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

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School of Engineering & Natural Sciences, University of Iceland
2022-04-29, RAISE WP2 Monthly Meeting April 2022, Online

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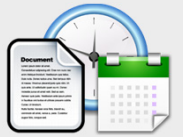
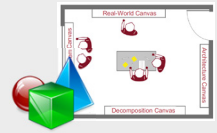
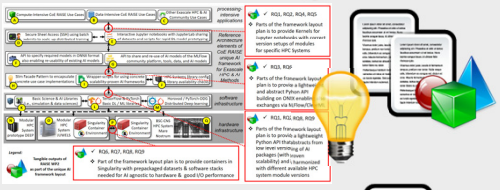
WP2 April – Welcome & Agenda

RAISE Center of Excellence

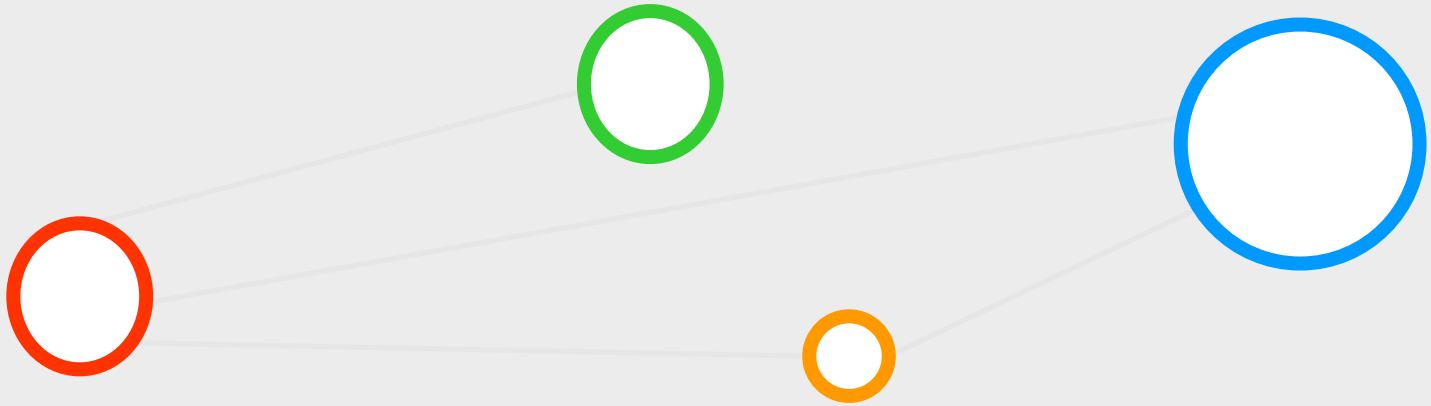
1. Approval of minutes from Monthly Meeting February 2022
   - (All), ~5 Min
2. Review WP2 Status on Interaction Rooms
   - (Morris Riedel, Matthias Book, Helmut Neukirchen), ~10 Min
3. Realization of the SW Framework
   - (Morris, Liang, Johannes et al.), ~20 Min
4. Upcoming Deliverables
   - (Morris et al.), ~5 Min
5. Status WP2 Training Plans
   - (Morris et al.), ~5 Min
6. Compelling Scoreboard Review & Next Steps
   - (All), ~15 Min



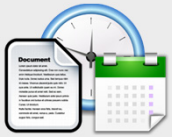




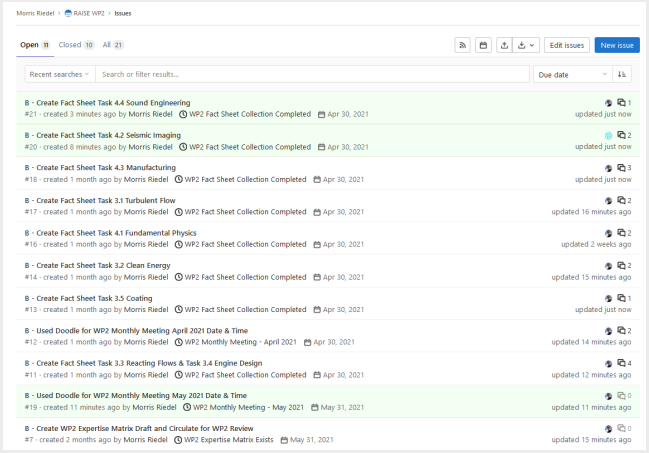
Agenda Item (1) – Minutes Approval – March 2022

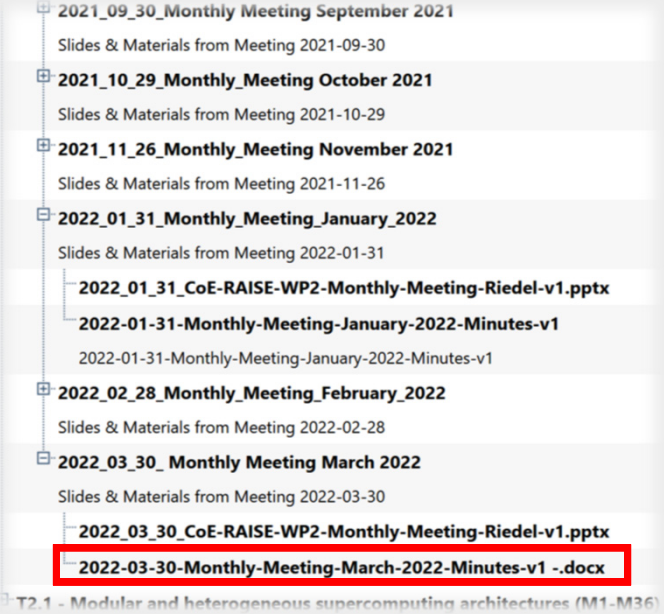


Minutes Approval – Monthly Meeting March 2022

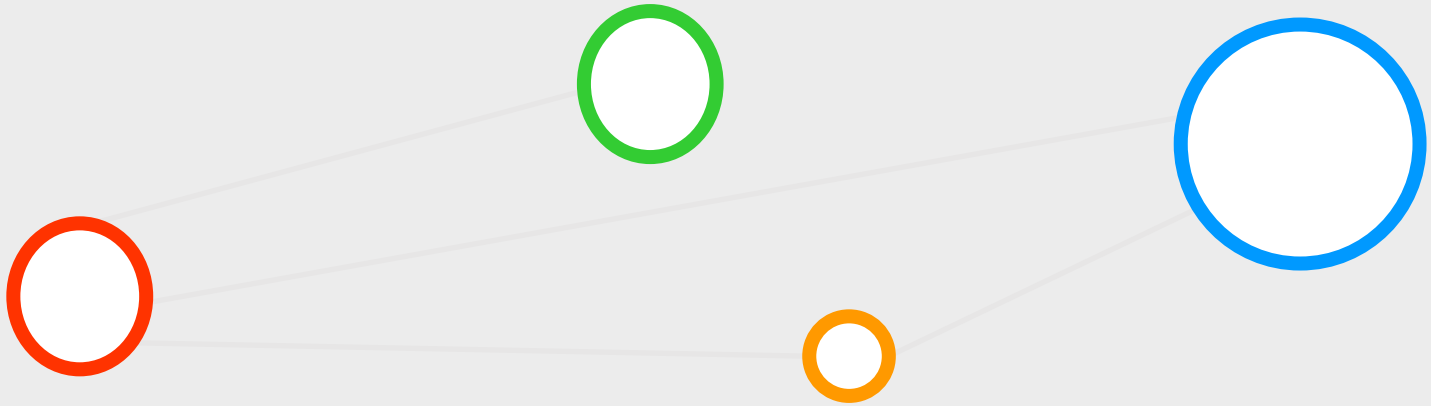


- Minutes available in BSCW
  - https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3340884
  - TBD(all): Any objections or additions/changes?

