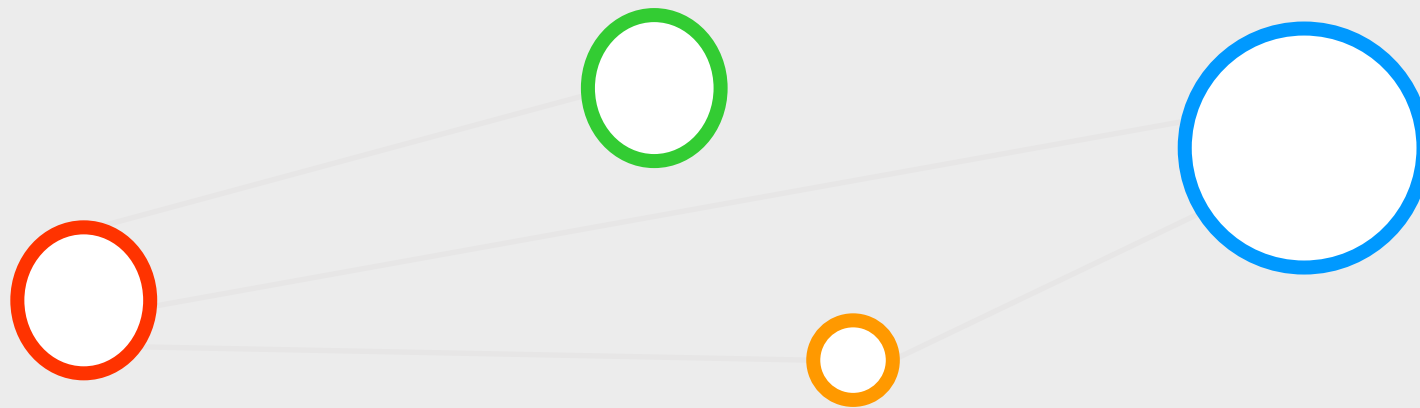


Discuss updates on DALI Data Loader, NumPy, Scikit-learn, Quantum, etc. DeepSpeed?



Continuously Updating!

