

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

Prof. Dr. – Ing. Morris Riedel et al.

School of Engineering & Natural Sciences, University of Iceland

2022-11-24, RAISE WP2 Monthly Meeting November 2022, Online



@ProfDrMorrisRiedel



@Morris Riedel



@MorrisRiedel



@MorrisRiedel



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



morris@hi.is



WP2 Meeting November – Welcome & Agenda

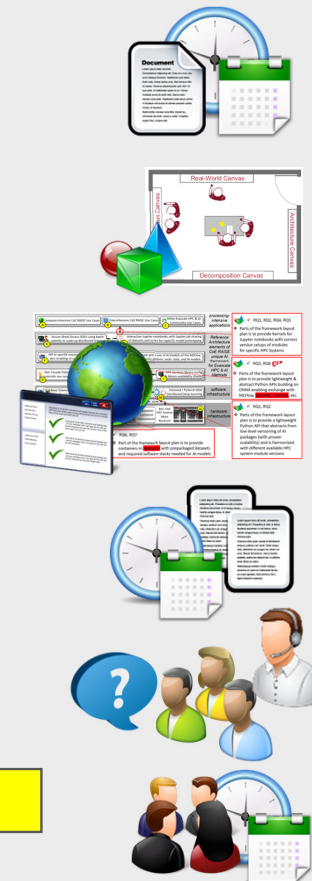


RAISE
Center of Excellence

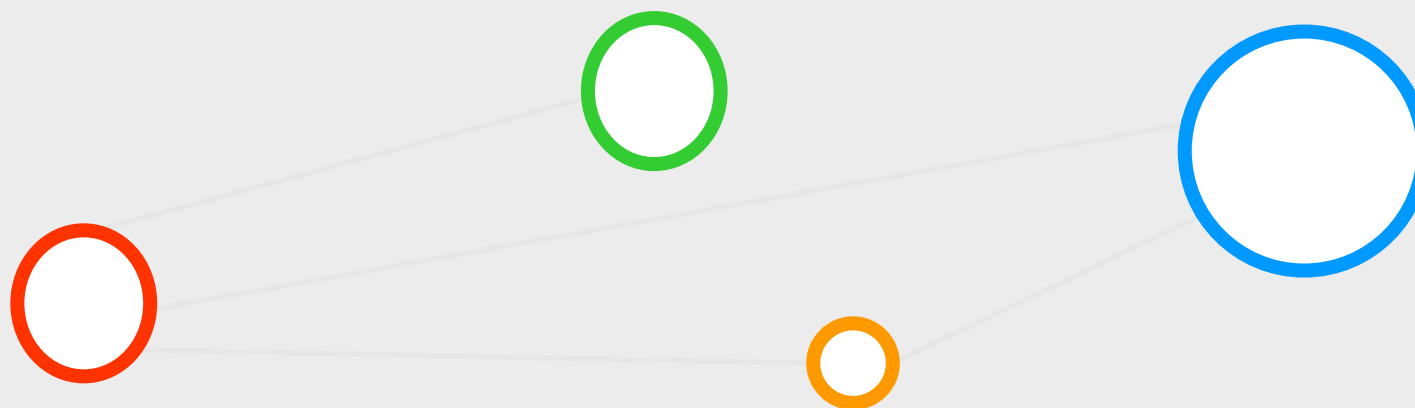
1. Approval of minutes from Monthly Meeting October 2022
 - (All), ~5 Min
2. Review WP2 Status on Interaction Rooms
 - (Morris Riedel, Matthias Book, Helmut Neukirchen), ~5 Min
3. Review Framework Adoption Status
 - (Morris, Andreas, et al.), ~10 Min
4. M24 Deliverable Status
 - (Morris, Rakesh, Guillaume/Cristobal, Fabian et al.), ~30 Min
5. Status WP2 Training Plans
 - (Morris et al.), ~5 Min
6. Compelling Scoreboard Review & Next Steps
 - (All), ~5 Min



