

# WP<sub>2</sub> AI- & HPC-Cross Methods at Exascale – Overview

Prof. Dr. – Ing. Morris Riedel et al.

School of Engineering & Natural Sciences, University of Iceland

2021-11-24, RAISE All Hands Meeting, Online



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

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# WP2 Agenda & Tasks



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Work package 2 presentations		13:15 – 14:25
<b>13:15 – 13:25</b>	WP2 (UOI): Introduction AI- and HPC-Cross Methods at Exascale	M. Riedel
<b>13:25 – 13:40</b>	Task 2.1 (BSC): Modular and heterogeneous supercomputing architectures	G. Houzeaux
<b>13:40 – 13:55</b>	Task 2.2 (FZJ): Hardware prototypes	E. Inanc
<b>13:55 – 14:10</b>	Task 2.4 (UOI): Software design of a unique AI framework	<b>NEW</b> M. Riedel
<b>14:10 – 14:25</b>	Task 2.5 (UOI): Cross-Sectional AI Methods	M. Riedel



# WP2 Deliverables – Status

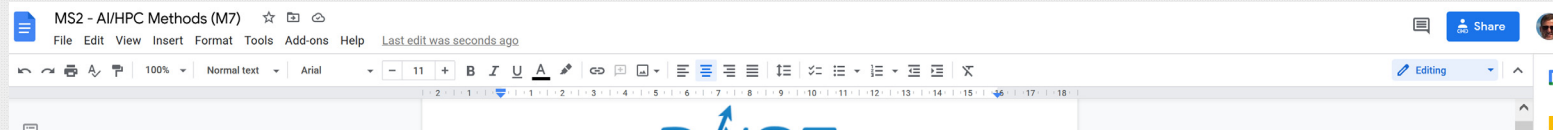


Del. No.	Delivery Name	Lead beneficiary	Type	Dis. Level	Del mo.	WP Leader	Responsible Editor, Authors	Internal Reviewers	Reviewers from PMT	Date draft av. for int. review	Deadline subm. to EC	Submitted to EU on
D2.1	Best practice guidelines/tutorials for MSA/heterogenous systems	BSC	R	PU	2	M. Riedel/ UOI	G. Houzeaux/ BSC	S. Richard/ SAFRAN	A. Lintermann/ FZJ	08.02.2021	28.02.2021	26.02.2021
D2.5	Best practice guidelines/tutorials prototype	FZJ	R	PU	2	M. Riedel/ UOI	A. Lintermann/ FZJ	V. Khristenko/ CERN	J. Lopez/ ParTec	08.02.2021	28.02.2021	26.02.2021
D2.6	Support report	FZJ	R	PU	6	M. Riedel/ UOI	E. Inanc/ FZJ	R. Heylen/ FM	I. Schmitz/ ParTec	09.06.2021	30.06.2021	25.06.2021
D2.12	Software framework layout plan	UOI	OTHER	PU	9	M. Riedel/ UOI	M. Book/ UOI	R. Speck/ FZJ	J. Lopez/ ParTec	09.09.2021	30.09.2021	30.09.2021
D2.2	Report on porting & performance engineering	BSC	R	PU	12	M. Riedel/ UOI	G. Houzeaux/ BSC	M. Meinke/ RWTH	A. Lintermann/ FZJ	29.11.2021	31.12.2021	
D2.14	Report on novel AI technologies	UOI	R	CO	12	M. Riedel/ UOI	M. Riedel/ UOI	S. Kesselheim/ FZJ	J.Lopez/ ParTec	29.11.2021	31.12.2021	
D3.1	Report on outcomes of WP3 use-cases	RWTH	R	CO	12	W. Schröder/ RWTH	M. Meinke/ RWTH	S. Schlimpert/ FM	J.Lopez/ ParTec	29.11.2021	31.12.2021	
D4.1	Report on outcomes of WP4 use-cases	CERN	R	CO	12	M.Girone/ CERN	E. Wulff/ CERN	H. Neukirchen/ UOI	I. Schmitz/ ParTec	29.11.2021	31.12.2021	

➤ **Talk of Task 2.4 (UOI): Software design of a unique AI framework includes interaction room process for co-design & more D2.12 details**



# WP2 Milestones – Status



Continuously Updating



## Plan for next 12 Month

- Revise factsheets over time & WP2 AI/HPC Methods matrix



H2020-INFRAEDI-2018-2020



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## BEFORE

Table 6: Use-case vs. AI-methods matrix.