Agenda Item (3) – Towards SW Framework Adoptions



Review Feedback & TCB Inputs



1. TCB Meeting Notes & Actions

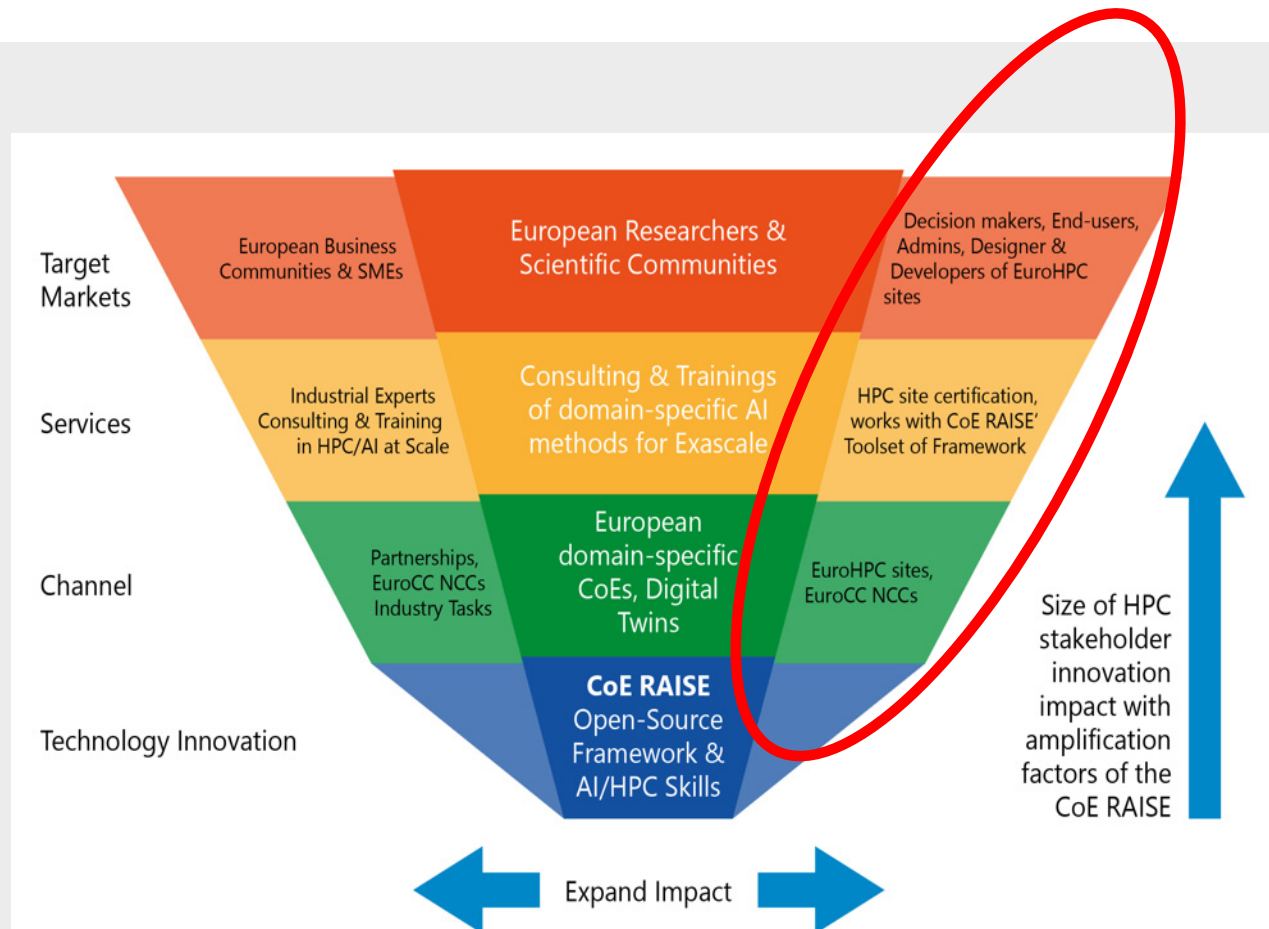
- Task leaders: think about who we might approach in industry, who might be close community allies that we can partner with.
- Identify target group, then reach out to them
- Research/WP leaders: prepare long-term funding outlook for strategy discussion in next years
- RAISE2: to be discussed at all-hands meeting @CERN in January
- WP2:
 - Perhaps industry conference presence?
 - Need to make our work open-source; create visibility of results, use for outreach.
 - Update website to add upcoming videos, promote visibility
 - Need to develop AI specific tools
 - TBD(HCH): Ask for Fortissimo



**EC Review Success:
Thanks to all WP2 members**



Towards SW Framework Adoptions



LUMI

LUMI is a pre-exascale EuroHPC supercomputer located in Kajaani, Finland. It is a Cray EX supercomputer supplied by Hewlett Packard Enterprise (HPE) and hosted by CSC – IT Center for Science.

LUMI supercomputer CSC

375 petaflops Sustained performance	550 petaflops Peak performance
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LEONARDO

Leonardo is a pre-exascale EuroHPC supercomputer currently built in the Bologna Technology, Italy. It is supplied by ATOS, based on a BullSequana XH2000 supercomputer and hosted by CINECA.

LEONARDO Supercomputer CINECA

249,47 petaflops Sustained performance	323,40 petaflops Peak performance
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MARENOSTRUM 5

Marenostrom 5 is a pre-exascale EuroHPC supercomputer to be located in Barcelona, Spain. The system is supplied by Bull SAS combining Bull Sequana XH2000 and Lenovo ThinkSystem architectures. Marenostrom 5 is hosted by Barcelona Supercomputing Center (BSC).