X-MAS fast approaching



Agenda Item (1) – Minutes Approval – October 2022



Minutes Approval – Monthly Meeting October 2022



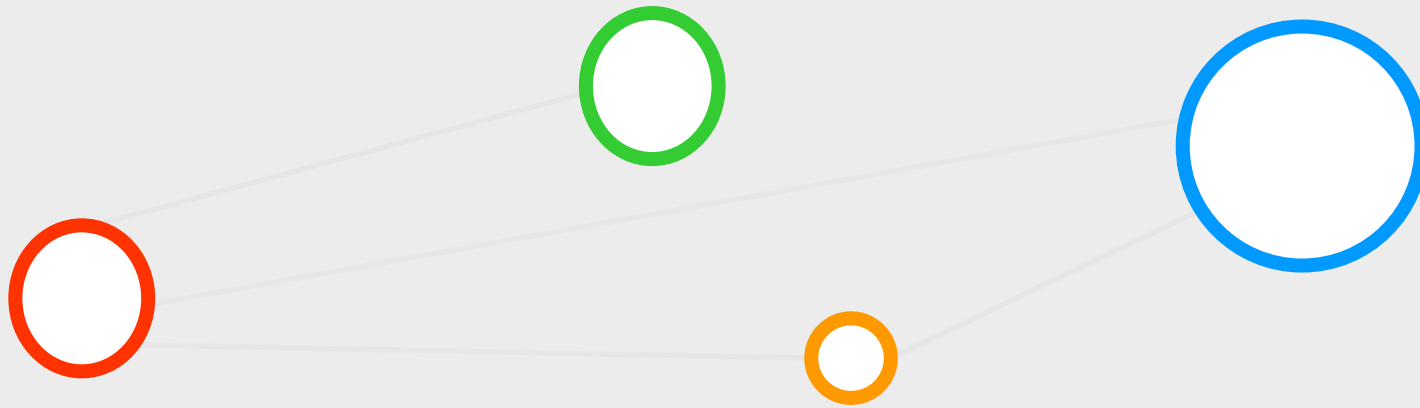
➤ Minutes available in BSCW

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

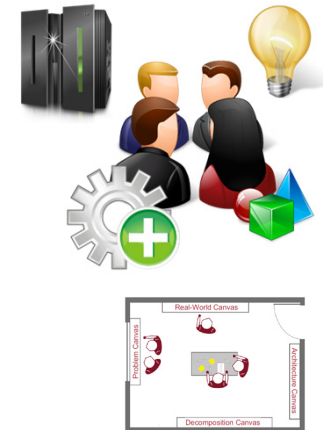
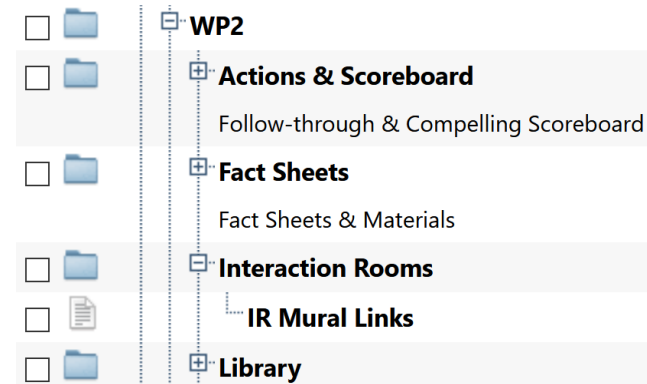
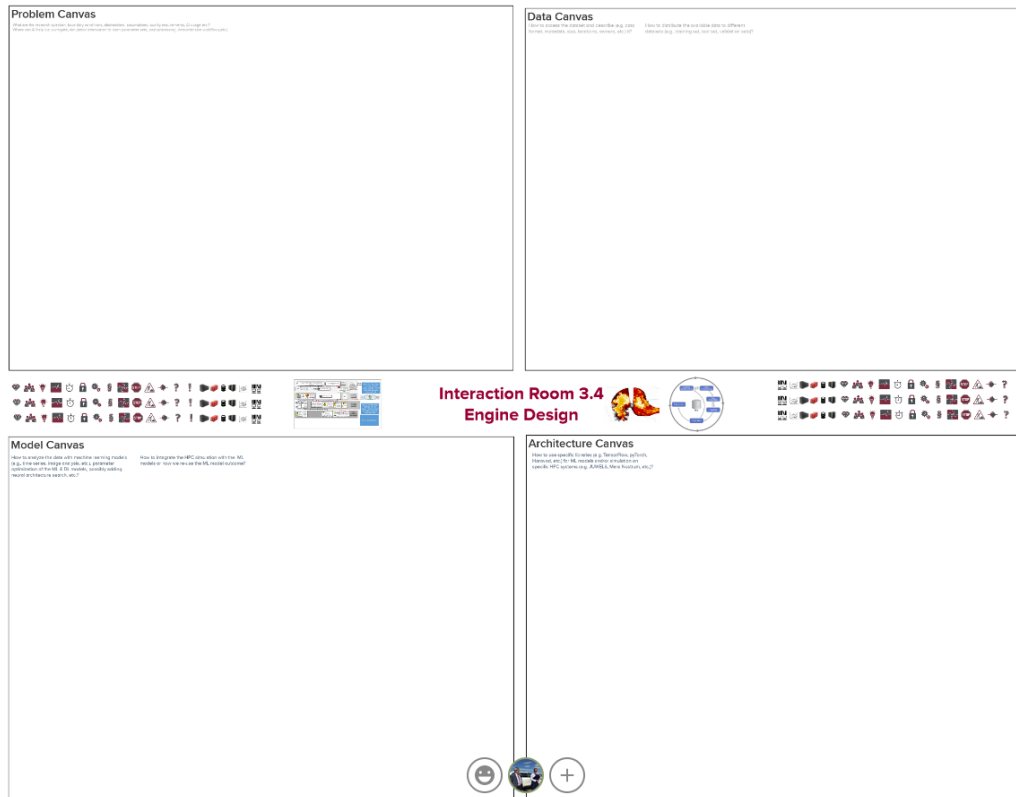
Slides & Materials from Meeting 2021-10-29			
<input type="checkbox"/>	2021_11_26_Monthly_Meeting_November_2021	2	M.Riedel
Slides & Materials from Meeting 2021-11-26			
<input type="checkbox"/>	2022_01_31_Monthly_Meeting_January_2022	2	M.Riedel
Slides & Materials from Meeting 2022-01-31			
<input type="checkbox"/>	2022_02_28_Monthly_Meeting_February_2022	2	M.Riedel
Slides & Materials from Meeting 2022-02-28			
<input type="checkbox"/>	2022_03_30_Monthly_Meeting_March_2022	2	Katrine
Slides & Materials from Meeting 2022-03-30			
<input type="checkbox"/>	2022_04_29_Monthly_Meeting_April_2022	2	M.Riedel
Slides & Materials from Meeting 2022-04-29			
<input type="checkbox"/>	2022_05_31_Monthly_Meeting_May_2022	2	Katrine
Slides & Materials from Meeting 2022-05-31			
<input type="checkbox"/>	2022_06_28_Monthly_Meeting_June_2022	2	M.Riedel
Slides & Materials from Meeting 2022-06-28			
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Slides & Materials from Meeting 2022-07-29			
<input type="checkbox"/>	2022_08_26_Monthly_Meeting_August_2022	1	Katrine
Slides & Materials from meeting 2022-08-26			
<input type="checkbox"/>	2022_09_30_Monthly_Meeting_September_2022	2	Katrine
Slides & Materials from meeting 2022-09-30			
<input type="checkbox"/>	2022_10_27_Monthly_Meeting_October_2022	2	Katrine
Slides & Materials from meeting 2022-10-27			
<input type="checkbox"/>	2022_11_24_Monthly_Meeting_November_2022	0	Katrine
Slides & Materials from meeting 2022-11-24			



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/cb44cca3eed3bb9964fbfa36a1f6b1bfcc085f?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/matthiasbook8855/1621377976343/8d7aba6be09af3b2fd305d2f709c53661ac889d?sender=u15e3008bb41d6628a5bb5701>
- IR3.5 Coating: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377991014/7a5d7e1ea230178342d1e1d4a84d656d9055d52?sender=u15e3008bb41d6628a5bb5701>
- IR4.1 Fundamental Physics: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378007335/6f0d5285feac3eaf315bd6676e84d8b4879d39?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/matthiasbook8855/1621378038069/93df6fa7a41093f4eaae7bc9d72979d2ba42b9d?sender=u15e3008bb41d6628a5bb5701>
- IR4.4 Sound Engineering: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa12219002404059f90a4bbb0101fa379a8503?sender=u15e3008bb41d6628a5bb5701>

- 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

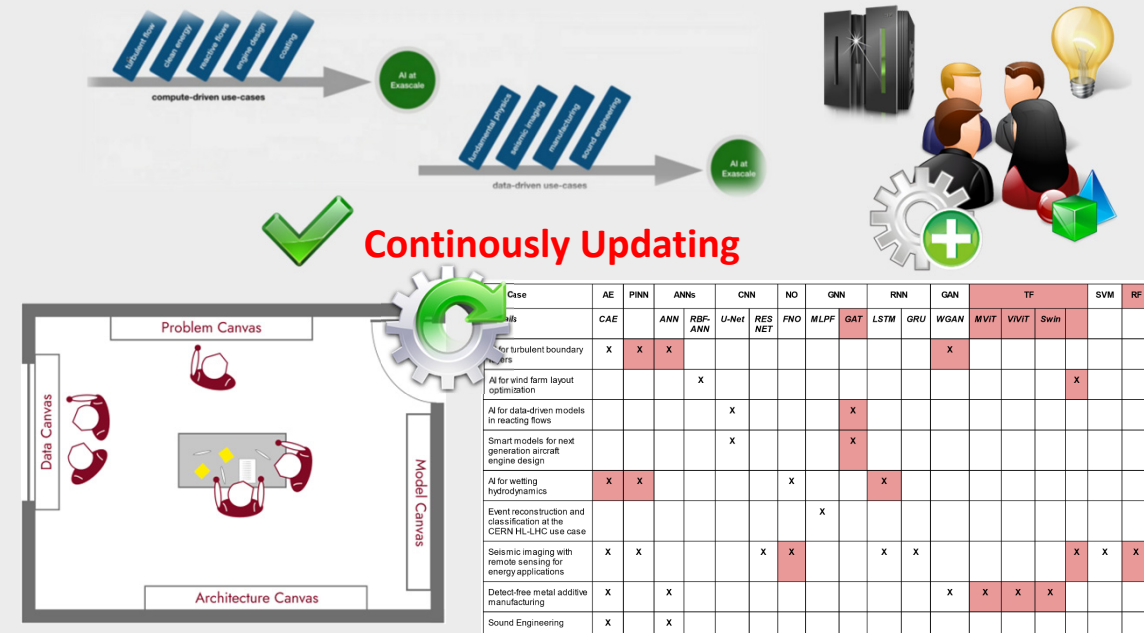
➤ WP3 (third round IRs)

- T3.1: Turbulent Flow → Dec/Jan
- T3.2: Clean Energy → Dec/Jan
- T3.3: Reactive Flows → Dec/Jan
- T3.4: Engine design → Dec/Jan
- T3.5: Coating → Dec/Jan

➤ WP4 (third round IRs)

- T4.1: Fundamental physics → Dec/Jan
- T4.2: Seismic imaging → Dec/Jan
- T4.3: Manufacturing → Dec/Jan
- T4.4: Sound engineering → Dec/Jan

