Earth system models of the future

Peter Dueben

Head of the Earth System Modelling Section



The strength of a common goal

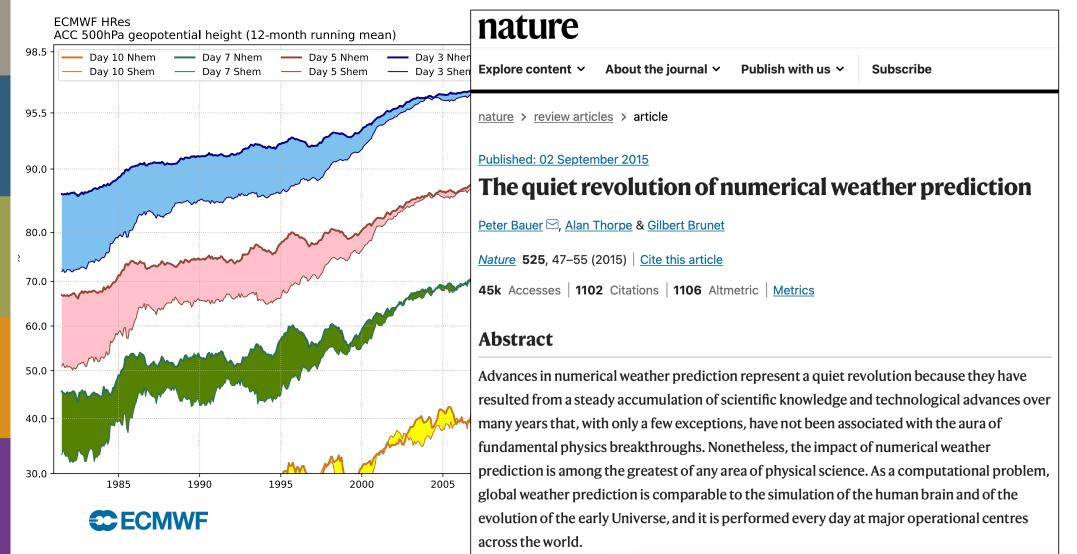




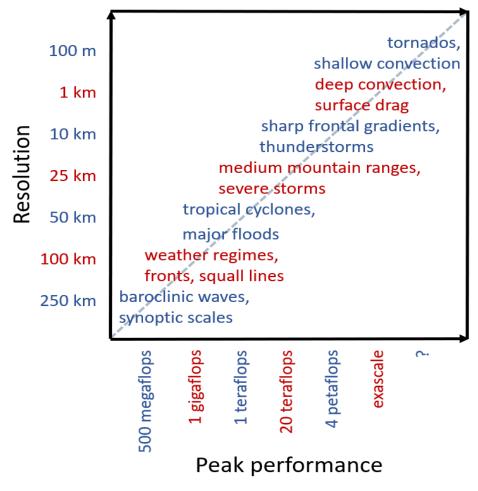
The MAELSTROM and ESiWACE projects have received funding from the EuroHPC-Joint Undertaking under grant agreement No 955513 and 101093054.

Earth system modelling is currently experiencing disruptive changes offering great opportunities.

