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

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2022-05-03, RAISE TCB Meeting, Online

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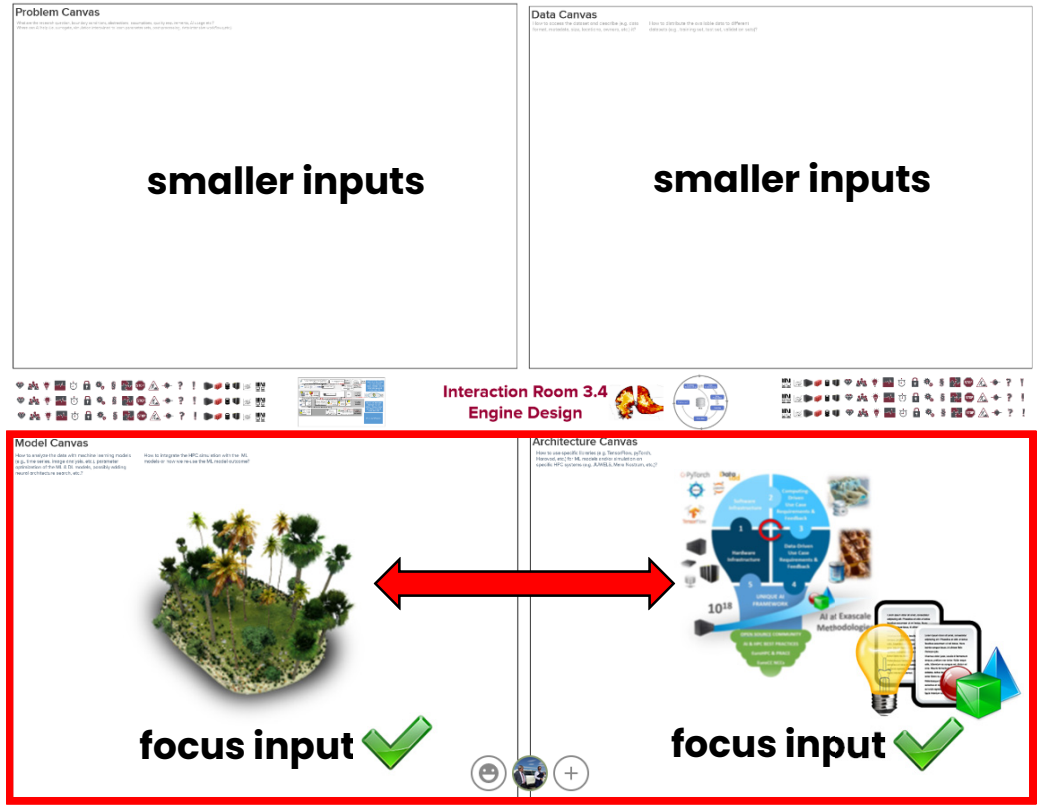
MURAL Board contents for Deliverables & Milestones



- 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/matthiasbook8855/1621378007553/6f0d5285fcacc5cafa515bd6676c84d8b4879d39?sender=u15e3008bb41d6628a5bb5701

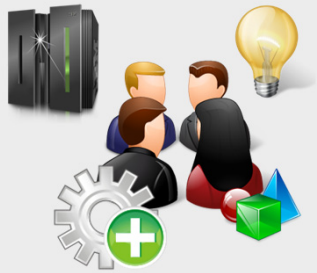
IR4.2 Seismic Imaging: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378023838/a0b9503abb837ae3e28af4bb8d9adbec33874998?sender=u15e3008bb41d6628a5bb5701

IR4.3 Manufacturing: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378038069/93df6fa7a41093f4eaae7be9d72979de2ba42b9d?sender=u15e3008bb41d6628a5bb5701

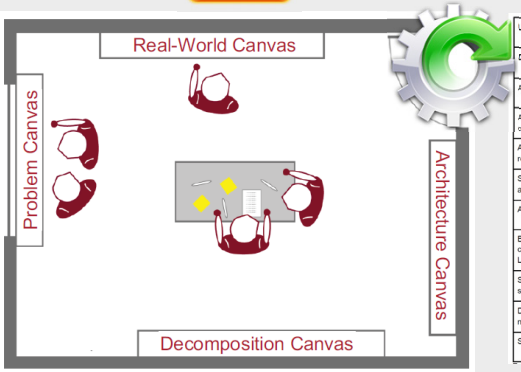
IR4.4 Sound Engineering: https://app.mural.co/t/matthiasbook8855/m/matthiasbook8855/1621378050431/b5fa122190024040 59f90a4bbb0101fa379a8503?sender=u15e3008bb41d6628a5bb5701

