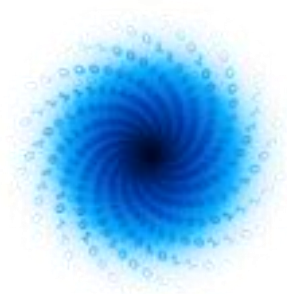




EuroHPC  
Joint Undertaking



# MAchinE Learning for Scalable meTeoROlogy and climate



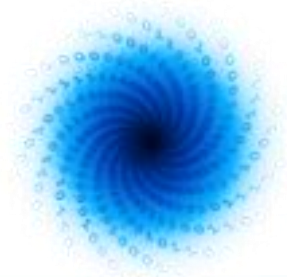
MAELSTROM

## Dissemination Workshop I

---

Jan Mirus, Peter Dueben

[www.maelstrom-eurohpc.eu](http://www.maelstrom-eurohpc.eu)



MAELSTROM

## D4.7 Dissemination Workshop I

<b>Author(s):</b>	Peter Dueben (ECMWF) Jan Mirus
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<b>Document Owner:</b>	ECMWF
<b>Contributors:</b>	All Partners
<b>Status:</b>	Final



# MAELSTROM

## Machine Learning for Scalable Meteorology and Climate

**Research and Innovation Action (RIA)**

**H2020-JTI-EuroHPC-2019-1: Towards Extreme Scale Technologies and Applications**

**Project Coordinator:** Dr Peter Dueben (ECMWF)

**Project Start Date:** 01/04/2021

**Project Duration:** 36 months

**Published by the MAELSTROM Consortium**

**Contact:**

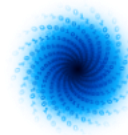
ECMWF, Shinfield Park, Reading, RG2 9AX, United Kingdom

[Peter.Dueben@ecmwf.int](mailto:Peter.Dueben@ecmwf.int)

The MAELSTROM project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 955513. The JU receives support from the European Union's Horizon 2020 research and innovation programme and United Kingdom, Germany, Italy, Luxembourg, Switzerland, Norway

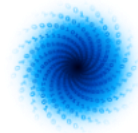


**EuroHPC**  
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## Contents

<b>1</b>	<b>EXECUTIVE SUMMARY .....</b>	<b>5</b>
<b>2</b>	<b>INTRODUCTION .....</b>	<b>6</b>
2.1	ABOUT MAELSTROM.....	6
2.2	SCOPE OF THIS DELIVERABLE .....	6
2.2.1	OBJECTIVES OF THIS DELIVERABLE.....	6
2.2.2	WORK PERFORMED IN THIS DELIVERABLE .....	7
2.2.3	DEVIATIONS AND COUNTER MEASURES.....	7
<b>3</b>	<b>PLANNING, PREPARATION, AND REALIZATION OF THE WORKSHOP.....</b>	<b>8</b>
3.1	SCHEDULING.....	8
3.2	INFRASTRUCTURE .....	8
3.3	TIMETABLE .....	9
3.4	PARTICIPATION .....	10
<b>4</b>	<b>RESONANCE AND RESULTS .....</b>	<b>11</b>
4.1	OVERALL RESONANCE AND QUESTIONS .....	11
4.2	POLL RESULTS AND CONCLUSIONS .....	11
<b>5</b>	<b>CONCLUSION .....</b>	<b>15</b>
<b>6</b>	<b>ANNEX: MAELSTROM PRESENTATION DECKS .....</b>	<b>17</b>
6.1	INTRODUCTION: PETER DUEBEN, ECMWF .....	17
6.2	WP1: GONG BING, JSC .....	19
6.3	WP2: FABIAN EMMERICH, 4CAST .....	21
6.4	WP3: DANIELE GREGORI, E4 .....	22
6.5	WP3: ANDREAS HERTEN, JSC .....	24



## 1 Executive Summary

On 28<sup>th</sup> March 2022, the first of two dissemination workshops was held with the objective not only to share the progress of project MAELSTROM with the high-performance computing, machine learning and weather & climate communities, but also to collect input on the needs of those communities. While restrictions due to the COVID pandemic are being lifted, it was still necessary to choose an online format for this workshop. Registrations soared up to over 200; over 60 people gathered in the virtual room.

The first part of the workshop was dedicated to Project MAELSTROM; each of the work packages introduced its motivation and goals and gave an overview on the achievements to date:

- WP1: Machine learning applications & datasets
- WP2: Machine learning workflow tools
- WP3: Hardware Systems

The second part of the workshop provided a stage for three of our EuroHPC partner projects:

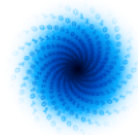
- TimeX: Time parallelization for eXascale computing
- DEEP-SEA: Programming Environment for European Exascale Systems
- RED-SEA: Network Solution for Exascale Architectures

The third part of the workshop featured external talks, giving insight into technologies with possible synergies or use cases within MAELSTROM's domains:

- MeteoSwiss: Time-consistent downscaling of atmospheric fields with GANs
- Pangeo: An open-source ecosystem for data-intensive science
- NVIDIA: Deep Learning for Earth Sciences in the HPC Context

Each part of the workshop led into an interactive phase, where a discussion was moderated by MAELSTROM; after the first part, feedback was collected in a series of polls.

The workshop was concluded MAELSTROM-internally, discussing conclusions and next steps.



## 2 Introduction

### 2.1 About MAELSTROM

To develop Europe's computer architecture of the future, MAELSTROM will co-design bespoke compute system designs for optimal application performance and energy efficiency, a software framework to optimise usability and training efficiency for machine learning at scale, and large-scale machine learning applications for the domain of weather and climate science.