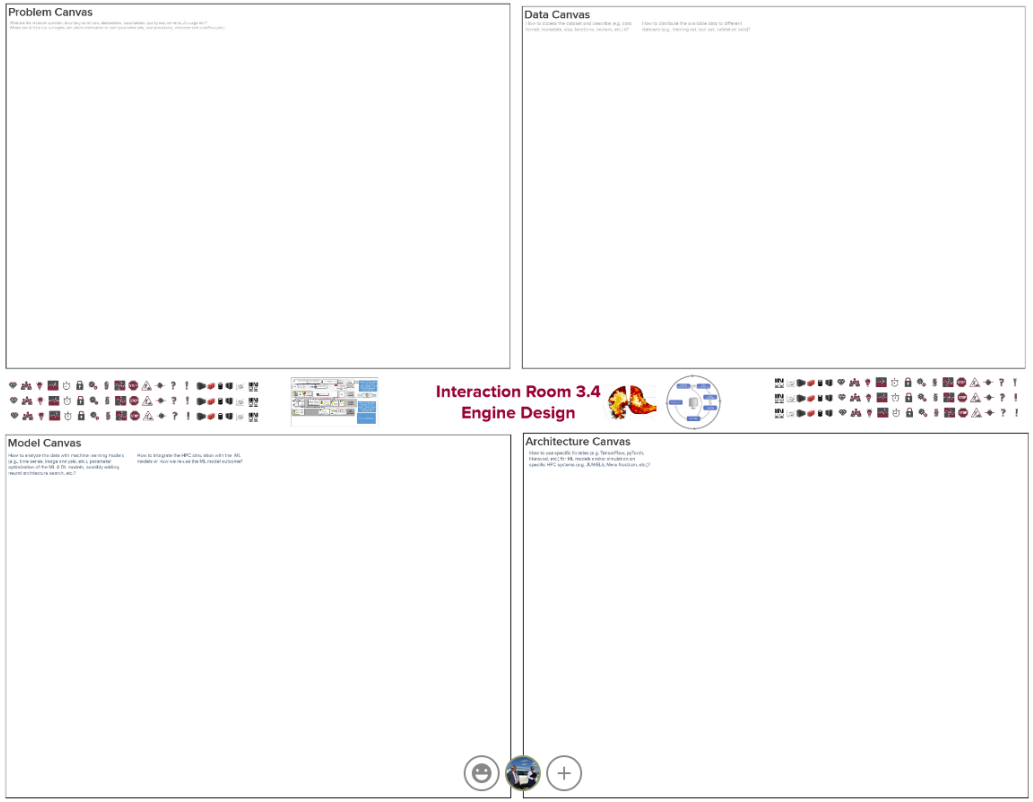


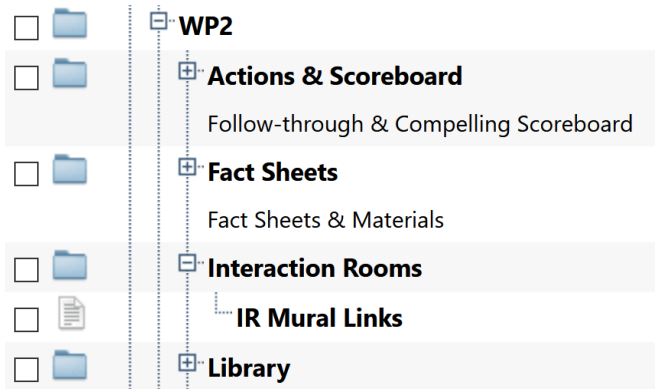


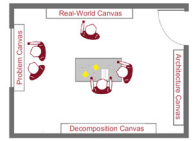
Agenda Item (2) – Review WP2 Status on Interaction Rooms



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

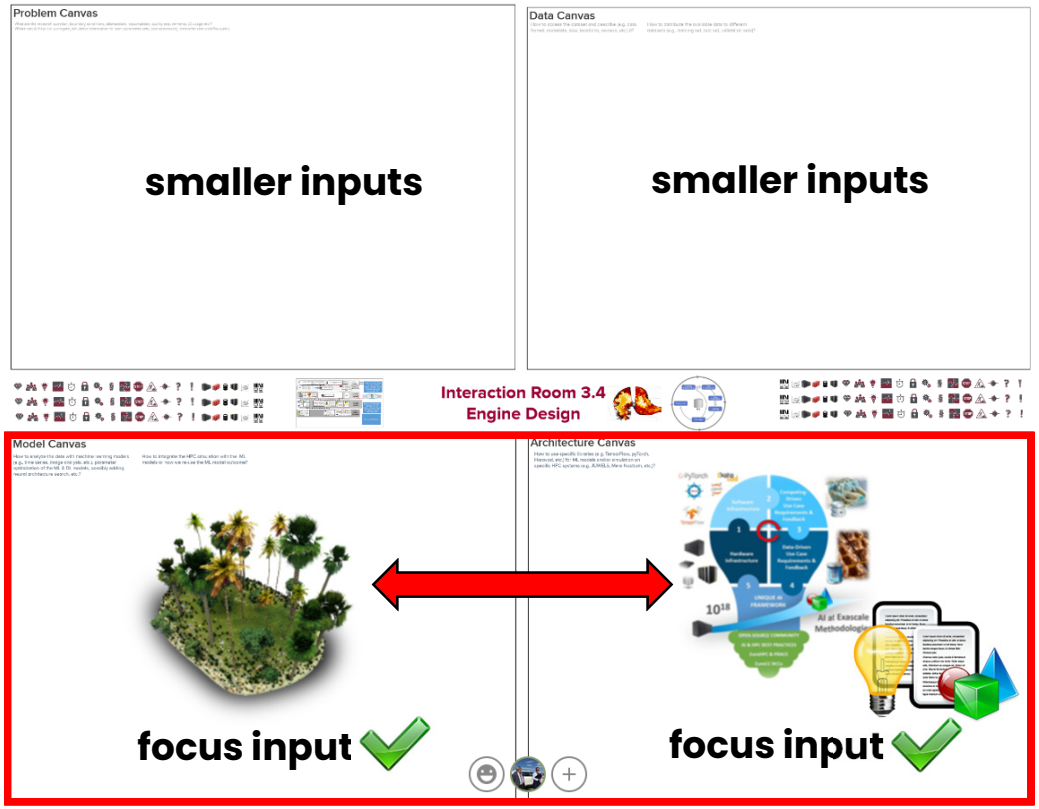
IR4.2 Seismic Imaging: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ae3e28af4bb8d9adbec33874998?sender=u15e3008bb41d6628a5bb5701

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
- 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=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

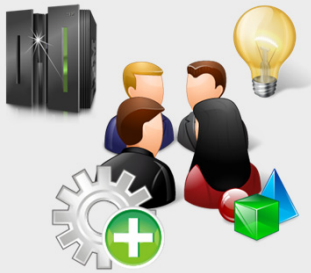
IR4.2 Seismic Imaging: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ae3e28af4bb8d9adbec33874998?sender=u15e3008bb41d6628a5bb5701