New BSC's data centre waiting to host MND supercomputer BSC

205 Petaflops Sustained performance	314 Petaflops Peak performance
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VEGA

Vega is a petascale EuroHPC supercomputer located in Maribor, Slovenia. It is supplied by Atos, based on the BullSequana XH2000 supercomputer and hosted by QUAM.

Cyprus: VEGA

6,92 petaflops Sustained performance	10,05 petaflops Peak performance
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MELUXINA

Meluxina is a petascale EuroHPC supercomputer located in Bissen, Luxembourg. It is supplied by Atos, based on the BullSequana XH2000 supercomputer platform and hosted by LuxProvide.

Par-Tec?

12,81petaflops Sustained performance	18,29 petaflops Peak performance
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KAROLINA

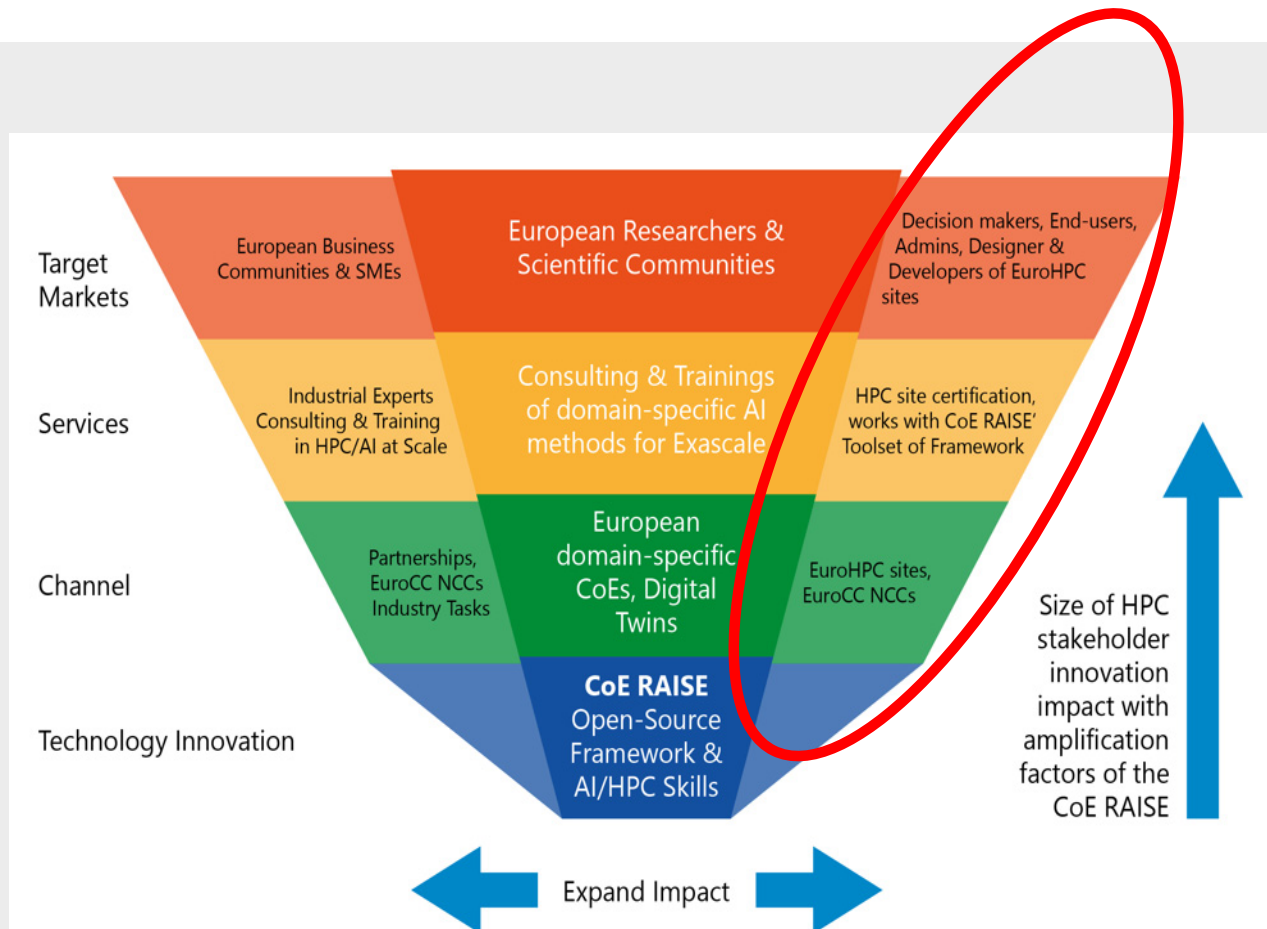
Karolina is a petascale EuroHPC supercomputer located in Ostrava, Czech Republic. It is supplied by Hewlett Packard Enterprise (HPE) Apollo 2000Gen10 Plus and hosted by IT4Innovations National Supercomputing Center.