The MAELSTROM compute system designs will benchmark the applications across a range of computing systems regarding energy consumption, time-to-solution, numerical precision and solution accuracy. Customised compute systems will be designed that are optimised for application needs to strengthen Europe's high-performance computing portfolio and to pull recent hardware developments, driven by general machine learning applications, toward needs of weather and climate applications.

The MAELSTROM software framework will enable scientists to apply and compare machine learning tools and libraries efficiently across a wide range of computer systems. A user interface will link application developers with compute system designers, and automated benchmarking and error detection of machine learning solutions will be performed during the development phase. Tools will be published as open source.

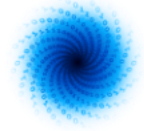
The MAELSTROM machine learning applications will cover all important components of the workflow of weather and climate predictions including the processing of observations, the assimilation of observations to generate initial and reference conditions, model simulations, as well as post-processing of model data and the development of forecast products. For each application, benchmark datasets with up to 10 terabytes of data will be published online for training and machine learning tool-developments at the scale of the fastest supercomputers in the world. MAELSTROM machine learning solutions will serve as blueprint for a wide range of machine learning applications on supercomputers in the future.

### 2.2 Scope of this deliverable

#### 2.2.1 Objectives of this deliverable

D4.7, the first dissemination workshop, aims to

- generate awareness in the scientific and technological communities of weather & climate science, machine learning and high-performance computing for the project Maelstrom, its mission, objectives, and products
- share MAELSTROM's progress and achievements after nearly one year of project runtime with the said audiences
- collect valuable input and feed-back, showing us where our products and outcomes resonate with the community, correspond to unmet needs, and are likely to spawn use cases.

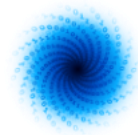


### 2.2.2 Work performed in this deliverable

The work to create the exploitation plan included collection of feedback from the partners in form of questionnaires and the identification of the relevant aspects pertaining to exploitation.

### 2.2.3 Deviations and counter measures

No deviations occurred; hence no counter measures were requisite.



### 3 Planning, preparation, and realization of the workshop

#### 3.1 Scheduling

The date for the workshop, Monday, 20<sup>th</sup> March 2022, was selected to join forces with the 4-day machine learning workshop held by ECMWF on the following four workdays of this week<sup>1</sup>.

#### 3.2 Infrastructure

Because of COVID restrictions, respectively because of the uncertainty that had existed beforehand about the regulations, it was advisable to hold this workshop online in a virtual room. Registration was required, to allow us to gauge the size of the audience and adjust our protocol accordingly.

The registration page and mechanism, just like the technical support for the webinar infrastructure, was shared with the said ECMWF workshop; an efficient solution for MAELSTROM.

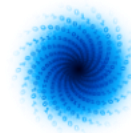
The workshop was announced on Twitter and on the MAELSTROM project website.

The workshop was held with Zoom Webinar, a tool specialized for larger audiences. Attendees were able to ask questions in a dedicated Q&A area. Another tool, Slido, was used to create live polls. The workshop has been recorded with the consent of all participants.

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<sup>1</sup> <https://events.ecmwf.int/event/294/>

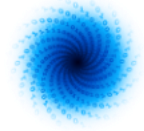




### 3.3 Timetable

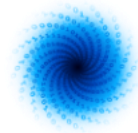
All times are GMT.

Part 1	Learn about MAELSTROM
8:30 → 08:50	<b>Introduction</b> Peter Dueben (ECMWF)
08:50 → 09:10	<b>WP1 Summary on Applications and Data Sets</b> Bing Gong (JSC)
09:10 → 09:30	<b>WP2 Summary on Software Tools</b> Greta Denisenko (4-cast)
09:30 → 09:50	<b>WP3 Summary on Hardware Benchmarks</b> Andreas Herten (JSC) and Daniele Gregori (E4)
09:50 → 10:30	<b>Possibility for general discussion</b>
10:30 → 11:00	<b>Coffee break</b>
Part 2	EuroHPC Partner Project Talks
11:00 → 11:20	<b>TimeX</b> Giovanni Samaey (KU Leuven) and Martin Schreiber (TU of Munich)
11:20 → 11:40	<b>Deep-Sea</b> Estela Suarez (JSC)
11:40 → 12:00	<b>Red-Sea</b> Nikos Xrysos (FORTH)
12:00 → 12:30	<b>Discussions between MAELSTROM and the speakers</b>
12:30 → 13:30	<b>Lunch break</b>
Part 3	External Science Talks
13:30 → 14:00	<b>Time-Consistent Downscaling of atmospheric fields with generative adversarial networks</b> Jussi Leinonen (MeteoSwiss)
14:00 → 14:30	<b>Pangeo: An open-source ecosystem for data-intensive science</b> Ryan Abernathey (Columbia University)
14:30 → 15:00	<b>Deep learning for earth sciences in the HPC context</b> Thorsten Kurth (NVIDIA)
15:00 → 15:30	<b>Discussions between MAELSTROM and the speakers</b>
15:30 → 16:00	<b>Coffee break</b>
16:00 → 17:30	<b>Possibility for further discussions between the working groups</b>



### 3.4 Participation

208 registrations were received. Eventually, up to 62 people participated at a single moment in time, i.e. speakers included. 34 participants contributed to the polls. The workshop started and ended as scheduled.



## 4 Resonance and results

### 4.1 Overall resonance and questions

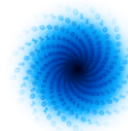
About 30 technical or scientific questions on the presented contents were collected through the Q&A tool, and either answered in verbally by the presenters, or in writing via the Q&A tool. The number, level and degree of detail of those inquiries demonstrated, that

- the presented contents, such as the objectives, approaches, achievements, and products of project MAELSTROM were well understood
- project MAELSTROM pursues objectives, that will have good chances to be adopted by the technology and science community, because they respond to relevant needs.