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

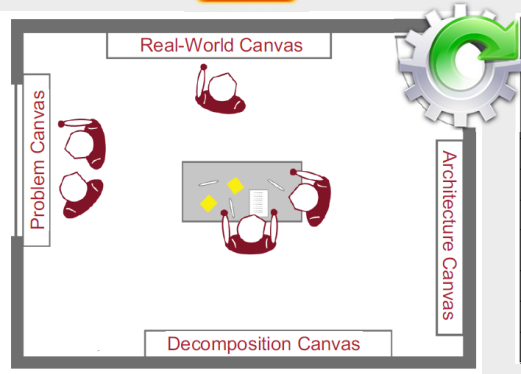
IR4.4 Sound Engineering: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa12219002404059f90a4bbb0101fa379a8503?sender=u15e3008bb41d6628a5bb5701

Interaction Room Status & Discussions – WP3/WP4 Overview

- WP3 (second round IRs)
  - T3.1: Turbulent Flow (asked) → later, needs RWTH
  - 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 (asked) → done
  - T4.2: Seismic imaging (started) → done
  - T4.3: Manufacturing (not started)
  - T4.4: Sound engineering (not started)
- TBD(Katrín): Schedule further meetings with Interaction Room teams



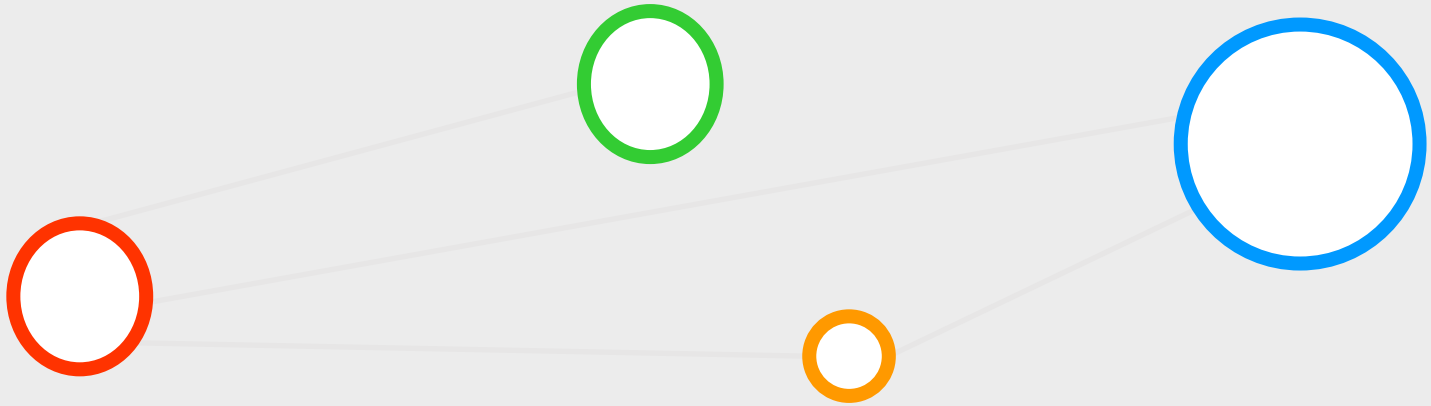
Continously Updating



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

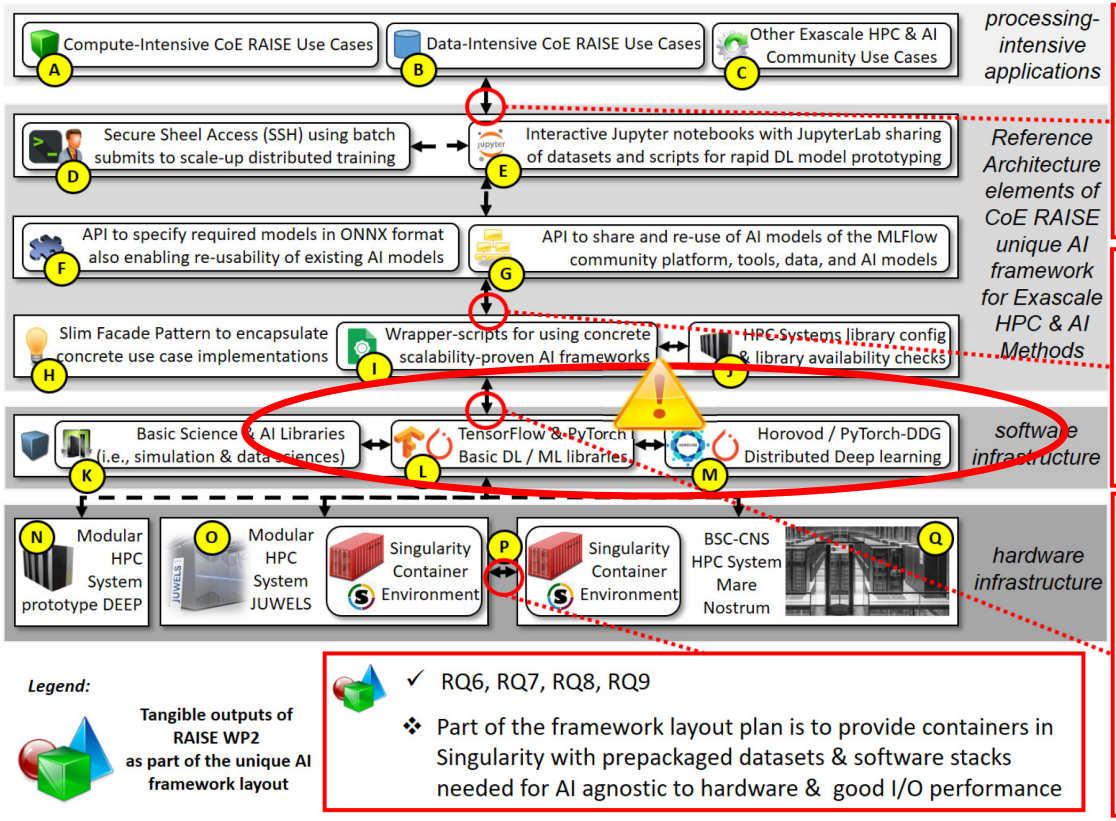
- Next round of Interaction Rooms with WP2
  - Carve out more details on AI/HPC methods
  - Contribute to the Unique AI Framework
  - Update our HPC/AI Methods Matrix