1980-2020: The quiet revolution



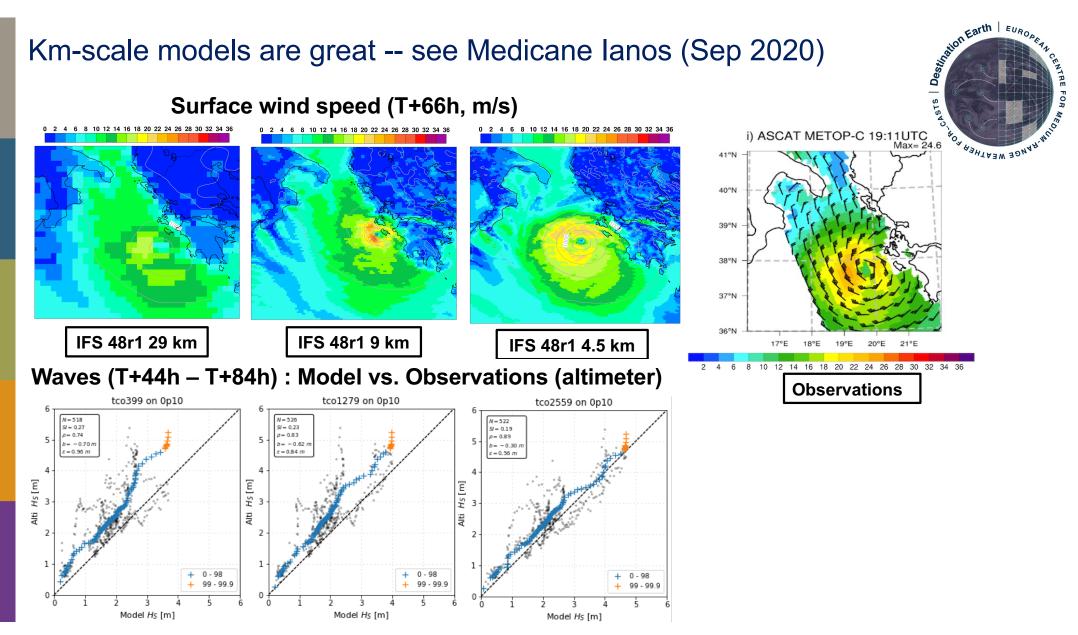
Km-scale models for better predictions



Adapted from Neumann, Dueben et al. Phil Trans A 2018

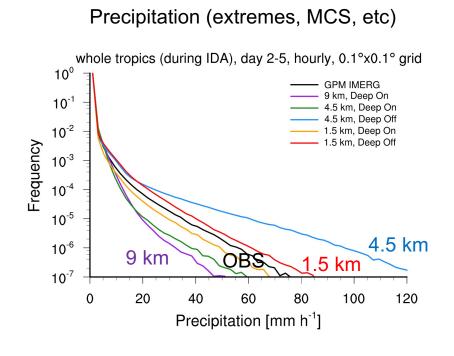
- More resolution more skill
- Better representation of topography and gravity wave drag
- Explicit representation of convection ("storm-resolving" models)
- Eddy resolving oceans + tides
- Same resolution as satellite measurements

Km-scale models are great -- see Medicane lanos (Sep 2020)

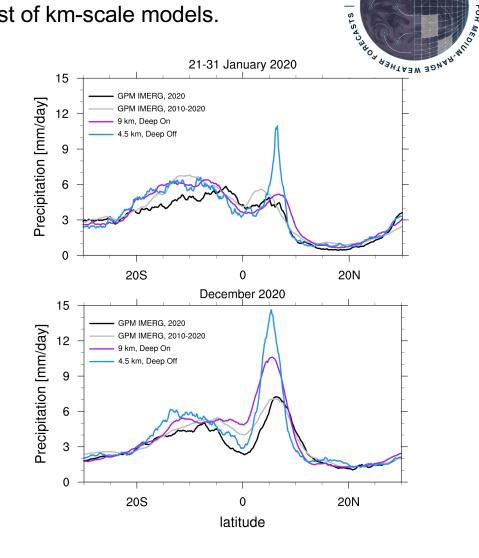


So let's push km-scale models to operations!? – Not out of the box

Scientific developments will be needed to make the most of km-scale models.



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So let's push km-scale models to operations!?

Climate is changing, \rightarrow we need better models now

Compute power? 9 km \rightarrow 1 km \rightarrow Factor 9³ = 729 compute power

Moore's law is the observation that the number of transistors in an integrated circuit doubles about every two years. $\rightarrow 2^9 = 512 \rightarrow \text{Let's wait for 18 years?}$

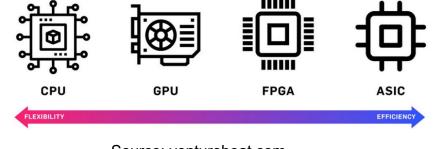
Data and storage? 9km: 6,599,680 points x 137 levels x10 variables \rightarrow 9 billion points \rightarrow > 0.5 TB

1.5km: 256,800,000 points x 137 levels x 10 variables \rightarrow 352 billion points \rightarrow > 20 TB

Uff...

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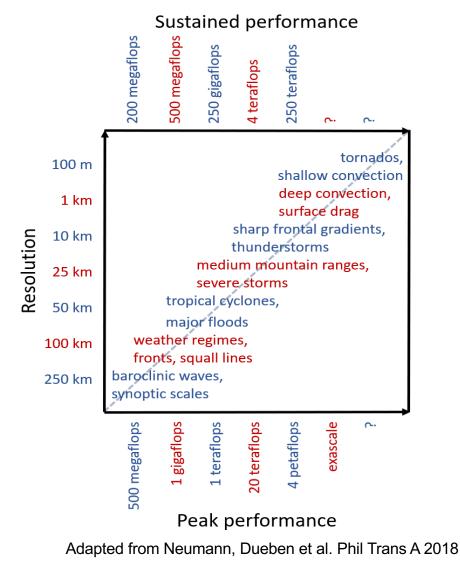


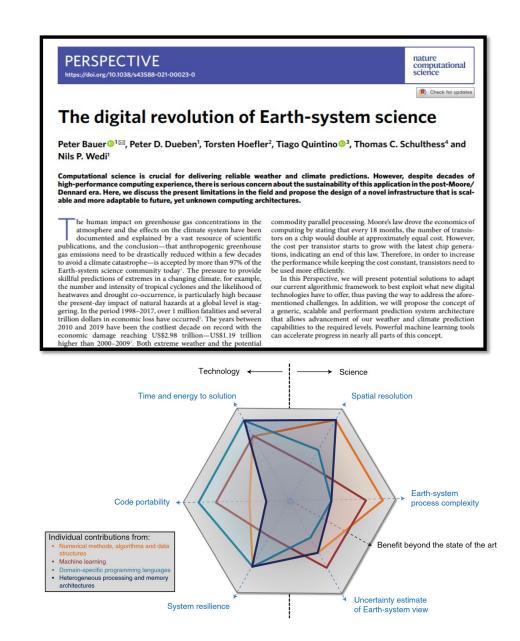


Source: venturebeat.com

- Individual processors will not be faster
 → Parallelisation / power consumption
- Hardware will be more heterogeneous \rightarrow CPUs / GPUs / FPGAs / ASICs
- Machine learning has strong impact on hardware development
 → High floprate at low precision