### 4.2 Poll results and conclusions

MAELSTROM had prepared 6 polls before the workshop, which were intended to jump-start a discussion, and enable the moderator (Peter Dueben) to structure this discussion. The questions were:

1. What's MAELSTROM's greatest idea for better forecasts? (Choice of 5 products of WP1)
2. What ML method will be most important for weather & climate prediction in the next 5 years? (open-ended)
3. What software tool are you missing most badly for ML? (open-ended)
4. Which ML workflow feature would delight you most? (Choice of 5 core features of WP2's workflow tools)
5. What hardware are you mostly working on?
6. What hardware will you be working on in 10 years?



### What's MAELSTROM's greatest idea for better forecasts?

25



Blend citizen observations and numerical weather forecasts



Incorporate social media data into prediction framework



Neural networks as emulator for radiative heating



Improved ensemble predictions in post-processing



ML for downscaling 2m temperature

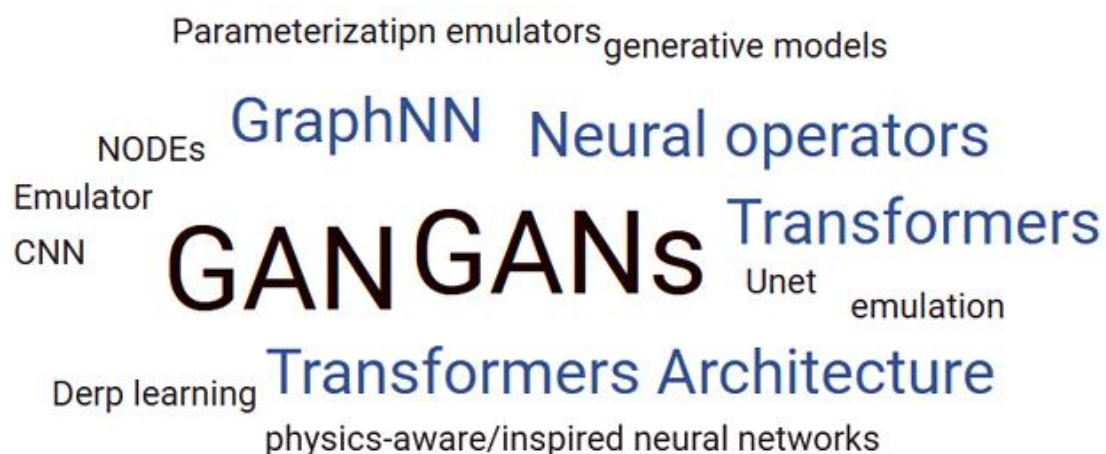


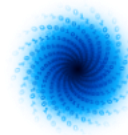
Yawn. None of that is great.



What ML method will be most important for weather & climate applications in next 5 years?

22





What software tool you are missing most badly for ML?

19 ...

interface between Xarray / ML libs

workflow management Tools to learn the methods

Testing bash Profiling Tool

# Efficient data loading

Accelerated data loading Easy parallelization

workflow management

verification

Reproducibility

Explainability tools

interpretability



Which ML workflow feature would delight you most?

22 ...

Reproducible ML solutions



Share ML solutions across user base



Recommendation of ML solutions to users with specific problems



Interface to cloud computing and HPC

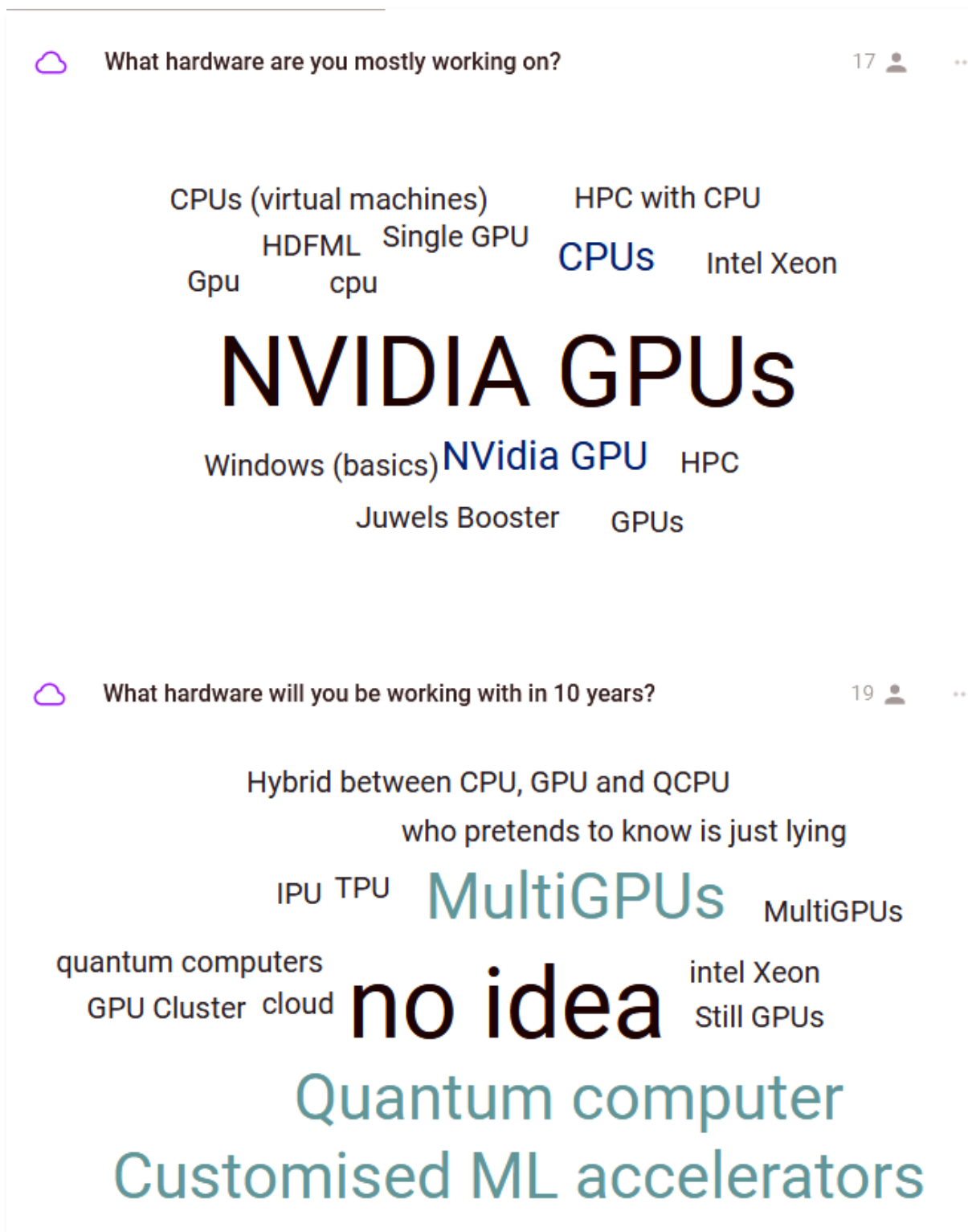
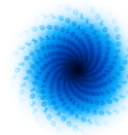