Agenda Item (3) – Realization of the SW Framework



Realization of SW Framework – Ideas of Web Page & Git Links

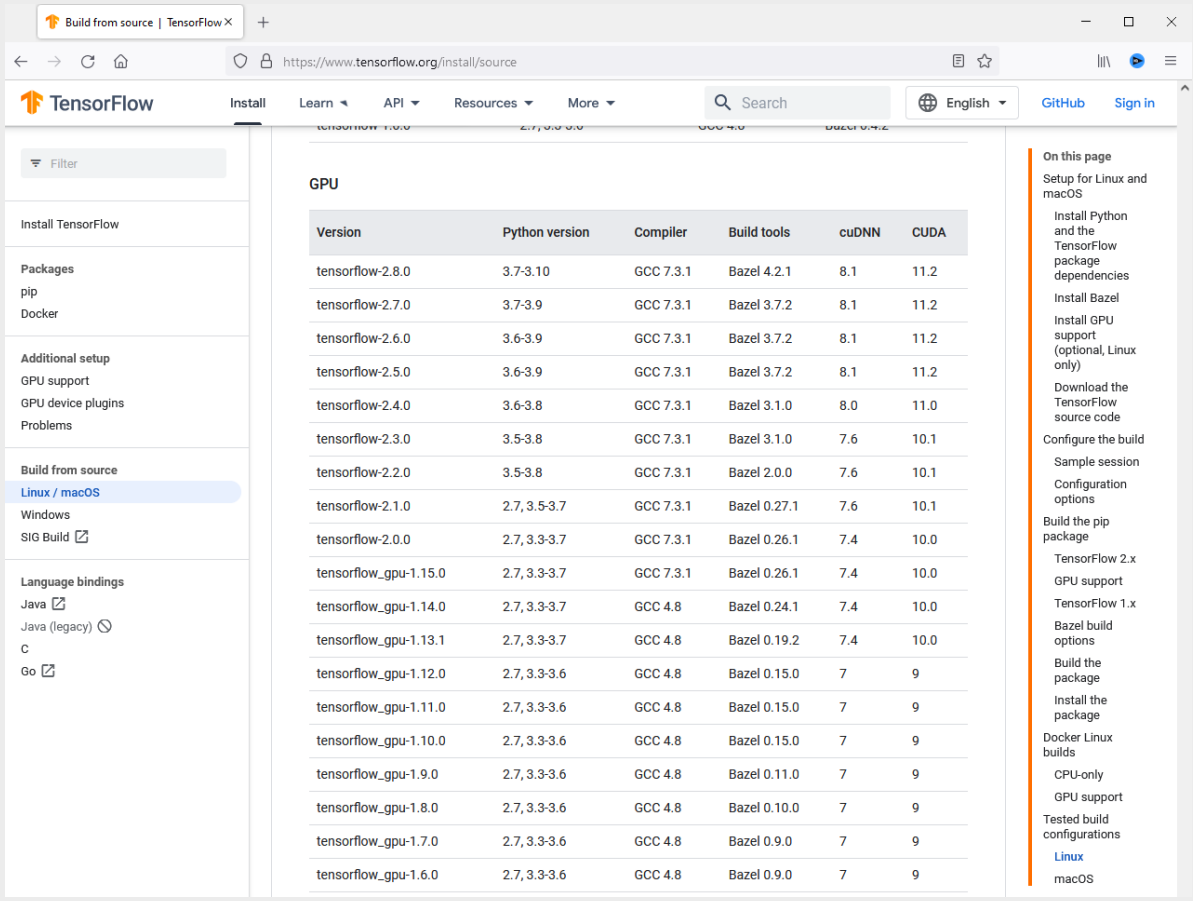
- Available in BSCW: https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3694045



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

Realization of SW Framework – Assess Challenges for Solutions

- Example: TensorFlow
  - Can we create an automated module checker for the SW Framework RAISE?
  - Specific versions of TensorFlow require specific versions of underlying HPC modules
  - Python versions must be correct as well
  - E.g., differences in Python 3.8.x and 3.9.x
  - Support AI developers with tool?



Version	Python version	Compiler	Build tools	cuDNN	CUDA
tensorflow-2.8.0	3.7-3.10	GCC 7.3.1	Bazel 4.2.1	8.1	11.2
tensorflow-2.7.0	3.7-3.9	GCC 7.3.1	Bazel 3.7.2	8.1	11.2
tensorflow-2.6.0	3.6-3.9	GCC 7.3.1	Bazel 3.7.2	8.1	11.2
tensorflow-2.5.0	3.6-3.9	GCC 7.3.1	Bazel 3.7.2	8.1	11.2
tensorflow-2.4.0	3.6-3.8	GCC 7.3.1	Bazel 3.1.0	8.0	11.0
tensorflow-2.3.0	3.5-3.8	GCC 7.3.1	Bazel 3.1.0	7.6	10.1
tensorflow-2.2.0	3.5-3.8	GCC 7.3.1	Bazel 2.0.0	7.6	10.1
tensorflow-2.1.0	2.7, 3.5-3.7	GCC 7.3.1	Bazel 0.27.1	7.6	10.1
tensorflow-2.0.0	2.7, 3.3-3.7	GCC 7.3.1	Bazel 0.26.1	7.4	10.0
tensorflow_gpu-1.15.0	2.7, 3.3-3.7	GCC 7.3.1	Bazel 0.26.1	7.4	10.0
tensorflow_gpu-1.14.0	2.7, 3.3-3.7	GCC 4.8	Bazel 0.24.1	7.4	10.0
tensorflow_gpu-1.13.1	2.7, 3.3-3.7	GCC 4.8	Bazel 0.19.2	7.4	10.0
tensorflow_gpu-1.12.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.15.0	7	9
tensorflow_gpu-1.11.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.15.0	7	9
tensorflow_gpu-1.10.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.15.0	7	9
tensorflow_gpu-1.9.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.11.0	7	9
tensorflow_gpu-1.8.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.10.0	7	9
tensorflow_gpu-1.7.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.9.0	7	9
tensorflow_gpu-1.6.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.9.0	7	9

Realization of SW Framework – Understanding Challenges

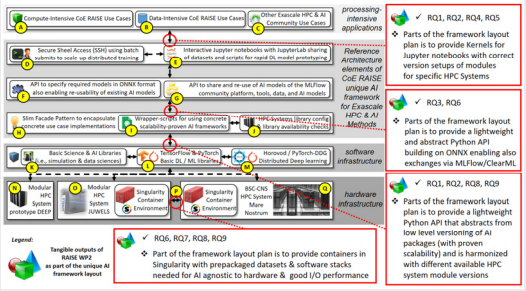
- Example of Setups
  - Many different versions / combinations
  - E.g. FZJ JSC DEEP-EST HPC System

```
[riedel1@dp-dam01 ~]$ module spider cudnn

---------------------------------------------------------------------------------------------------------------------------------------------------------------
  cuDNN:
---------------------------------------------------------------------------------------------------------------------------------------------------------------
     Description:
       The NVIDIA CUDA Deep Neural Network library (cuDNN) is a GPU-accelerated library of primitives for deep neural networks.

     Versions:
        cuDNN/7.4.1.5-CUDA-9.2.88
        cuDNN/7.5.1.10-CUDA-10.1.105
        cuDNN/7.6.4.38-CUDA-10.1.105
        cuDNN/7.6.5.32-CUDA-10.2.89
        cuDNN/8.0.2.39-CUDA-11.0
        cuDNN/8.2.1.32-CUDA-11.3
        cuDNN/8.3.1.22-CUDA-11.5

---------------------------------------------------------------------------------------------------------------------------------------------------------------
  For detailed information about a specific "cuDNN" module (including how to load the modules) use the module's full name.
  For example:

     $ module spider cuDNN/7.6.5.32-CUDA-10.2.89
---------------------------------------------------------------------------------------------------------------------------------------------------------------
```

```
[riedel1@dp-dam01 ~]$ module spider nccl

---------------------------------------------------------------------------------------------------------------------------------------------------------------
  NCCL:
---------------------------------------------------------------------------------------------------------------------------------------------------------------
     Description:
       The NVIDIA Collective Communications Library (NCCL) implements multi-GPU and multi-node collective communication primitives that are performance optimized for NVIDIA GPUs.

     Versions:
        NCCL/2.4.2-1-CUDA-9.2.88
        NCCL/2.4.6-1-CUDA-10.1.105
        NCCL/2.4.8-CUDA-10.1.105
        NCCL/2.4.8
        NCCL/2.7.3-1-CUDA-10.2.89
        NCCL/2.8.3-1-CUDA-11.0
        NCCL/2.8.3-1-CUDA-11.3
        NCCL/2.10.3-1-CUDA-11.3
        NCCL/2.11.4-CUDA-11.5

---------------------------------------------------------------------------------------------------------------------------------------------------------------
  For detailed information about a specific "NCCL" module (including how to load the modules) use the module's full name.
  For example:

     $ module spider NCCL/2.7.3-1-CUDA-10.2.89
---------------------------------------------------------------------------------------------------------------------------------------------------------------
```

