



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

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School of Engineering & Natural Sciences, University of Iceland

*2022-03-30, RAISE WP2 Monthly Meeting March 2022, Online*



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@Morris Riedel



@MorrisRiedel



@MorrisRiedel



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



morris@hi.is

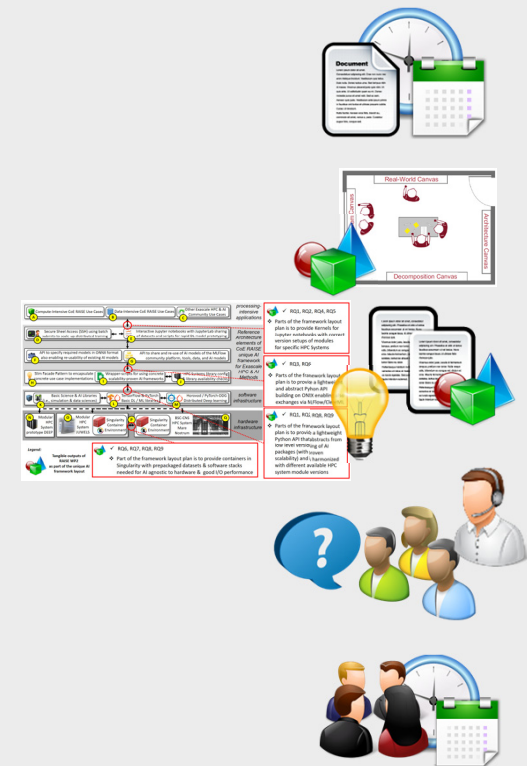


# WP2 February March – Welcome & Agenda

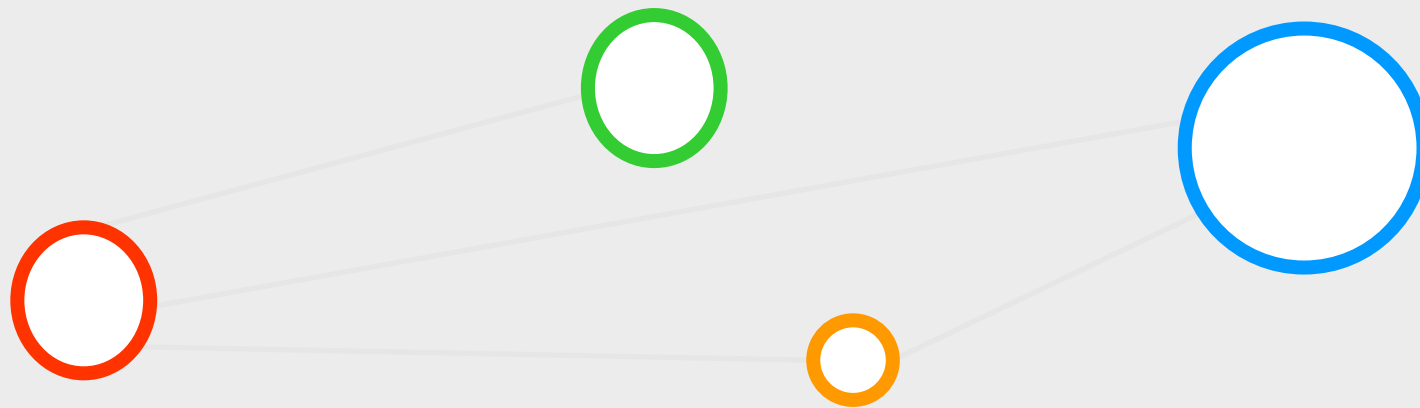


**RAISE**  
Center of Excellence

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. Status WP2 Seminar Plans
  - (Morris et al.), ~10 Min
5. Compelling Scoreboard Review & Next Steps
  - (All), ~15 Min



# Agenda Item (1) – Minutes Approval – Meeting February 2022



# Minutes Approval – Monthly Meeting February 2022

## ➤ Minutes available in BSCW

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

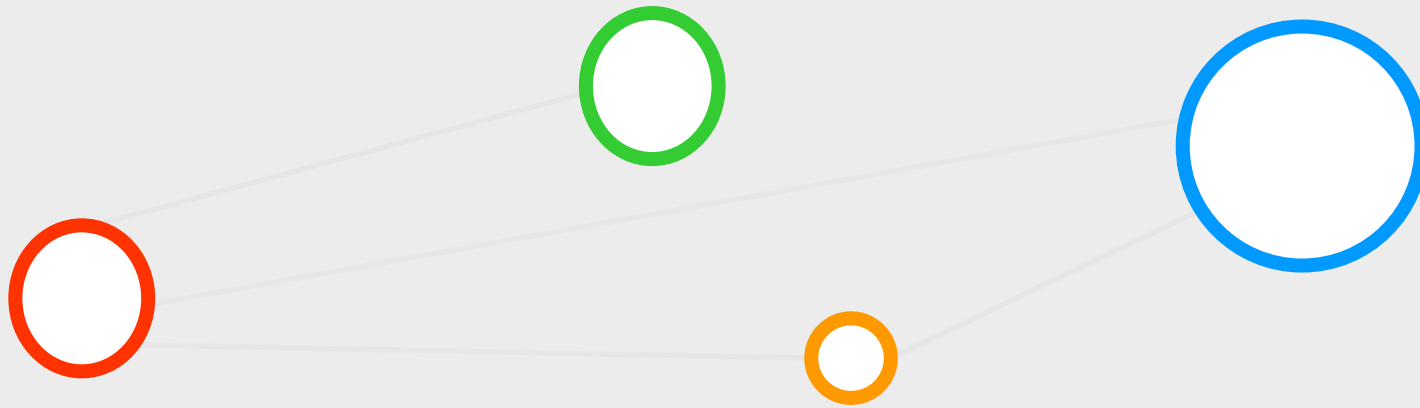


Morris Riedel - RAISE WP2 - Issues		
Open	Closed	All (2)
Recent searches - Search or filter results...		
Due date - 1h		
B - Create Fact Sheet Task 4.4 Sound Engineering		
#21 - created 3 minutes ago by Morris Riedel	WP2 Fact Sheet Collection Completed	Apr 30, 2021
		updated just now
B - Create Fact Sheet Task 4.3 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