2015-today: The digital revolution



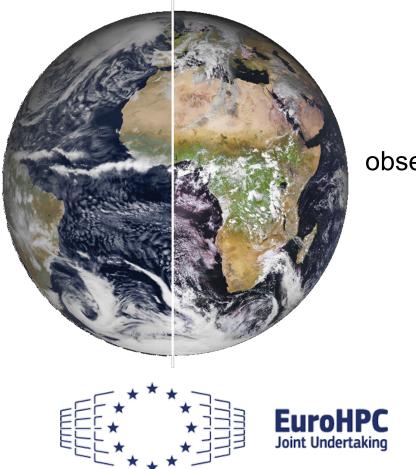


EU's Destination Earth (DestinE) initiative

simulations

(ECMWF IFS 1.4 km)

Towards a Digital Twin Earth



observations





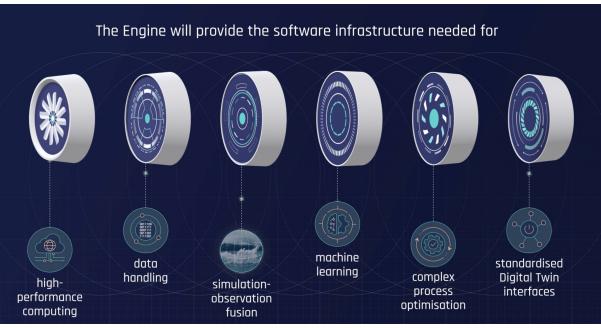
Funded by the European Union

DestinE's Digital Twin Engine

Framework for Digital Twin Workflows

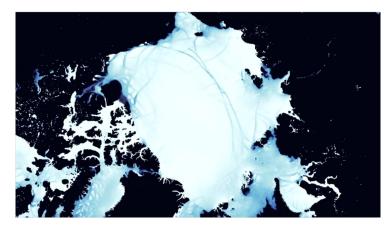
- High Performance Computing adaptation / Digital Twin optimisation
- · IO and data workflows
- Software management, controlling workflows, cloud environments
- Visualization

A Game Engine type framework but for Earth Systems...

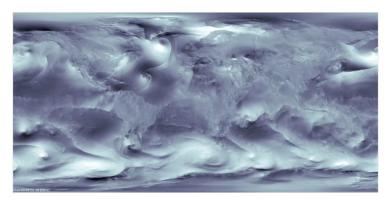


HPC Medicine List of ingredients: workflow manager, data structures/parallelization library, model plugin architecture for interactive capabilities, key-value object storage with semantic, data access API, IO-Server API, on-the-fly post-processing API, data notification system, data cube API, visualisation & rendering services

2015-today: The digital revolution to allow for km-scale models



More realistic at local scale



More realistic at global scale



Better results via a coupled model system





Global km-scale models will improve realism of simulations significantly and are now becoming available.

Machine learned weather models



Explore the space of machine learning for weather and climate modelling

Improve understanding

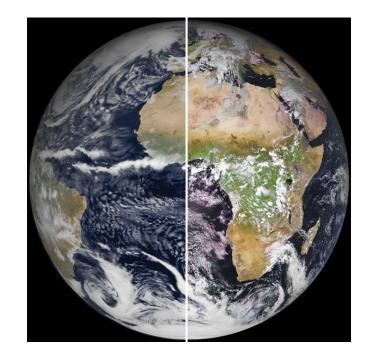
- Fuse information content from different datasources
- Unsupervised learning
- Causal discovery
- Al powered visualisation
- Uncertainty quantification
- ...

Speed up simulations

- Emulate model components
- Port emulators to heterogeneous hardware
- Use reduced numerical precision and sparse machine learning
- Optimise HPC and data workflow
- Data compression
- .

Improve models

- Learn components from observations
- Correct biases
- Quality control of observations and observation operators
- Feature detection
- •



Link communities

- Health e.g. for predictions of risks
- Energy e.g. for local downscaling
- Transport e.g. to combine weather and IoT data
- Pollution e.g. to detect sources
- Extremes e.g. to predict wild fires
- ...

Weather and climate modelling centres mostly explore the "hybrid space" coupling machine learning to conventional models.

Can we replace conventional Earth System models by deep learning?

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- If Hamlet were a musical comedy, rather than a tragedy, how would it have ended? Describe the plot.
- If Hamlet were a musical comedy, rather than a tragedy, the ending would likely be much happier and more lighthearted. Instead of ending in a violent and tragic showdown, with the deaths of several major characters, the play would likely have a more comedic and satisfying resolution.

For example, the play could end with Hamlet successfully avenging his father's death, but then choosing to forgive and reconcile with his uncle, the new king. This would allow Hamlet to put aside his grudges and bitterness, and to find peace and happiness.

As part of this resolution, there could be a big, energetic finale song, where the characters sing and dance together, expressing their newfound sense of joy and unity. This could be a lively and upbeat number, with a catchy and infectious melody, and lyrics that reflect the themes and events of the play, while also expressing a sense of hope and optimism for the future.

Overall, a musical comedy version of Hamlet would likely have a more uplifting and optimistic ending, with the main character achieving a sense of closure and resolution, and moving on with his life in a positive and fulfilling way.