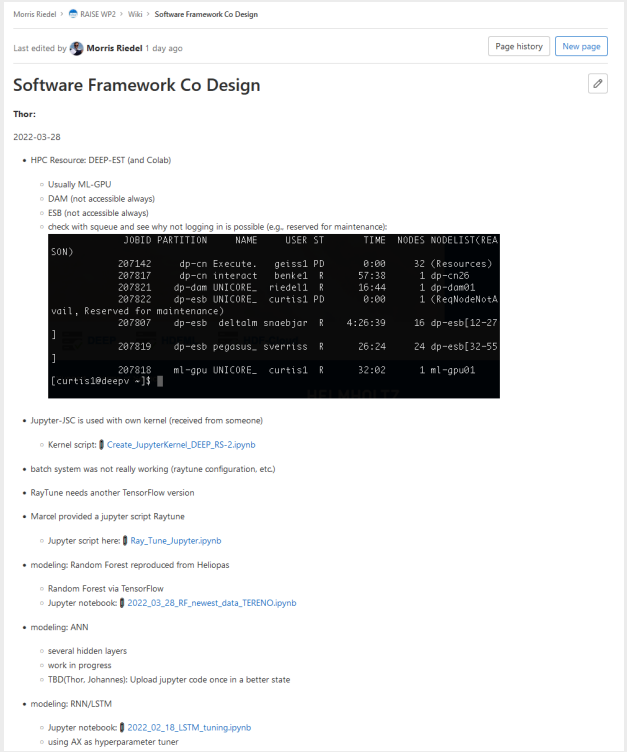
```
[riedel1@dp-dam01 ~]$ module spider tensorflow

---------------------------------------------------------------------------------------------------------------------------------------------------------------
  TensorFlow:
---------------------------------------------------------------------------------------------------------------------------------------------------------------
     Description:
       An open-source software library for Machine Intelligence

     Versions:
        TensorFlow/1.12.0-GPU-Python-2.7.15
        TensorFlow/1.12.0-GPU-Python-3.6.6
        TensorFlow/1.13.1-GPU-Python-3.6.8
        TensorFlow/2.2.0-GPU-Python-3.6.8-1
        TensorFlow/2.3.1-Python-3.8.5
        TensorFlow/2.5.0-Python-3.8.5
        TensorFlow/2.6.0-CUDA-11.5

---------------------------------------------------------------------------------------------------------------------------------------------------------------
  For detailed information about a specific "TensorFlow" module (including how to load the modules) use the module's full name.
  For example:

     $ module spider TensorFlow/2.2.0-GPU-Python-3.6.8-1
---------------------------------------------------------------------------------------------------------------------------------------------------------------
```


```
[riedel1@dp-dam01 ~]$ module spider cuda

---------------------------------------------------------------------------------------------------------------------------------------------------------------
  CUDA:
---------------------------------------------------------------------------------------------------------------------------------------------------------------
     Description:
       CUDA (formerly Compute Unified Device Architecture) is a parallel computing platform and programming model created by NVIDIA and implemented by the graphics processing units (GPUs) that they produce. CUDA gives developers access
       to the virtual instruction set and memory of the parallel computational elements in CUDA GPUs.

     Versions:
        CUDA/9.2.88
        CUDA/10.1.105
        CUDA/10.2.89
        CUDA/11.0
        CUDA/11.0.207
        CUDA/11.3
        CUDA/11.5

---------------------------------------------------------------------------------------------------------------------------------------------------------------
  For detailed information about a specific "CUDA" module (including how to load the modules) use the module's full name.
  For example:

     $ module spider CUDA/11.0.207
---------------------------------------------------------------------------------------------------------------------------------------------------------------
```



Realization of SW Framework – Ideas of Web Page & Artefacts

- Initial ideas collected on WP2 RAISE
  - Should be transformed in a proper GIT structure (new WP2 RAISE programmer & RAISE folks → next slide)
  - Selected artefacts of different types: Jupyter notebooks of AI codes, Kernel for Jupyter notebooks, infos links to Nvidia drivers
  - Context: Concrete HPC machines (e.g., DEEP-EST DAM, ESB, ML-GPU)
  - Practice & experience: Shows highly unstable environments for AI configuration and setups (not deterministic behaviours) → room for framework idea
  - Lessons learned: Invested many hours to identify issues in kernel developments with new stages and new python versions → we need improvements!
  - Wiki page for now with attachment: https://gitlab.jsc.fz-juelich.de/riedel1/raise-wp2/-/wikis/Software-Framework-Co-Design



Morris Riedel › RAISE WP2 › Wiki › Software Framework Co Design

Last edited by **Morris Riedel** 1 day ago — Page history — New page

Software Framework Co Design

Thor:

2022-03-28

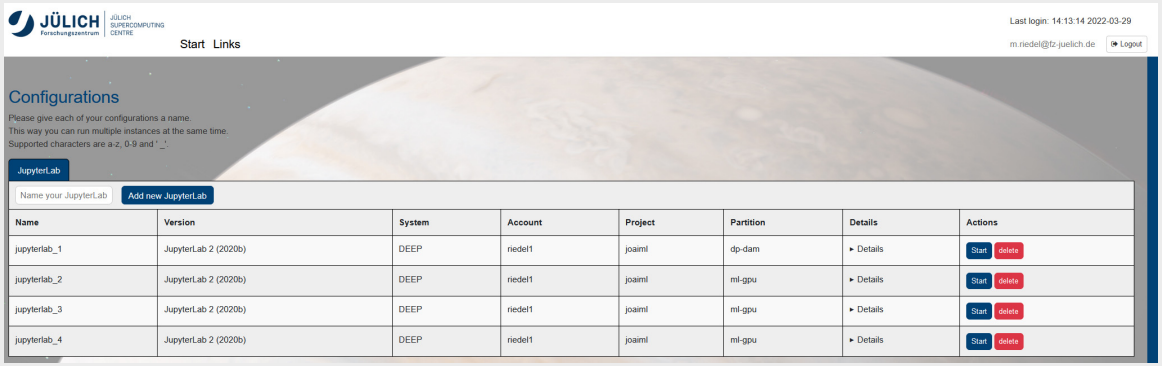
- HPC Resource: DEEP-EST (and Colab)
  - Usually ML-GPU
  - DAM (not accessible always)
  - ESB (not accessible always)
  - check with squeue and see why not logging in is possible (e.g., reserved for maintenance):

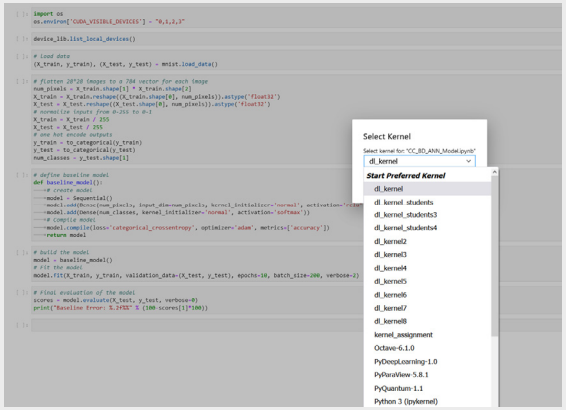
```
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
            207142     dp-cn Execute.    geiss1 PD       0:00     32 (Resources)
            207817     dp-cn interact    benkel  R      57:38      1 dp-cn26
            207821    dp-dam UNICORE_   riedel1  R      16:44      1 dp-dam01
            207822    dp-esb UNICORE_   curtis1 PD       0:00      1 (ReqNodeNotAvail, Reserved for maintenance)
            207807    dp-esb  deltalm snaebjar  R    4:26:39     16 dp-esb[12-27]
            207819    dp-esb pegasus_ sverriss  R      26:24     24 dp-esb[32-55]
            207818    ml-gpu UNICORE_   curtis1  R      32:02      1 ml-gpu01
[curtis10@deepv ~]$
```