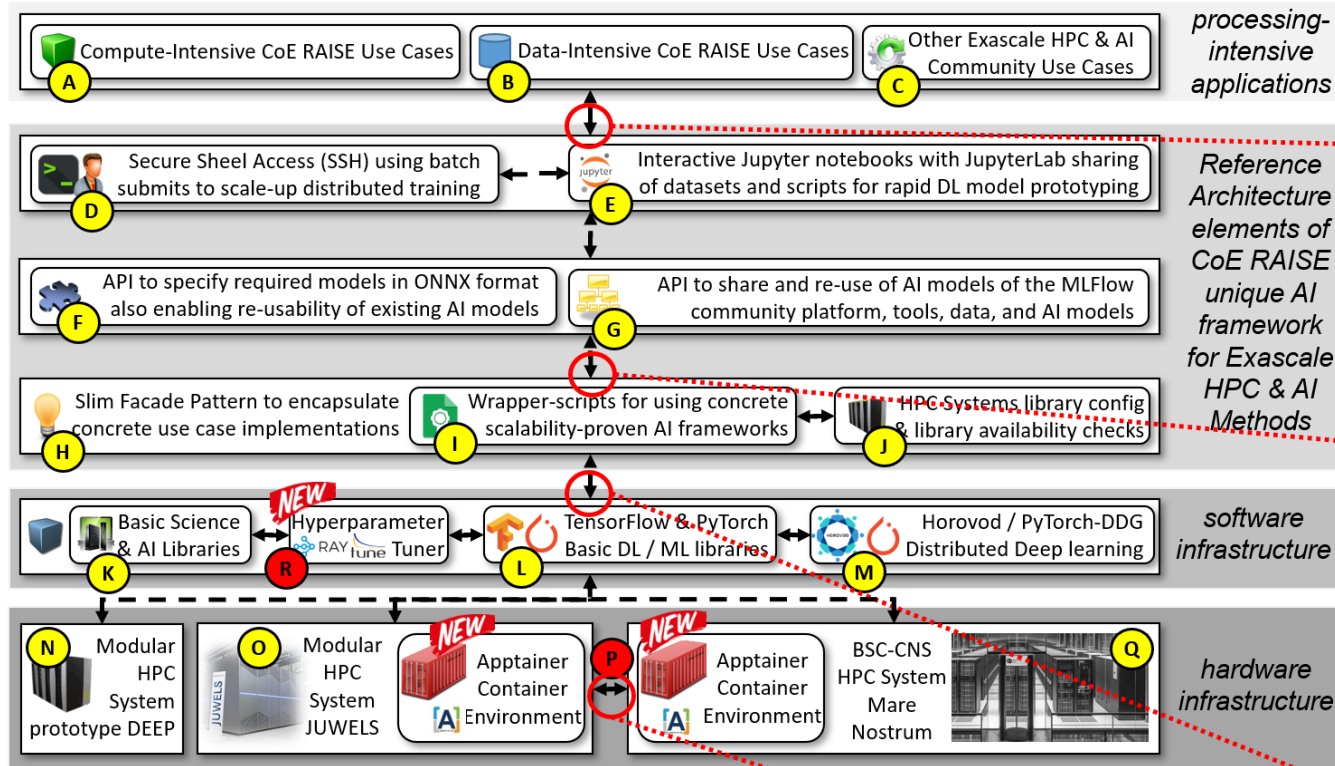
➤ 3rd iteration of Interaction Rooms → schedule



➤ 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



✓ 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

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



✓ 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

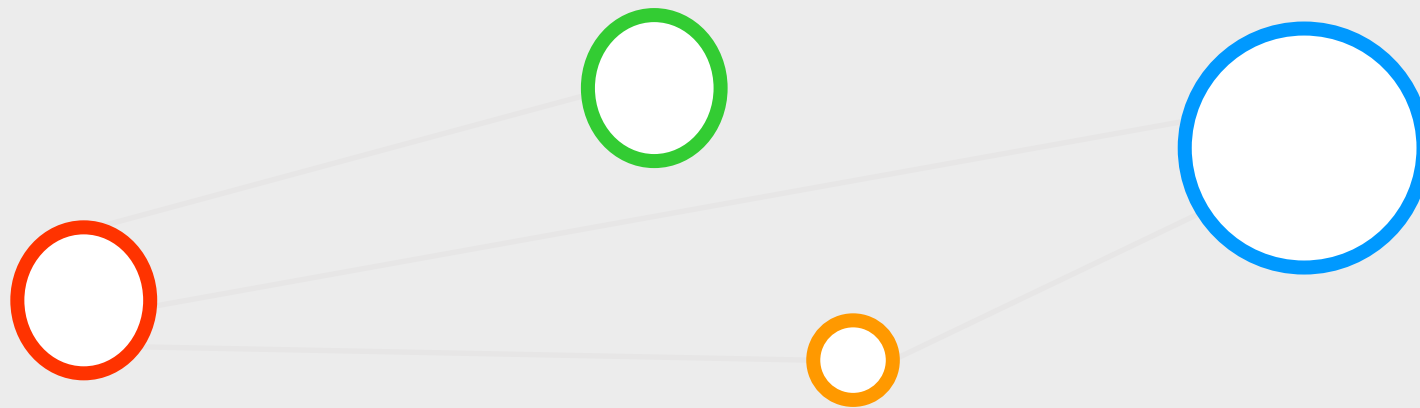


Discuss updates on DALI Data Loader, NumPy, Scikit-learn, Quantum, etc. DeepSpeed, DeepHyper, Google JAX?