Prague meeting CoE RAISE

9,59 petaflops Sustained performance	12,91 petaflops Peak performance
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Towards SW Framework Adoptions



DISCOVERER

Discoverer is a petascale EuroHPC supercomputer located in Sofia, Bulgaria. It is supplied by Alos, based on the Bullsequana XH2020 supercomputer and hosted by Sofia Tech Park.

Discoverer supercomputer Sofia Tech Park

4,51 petaflops	5,94 petaflops
Sustained performance	Peak performance

DEUCALION

Deucalion is a petascale EuroHPC supercomputer currently built in Guimarães, Portugal. It is supplied by Fujitsu combining a Fujitsu PRIMERGY X8600 (partition) and Alos Bull Sequana (x86 partitions). Deucalion is hosted by MACC.

Deucalion supercomputer MACC

7,22 petaflops	10 petaflops
Sustained performance	Peak performance

- TBD: Other project partner sites?
 - RTU system
 - DEEP system
 - JUELICH Systems
- Vit Vondrak (IT4Innovation),
 - Tomas

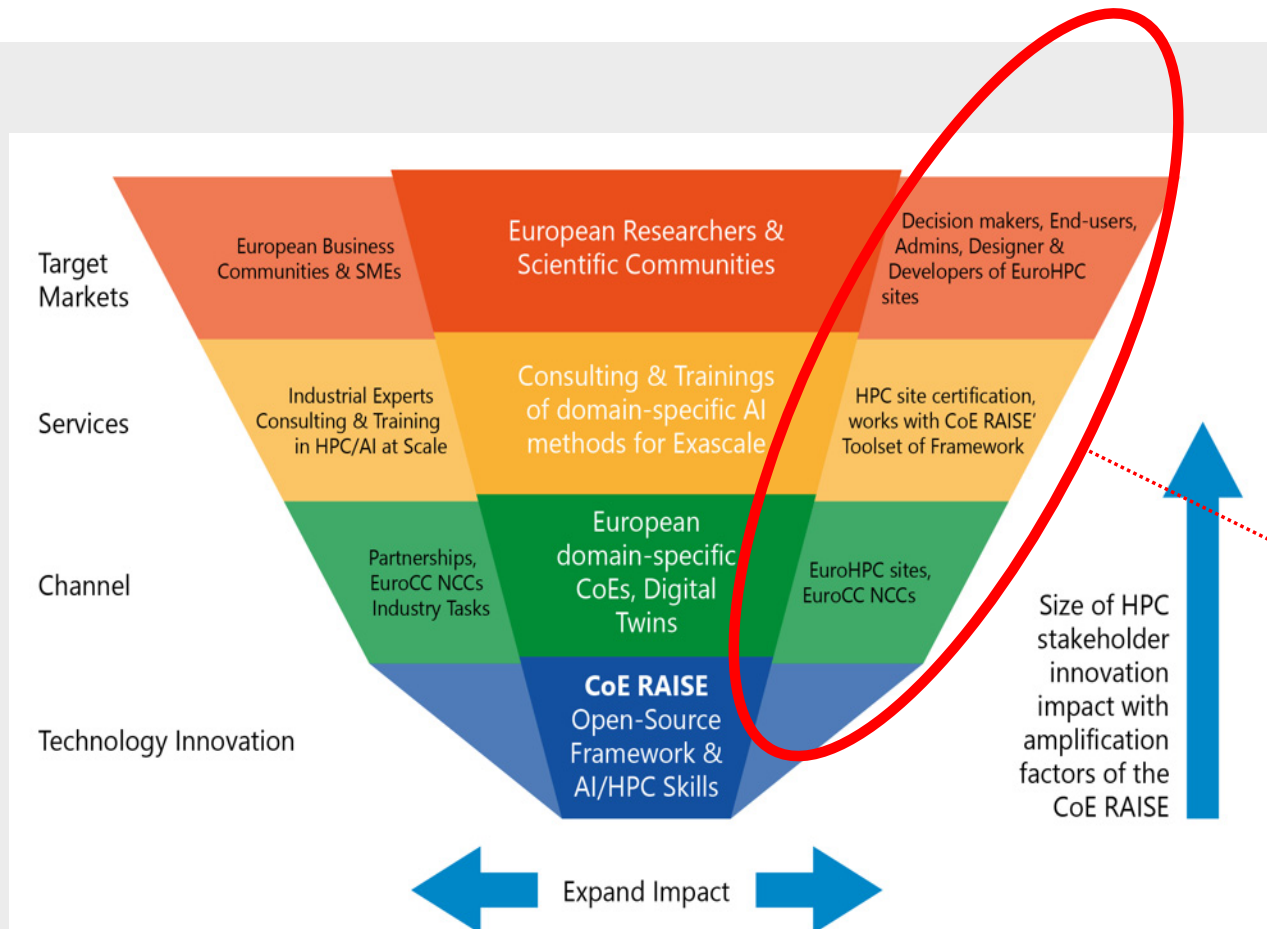


Towards SW Framework Adoptions



EuroHPC
Joint Undertaking

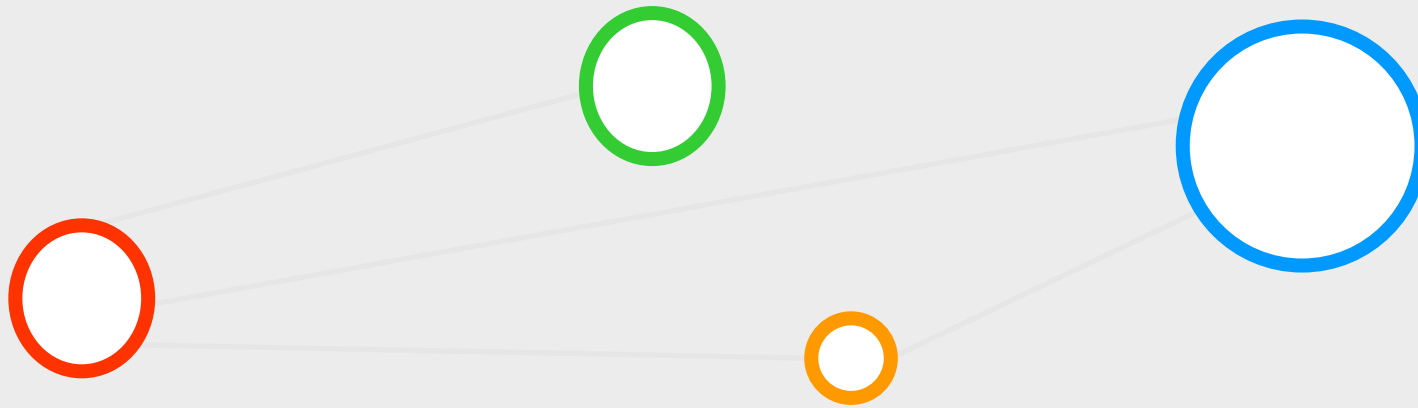
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- 1. Goal Project Sites
 - Talk to administrators of AI tools & technologies about framework
 - Assumption: many tools already deployed, but in different modules
- BSC
 - Contact received – Thanks!
- LUMI
 - Contact existing (2 PhDs work on LUMI already)
- RTU
 - TBD(Lauris, etc.): ask him
- 2. Goal: Vega, Meluxina, Contacts?