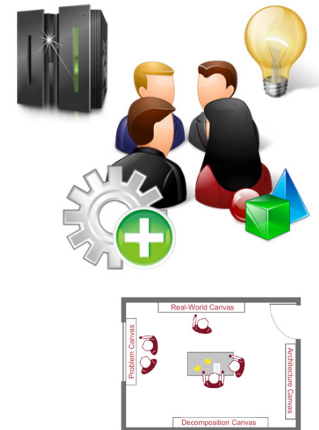
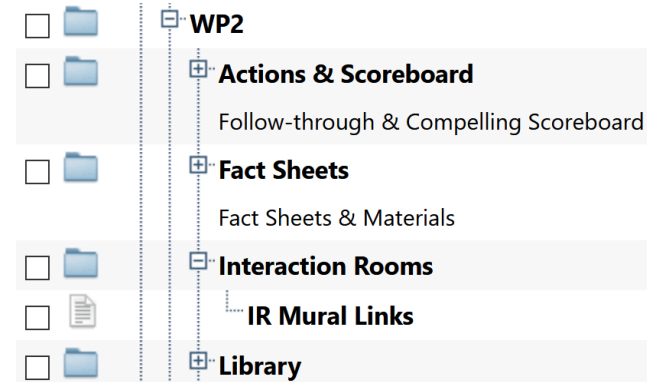
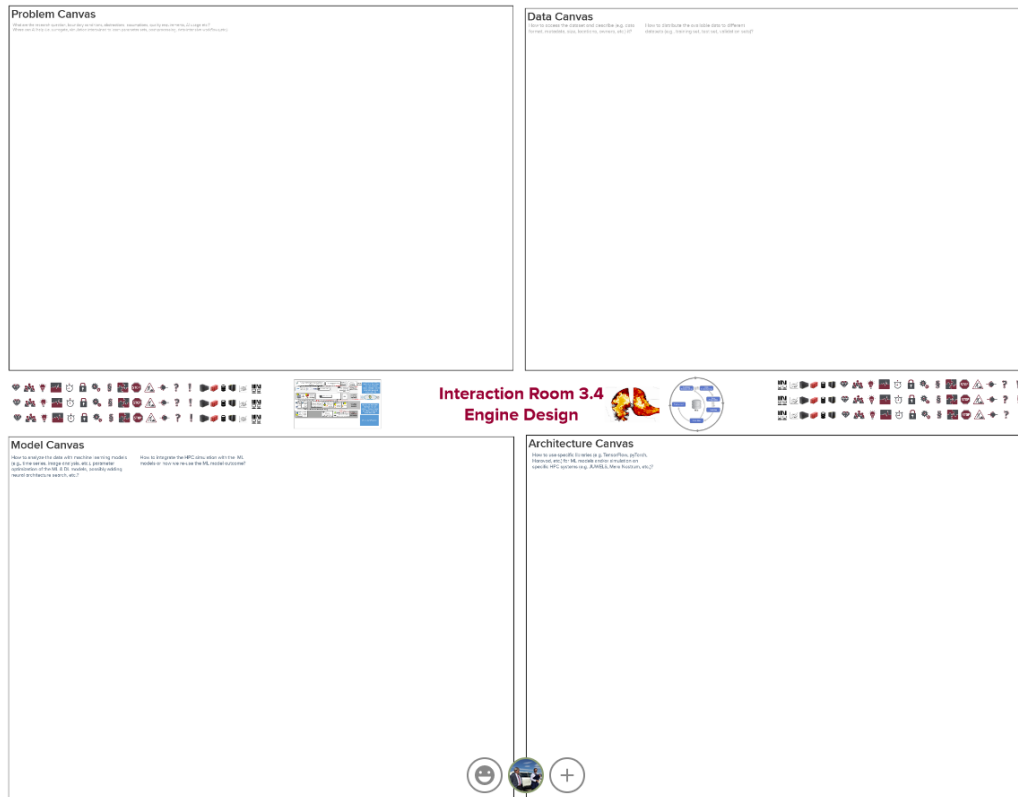
2021_06_29_Monthly_Meeting_June 2021	Slides & Materials from meeting 2021-06-29
2021_07_22_Monthly_Meeting_July 2021	Slides & Materials from meeting 2021-07-22
2021_08_30_Monthly_Meeting_August 2021	Slides & Materials from meeting 2021-08-30
2021_09_30_Monthly_Meeting_September 2021	Slides & Materials from Meeting 2021-09-30
2021_10_29_Monthly_Meeting_October 2021	Slides & Materials from Meeting 2021-10-29
2021_11_26_Monthly_Meeting_November 2021	Slides & Materials from Meeting 2021-11-26
2022_01_31_Monthly_Meeting_January 2022	Slides & Materials from Meeting 2022-01-31
2022_01_31_CoE-RAISE-WP2-Monthly-Meeting-Riedel-v1.pptx	
2022-01-31-Monthly-Meeting-January-2022-Minutes-v1	
2022-01-31-Monthly-Meeting-January-2022-Minutes-v1	
2022_02_28_Monthly_Meeting_February 2022	Slides & Materials from Meeting 2022-02-28