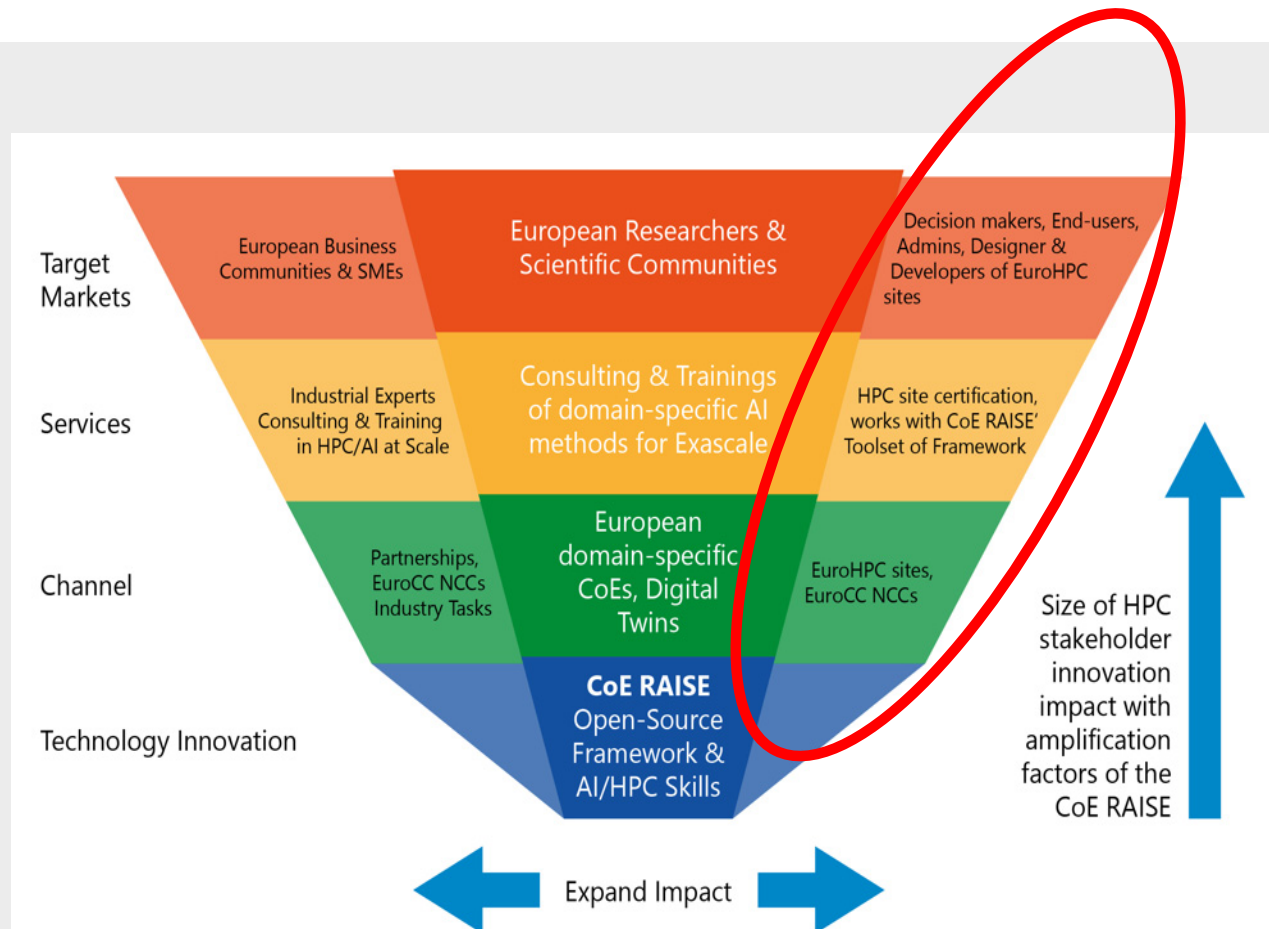


Continuously Updating!

Agenda Item (3) – Review Framework Adoption Status




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.

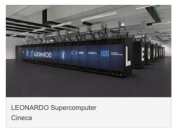


LUMI supercomputer CSC

375 petaflops	550 petaflops
Sustained performance	Peak performance

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	323,40 petaflops
Sustained performance	Peak performance

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	314 Petaflops
Sustained performance	Peak performance

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 GUM.



Atos VEGA

Cyprus: VEGA

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

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.




Meluxina supercomputer LuxProvide

Par-Tec?

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

KAROLINA

Karolina is a petascale EuroHPC supercomputer located in Opatowitz, Czech Republic. It is supplied by Hewlett Packard Enterprise (HPE) and hosted by IT4Innovations.

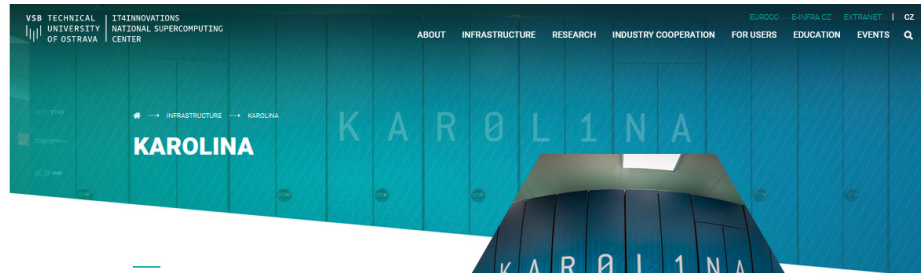


Karolina supercomputer IT4Innovations

Prague meeting CoE RAISE



SW Framework Adoption: Check Karolina in Prague Meeting



The petascale system Karolina, acquired as part of the EuroHPC Joint Undertaking, was installed in 2021. In the TOP500 list, which evaluates supercomputers in terms of their performance, it ranked 69th worldwide, 19th in Europe, and in the Green500 list of the most energy-efficient supercomputers, it even ranked 8th in 2021. The HPC system is designed to respond coherently to the needs of its user communities, addressing complex scientific and industrial challenges, including standard numerical simulations, demanding data analysis, and artificial intelligence applications.

The new supercomputer reaches theoretical peak performance of 15.7 PFlop/s, which corresponds to 15.7 quadrillion floating-point operations per second.

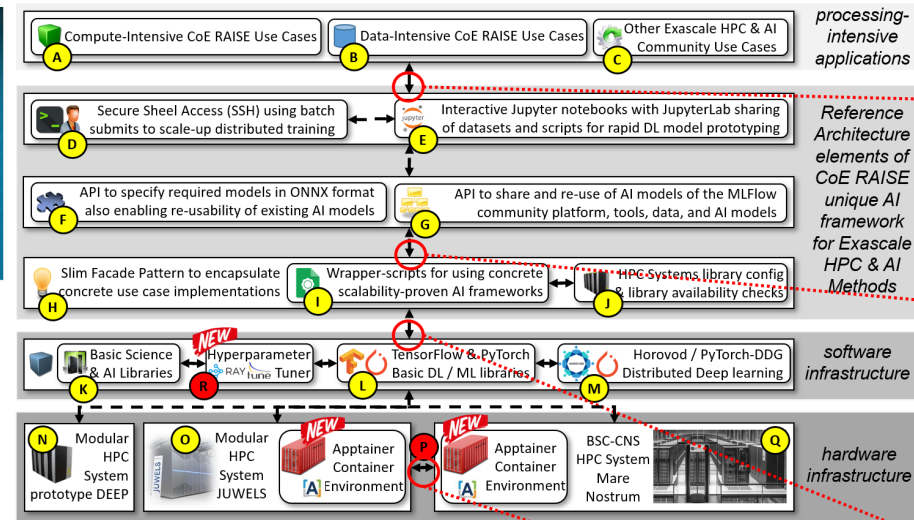
The supercomputer consists of 6 main parts:

- a universal part for standard numerical simulations, which consists of approximately 720 computer servers with a theoretical peak performance of 3.9 PFlop/s,
- an accelerated part with 72 servers and each of them is equipped with 8 GPU accelerators providing a performance of 11.6 PFlop/s for standard HPC simulations and up to 360 PFlop/s for artificial intelligence computations,
- a part designated for large dataset processing that provides a shared memory of as high as 24 TB, and a performance of 74 TFlop/s,
- 36 servers with a performance of 192 TFlop/s are dedicated to providing cloud services,
- data storage that provides space for 1.4 PB of user data processing and also include high-speed data storage with a speed of 1 TB/s for simulations as well as computations in the fields of advanced data analysis and artificial intelligence.

15.7
PFlop/s
THEORETICAL PEAK

1.4
PB
STORAGE

200
Gb/s
INTERCONNECT



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

✓ 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

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

✓ 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.