Agenda Item (4) – DALI Data Loader Update

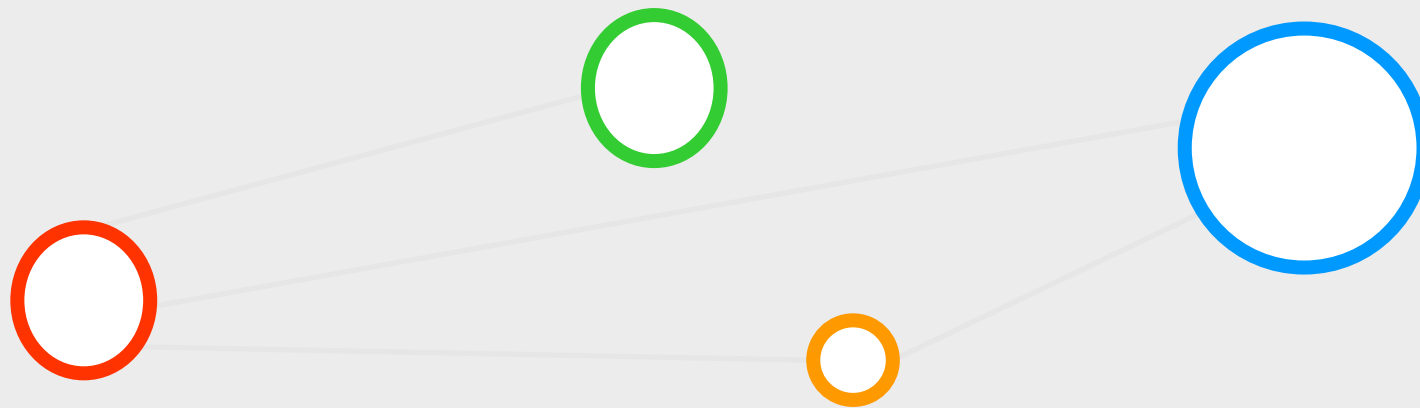


SW Framework Component DALI Data Loader Update

➤ Slides Marcel (~10 Min)



Agenda Item (5) – Status WP2 Training Plans



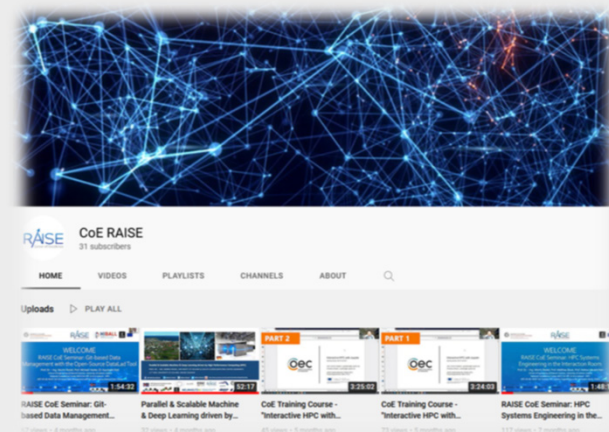
WP2 Monthly Trainings – Review & Plan



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Center of Excellence

➤ 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

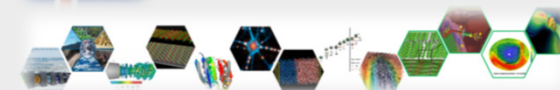


Plan for next months

- 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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EUROPEAN UNION

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](#)
<https://www.youtube.com/watch?v=UVCWCVWvL4Zg> [@MorrisRiedel](#)

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

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RAISE
Center of Excellence
HIBALL
HELMHOLTZ INSTITUTE FOR
DATA-DRIVEN SCIENCE
EUROPEAN UNION