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



# Interaction Rooms via MURAL Boards & Milestone Inputs

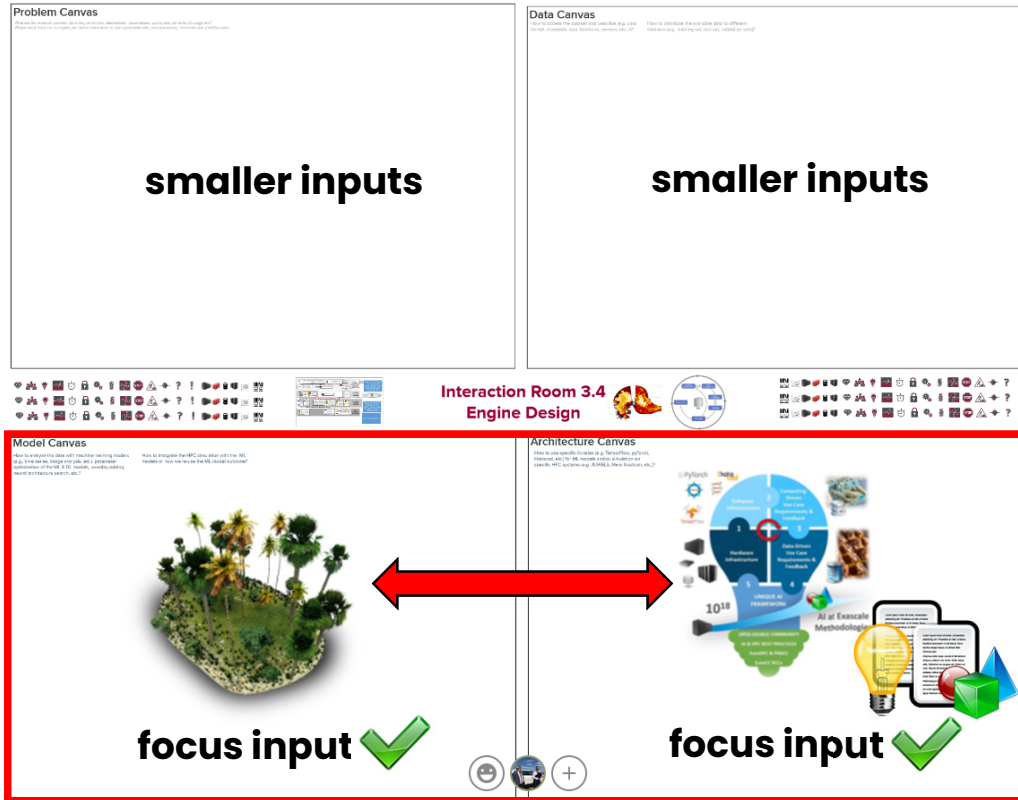


## IR Mural Links

- IR3.1 Turbulent Flow: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377866397/8613c384d54f66fb5e78599ff307a4ce8a9090c0?sender=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/matthiasbook8855/1621377991014/7a5d7e1ea7230178342d1e1d4a84d656d905d52?sender=u15c3008bb41d6628a5bb5701>
- IR4.1 Fundamental Physics: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378007335/6f0d5285feaec3eaf515bd6676e84d8b4879d39?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/matthiasbook8855/1621378038069/93df6fa7a41093f4eaae7bc9d72979dc2ba42b9d?sender=u15c3008bb41d6628a5bb5701>
- IR4.4 Sound Engineering: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa12219002404059f90a4bbb0101fa379a8503?sender=u15c3008bb41d6628a5bb5701>

- 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=u15c3008bb41d6628a5bb5701>
- IR3.2 Clean Energy: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377887905/cb44cca3eed3bb9964fbfa36af16b1bfcc085f?sender=u15c3008bb41d6628a5bb5701>
- IR3.3 Reactive Flows: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377959022/0c363886f24833eeb19b025d87324b57fd50e2db?sender=u15c3008bb41d6628a5bb5701>
- IR3.4 Engine Design: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377976343/8d7aba6be09af3b2fd305d2f709e53661ac889d?sender=u15c3008bb41d6628a5bb5701>
- IR3.5 Coating: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621377991014/7a5d7e1eaf230178342d1e1d4a84d656d9055d52?sender=u15c3008bb41d6628a5bb5701>
- IR4.1 Fundamental Physics: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378007335/6f0d3283f6aec3eaf315bd6676e84d8b4879d39?sender=u15c3008bb41d6628a5bb5701>
- IR4.2 Seismic Imaging: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ac3e28a4fbb8d9adbec33874998?sender=u15c3008bb41d6628a5bb5701>
- IR4.3 Manufacturing: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378038069/93df6fa7a41093f4eaae7be9d72979dc2ba42b9d?sender=u15c3008bb41d6628a5bb5701>
- IR4.4 Sound Engineering: <https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa12219002404059f90a4bbb0101fa379a8503?sender=u15c3008bb41d6628a5bb5701>