software infrastructure

hardware infrastructure

✓ RQ1, RQ2

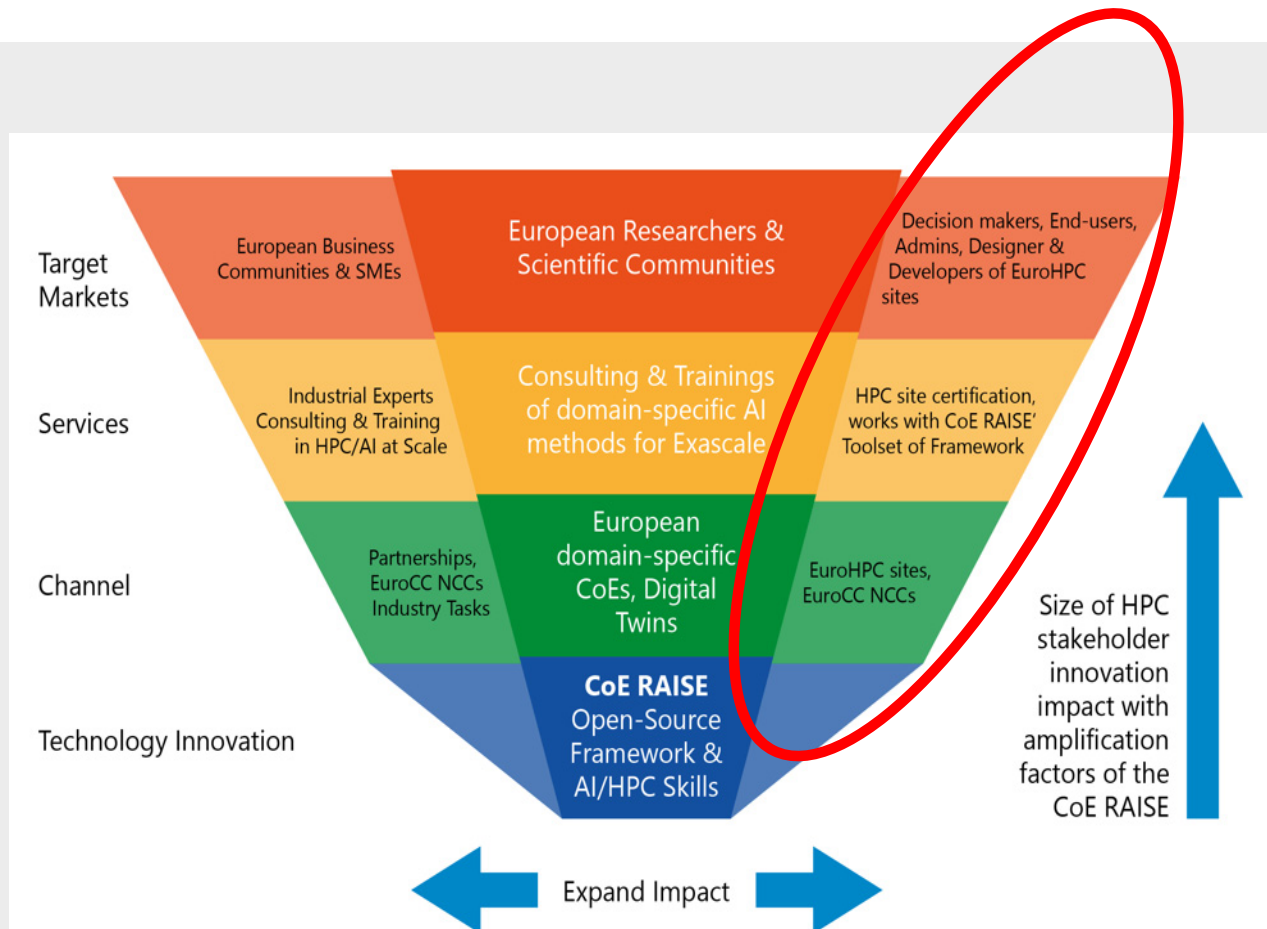
- ❖ Parts of the framework layout plan is to provide a lightweight Python API that abstracts from low level versioning of AI packages (with proven scalability) and is harmonized with different available HPC system module versions

➤ IT4Innovation

- Vit Vondrak (not in workshop)
- Tomas (hopefully in workshop)
- TBD: Check what SW already installed & clarify access for CoE RAISE WP2 folks



Towards SW Framework Adoptions



DISCOVERER

Discoverer is a petascale EuroHPC supercomputer located in Sofia, Bulgaria. It is supplied by Alos, based on the BullSequana XH2000 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 X800 (partition) and Alos Bull Sequana (x86 partitions). Deucalion is hosted by MACC.

Deucalion supercomputer MACC

7,22 petaflops	10 petaflops
Sustained performance	Peak performance

- Other project partner sites?
 - RTU system → Lauris
 - DEEP system → Morris
 - JUELICH Systems → Morris
 - LUMI → CERN?
- Vit Vondrak (IT4Innovation),
 - Tomas