Use-Case vs. AI-Methods	DA	NAS	AE	TL	PF	PIDL	LSTM
Turbulent boundary layers	X	X	X	X	X	X	
Wind farm layout optimization	X			X		X	
AI for data-driven models in reacting flows				X		X	
Smart models for next-generation aircraft engine design	X	X		X		X	
Wetting hydrodynamics		X	X			X	X
Event reconstruction and classification at the CERN HL-LHC		X		X			X
Seismic imaging with remote sensing - oil and gas exploration and well maintenance	X	X		X			
Defect-free metal additive manufacturing		X				X	X
Sound engineering	X	X		X			X

Center of Excellence "Research on AI- and Simulation-Based Engineering at Exascale"

Grant Agreement Number: 951733

MS2

AI/HPC Methods

Draft



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

➤ Talk of Task 2.5 (UOI): Cross-Sectional AI Methods includes details on how to move ahead with identifying cross-sectional techniques





# WP2 Monthly Meetings – Review & Plan



## ➤ Monthly WP2 Meetings

- Performed since the beginning of the project (Feb 2021)
- Selected dates via doodle usually end of each months
- Used as major synchronisation of WP2 members
- Having one hour meetings seem to be enough (in addition with interaction rooms & task-wise meetings)
- Check available meeting minutes on BSCW:  
<https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/3340884>

### Plan for next 12 Month

- Carry on with monthly WP2 meetings in the same style, but perform doodle earlier to plan better

## Meetings

### Monthly Meetings

- 2021-02-11\_Monthly Meeting February 2021  
Slides & Materials from meeting 2021-02-11
- 2021-03-15\_Monthly Meeting March 2021  
Slides & Materials from meeting 2021-03-15
- 2021-04-30\_Monthly Meeting April 2021  
Slides & Materials from meeting 2021-4-30
- 2021\_05\_28\_Monthly\_Meeting May 2021  
Slides & Materials from meeting 2021-05-28
- 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



# 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](#)

<https://www.youtube.com/watch?v=UVCWCVWvL4Qg>

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

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<https://www.youtube.com/watch?v=UVCWCVWvL4Qg>

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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](#)

<https://www.youtube.com/watch?v=UVCWCVWvL4Qg>

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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](#)

<https://www.youtube.com/watch?v=UVCWCVWvL4Qg>

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WELCOME  
RAISE CoE Seminar:  
Brief Introduction to Autoencoders

Prof. Dr. – Ing. Morris Riedel et al.  
School of Engineering & Natural Sciences, University of Iceland, Iceland  
National Competence Center (NCC) for HPC & AI in Iceland – IHPC  
2021-08-31, RAISE CoE Seminar Brief Introduction to Autoencoders, Online

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<https://www.youtube.com/watch?v=UVCWCVWvL4Qg>

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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](#)

<https://www.youtube.com/watch?v=UVCWCVWvL4Qg>

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# WP2 Monthly Seminars – Review & Plan





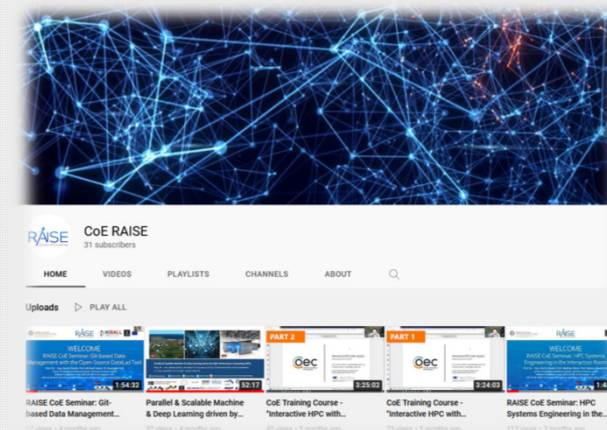
# WP2 Monthly Seminars – Review & Plan



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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
- Participated seminar speakers are project external & internal
- 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>