# Interaction Room Status & Discussions – WP3/WP4 Overview

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

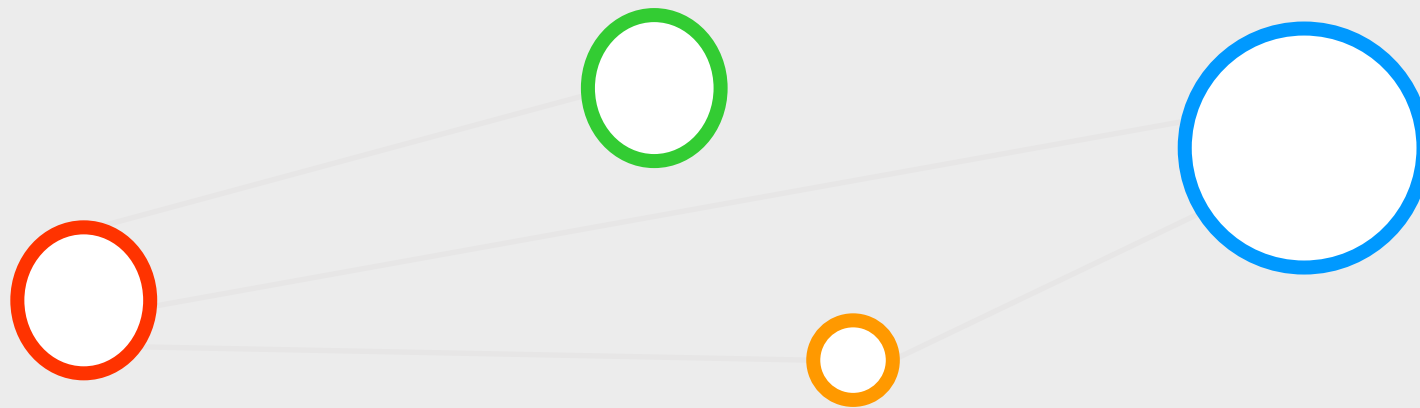


Use Case	AE	PIML	ANNs	CNN	NO	SMs	GNN	IN	LSTM	GRU
Details	CAE	RBP-ANN	U-Net	RESNET	FNO	AR	ARMA	ARIMA	JEDI-net	
AI for turbulent boundary layers	X	X								
AI for wind farm layout optimization			X			X	X	X		
AI for data-driven models in reacting flows			X					X		
Smart models for next generation aircraft 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

- **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

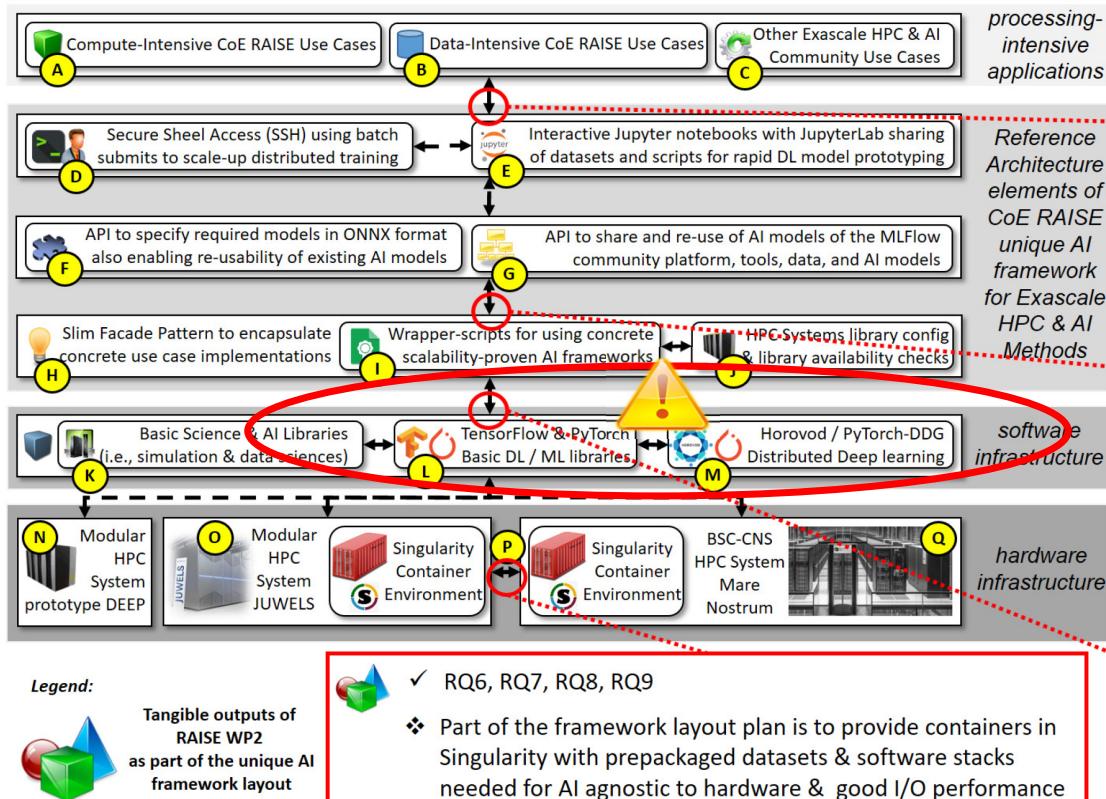


## Agenda Item (3) – Realization of the SW Framework



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

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



**Continuously 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?

The screenshot shows the TensorFlow website's 'Build from source' page. The left sidebar contains navigation links: 'Install TensorFlow', 'Packages' (pip, Docker), 'Additional setup' (GPU support, GPU device plugins, Problems), 'Build from source' (Linux / macOS, Windows, SIG Build), and 'Language bindings' (Java, Java (legacy), C, Go). The main content area is titled 'GPU' and contains a table with columns: Version, Python version, Compiler, Build tools, cuDNN, and CUDA. The table lists various TensorFlow versions and their corresponding dependencies. On the right, a sidebar titled 'On this page' lists links to setup instructions for Linux and macOS, installation of Python and TensorFlow dependencies, Bazel, GPU support, source code download, build configuration, sample session, pip package build, TensorFlow 2.x GPU support, TensorFlow 1.x Bazel build options, package build and installation, Docker Linux builds, CPU-only GPU support, and tested build configurations for Linux and macOS.