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 Git-based Data Management with the Open-Source DataLad Tool, Online

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<https://www.youtube.com/watch?v=UVCWCVWvL4Zg> [@MorrisRiedel](#)

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

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HEAT
HELMHOLTZ ANALYTICS TOOLKIT
EUROPEAN UNION

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

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<https://www.youtube.com/watch?v=UVCWCVWvL4Zg> [@MorrisRiedel](#)

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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=UVCWCVWvL4Zg> [@MorrisRiedel](#)

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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

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<https://www.youtube.com/watch?v=UVCWCVWvL4Zg> [@MorrisRiedel](#)

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WELCOME

RAISE CoE Seminar: MLOps with ClearML

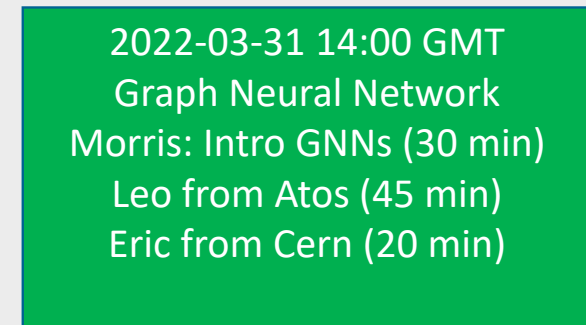
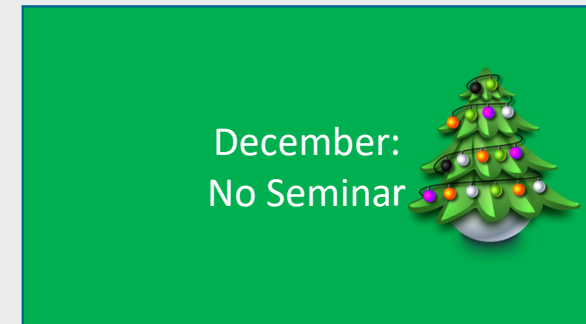
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National Competence Center (NCC) for HPC & AI in Iceland – IHPC
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<https://www.youtube.com/watch?v=UVCWCVWvL4Zg> [@MorrisRiedel](#)

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



WP2 Monthly Trainings – Review & Plan



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)



August:
SW Framework

September:
Transformer Models

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:

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

ATOS: affects of
change in persons?



November:
Project Partners?

December:
Project Partners?

January:
Project Partners?

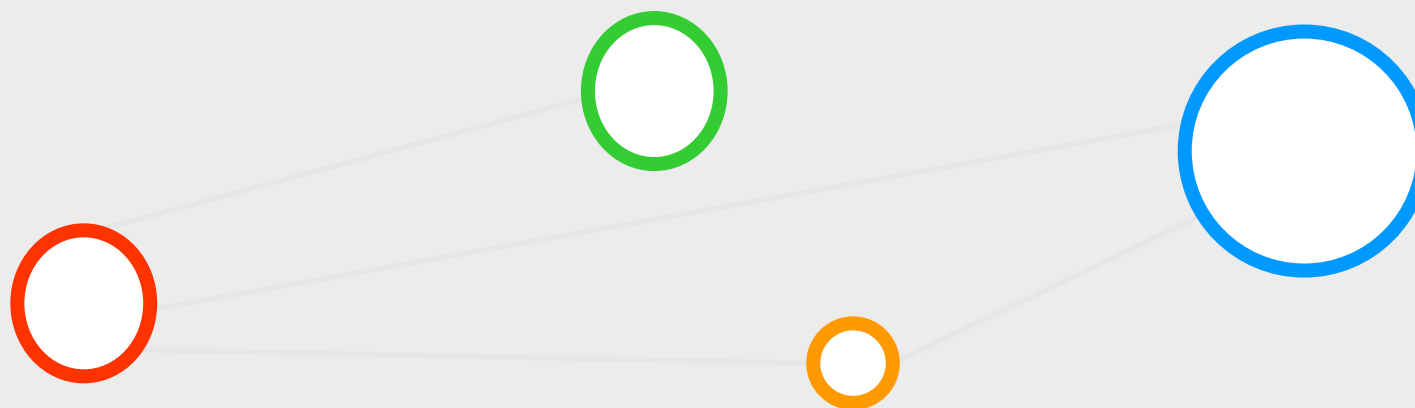
February:
Project Partners?