- Jupyter-JSC is used with own kernel (received from someone)
  - Kernel script: Create_JupyterKernel_DEEP_RS-2.ipynb
- batch system was not really working (raytune configuration, etc.)
- RayTune needs another TensorFlow version
- Marcel provided a jupyter script Raytune
  - Jupyter script here: Ray_Tune_Jupyter.ipynb
- modeling: Random Forest reproduced from Heliopas
  - Random Forest via TensorFlow
  - Jupyter notebook: 2022_03_28_RF_newest_data_TERENO.ipynb
- modeling: ANN
  - several hidden layers
  - work in progress
  - TBD(Thor, Johannes): Upload jupyter code once in a better state
- modeling: RNN/LSTM
  - Jupyter notebook: 2022_02_18_LSTM_tuning.ipynb
  - using AX as hyperparameter tuner

Realization of SW Framework – Ideas of Web Page & Artefacts

- Example of Setups
  - Tried many varieties of kernels
  - Developers / PhD Students loose ~3-4 hours average by trying new HPC machine just to get new modules right and/or setup kernels that work with modules
  - Selected debug/solution tools not known always, e.g., nvidia-smi, etc.
  - Note: Jupyter-JSC itself seems not to be the problem, rather complex hardware/software configurations
  - E.g., DEEP-EST DAM different nodes: FPGAs and GPUs?! ML-GPU worked better

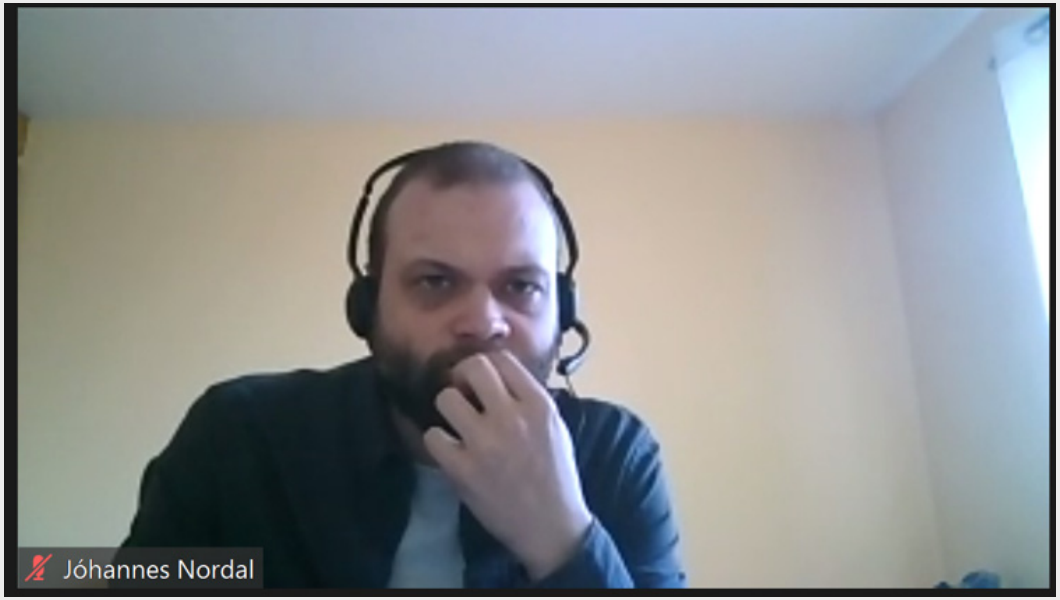




New WP2 Programmer - Jóhannes Nordal

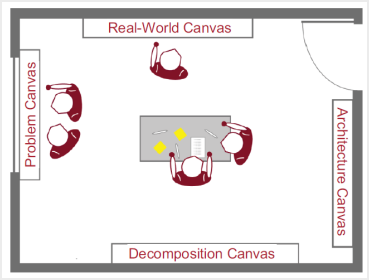
- WP2 Programmer with experience in C/UNIX/HPC
  - University of Iceland
- Should be involved in all RAISE relevant programming aspects to collect and curate artefacts for the SW framework co-design efforts
- Email: jon8@hi.is

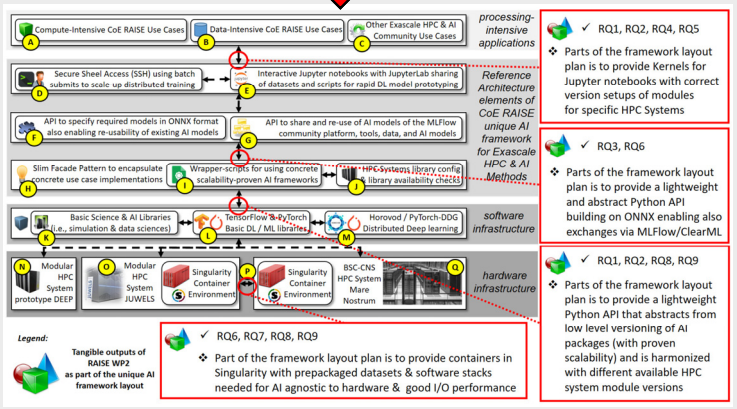
- WELCOME!



Realization of SW Framework – Interaction Room Results (1)

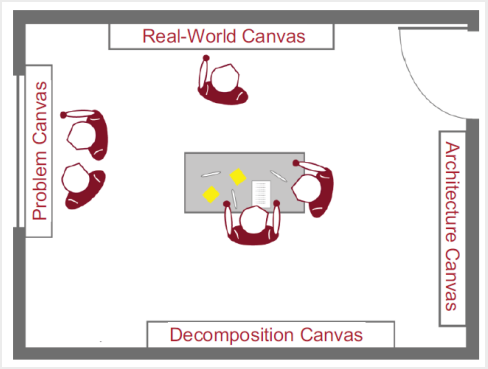
- ✓ Interaction Room Seismic Imaging
  - Pipeline activities relevant for the SW Framework Co-Design
  - Updates from Johannes (WP2) & Liang (WP4)
- ✓ Interaction Room Event Reconstruction & Classification at the CERN-LHC
  - Official Repository exists, no need to put elements into github
  - Includes also job scripts, AI model scripts, etc.
  - Very specific model in the community „MLPF“, perhaps limited use for other communities
  - Good to share for world-wide LHC collaboration
  - TBD(): Adding Raytune to SW framework relevant and Rapids.AI (e.g., for memory management)

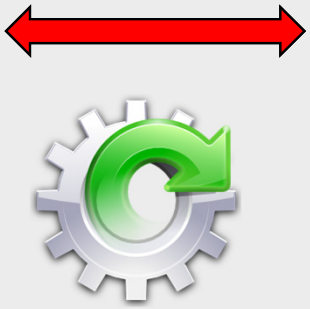




Realization of SW Framework – Interaction Room Results (2)