Manipulation of execution graphs leading to optimal execution of W&C workflows

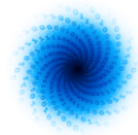


Meh. None of this is new or useful.





The results were discussed among and between MAELSTROM work package teams following the public part of the workshop.



## 5 Conclusion

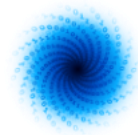
With over 60 participants and a rich level of questions and discussions, MAELSTROM's first dissemination workshop can be considered successful. The format of the panel – MAELSTROM, partner projects, and relevant talks from the wider science community – has proven to be suitable and can serve as a model for the coming second dissemination workshop.

Learning from this workshop will help us develop the interactive parts – polling, discussion – further for the coming hackathons and dissemination workshop II.

A recording of the workshop, MAELSTROM presentation decks and poll results will be made available on the MAELSTROM project website. Recording for some of the talks as well as the slides are already available on Machine Learning Workshop webpage<sup>2</sup>.

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<sup>2</sup> <https://events.ecmwf.int/event/294/timetable/>



## Document History

Version	Author(s)	Date	Changes
<b>0.1</b>	Jan Mirus	30/03/2022	Initial version
<b>1.0</b>	Peter Dueben (ECMWF)	30/03/2022	Final version

## Internal Review History

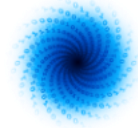
Internal Reviewers	Date	Comments
<b>Peter Dueben (ECMWF)</b>	30/03/2022	Approved with comments

## Estimated Effort Contribution per Partner

Partner	Effort
<b>Jan Mirus</b>	0.25
<b>ECMWF</b>	0.25
<b>Total</b>	<b>0.5</b>

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## 6 Annex: MAELSTROM presentation decks

### 6.1 Introduction: Peter Dueben, ECMWF

Empowering weather & climate forecast.

**ML Apps & Datasets**

**ML Workflow Tools**

**Hardware Systems**

**Welcome & Introduction**  
Peter Dueben (ECMWF)

"The MAELSTROM project has received funding from the European HighPerformance Computing Joint Undertaking (JU) under grant agreement No 101015133. The JU receives support from the European Union's Horizon 2020 research and innovation programme and United Kingdom, Germany, Italy, Luxembourg, Switzerland, Norway".

ECMWF

**Timetable**

MAELSTROM	Our sister projects	External science talks
<b>8:30 GMT</b>	<b>10:30</b>	<b>11:00</b>
<b>Introduction</b> Peter Dueben (ECMWF)	<b>TimeX</b> Giovanni Samay (RJ Leaver)	<b>Time-consistent downscaling of atmospheric fields with generative adversarial networks</b> Jussi Leronen (MeteoSwiss)
<b>ML Apps &amp; Datasets</b> Bing Gong (JSC)	<b>Deep-Sea</b> Estela Suarez (JSC)	<b>Pangloss: an OS ecosystem for data-intensive science</b> Ryan Abernethy (Columbia)
<b>ML Workflow Tools</b> Fabian Emmert (Kead)	<b>Red-Sea</b> Nikos Xysois (FORTH)	<b>Deep learning for earth sciences in the HPC context</b> Thorsten Kurth (NVIDIA)
<b>Hardware Systems</b> Daniela Gregori (E4)	<b>Interactive part</b>	<b>Interactive part</b>
<b>Interactive part</b>		
	<b>12:30</b>	<b>13:30</b>
	<b>Lunch break</b>	<b>Coffee break and more time for discussion</b>
		<b>15:30 → 17:30</b>

#### Housekeeping

- As an attendee you only have facility to view the webinar and will not have video or audio functionality
- To submit your questions, please use the Q&A function in the bottom toolbar
- If you wish to ask a question verbally, please raise your hand and we will invite you to speak. A prompt will appear on your screen to allow you to unmute yourself.
- There will be various polls throughout the webinar using Slido. Please scan the QR when it appears on screen. Alternatively you can access via slido.com using the code #MSD2022



EUROPEAN CENTRE FOR MEDIAN-SCALE WEATHER FORECASTS

3

#### Housekeeping

As an attendee you can view the webinar but will not have video or audio functionality

Please ask questions via the Q&A option

Please raise your hands if you want to ask a question verbally and wait for a prompt to appear on your screen to allow you to unmute yourself.