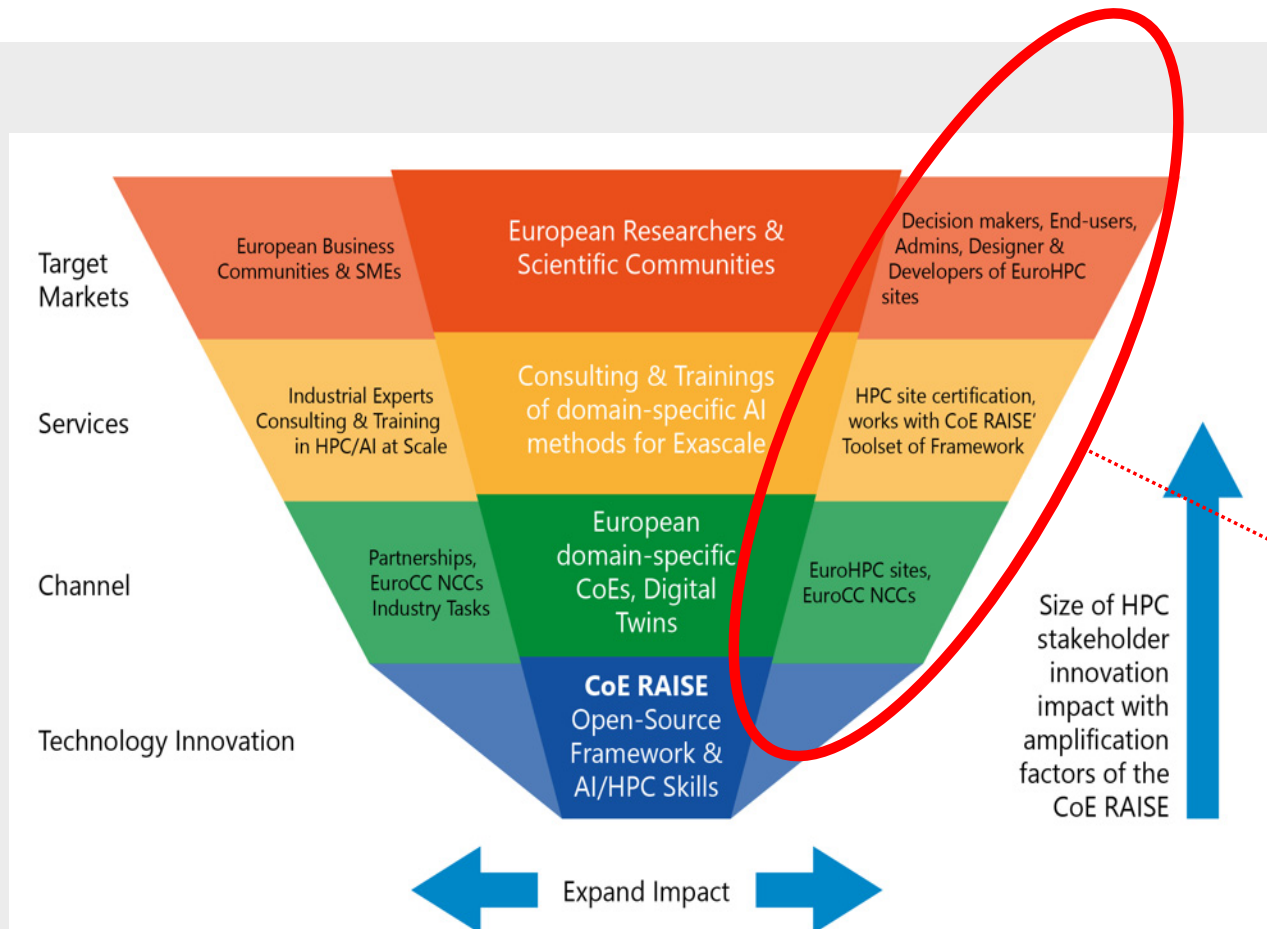


Towards SW Framework Adoptions



EuroHPC
Joint Undertaking

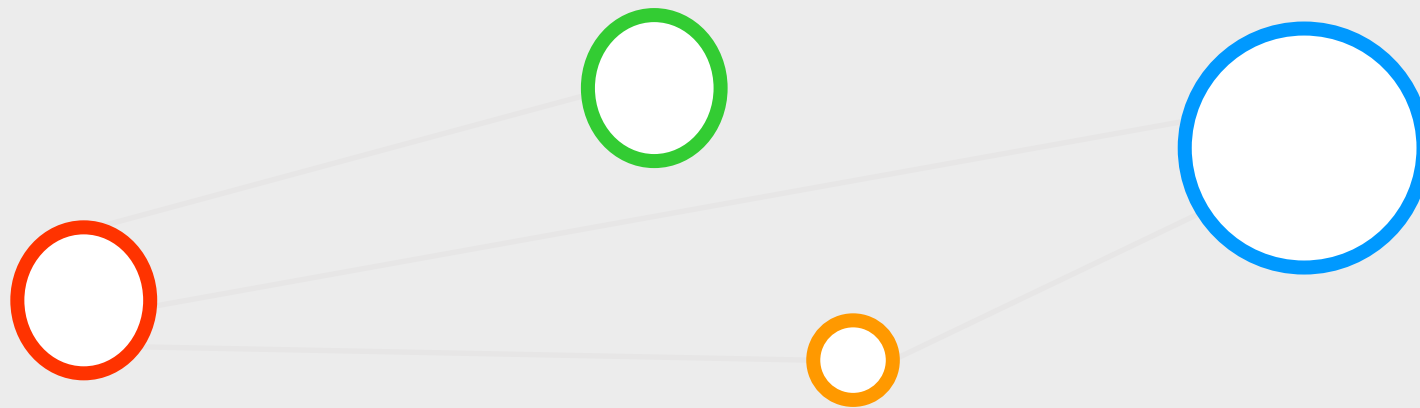
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- 1. Goal Project Sites
 - Talk to administrators of AI tools & technologies about framework
 - Assumption: many tools already deployed, but in different modules
- BSC
 - Contact received – Thanks!
- LUMI
 - Contact existing (2 PhDs work on LUMI already)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



Agenda Item (4) – M24 Deliverable Status



M24 Deliverable Timelines



From: Andreas Lintermann <A.Lintermann@fz-juelich.de>

Sent: Thursday, October 20, 2022 1:15 PM

To: Morris Riedel <m.riedel@fz-juelich.de>; Katrin Ólöf Egilsdóttir - HI <katrine@hi.is>; Lapeyre Corentin <corentin.lapeyre@cerfacs.fr>; Maria Giron <Maria.Giron@cern.ch>; Lammens Wouter <wouter.lammens@flandersmake.be>; Rose Gregorio <rose.gregorio@bsc.es>; Houzeaux Guillaume <guillaume.houzeaux@bsc.es>; Sarma Rakesh <r.sarma@fz-juelich.de>; Meinke Matthias <M.Meinke@aia.rwth-aachen.de>; Wiechol Monika <office@aia.rwth-aachen.de>; Eric Wulff <eric.wulff@cern.ch>; Hans-Christian Hoppe <hans-christian.hoppe@par-tec.com>; Ilmārs Slaidiņš <Ilmars.Slaidins@rtu.lv>; Bresser, Michael <m.bresser@fz-juelich.de>; leo.nicoletti@atos.net>; Matthias Book - HI <book@hi.is>; REMI DRUILHE <remi.druihe@atos.net>; Albers Marian <M.Albers@aia.rwth-aachen.de>; RICHARD Stephane (SAFRAN HELICOPTER ENGINES) <stephane.richard@safrangroup.com>; Joan Farnos <joan.farnos@bsc.es>; Lintermann Andreas <A.Lintermann@fz-juelich.de>; Jennifer Lopez Barrilao <lopez@par-tec.com>; Schmitz Ina <schmitz@par-tec.com>; Speck Robert <r.speck@fz-juelich.de>; Göbbert Jens Henrik <j.goebbert@fz-juelich.de>; CASA <cristobal.samaniego@bsc.es>

Cc: FM-raise_pmt <raise_pmt@fz-juelich.de>

Subject: RAISE: Roadmap M24 Deliverables

Dear All,

Since we have been successful in delivering last year's Christmas deliverables on time, I would like to stick this year again to the same procedure such that everyone can go into the Christmas break without worries :)...

You are receiving this mail because you are either a responsible WP leader, a responsible deliverable author, or an internal reviewer for the upcoming M24 deliverables in December (see your responsibility in https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/d3287337/CoE%20RAISE_Deliverables_Status.xls - Note that there will be some updates to this document in the very near future!).

As we have 8 Deliverables coming up and with the Christmas holidays in mind, we would like to start with the preparation of the deliverables earlier. We are now looking at the following time schedule:

- 29.11.2022:

The author(s) upload(s) the Deliverable to the BSCW server to CoE RAISE / Reports and Deliverables / In progress / DX.Y. The author(s) inform(s) the WP leader, the internal reviewer, and the PMT about the uploaded document. The document name includes the term "Draft".

- 06.12.2022:

The internal reviewer returns the document with comments and suggestions in track-changes mode to the author(s). The reviewed document is placed into the same folder on the BSCW as the original document and the PMT and WP leaders are informed in addition to the author(s).

- 06.12.2022 - 14.12.2022:

Continuous exchange between the author(s) and the reviewer (the PMT can already be involved). When a final version is ready for the PMT to review, the author(s) uploads the revised Deliverable to the BSCW server and informs the WP leader, the internal reviewer, and the PMT. The PMT starts to review the Deliverable and keeps track of all changes.

- 14.12.2022:

The PMT uploads the commented version to the BSCW server and informs the author(s) and the WP leader.

- 14.12.2022 - 21.12.2022:

Continuous exchange between the author(s), the reviewer, and the author(s). At the end, all corrections requested by the PMT have been included and the document is uploaded to the BSCW server. The file name includes the term "Final".

- 21.12.2022 - 22.12.2022:

The PMT generates the final PDF.

- 23.12.2022:

The Coordinator submits the Deliverable to the EC and places the finally submitted version into the BSCW folder CoE RAISE / Reports and Deliverables / EC submitted.



M24 Deliverable Content Strategy WP3/WP4

Participants:

Maria Girone, Morris Riedel, Corentin Lapeyre, Rakesh Sarma, Andreas Lintermann



- D3.2 and D4.2
 - will have the same structure (template was sent around by Maria)
 - content per use case
 - current status incl. review of M12 achievements (to highlight the progress)
 - generalizable methods beneficial across use cases
 - results section specific to the use case results (with a reduced description of the AI/HPC methodologies)
 - plan for exascale execution
- D4.2 Tk 4.1
 - will link in the generalizable section to the general quantum methods to be described in D2.8
 - hyperparameter optimization will be mentioned but explained in WP2 deliverables

https://docs.google.com/document/d/15bo6dkj0AHpP7sy_XVmgacOFLuC359r_rGWOecbJIEA/edit?usp=sharing



M24 Deliverable Content Strategy WP2



Guillaume /
Cristobal

D2.3 Report on porting & performance engineering

- Morris talks to Guillaume about the content
- Andi is on the contract for AVBP usage at FZJ (benchmarking hopefully to become a part of D2.3)
- Guillaume to report on successful compute-time applications (LUMI-Q, LUMI-G, other projects, PRACE, etc.)
- news from Alya and m-AIA (latter GPU porting activities?!): Alya porting and performance test on graviton3 (CPU configuration similar to the grace one which will be part of MN5).

Rakesh

D2.8 Benchmarking & support report

- reports on the general methods (QSVR, QSVM)
- will have a contribution from the RS use case
- will have a contribution from CERN

Morris

D2.15 Novel AI Methods Report (Update)

- similar to last year's deliverable
- will report on the AI technologies and update the AI matrix

Fabian?