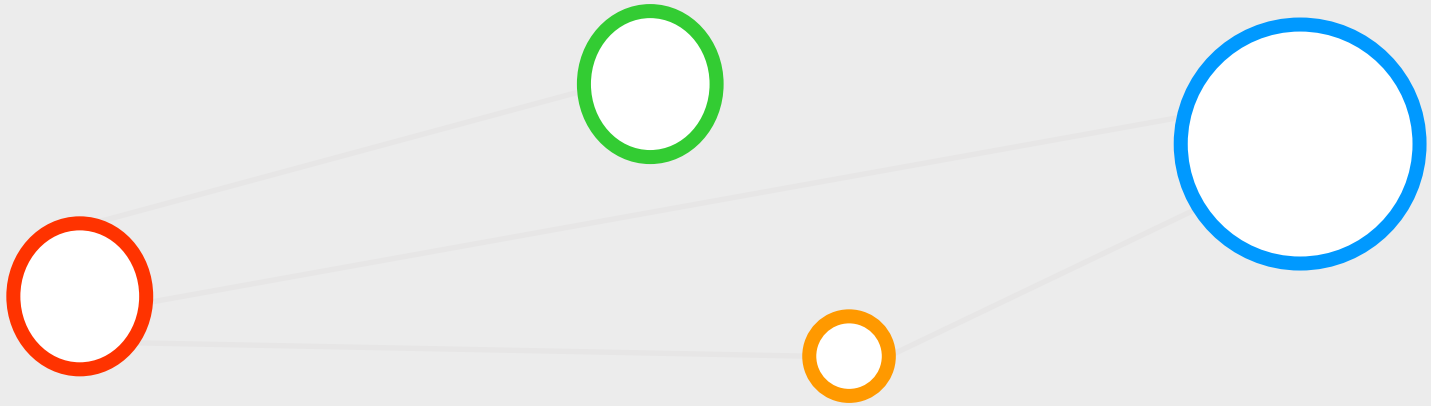
- ✓ Interaction Room Event Reconstruction & Classification at the CERN-LHC
  - ✓ Initial set of models analyzed, but not used in RAISE
  - ➢ Removal of Statistical Methods
  - ➢ Removal of Jedi-NET
  - ➢ Update of Matrix





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

Agenda Item (4) – Upcoming Deliverables



Upcoming Deliverables

- Time to start with selected deliverables

D2.7	Support report	FZJ	R	PU	18	M. Riedel/ UOI	E. Inanc/ FZJ	Thomas Jaravel/ CERFACS	I. Schmitz/ ParTec	09.06.2022	30.06.2022
D2.10	Monitoring report	UOI	R	CO	18	M. Riedel/ UOI	M. Book/ UOI	M. Nicolaou/ CYI	A. Lintermann/ FZJ	09.06.2022	30.06.2022
D5.1	Market analysis report; innovation plan	FM	R	CO	18	W. Lammens/ FM	W. Lammens/ FM	A. Lektauers/ RTU	K. Pausch / FZJ	09.06.2022	30.06.2022
D6.6	Network evaluation document	BSC	R	PU	18	R. Gregorio/ BSC	G. Houzeaux/ BSC	R. Heylen/ FM	J. Lopez/ ParTec	09.06.2022	30.06.2022
D2.3	Report on porting & performance engineering	BSC	R	PU	24	M. Riedel/ UOI	G. Houzeaux/ BSC	L. Nicoletti/ BULL	A. Lintermann/ FZJ	28.11.2022	31.12.2022
D2.8	Benchmarking & support report	FZJ	R	PU	24	M. Riedel/ UOI	K. Michielsen/ FZJ	Guillermo Oyarzun/ BSC	J.Lopez/ ParTec	28.11.2022	31.12.2022
D2.15	Report on novel AI technologies	UOI	R	CO	24	M. Riedel/ UOI	M. Riedel/ UOI	C. Lapeyre/ CERFACS	I. Schmitz/ ParTec	28.11.2022	31.12.2022
D3.2	Report on outcomes of WP3 use-cases	RWTH	R	CO	24	C. Lapeyre/ CERFACS	M. Meinke/ RWTH	Matthias Book/ UOI	A. Lintermann/ FZJ	28.11.2022	31.12.2022

Upcoming Deliverables

- Time to start with selected deliverables

Task 2.2 Hardware prototypes <Leader: FZJ> <M1-M18>

Contributors: FZJ & ParTec, UOI, RTU Outputs: ***D2.5, D2.6, D2.7***

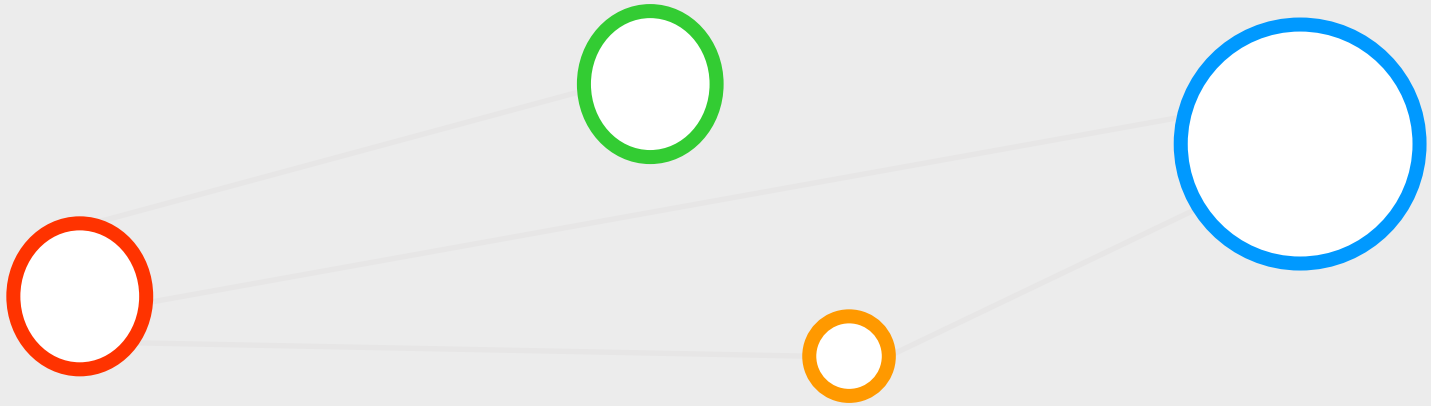
FZJ gives access to hardware prototypes that are developed in the DEEP-projects via corresponding "Early Access Programs". At FZJ, this means provision of access to the DEEP-EST prototype, which consist of a x86-based Cluster module, an NVIDIA-GPGPU-based Booster module, and a x86-, NVIDIA-GPGPU-, and FPGA-based Data Analytics module. The prototypes also include technologies for NAMs, NVMs, and non-x86-based solutions like ARM architectures. Furthermore, the D-Wave Quantum Annealing machine is integrated into FZJ's MSA environment when it becomes available. At BSC, other prototype facilities, described in Sec. 4.1.5, are available for running the use-cases proposed by BSC. In case of additional user-requirements, FZJ & ParTec, and BSC provide solutions for integrating the aforementioned technologies as well as support, training, best practice guidelines, and manuals in using these new technologies for the AISee partners.

Task 2.4 Software design of a unique AI framework <Leader: UOI> <M7-M36>

Contributors: FZJ, UOI, RTU Outputs: ***D2.10, D2.11, D2.12***

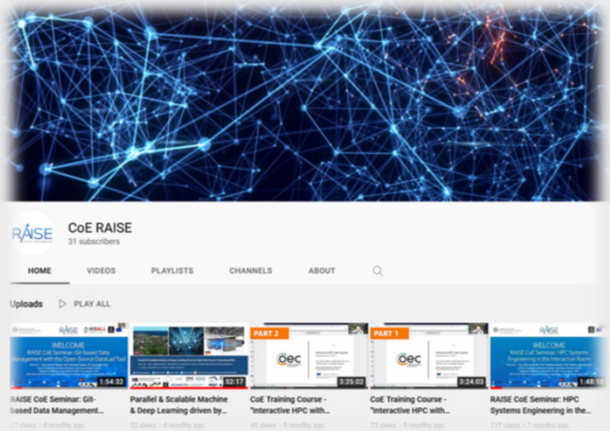
In this task, the software design of a unique use-case-driven AI framework is commenced within the frame of a planning and strategy layout phase. Therefore, the task contributors perform a use-case requirement analysis to decide on a generalized layout of the framework that includes all necessary components coming from the use-cases. It ensures that the developments in the use-cases are in line with a future integration into a generalized software framework by continuously monitoring them. A lively interaction between the framework designers and the use-case developers is necessary to find a layout, which is suitable for a generalized approach. Interfaces and APIs are described in detail together with the use-case providers to ensure the generalized approach and future sustainability of the framework as well as its easy application. It is ensured that use-case results are furthermore in line with the Design and Development of new Service prototypes task of PRACE 5IP/WP6. Suitable use-cases will be contributed to the PRACE GitLab Data Analytics project.