We will use Slido for Polls and Surveys (anonymously)  
Please scan the QR code or access via slido.com using #MSC2022



#### Weather and Climate, High-Performance Computing and Machine Learning

Predictions of weather and climate are difficult as the Earth system is huge, complex and chaotic, and as the resolution of our models is limited

However, we have a several hundred peta-byte of Earth system data from observations and model output

- There are many application areas for machine learning in numerical weather predictions



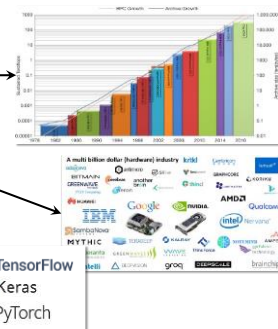
#### MAELSTROM – Why now?

**Increase in data volume**

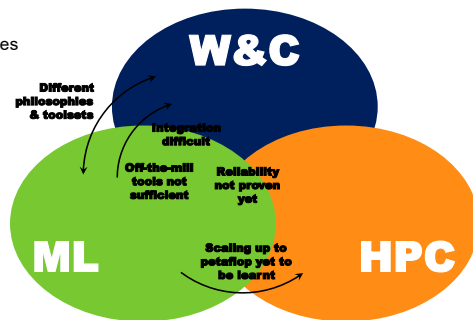
**New computing hardware**

**New machine learning software**

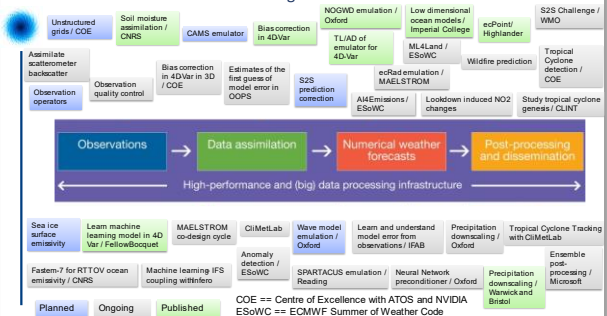
**Increase in knowledge**

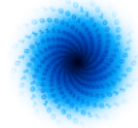


#### Challenges

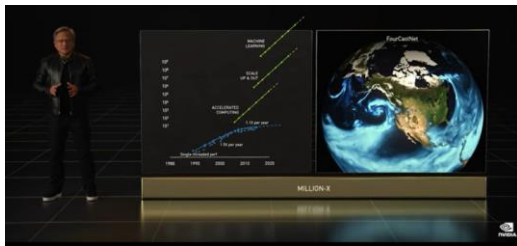


#### The state-of-the-art – Machine learning at ECMWF





### The perspective – Full ML models for weather and climate?



NVIDIA's Earth-2 is coming with FourCastNet – see Thorsten's talk Climate?

### A myriad of options...

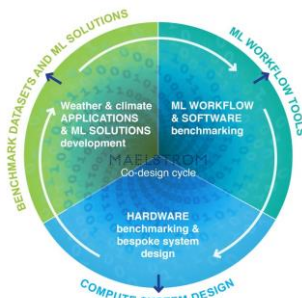
#### A myriad of options for machine learning approaches

Dense Neural Networks, LSTMs, ConvGru, Attention Layers, Transformer networks, # of hidden layers, different normalisation of inputs, batch normalisation, tanh, relu, gelu, softplus, elu, selu, leaky relu, softmax, sigmoid function, generative adversarial networks, recurrent neural networks, encoding/decoding networks, random forests, boosting methods, clustering techniques, singular vector decomposition, causal discovery, ablation studies, root mean square error, variational auto encoder, gradient descent, stochastic gradient descent, adagrad, adadelata, RMSprop, Adam, # of epochs, # of batches, learning rate, overfitting, dropout, Bayesian networks, Gaussian processes, half precision, sparse networks .... Argh...

#### + a myriad of options for machine learning hardware

= confused scientists

### The MAELSTROM approach



### We are MAELSTROM



### MAELSTROM – How to get involved?

- Visit our [project webpage](http://project webpage): [www.maelstrom-eurohpc.eu](http://www.maelstrom-eurohpc.eu)
- Use our [benchmark datasets](#)
- Use our [machine learning blueprints](#) for other applications
- Use of [machine learning workflow tools](#)
- Use of [compute system designs](#)
- [Talks, deliverables and publications](#)
- Two [dissemination workshops](#) are planned for April 2022 and Spring 2024 at ECMWF
- Two [hackathons](#) foreseen (2022 in Juelich and 2023 at ECMWF)

#### Our partners have a special interest in collaborations regarding:

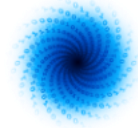
Machine learning, data movement and IO, approximate computing and mixed precision, hardware accelerators and co-design, hardware and software benchmarks and many other topics.

### Questions?

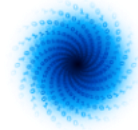
Please also join us for the ECMWF Machine Learning Workshop Tu -Fr  
<https://events.ecmwf.int/event/294/>



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## 6.2 WP1: Gong Bing, JSC



### App 4: Improved ensemble predictions in forecast post-processing

**Why improve ensemble prediction by ML?**

- Weather is a chaotic system. Minor perturbations affect the outcome the further into the future we predict  
→ ensemble prediction predicts weather as a probability distribution.
- ML solution should be applied to uncertainty quantification and bias corrections.