The New York Times

THE SHIFT

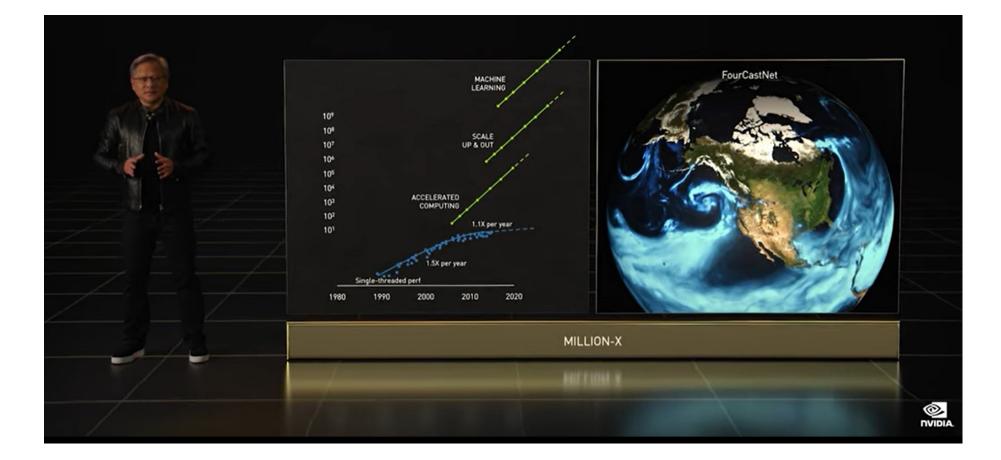
An A.I.-Generated Picture Won an Art Prize. Artists Aren't Happy. "I won, and I didn't break any rules," the artwork's creator says.

🛱 Give this article 🏟 📮 🖵 1.5K



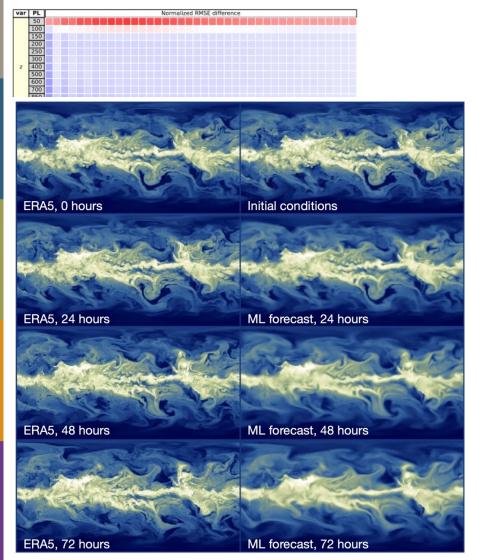
Jason Allen's A.I.-generated work, "Théâtre D'opéra Spatial," took first place in the digital category at the Colorado State Fair. via Jason Allen

Can we replace conventional Earth System models by deep learning?



NIVIDA's Earth-2 is coming with FourCastNet

2022-today: The machine learning revolution



GraphCast from Google/Deepmind and Fourcastnet from NVIDIA are beating conventional weather forecast model in deterministic scores and are orders of magnitudes faster.

But how do these models actually work?

They get the best results when using very large timesteps.

They are trained for a small Root Mean Square Error. \rightarrow They smear out for large lead times.

Many questions remain: Can the models extrapolate? Can they represent extreme events? Can they learn uncertainty? Can they be trained from observations? Can they represent physical consistency?

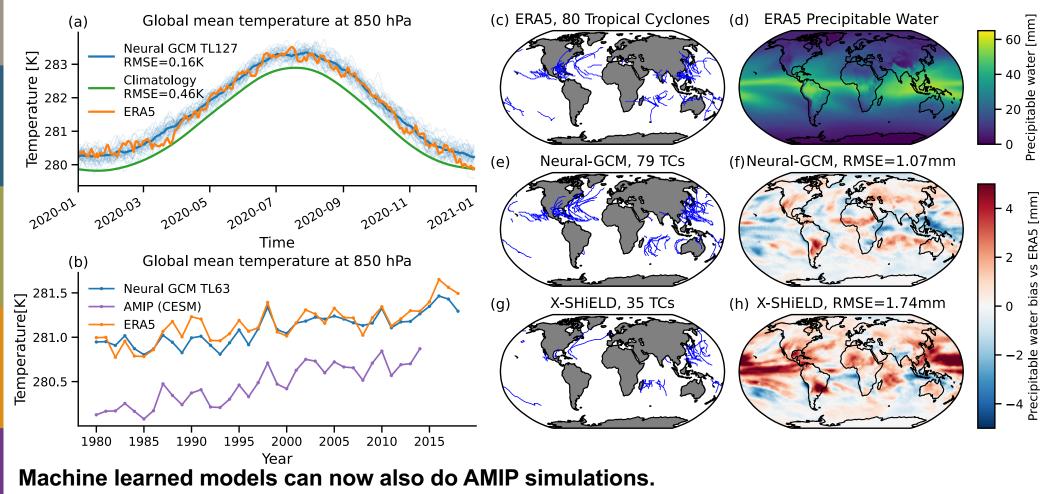
Images from Keisler (2022)

2022-today: The machine learning revolution

What machine learned models can and cannot do?

- Conventional models will not be replaced by machine learning models entirely.
- Within the next couple of years most weather predictions will come from machine learning models.
- Machine learning will be the perfect glue between models and observations.
- Km-scale models will make a difference for the generation of training datasets.
- Machine learning models have also potential for climate projections despite the extrapolation problem.

2022-today: The machine learning revolution



Kochokov et al. @Google in preparation

And Foundation Models will enter the domain...

Dude, when does he finally start to talk about correctness and reproducibility?