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 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/2.4.4-1-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
-----
```

```
[riedell@sp-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:

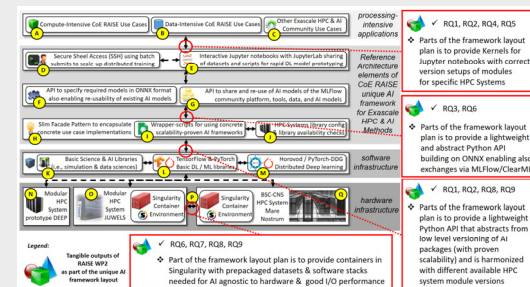
  $ module spider CUDA/11.0.207
-----
```

```
[riedell@dp-dan01 ~]$ 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/7.6.1.8-CUDA-9.2.88
  cudNN/7.5.1.15-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/8.3.1.32-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
```

```
[riedell@dgp-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
```



# 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	MODEL
207142	dp-cn	Esacuta	geisel	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	(ReqModelNotA
207807	dp-esb	deltalm	snaebjor	R	4:26:39	16	dp-esb[12-27
207819	dp-esb	pegdsus	sverriss	R	26:24	24	dp-esb[32-55
207818	ml-gpu	UNICORE	curtis1	R	32:02	1	ml-gpu01

[curtis1@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 Heliosas
  - 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

## ➤ 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

**JÜLICH**  
Forschungszentrum  
FUTURES COMPUTING CENTRE

Last login: 14:13:14 2022-03-29  
m.riedel@fz-juelich.de Logout

### Configurations

Please give each of your configurations a name.  
This way you can run multiple instances at the same time.  
Supported characters are a-z, 0-9 and " \_ - . , : ; \* & % ^ ` ~ ! @ # \$ % & ' \"

Name	Version	System	Account	Project	Partition	Details	Actions
jupyterlab_1	JupyterLab 2 (2020b)	DEEP	niede1t	joaiml	dp-dam	► Details	[Start] [Delete]
jupyterlab_2	JupyterLab 2 (2020b)	DEEP	niede1t	joaiml	m1-gpu	► Details	[Start] [Delete]
jupyterlab_3	JupyterLab 2 (2020b)	DEEP	niede1t	joaiml	m1-gpu	► Details	[Start] [Delete]
jupyterlab_4	JupyterLab 2 (2020b)	DEEP	niede1t	joaiml	m1-gpu	► Details	[Start] [Delete]