March
Project Partners?

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



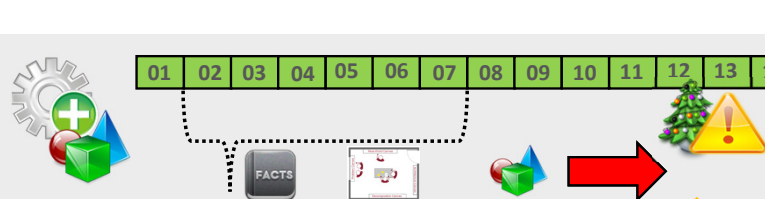
Agenda Item (6) – Compelling Scoreboard Review



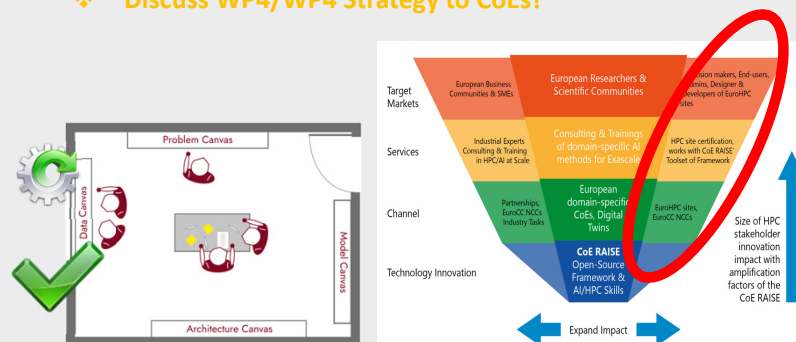
Compelling Scoreboard Review – Use Case Progress



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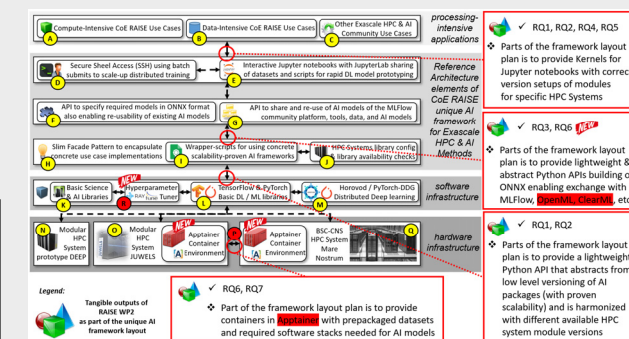


- ❖ Realization of SW framework design started → initial collection in WP2 Wiki page RAISE (Jupyter notebooks, etc.)
- ❖ Adoption of SW Framework started: first friendly EuroHPC JU sites & project partners:
- ❖ Discuss WP4/WP4 Strategy to CoEs?



Use Case	AE	PINN	ANNs		CNN	NO	GNN		RNN		GAN	TF			SVM	RF
Details	CAE		ANN	RBF-ANN	U-Net	RES NET	FNO	MLP	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
Detect-free metal additive manufacturing	X		X									X	X	X	X	
Sound Engineering	X		X													

Meetings with administrators in next months to encourage adoption at EuroHPC JU Hosting Sites





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)
 - Ahti
- CoEC
 - Combustion AI Training → Contact
 - JUELICH, BSC, RWTH (Heinz Pitch)
- Excellerat2: one task with ML (BSC, KTH, OVGU)
 - In excellerat2, ML is for physical modeling while in CEEC it's on machine learning and physics-informed data analytics
- CEEC (KTH)
 - CEEC: One task (UL, KTH, BSC, RWTH, CINECA, FhG)
- HI
 - CoE CHEESE1+2



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