Change of gear

Workmode of 2010:

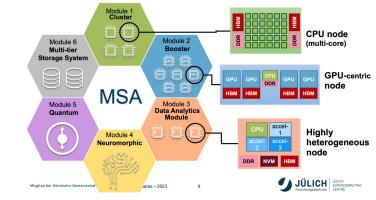
- A single scientist can understand the whole Earth system model
- Earth system models consist of 100,000 lines of Fortran Code
- Code is shared via tarballs, data is stored locally
- Models run on CPUs and Moore's law is still working

Workmode of 2020:

- A single scientist cannot understand the whole Earth system model anymore
- A team of software developers is needed to use heterogeneous hardware
- Models start to run on GPUs, Moore's law is dying
- Data is stored locally but meta information is available online
- Online code repositories are used to control quality and share model code

Workmode of 2030:

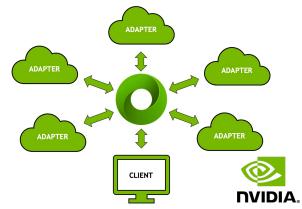
- Machine learning models of 2,000 lines of Python code compete with conventional models
- There are hundreds of models and many of them with specific tasks
- HPC is federated
- Data is federated





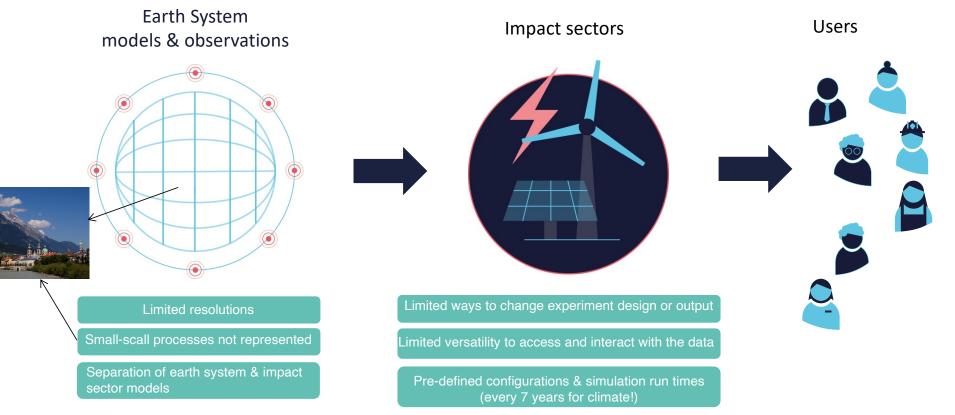


Tim Palmer's A380 comparison



ECMWF - DESTINATION EARTH

Current Systems

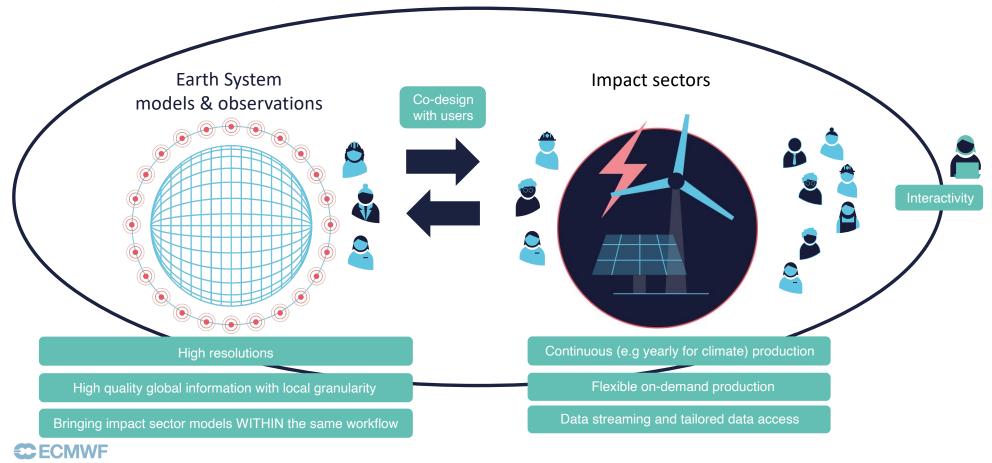


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DestinE builds Digital Twins of the Earth



Reproducibility – So much room for pessimism

- In 2020, the IFS ran in production on ECMWF's supercomputer and on a handful other computers for research. In 2024, the IFS will generate semi-operational predictions on several of the EuruHPC supercomputers as part of DestinE.
- Today's high-end models use several tools for portability (OpenACC, HIP, CUDA, DSLs such as GT4Py, Loki and Psyclone...).
- Machine learning models add new dimensions of complexity:
 - Retrained models can be very different
 - Use of pre-trained models
 - Use of transfer learning
 - Use of Foundation models in the future
 - Need to define and keep track of dataset and data manipulations