```

2 import os
3 os.environ["CUDA_VISIBLE_DEVICES"] = "0,1,2,3"
4
5 device_lib_list_local_devices()
6
7 # Load data
8 (X_train, y_train), (X_test, y_test) = mnist.load_data()
9
10 # Flatten 28x28 images to a 1D vector for each image
11 num_train = X_train.shape[0] * X_train.shape[1]
12 X_train = X_train.reshape(X_train.shape[0], num_train).astype('float32')
13 X_test = X_test.reshape(X_test.shape[0], num_test).astype('float32')
14 # normalize data (inputs from 0-255 to 0-1)
15 X_train = X_train / 255
16 X_test = X_test / 255
17 # One-hot labels
18 y_train = to_categorical(y_train, num_classes)
19 y_test = to_categorical(y_test, num_classes)
20 y_train = y_train.reshape(-1)
21 y_test = y_test.reshape(-1)
22
23 # Define baseline model
24 def baseline_model():
25     # create model
26     model = Sequential()
27     model.add(Dense(num_train, input_dim=num_train, kernel_initializer='normal', activation='relu'))
28     model.add(Dense(num_test, input_dim=num_test, kernel_initializer='normal', activation='relu'))
29     # compile model
30     model.compile(loss='categorical_crossentropy', optimizer='adam', metrics=['accuracy'])
31     return model
32
33 # Fit the model
34 model = baseline_model()
35 # Fit the model
36 model.fit(X_train, y_train, validation_data=(X_test, y_test), epochs=10, batch_size=32, verbose=2)
37
38 # Final evaluation of the model
39 scores = model.evaluate(X_test, y_test, verbose=0)
40 print("Baseline Error: %.2f%% (%.3f score) (%.100s)"

```



# 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](mailto:jon8@hi.is)



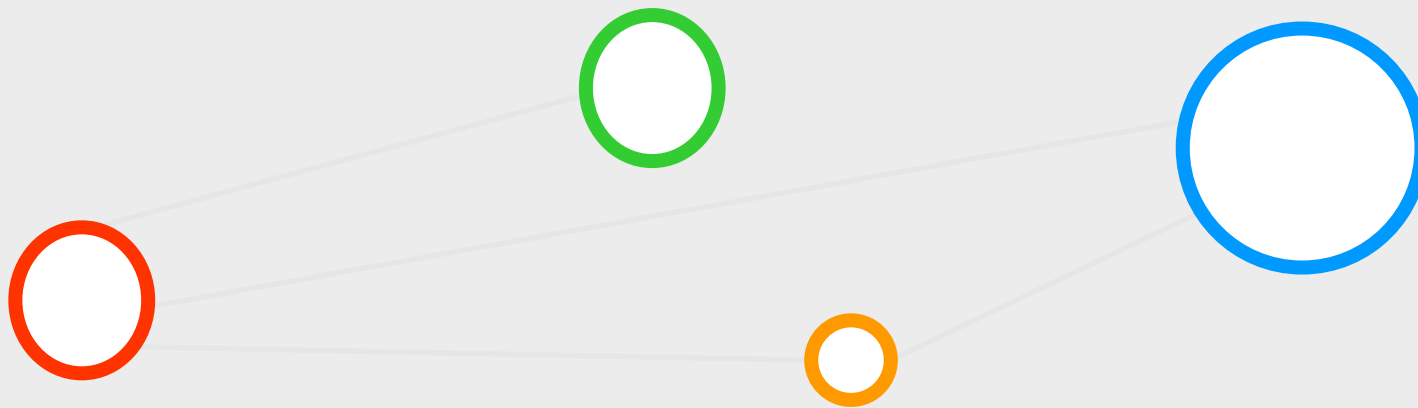
➤ **WELCOME!**



# Realization of SW Framework – Interaction Room Seismic Imaging

- Pipeline activities relevant for the SW Framework Co-Design
  - Updates from Johannes (WP2) & Liang (WP3)
  - TBD: presentation by Johannes/Liang

## Agenda Item (4) – Status WP2 Seminar Plans



# WP2 Monthly Seminars – Review & Plan



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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 @ProfDrMorrisRiedel](#) [in @MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#)

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

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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 @ProfDrMorrisRiedel](#) [in @MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#)

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

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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 @ProfDrMorrisRiedel](#) [in @MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#)

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

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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

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

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

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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 @ProfDrMorrisRiedel](#) [in @MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#)

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

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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 @ProfDrMorrisRiedel](#) [in @MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#) [@MorrisRiedel](#)