**ML solutions and achievement:**

- Goal: Predict T850, Z500 as a probability distribution
- Solutions: inception-style network for Uncertainty Quantification

Observations  
Data assimilation  
Numerical weather forecasts  
Post processing ensemble output  
Product generation

ETH zürich Salehkhooos

### App 5: Improved local weather predictions in forecast post-processing

**Why ML for downscaling 2m temperature?**

- High spatial variability of T2m in complex terrain
- Local variations in T2m with adverse effects (e.g., Traffic hazards, Loss in agriculture)
- increase in spatial resolution  
→ Computation cost  
→ Challenges across gray-zone resolutions

**ML solutions and achievement:**

- Goal: Mapping from (coarsened) 0.8° to 0.1° grid
- Solutions: U-Net
- Results: (RMSE: )

Observations  
Data assimilation  
Numerical weather forecasts  
Post processing ensemble output  
Product generation

JÜLICH Michael Langguth & Bing Gong

### App 6: Bespoke weather forecasts to support energy production in Europe

**Why ML for energy generation forecast?**

- Allow large market share of renewable energies by optimal efficiency throughout all providers (solar, wind, biogas, storage capacities, ...)  
→ requirement of accurate forecasts for energy generation
- Increase of renewable energy generation important for mitigation to climate change
- Predictions for the exact location of wind/solar parks can only be achieved by ML algorithms

**ML solutions and achievement:**

- Goal: Power production forecasts
- Solutions: Gradient boosting (intraday/day ahead) Neural Networks (intraday)
- Results: NMAE approximately: Wind 12%; Solar 7%

Observations  
Data assimilation  
Numerical weather forecasts  
Post processing ensemble output  
Product generation

acast Dr. Markus Abel, Greta Denisenko, Fabian Emmert

### Delivered: Tier 1 datasets

ClimateLab manages the downloading and loading of data, for a variety of datasets, dubbed plugins.

```

(pip install climetlab climetlab-maelstrom-radiation
import climetlab as cml
cmls = cml.load_dataset('maelstrom-radiation')
ds = cmls.to_xarray())

```

Application	Res.	Grid size	Data size	Data format	Pip package name	CML dataset name
A1: Postprocessing	1 km	1799x2321	~ 5 TB	NetCDF	climetlab-maelstrom	'maelstrom'
A3: Radiation	40 km	137 vertical levels	~ 2 TB	NetCDF/FFRecon	climetlab-maelstrom-radiation	'maelstrom-radiation'
A4: ENS10	0.5°	720x361x11x11	~ 2.6 TB	GRIB/NetCDF	climetlab-maelstrom-ens10	'maelstrom-ens10'
A5: Downscaling	0.1°	96x128	~ 300 MB	NetCDF	climetlab-maelstrom-downscaling	'maelstrom-downscaling'
A6: Power production	0.1°	351x551 10 vertical levels	~ 0 (TB)	NetCDF	climetlab-maelstrom-power-production	'maelstrom-constant-a-0', 'maelstrom-power-production', 'maelstrom-weathermodel-level', 'maelstrom-weathermodel-level'

### Delivered: ML with customized loss function for weather forecasts applications

Quantile Scores:  $S_\tau(u) = \begin{cases} u(\tau-1), & u < 0 \\ u\tau, & u \geq 0 \end{cases} \rightarrow \text{AP1}$

Latitude-Weighted Mean Square Error:  $MSE_{lat} = \frac{1}{L} \sum_{l=1}^L (\hat{Y}_l - Y_l)^2 L(l) \rightarrow \text{AP2, AP6}$

The Ranked Probability Score (CRPS):  $CRPS(F, y) = \int_{-\infty}^{\infty} [F(x) - 1_{x>y}]^2 dx \rightarrow \text{AP4}$

Adversarial loss:  $\min_D \max_G (D, G) = E_{x \sim p_{data}(x)} [\log(D(x))] + E_{x \sim p_G(x)} [\log(1 - D(G(x)))] \rightarrow \text{AP1, AP5}$

- Other loss functions: Structural Similarity Index (SSIM), Mean Square Error (MSE) and Mean Absolute Error (MAE)

Jupyter notebooks have been created to explore the datasets and demonstrate simple machine learning solutions to act as first benchmarks → <https://www.maelstrom-eurohpc.eu/deliverables>

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### Outlook to the next two years

Towards Tier 2 Datasets → Large data

Use ML tools → Integrate ML solutions with workflow tools

Hardware Testing → Parallelizing ML solutions on HPC

Scientific aspects → Further ML solution developments for all applications

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[www.maelstrom-eurohpc.eu](http://www.maelstrom-eurohpc.eu)