Make machine learning developments comparable via benchmark datasets

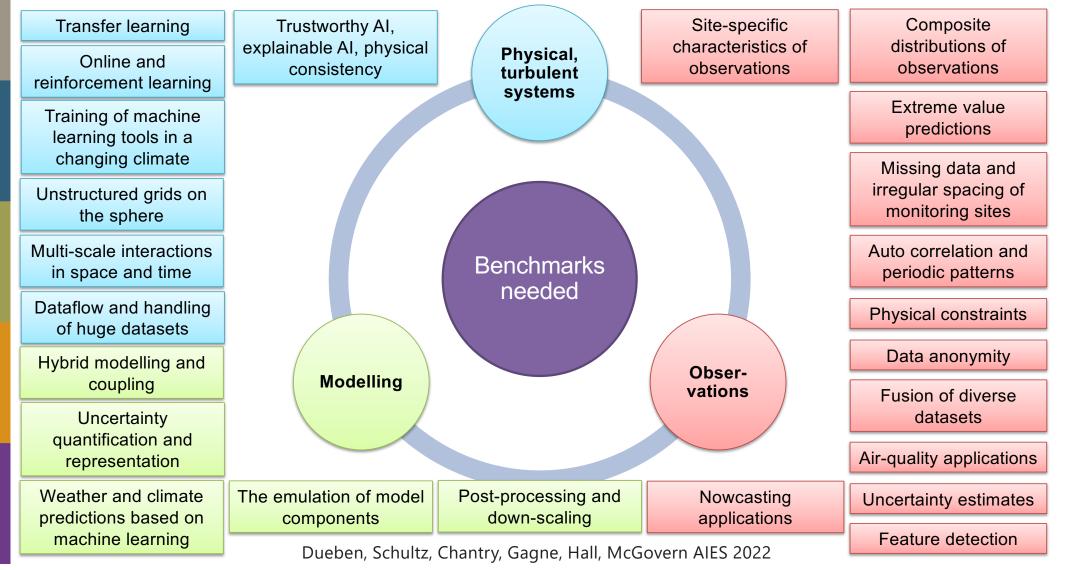
Benchmark datasets include:

- A problem statement
- Data that is available online
- Python code or Jupyter notebooks
- A reference machine learning solution
- Quantitative evaluation metrics
- Visualisation, diagnostics and robustness tests
- Computational benchmarks

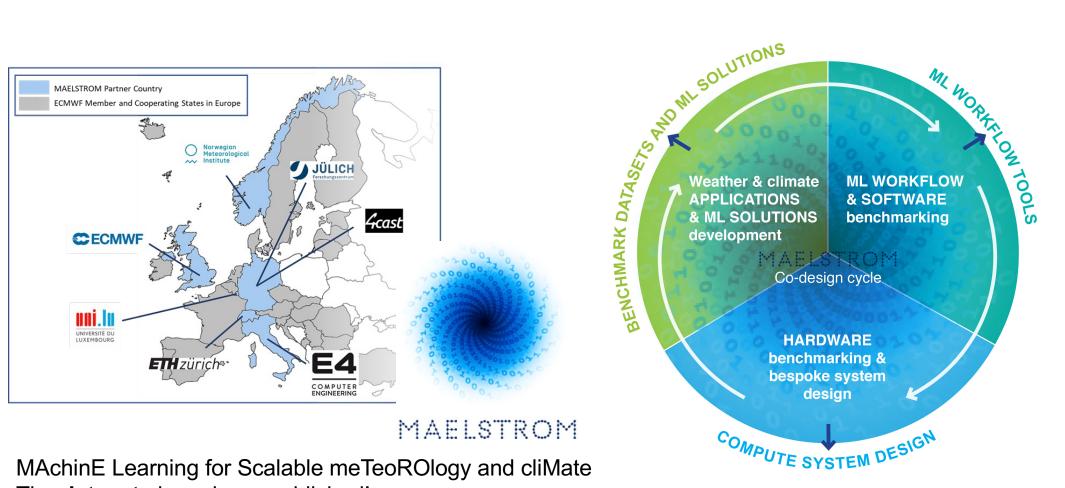
Benchmark datasets are useful because:

- They allow a quantitative evaluation of machine learning approaches
- They reduce data access and help scientists to get access to relevant data
- They allow for a separation of concerns between domain sciences and machine learning experts
- They allow for a separation of concerns between domain sciences and HPC experts

Missing machine learning benchmark datasets for atmospheric sciences

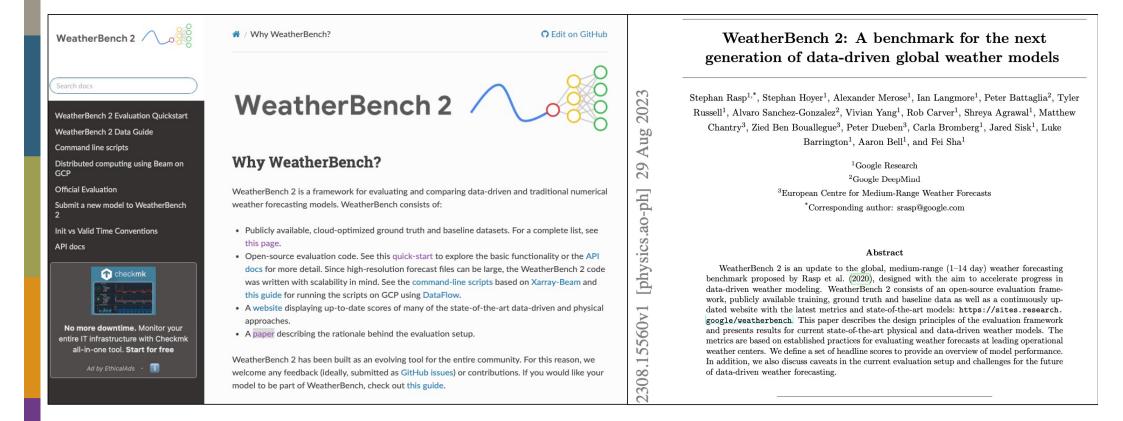


Learn how to use machine learning at scale \rightarrow The MAELSTROM project



The **datasets** have been published! https://www.maelstrom-eurohpc.eu/content/docs/uploads/doc6.pdf https://www.maelstrom-eurohpc.eu/ @MAELSTROM_EU