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

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

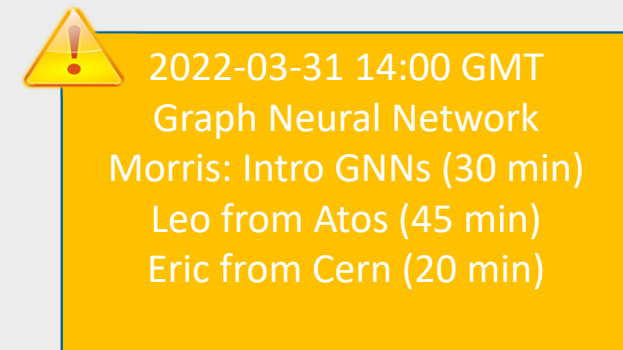
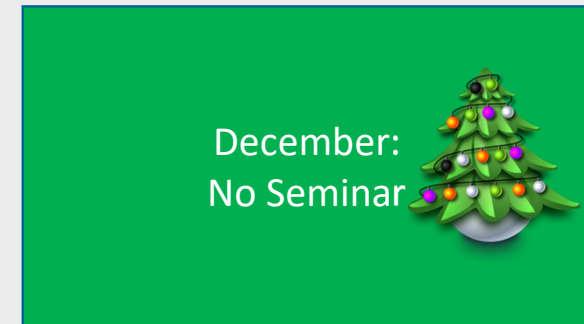


2022-03-30 RAISE WP2 Monthly Meeting March 2022

# WP2 Monthly Seminars – 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 Seminars – Review & Plan



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

May:  
Request Project Partners?  
ONNX / OpenML  
Interoperable formats

June:  
Morris: GPUs in general  
Arnis & Cuda @ RTU

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

August:  
Request Project Partners?  
Gael (continuous 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



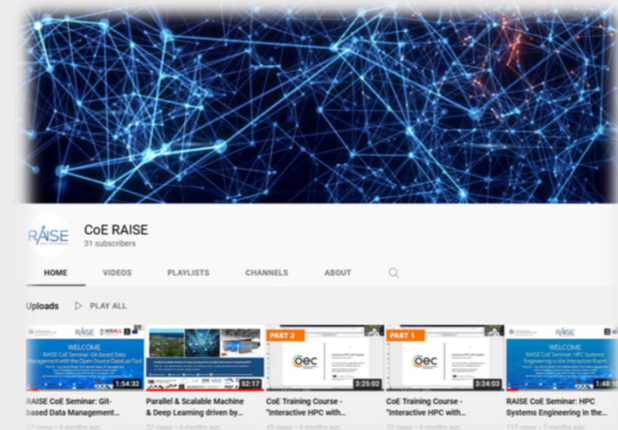
# WP2 Monthly Seminars – Review & Plan



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## ➤ Monthly WP2 Seminars

- Co-organized with Icelandic National Competence Center (NCC) funded by the EuroCC project: <http://ihpc.is>
- Performed since Quarter 2 of the project (April 2021)
- Selected dates via agreement of availability of speakers
- 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 Seminar series with speakers

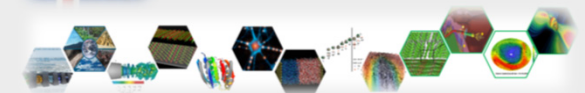


### Plan for next 12 Month

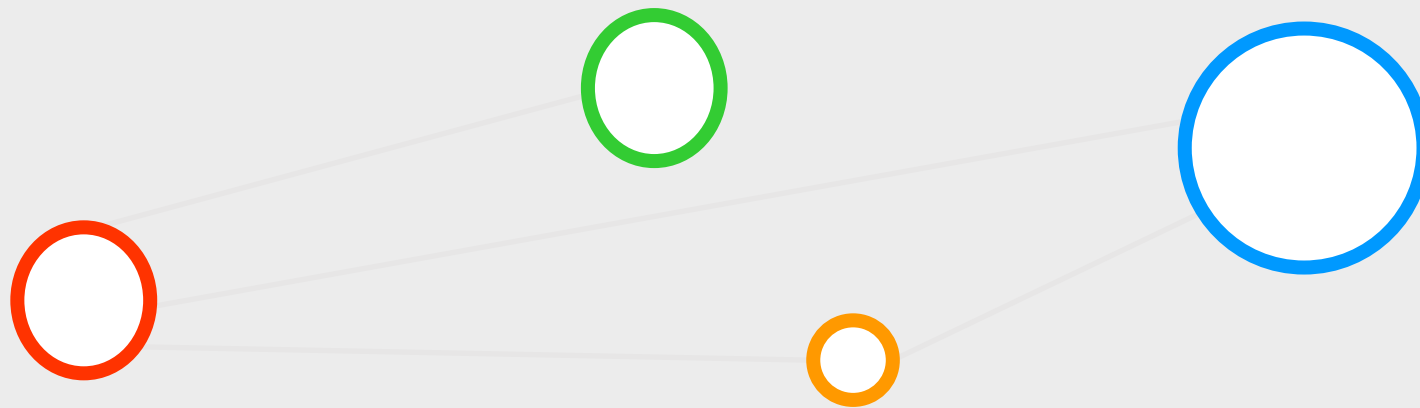
- Carry on with monthly WP2 seminars in the same style, but schedule on 3-4 month horizons
- Repeat certain seminars with advanced content and updates of activities (e.g., GraphCore & ATOS)
- Work better together with WP6 on releasing seminars on YouTube channel more regularly
- Collect slides of speakers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



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



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

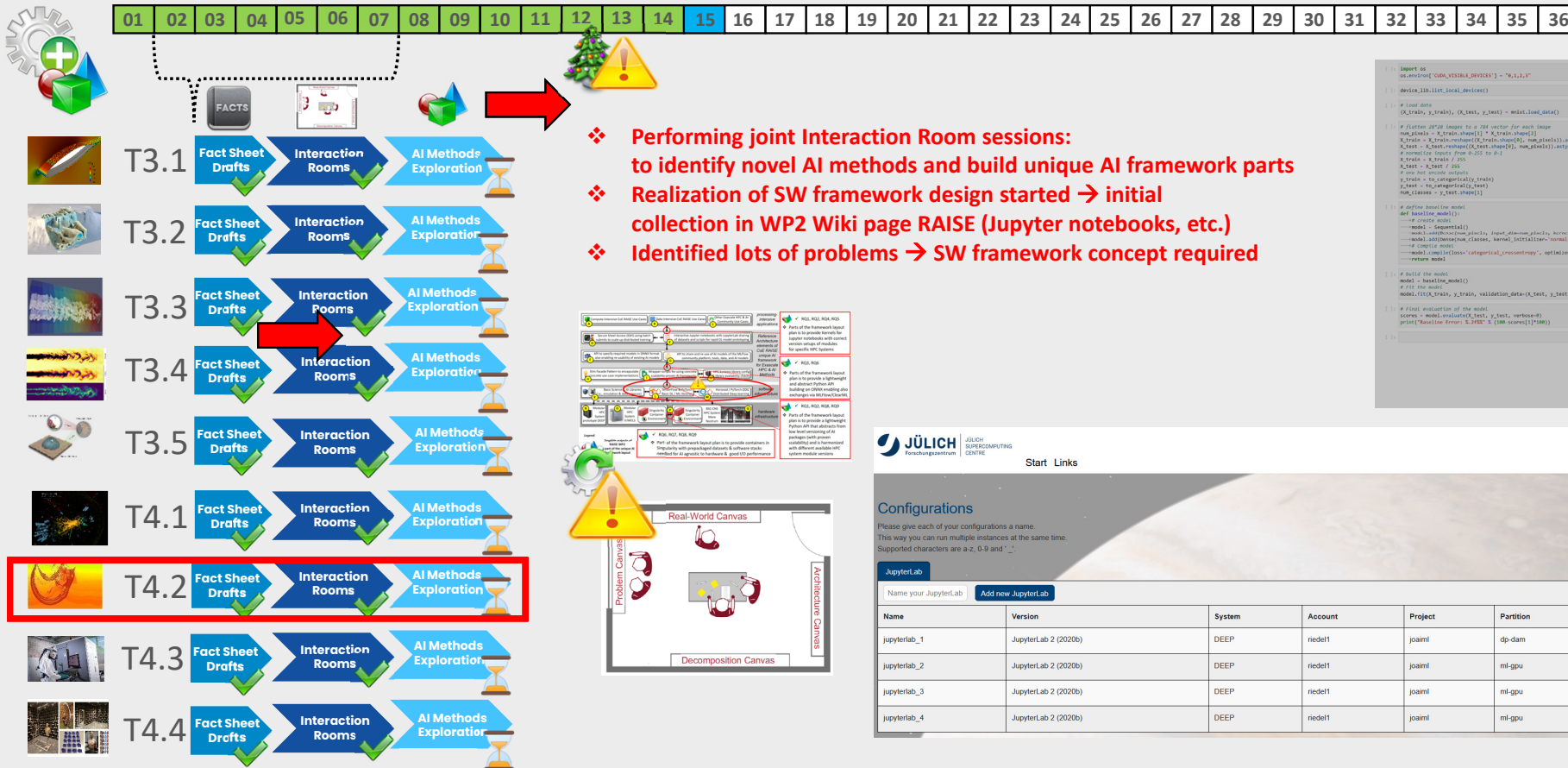




# Compelling Scoreboard Review – Use Case Progress



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```

import os
os.environ["CUDA_VISIBLE_DEVICES"] = "0,1,2,3"

DEVICE_ID_LIST_LOCAL_DEVICES()

# Load data
(X_train, y_train), (X_test, y_test) = mnist.load_data()

# Flatten input to a 784 vector for each image
num_pixels = X_train.shape[1] * X_train.shape[2]
X_train = X_train.reshape((X_train.shape[0], num_pixels)).astype('float32')
X_test = X_test.reshape((X_test.shape[0], num_pixels)).astype('float32')
# normalize inputs from 0-255 to 0-1
X_train = X_train / 255
X_test = X_test / 255

# one-hot encode output
y_train = np_categorical(y_train)
y_test = np_categorical(y_test)
num_classes = y_test.shape[1]

# Define baseline model
def baseline_model():
    model = Sequential()
    model.add(Dense(num_pixels, input_dim=num_pixels, kernel_initializer='normal', activation='relu'))
    model.add(Dense(num_classes, kernel_initializer='normal', activation='softmax'))
    model.compile(loss='categorical_crossentropy', optimizer='adam', metrics=['accuracy'])
    return model

# Build the model
model = baseline_model()
# Fit the model
Model.fit(X_train, y_train, validation_data=(X_test, y_test), epochs=50, batch_size=200, verbose=2)

# Find evaluation of the model
scores = model.evaluate(X_test, y_test, verbose=0)
print("Baseline Error: %.2f%% (%.3f score) (%.1f%%)"
    )
    
```