Agenda Item (5) – Status WP2 Training Plans



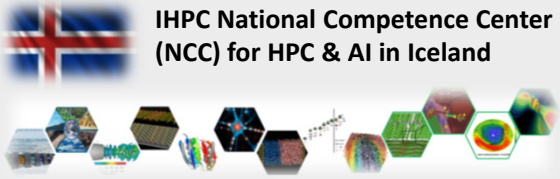
WP2 Monthly Trainings – Review & Plan

- 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/UCAdIZ-v6cWwGdapwYxdN7dg
  - TBD(Katrín): Schedule the YouTube Training series with speakers



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

WP2 Monthly Trainings – Review & Plan

December:
No Seminar

January:
RTU CUDA Seminar
(THANKS!)

February:
none

2022-03-31 14:00 GMT
Graph Neural Network
Morris: Intro GNNs (30 min)
Leo from Atos (45 min)
Eric from Cern (20 min)

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

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

May:
Request Project Partners?
ONNX / OpenML
Interoperable formats

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

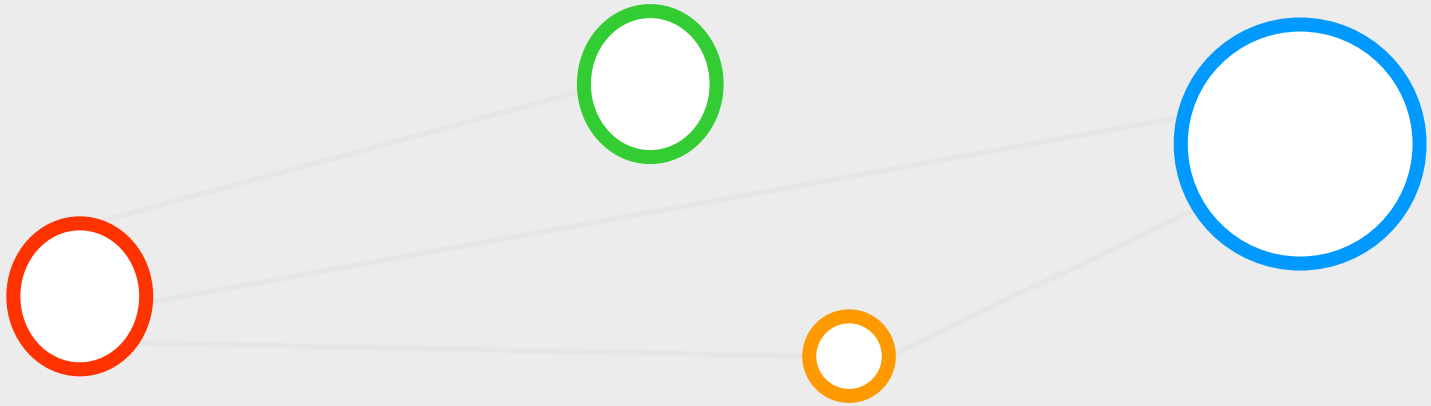
July:
Request Project Partners?
(Deliverables maybe in WP2)

August:
Request Project Partners?
Gael (continous integration ATOS)???
Eray: Tooling with modules???

September:
Request Project Partners?

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

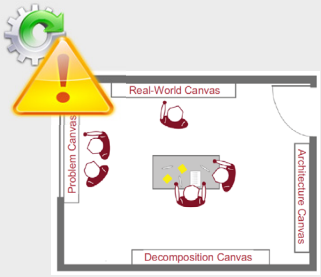
Agenda Item (6) – Compelling Scoreboard Review



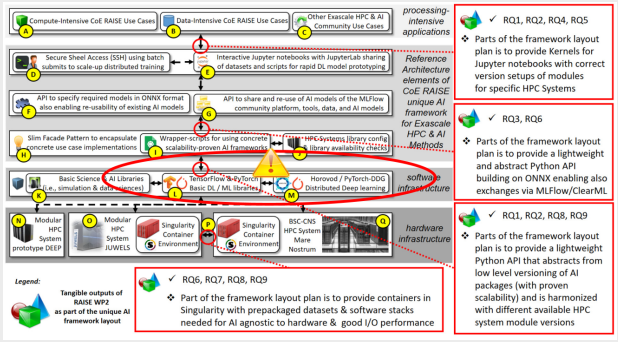
Compelling Scoreboard Review – Use Case Progress

RAISE Center of Excellence

- 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



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



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

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

SC21


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

✓ Quantum SVM Training 2022-04-21

❖ Monthly Meeting April

✓ AHM Meeting 2021-11-24/25

✓ Graph Neural Networks Training 2022-03-31

✓ GraphCore Seminar 2021-11-23

✓ Monthly Meeting March

✓ Monthly Meeting November

✓ Monthly Meeting February

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

✓ Monthly Meeting January

✓ CUDA Seminar January 2022-01-19/20

✓ Monthly Meeting October

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

✓ MLOps with ClearML Seminar ~end Sep

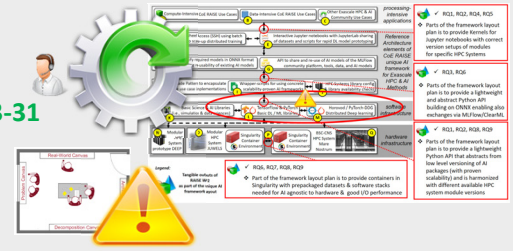
✓ Monthly Meeting September

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

✓ Monthly Meeting August

✓ Autoencoder Seminar ~end August

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



- Next Steps
- Interaction Room 2nd Round → Discuss & Implement framework
- Upcoming Deliverables

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

1. RWTH Aachen
    1. Marian leaved (temporarily), Fabian Hübenthal (new in April), another PhD student might join (together with Eray, Rakesh), VAE
    2. RWTH -> Christian Terboven for QR
2. AOB: Plan a continous integration and toolset support for underlying module environment that works for specific HPC systems in RAISE (including MPI versions, for coupling, etc.)
    1. ATOS
3. AOB: Documentation of systems of FZJ, BSC: automation of modules that work
    1. Still challenges with on top libraries, horovod, pip install tensorflow
    - WP2 Eray → more automated over time (e.g., what happens with LUMI AMD roc toolkits)

- AOB: PRACE Calls for Access
- AOB: Extension of RAISE Data Project
    - 200 TB, not used 10%,
    - Interaction Room, Liang,
    - Promote data project, CFD
- 09.06.2022
    - Training RTU
- 09.09.2022 (Review)
    - One day full event in Juelich
    - WP leaders, not really task leaders
    - One day rehearsal

drive. enable. innovate.

RAISE Center of Excellence

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the European Union's Horizon 2020 –
Research and Innovation Framework Programme
H2020-INFRAEDI-2019-1 under grant agreement no. 951733

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