Morris

D2.12 (due in M26) needs to be discussed later → SW Framework Update (M26)

https://docs.google.com/document/d/15bo6dkj0AHpP7sy_XVmgacOFLuC359r_rGWOecbJIEA/edit?usp=sharing



M24 Deliverable Status D2.3 → Guillaume/Cristobal



Guillaume /
Cristobal

D2.3

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Rakesh

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M24 Deliverable Status D2.8 → Rakesh

Guillaume /
Cristobal

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M24 Deliverable Status D2.15 → Morris

Guillaume /
Cristobal

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D2.8

- reports on the general methods (QSVR, QSVM)
- will have a contribution from the RS use case
- will have a contribution from CERN

Morris

D2.15

Fabian?

- similar to last year's deliverable
- will report on the AI technologies and update the AI matrix

Morris

D2.12 (due in M26) needs to be discussed later

https://docs.google.com/document/d/15bo6dkj0AHpP7sy_XVmgacOFLuC359r_rGWOecbJIEA/edit?usp=sharing

M24 Deliverable Status D2.15 → Review History



(M12)

In D2.14 (Novel AI Methods Report), we reported the AI methods details of our HPC/AI matrix at M12.



(M18)

We then briefly described the updated matrix in D2.10 (Monitoring report) at M18.



(M24 - ~NOW)

For our coming deliverable D2.15 (Novel AI Methods Report Update), we will go into details of methods again for M24.

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Use Case	AE	PINN	ANNs	CNN	NO	GNN	RNN	GAN	TF				SVM	RF	
Details	CAE		ANN	RBF/ANN	RES/NET	MLPP	GAT	LSTM	GRU	WDAN	WVIT	VFIT	Swit		
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
Defect-free metal additive manufacturing	X	X								X	X	X	X		
Sound Engineering	X		X												

M24 Deliverable Status D2.15 → Review Input Status

Maybe a thin deliverable

- Task 3.1 → Input received (new content)
- Task 3.2 → Reminder done
- Task 3.3/3.4 → Answer (no new content)
- Task 3.5 → Reminder done
- Task 4.1 → Answer (no new content)
- Task 4.2 → Reminder done
- Task 4.3 → Partly input received (new content)
- Task 4.4 → Input received (no new content)

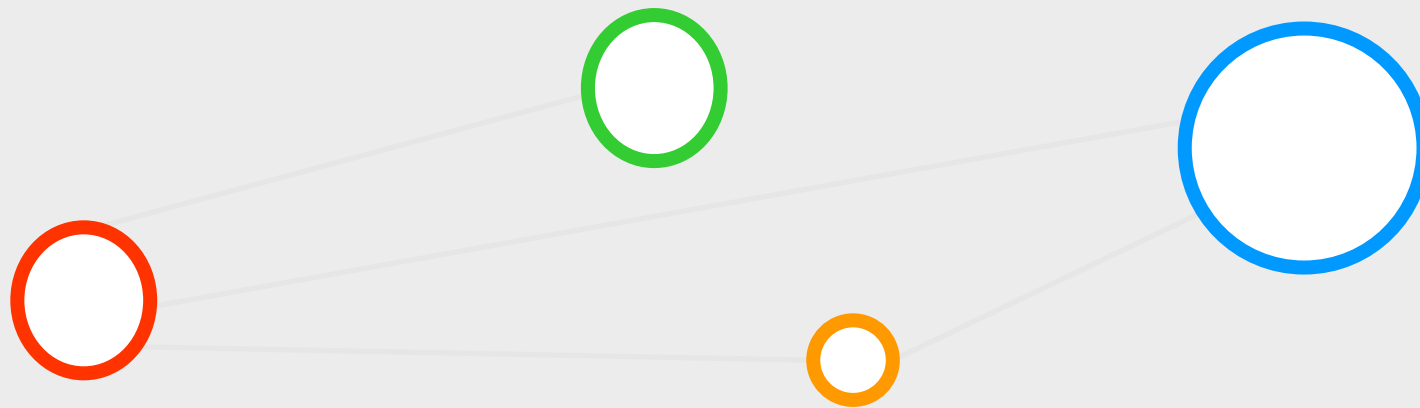
Work on
ClearML (FM)
in D2.12 (M26)

Fabian Contents?
Adoption Task working with other projects
→ D2.15 NHR Coupler X
→ D2.8/D2.3 Inputs



Use Case	AE	PINN	ANNs		CNN		NO	GNN		RNN		GAN	TF			SVM	RF	Coupling CFD
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	
Detect-free metal additive manufacturing	X		X									X	X	X	X			
Sound Engineering	X		X															
NHR Use Case																		X
Covid Use Case																		

Agenda Item (5) – Status WP2 Training Plans



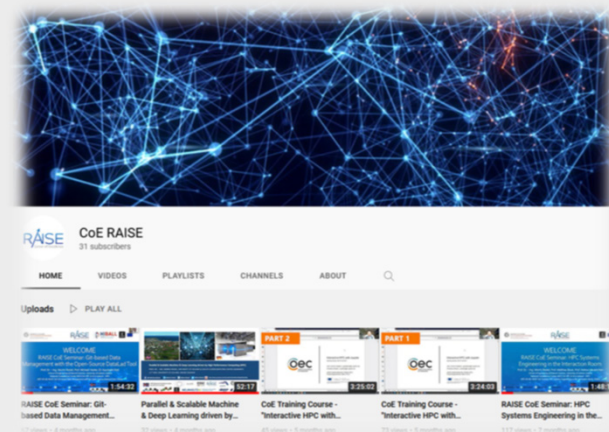
WP2 Monthly Trainings – Review & Plan



RAISE
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

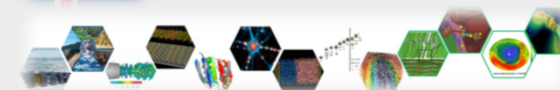


Plan for next months

- 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



RAISE
Center of Excellence

UNIVERSITY OF ICELAND
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=UVCWCVWvL4g>

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

UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES
RAISE
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=UVCWCVWvL4g>

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RAISE
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=UVCWCVWvL4g>

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SCHOOL OF ENGINEERING AND NATURAL SCIENCES
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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

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

<https://www.youtube.com/watch?v=UVCWCVWvL4g>

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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=UVCWCVWvL4g>

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

UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES
RAISE
Center of Excellence

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=UVCWCVWvL4g>

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

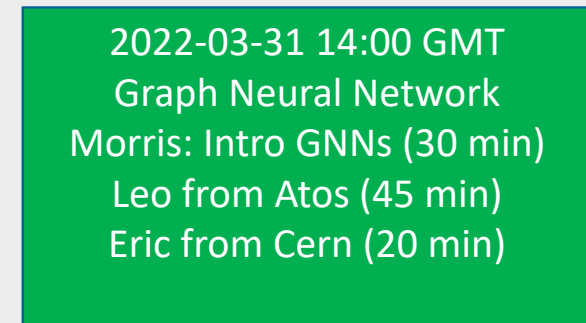
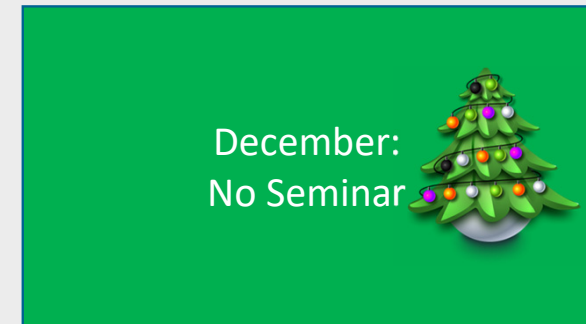


2022-11-24 RAISE WP2 Monthly Meeting November 2022

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)



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:

LSTM & GRU in CFD

November:

Matlab – Parallel Toolbox? RTU
HPC Machine?
Plus external speaker,
Mathworks?

Alternative SVM lecture
(UOI) + QSVM (FZJ)?

ATOS: affects of
change in persons?

February:

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

January:

Project Partners?

Shifted RTU Matlab (chadi)
Training, etc.