**JÜLICH** SUPERCOMPUTING CENTRE

Start Links

Configurations

Please give each of your configurations a name. This way you can run multiple instances at the same time. Supported characters are a-z, 0-9 and '-'.

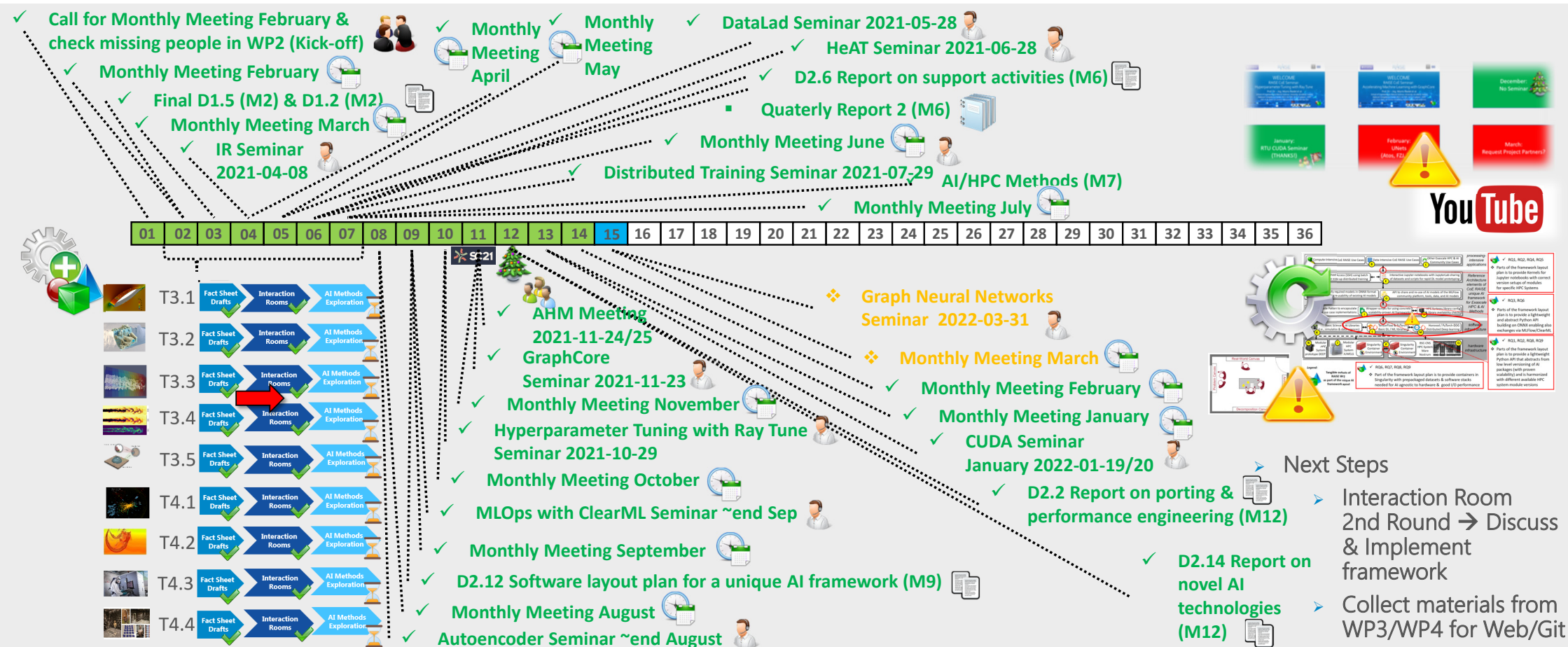
Name	Version	System	Account	Project	Partition	Details	Actions
jupyterlab_1	JupyterLab 2 (2020b)	DEEP	riedel1	joaimi	dp-dam	► Details	<a href="#">Start</a> <a href="#">delete</a>
jupyterlab_2	JupyterLab 2 (2020b)	DEEP	riedel1	joaimi	ml-gpu	► Details	<a href="#">Start</a> <a href="#">delete</a>
jupyterlab_3	JupyterLab 2 (2020b)	DEEP	riedel1	joaimi	ml-gpu	► Details	<a href="#">Start</a> <a href="#">delete</a>
jupyterlab_4	JupyterLab 2 (2020b)	DEEP	riedel1	joaimi	ml-gpu	► Details	<a href="#">Start</a> <a href="#">delete</a>



# Compelling Scoreboard Review & Next Steps



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2022-03-30 RAISE WP2 Monthly Meeting March 2022

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

1. AOB (Andi): Review Dates & Agenda?
2. AOB: Plan a continuous 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)



# 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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