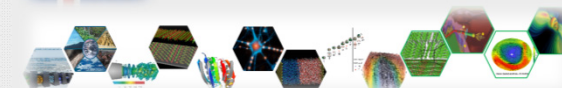


### Plan for next 12 Month

- Carry on with monthly WP2 seminars in the same style, but schedule on 3-4 month horizons
- RTU plans special training on GPUs & porting
- 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



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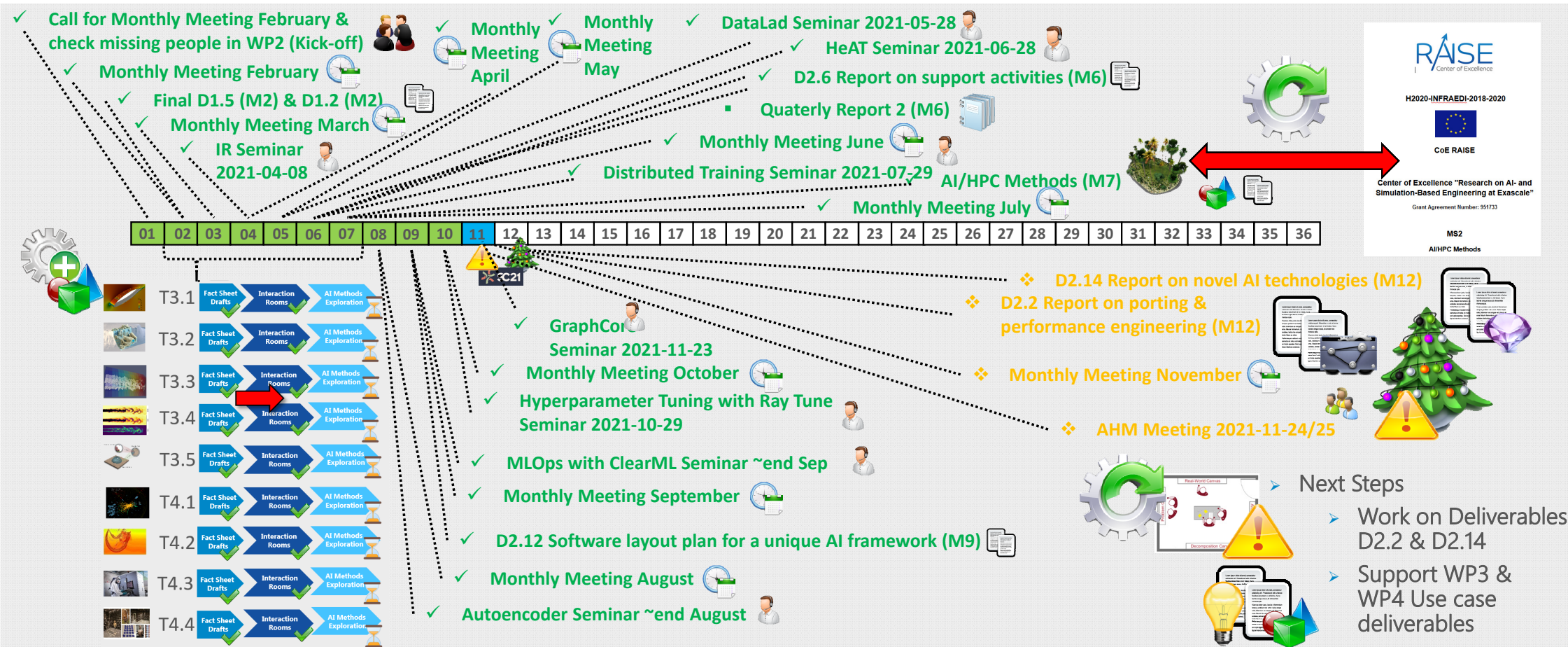




# Compelling Scoreboard Review & Next Steps



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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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