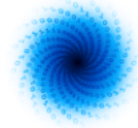
MAELSTROM

## Thank you

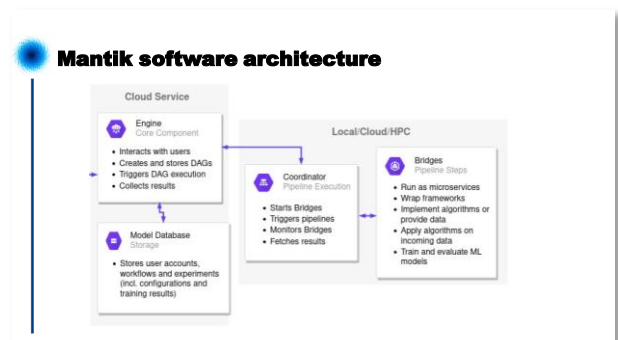
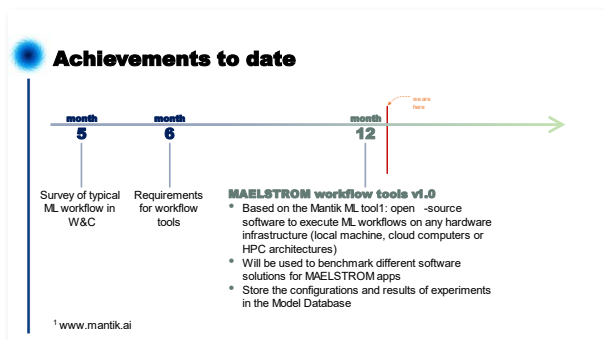
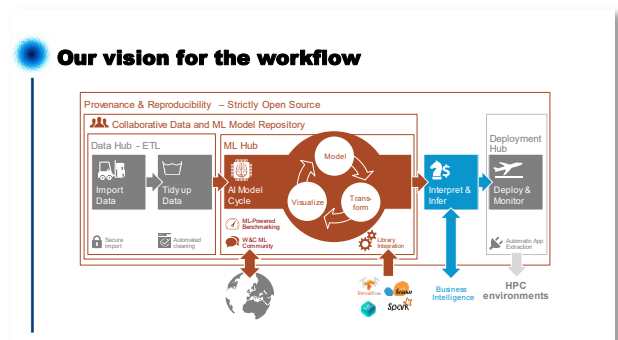
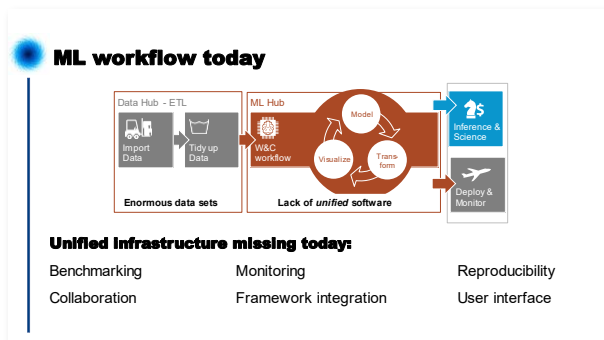
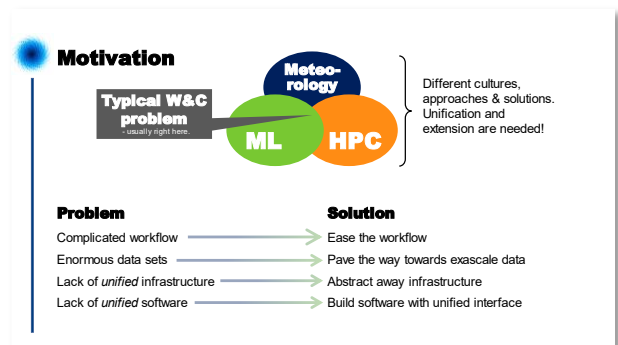
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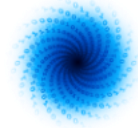
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## 6.3 WP2: Fabian Emmerich, 4cast







### Workflow tools key features

- Reproducible ML solutions
- Share ML solutions across user base
- Recommendation of ML solutions to users with specific problems
- Interface to cloud computing and HPC
- Manipulation of execution graphs leading to optimal execution of W&C workflows

### Current Interfaces

MAELSTROM platform as a ML workflow platform

- Command Line Interface
- Model Database
- HPC interface
- GUI for Executor and Job Status

### Vision for the next two years

Timeline milestones:

- Month 6: MAELSTROM protocol and ML requirements
- Month 12: Workflow tools v1.0
- Month 30: Improved data processing tools and weather data loading pipeline
- Month 36: Final version of workflow tools

Software performance benchmarking

### MAELSTROM

## Questions?

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## 6.4 WP3: Daniele Gregori, E4

### MAELSTROM

Empowering weather & climate forecast

- ML Apps & Datasets
- ML Workflow Tools
- Hardware Systems

Daniele Gregori E4

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### Agenda

- ML Apps & Datasets
- ML Workflow Tools
- Hardware Systems

Codesign Approach

Adopted Computing Infrastructure

E4 FZJ

New Infrastructure

E4 FZJ

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### Codesign Approach

Aim of Codesign: guide developers to the infrastructure that maximizes performance -

- Time-to-Solution
- Energy-to-solution.

Developer: ML Application to benchmark (installation in user space)

HPC System

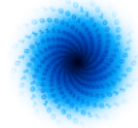
Environment Set up to improve performance (i.e. driver, bios,...)

Hardware set up (i.e. GPU, FPGA, RiscV,...)

### Codesign Approach

An aspect of fundamental importance is the availability of different hardware systems in terms of:

- Architecture: Amd, Intel, ARM,...
- Accelerator: GPU NVIDIA, GPU AMD, GPU Intel, IPU, FPGA, ...
- Network: Ethernet, Infiniband
- Storage: Local, NFS, Parallel Storage



## Adopted Infrastructure @ FZJ

- JUWELS Cluster (2018)
  - 2511 computing nodes (2 x Skylake)
  - 48 GPU nodes (4 x NVIDIA V100 with NVLINK)
  - Mellanox 100 Gbit/s Fat Tree Topology (1:2 blocking factor)
  - 12 PFLOPs



- JUWELS Booster (2020)
  - JUWELS Booster consists of
    - 936 compute nodes,
    - each equipped with 4 NVIDIA A100 GPUs, 4 HDR200 adaptor.
    - The GPUs are hosted by AMD EPYC Rome 7402 dual socket CPUs.
    - The compute nodes are connected with HDR200 InfiniBand in a DragonFly+ topology.
  - 73 PFLOPs



Top500 Nov-2020  
 #1 Europe  
 #7 World  
 #1 "Green500"

## Adopted Infrastructure @ FZJ

- JUWELS Cluster (2018)
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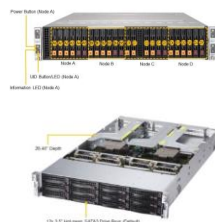
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  - 73 PFLOPs



Top500 Nov-2020  
 #1 Europe  
 #7 World  
 #1 "Green500"

## New Infrastructure @ E4

- AMD Cluster (Cervia)
  - 1 login node (Virtual Machine)
  - 4 nodes in a single chassis (twin square) 2U
    - OS Red Hat Enterprise Linux release 8.5 (Dotopa), with linux kernel 4.18.0-305
    - Dual socket
    - 2x AMD EPYC 7313 16-Core Processor @3GHz
    - 256 GB RAM
    - connected via InfiniBand 100 Gb/s network.
  - 2 nodes single server 2U
    - OS Red Hat Enterprise Linux release 8.5 (Dotopa), with linux kernel 4.18.0-305
    - Dual socket
    - 2x AMD EPYC 7313 16-Core Processor @3GHz
    - 512 GB RAM
    - connected via InfiniBand 100 Gb/s
    - 3x AMD MI100 GPU