Data is open, diagnostics are at hand – A new way to verify correctness



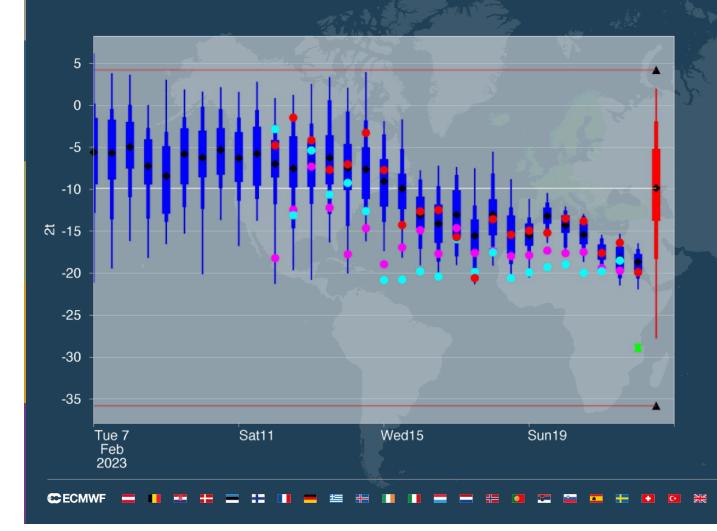
Data is open, diagnostics are at hand – A new way to verify correctness

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[Submitted on 19 Jul 2023]	
The rise of data-driven we	
Zied Ben-Bouallegue, Mariana C A Clare,	ECMWF unveils alpha version of new ML
Dramsch, Simon T K Lang, Baudouin Rao Data-driven modeling based on machine lea some applications. The uptake of ML methor revolution' of weather forecasting. The com increasing model resolution and ensemble s forecasts that require much lower computat standard NWP-based forecasts in an operat verification tools to assess to what extent a of a forecast from one of the leading global when verified against both the operational a drawbacks of ML-based forecasts. A new NV initialization and model training.	In focus Science blog Key facts and figure Media resources Videos ECMWF is today launching a newborn companion to the IFS (Integrated Forecasting System), the AIFS, our Artificial Intelligence/Integrated Forecasting System (one "I" covering both Intelligence and Integrated) Recent posts
Subjects: Atmospheric and Oceanic Physics (physic Cite as: arXiv:2307.10128 [physics.ao-ph] (or arXiv:2307.10128v1 [physics.ao-ph] fo	been navigating for a few years now. The AIFS forms one of three components of our new ML project, which began in summer 2023 and aims to expand our applications of machine learning to Earth system modelling.
https://doi.org/10.48550/arXiv.2307.1012 Submission history From: Zied Ben Bouallegue [view email]	https://www.ecmwf.int/en/about/media-centre/news/2023/how-ai-models-are- transforming-weather-forecasting-showcase-data

[v1] Wed, 19 Jul 2023 16:51:08 UTC (18,531 KB)

https://www.ecmwf.int/en/about/media-centre/aifs-blog/2023/ECMWF-unveilsalpha-version-of-new-ML-model

What the forecasts are showing: Severe Cold / Sodankylä, Finland, 22 Feb 00UTC



To explore the ability of data-driven models to capture extreme events we examine a case study from Finland from earlier this year, when -29C was observed.

We find that Pangu and FourCastNet recognised the severity of this event earlier, however all models underestimated the temperature significantly, to a similar degree.

29

Observation – green hourglass IFS HRES – red dot IFS ENS - blue Pangu – cyan dot FourCastNet – magenta dot Climatology – red box plot

Figure from Zied Ben-Bouallegue

Data is open, diagnostics are at hand – A new way to verify correctness

Why was the approach of global machine learning models so successful?

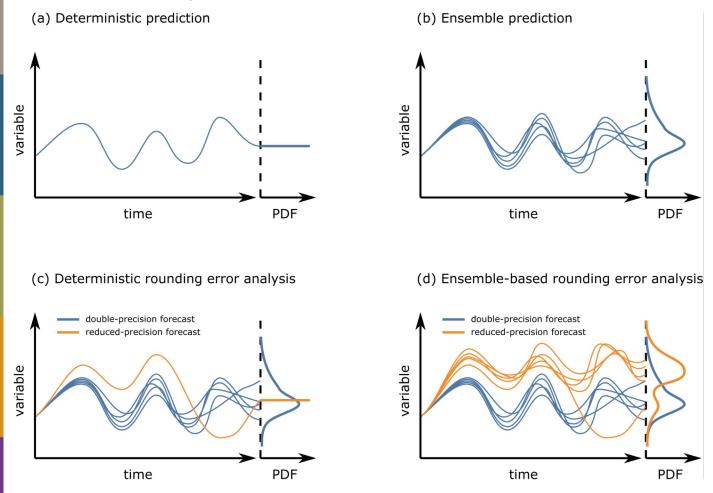
- Because there was a very large unified training dataset available with ERA5 from Copernicus.
- Open benchmark datasets are needed to allow for quantitative comparisons and to bridge communities.
- Km-scale models will make a difference for the generation of training datasets.