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

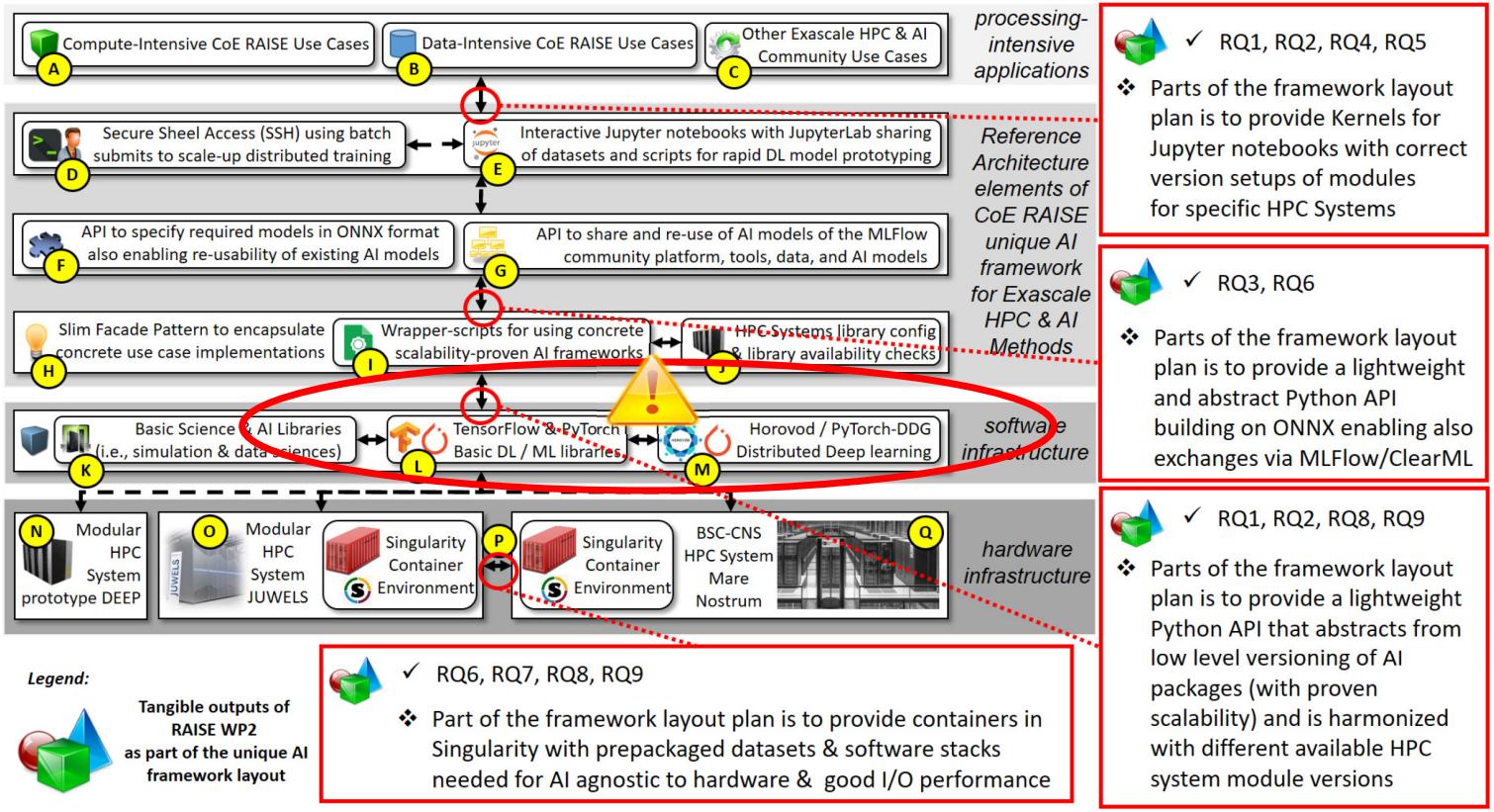


Use Case	AE	PIML	ANNs	CNN		NO	SMs			GNN	IN	LSTM	GRU
Details	*CAE*		*RBF-ANN*	*U-Net*	*RESNET*	*FNO*	*AR*	*ARMA*	*ARIMA*		*JEDI-net*		
AI for turbulent boundary layers	X	X											
AI for wind farm layout optimization			X				X	X	X				
AI for data-driven models in reacting flows				X						X			
Smart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

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

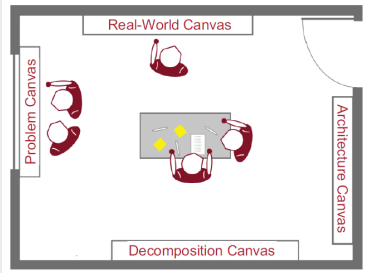
- Available in BSCW: https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3694045

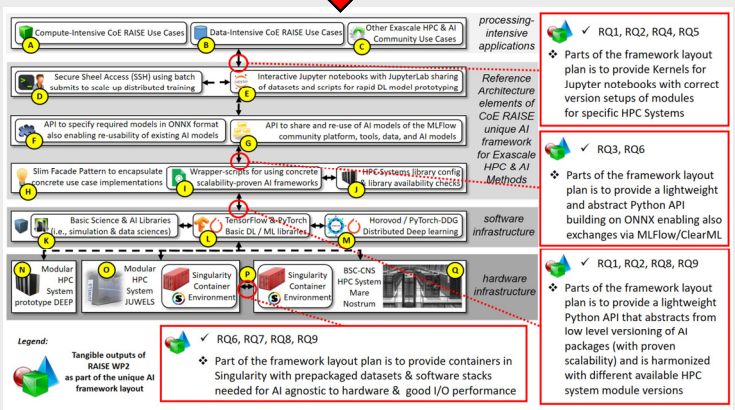


Continously Updating: e.g., add hyper-parameter optimization tools, pipelines?!

Realization of SW Framework – Interaction Room Results (1)

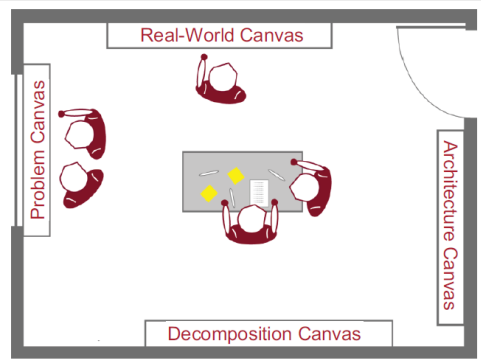
- ✓ Interaction Room Seismic Imaging
  - Pipeline activities relevant for the SW Framework Co-Design
  - Updates from Johannes (WP2) & Liang (WP4)
- ✓ Interaction Room Event Reconstruction & Classification at the CERN-LHC
  - Official Repository exists, no need to put elements into github
  - Includes 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
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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

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