ARM Cluster Based on Ampere Altra Max CPU  
 New Accelerator: Intel Ponte Vecchio (end 2022), FPGA

## New Infrastructure @ FZJ

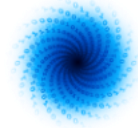
- JURECA DC
  - Total: 768 compute nodes (AMD EPYC 7742, 2 x 64 cores; 512 GB; InfiniBand HDR-100)
  - 192 accelerated nodes: 4 x NVIDIA A100 GPUs
- Evaluation nodes
  - 2 x AMD MI250
  - 2 x Arm+A100 (NVIDIA HPC Devkit)
  - Graphcore IPU Accelerator



## Questions?



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## 6.5 WP3: Andreas Herten, JSC

**MAELSTROM**

Empowering weather & climate forecasts:

**ML Apps & Datasets**  
**ML Workflow Tools**  
**Hardware Systems**

**Andreas Herten, Stepan Nassyr**  
Julich Supercomputing Centre

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## Metrics



## Time-related

- Total runtime
- Total training time
- Training time per epoch (avg, min, max)
- Training time per iteration (avg, min, max)
- Training time of first epoch
- Model saving time



## Learning-related

- Final loss (training, validation)



## Energy-related

- GPU power draw (max)
- Energy consumption (GPU, node)

30.03.2022

Project MAELSTROM to 2025-2026, Project to 2025-2026, Project to 2025-2026

3

## Result Highlights: AP1

## JUWELS Booster

- 10 experiments
- 350 s per experiment; 1/3 training, 2/3 data loading, 2% other

## JUWELS Cluster

- 3 experiments
- 700 s per experiment, similar distribution

## E4

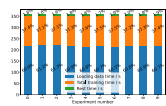
- 5 experiments
- 450 s per experiment, 28% training, 72% data loading, 1% other

Mostly stable results over various experiments; first epoch always ~30% (JUWELS) / 2 × (E4) slower

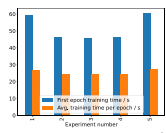
**Summary:** Bound by filesystem, not using GPUs very efficiently; GPFS > NFS; E4-A100 slower than JSC-A100

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JUWELS Booster Total Time Split



E4 Epoch Comparison



4

## Result Highlights: AP3

## JUWELS Booster

- 440 s runtime; 98% training time; largely stable over 3 repetitions
- Experiments with various configurations: synthetic data; disabled cache in TensorFlow; different GPU number (1 or 2); different batch size (12 or 1024)
  - Disable cache: runtime increase 20%
  - GPU batch size: runtime decrease 25%
- Energy: 9.25 Wh/GPU (2-1024) vs 12.32 Wh/GPU (1-512)

## JUWELS Cluster

- 824 s runtime, ~85% slower than A100

## E4

- Slightly faster; 390 s runtime
- Extra experiment: clear filesystem (NFS) cache by rebooting → 2.5 × slower; benefits from streaming data

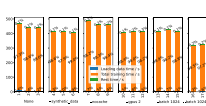
Additional tests with inference on JUWELS Booster

## Summary:

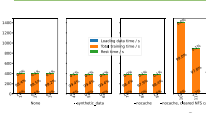
- Compute-intensive application (little I/O impact)
- 2-GPU study (benefits from larger batch size);
- Caches used during streaming data important

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JUWELS Booster Experiment Overview



E4 Epoch Overview, NFS Cache



5

## Result Highlights: AP4

## JUWELS Booster

- 6400 s runtime; 70% training time, significant unaccounted time
- 150 Wh energy consumed, GPU max draw 400 W

## E4

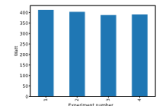
- Batch size: 2 (JUWELS Booster: 1)
- 25 729 s runtime; 88% training time

## Summary:

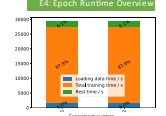
- Long runtime for easy statistical measurements;
- Good GPU usage;
- Investigate run 1 outlier

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JUWELS Booster: Max Power Data



E4 Epoch Runtime Overview



6

## Result Highlights: AP5

## JUWELS Booster

- Small data set: 75 s runtime, 92% training
- Large data set: 1500 s runtime, 98% training
- First epoch 1.75 × (large) / 20 × (small) slower
- 300 W max, 45 Wh consumed

## JUWELS Cluster

- Large data set: 2700 s runtime
- 300 W max, 190 Wh

## E4

- Various experiments
- Large data set: 1600 s runtime, 94% training

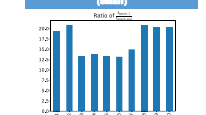
Additional tests with inference on JUWELS Booster

## Summary:

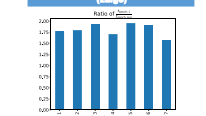
- Small data set: Too short runtimes with curious behaviors
- Faster GPU, less energy

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JUWELS Booster Epoch Time Ratio (Small)



JUWELS Booster Epoch Time Ratio (Large)



7

## Conclusion

Examples shown of selected MAELSTROM application benchmarks

Applications × Configurations × Hardware = Many data points

Investigation ongoing, already many specific (and interesting!) features identified

Also spotted curiosities for further investigation

Much more data and results then presented here!

→ See [maelstrom-eurohpc.eu](https://maelstrom-eurohpc.eu) website for D3.4, soon

30.03.2022

Thank you  
for your attention!  
a.herten@fzjuelich.de // @Andri  
nassyr@fzjuelich.de

8

**MAELSTROM**

**Questions?**

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