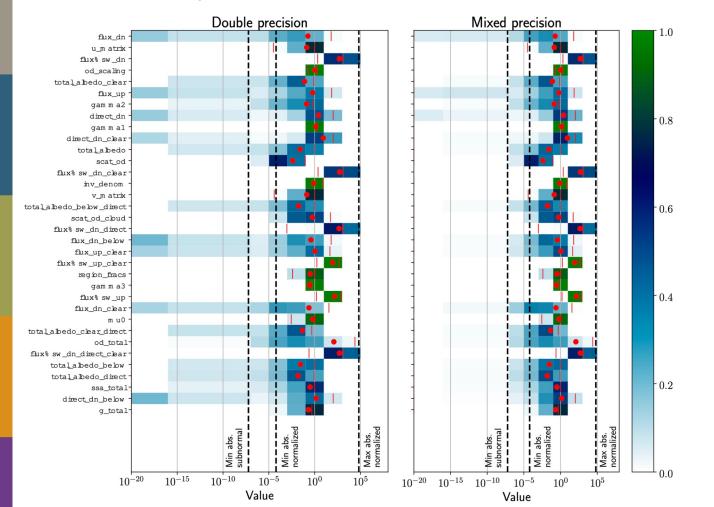
Reproducibility – So much room for optimism

- Git is standard, CI tests are getting better, model code is unified via DSLs
- Many datasets are nowadays open and Journals require open data and source code
- Most machine learning models and training datasets are published with the papers as open source
- Bit-wise reproducibility may not be as important anymore when compared to the ability to fulfil loss functions and complex diagnostics as we approach a new era in model comparison
- Compute and data handling will (hopefully) be more unified as we approach federated data and computing

The best way to check correctness is via automated tools



Pershin, Chantry, Dueben, Hogan, Palmer ESS Open Archive 2023



The best way to check correctness is via automated tools

Pershin, Chantry, Dueben, Hogan, Palmer ESS Open Archive 2023

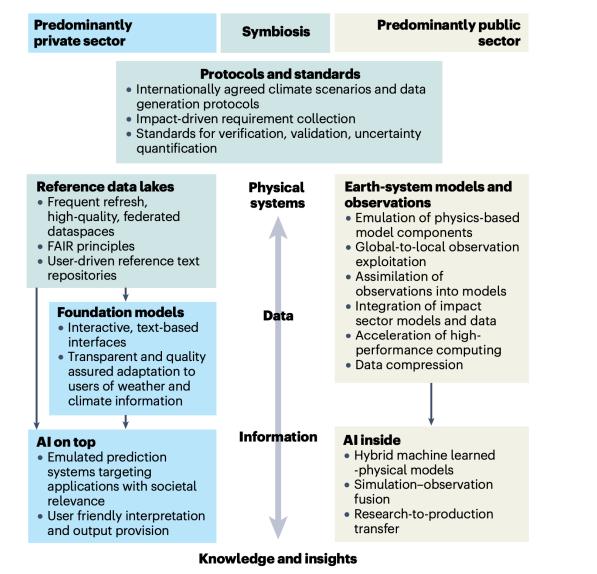
What is our aim today? – Imagine if...

- ...all model output, reanalysis data and all observations from the past and presence would be available online via federated data storage and next to federated computing and with a uniform API and as uniform packages
- ...there would be conventional Earth system models and machine learning models that can be used off-the-shelf to analyse and extend those datasets
- ...all of these tools would be scalable and easy to use on laptops and supercomputers from various computing languages
- ...there would be off-the-shelf tools to interpret physical reasoning and causality via unsupervised machine learning, to perform uncertainty quantification, and to perform state-of-the-art visualisation
- ...there are off-the shelf machine learning solutions, and unit testing would be standard

We need to fight complexity and diversity of software with centralised infrastructure efforts and norms.

We need world-wide collaboration on data and infrastructure developments to achieve this. First approaches already exist with Destination Earth, Earth-2 and EVE

How will machine learning for weather and climate evolve in a public/private partnership?



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Deep learning and a changing economy in weather and climate prediction

Peter Bauer ⊠, Peter Dueben, Matthew Chantry, Francisco Doblas-Reyes, Torsten Hoefler, Amy McGovern & Bjorn Stevens

Nature Reviews Earth & Environment 4, 507-509 (2023) Cite this article

638 Accesses | 34 Altmetric | Metrics

The rapid emergence of deep learning is attracting growing private interest in the traditionally public enterprise of numerical weather and climate prediction. A public-private partnership would be a pioneering step to bridge between physics- and data-based methods, and necessary to effectively address future societal challenges.

What have we learned?

The quiet revolution (1980-2020):

• Steady investment into Earth system modelling and Earth system observations made a difference.

The digital revolution (2015-today):

- Conventional models need to be made future proof via new software and hardware standards.
- Large scale efforts make km-scale models possible today and they will make a difference.

The machine learning revolution (2022-today):

- A PhD student can write a machine learning tool that can beat the best weather prediction model in the world based on hundreds of person years of developments.
- Data needs to be open and easy to use to make progress.

The next step: Models will be better, tools will be easier, and data/HPC will be federated

• To achieve this needs programmes such as Destination Earth, Earth-2 and EVE.

Many thanks!

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@PDueben



The strength of a common goal