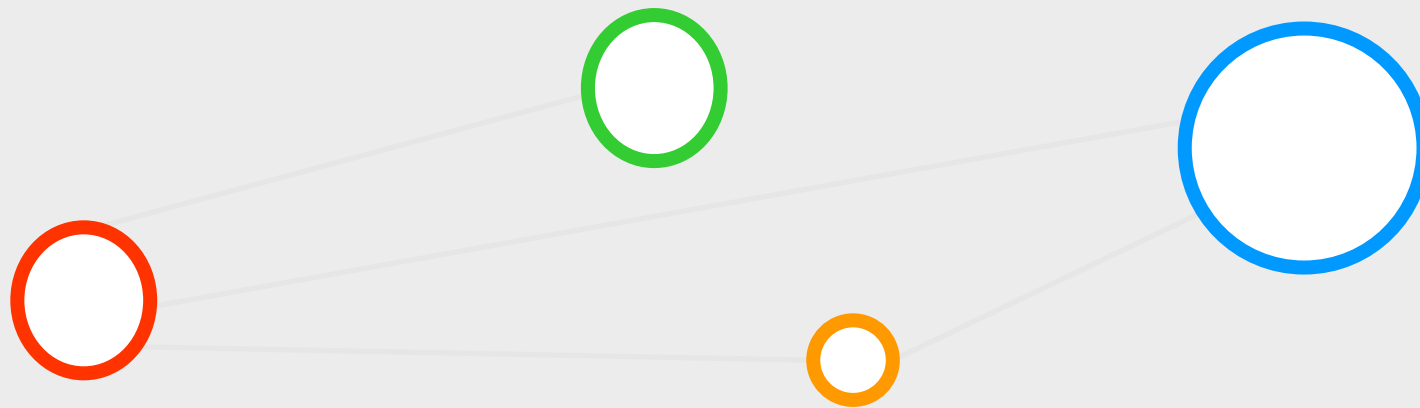
December:
Project Partners?

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

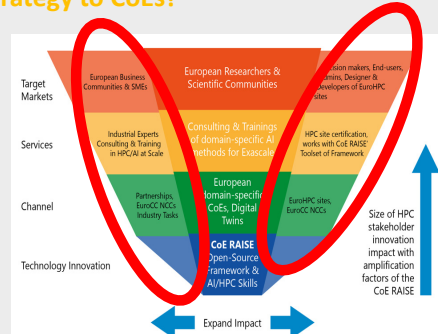
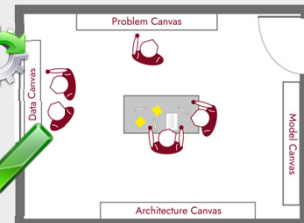
Fact Sheet Drafts Interaction Rooms AI Methods Exploration



T4.4

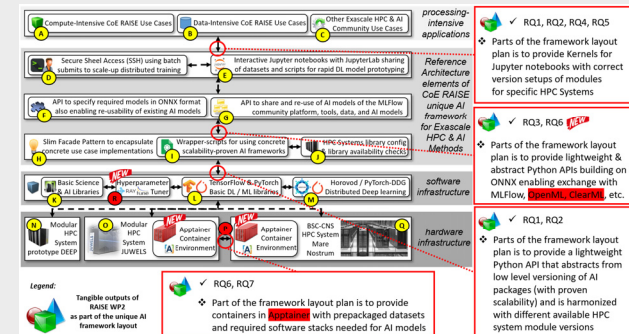
Fact Sheet Drafts Interaction Rooms AI Methods Exploration

- ❖ Focus on the deliverable wave
- ❖ 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?



Meetings with administrators in next months to encourage adoption at EuroHPC JU Hosting Sites: LUMI, BSC, etc. → Prague meeting next (Katalina)

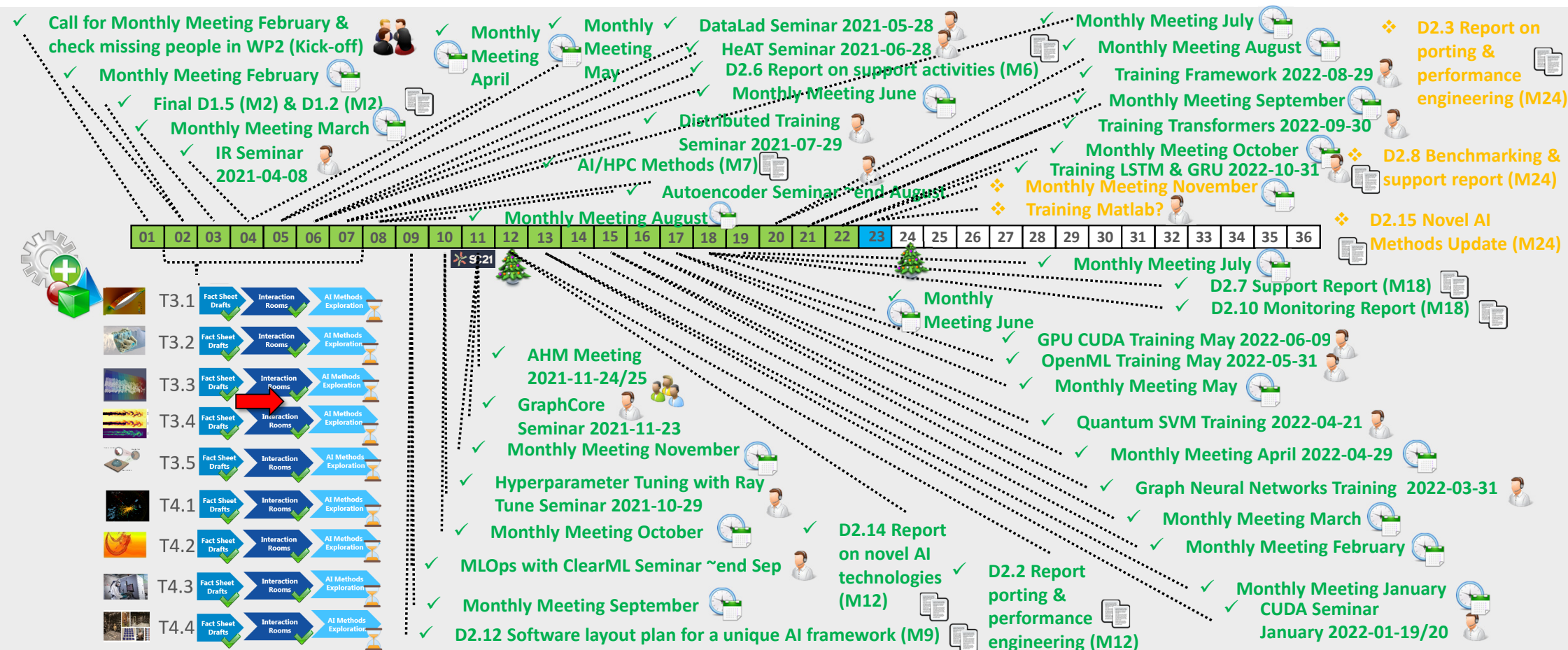
Use Case	AE	PINN	ANNs		CNN		NO	GNN		RNN		GAN	TF			SVM	RF
Details	CAE		ANN	RBF-ANN	U-Net	RES NET	FNO	MLPF	GAT	LSTM	GRU	WGAN	MVIT	VIVIT	Swin		
AI for turbulent boundary layers	X	X	X									X					
AI for wind farm layout optimization				X											X		
AI for data-driven models in reacting flows					X				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
Detect-free metal additive manufacturing	X		X									X	X	X	X		
Sound Engineering	X		X														



Compelling Scoreboard Review & Next Steps



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



➤ 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
- Current trouble with getting no LUMI consortium member an access, work-in-progress
- Status of LUMI access for BSC? Handled via CERN?

➤ Contacts to CoEs

- 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



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

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