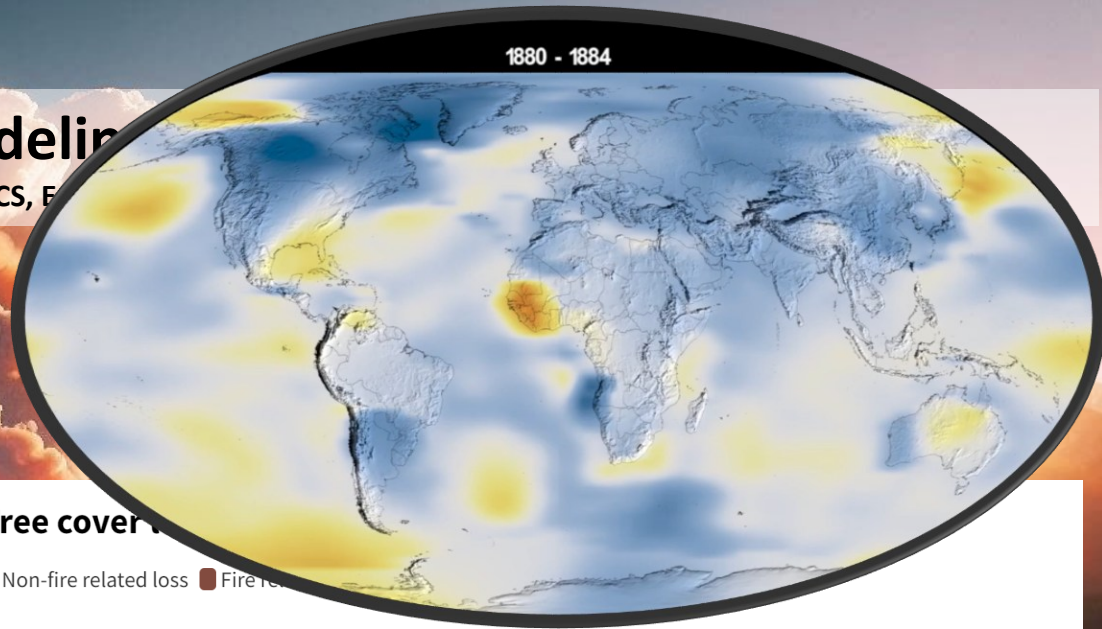


T. HOEFLER

AI for Climate Data Generation, Assimilation, and Modeling

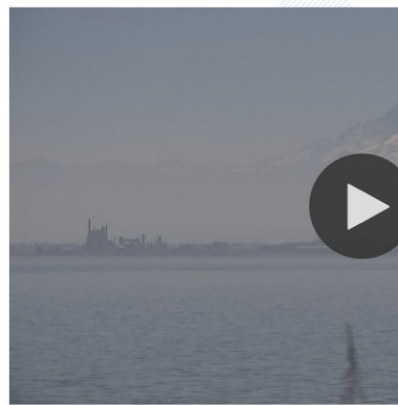
with contributions by B. Stevens, L. Huang, O. Fuhrer, P. Dueben, S. Schemm, and the whole SPCL team, CSCS, ETH Zurich

Keynote at HPC-CH Meeting, Lugano, Switzerland, Oct. 2024



Seeing hazy skies? Seattle area's air quality was among worst in US Friday morning

Seattle, Kirkland and Bothell were seeing the worst air quality in western Washington the morning after F...
MYNORTHWEST WEATHER



Author: Alex Didion
Published: 7:08 AM PDT July 5, 2024
Updated: 6:43 PM PDT July 5, 2024

Brace yourself for weeks of poor air quality in 2024, Seattle residents

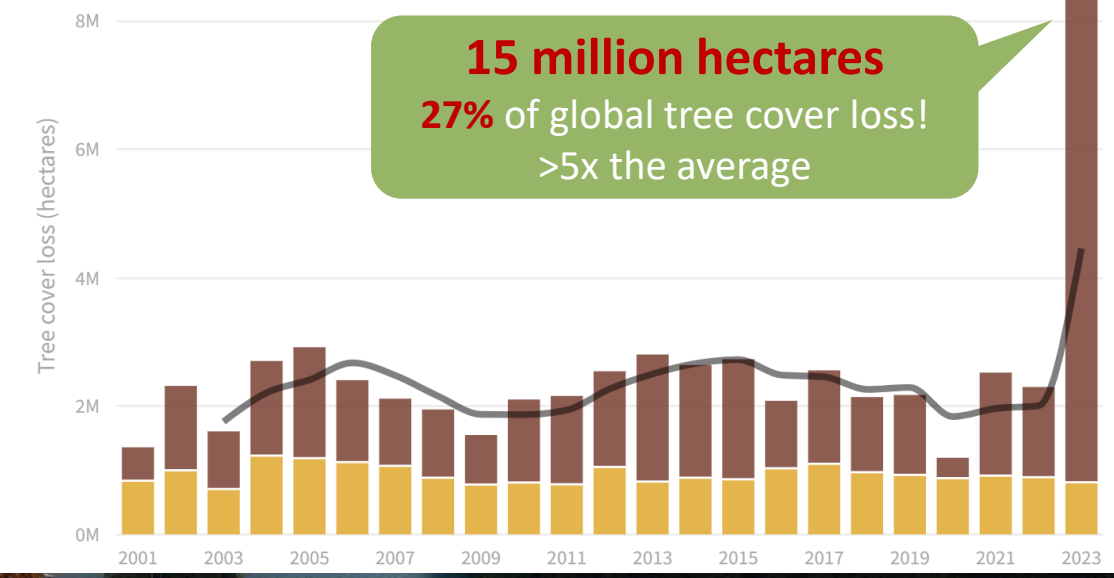
Apr 16, 2024, 3:29 PM | Updated: Apr 17, 2024, 12:32 pm



Smoke from wildfires fills the air along Alaskan Way on September 12, 2020 in Seattle, Washington. (Photo by Lindsey Wasson, Getty Images)

Tree cover loss

■ Non-fire related loss ■ Fire related loss



15 million hectares
27% of global tree cover loss!
>5x the average

T. HOEFLER

AI for Climate Data Generation, Assimilation, and Modeling

with contributions by B. Stevens, L. Huang, O. Fuhrer, P. Dueben, S. Schemm, and the whole SPCL team, CSCS, ECMWF, the EVE Summit Attendees, industry friends, and others

Keynote at HPC-CH Meeting, Lugano, Switzerland, Oct. 2024



“Climate simulation is basically impossible today.”
 “Predicting the average temperature is possible. However, the world doesn’t care about average. You care about your own region.” (Huang, Nov. 2023)



21% of global tree cover loss!

What can WE do about this?

Smoke from wildfires fills the air along Alaskan Way on September 12, 2020 in Seattle, Washington. (Photo by Lindsey Wasson, Getty Images)

Alps, the 6th fastest publicly known supercomputer on the planet - #2 in Europe (maybe soon #1!)

10,752 H100 GPUs and Grace CPUs	~10 Exaflop (10^{18}) BF16 performance	~40 years of humanity-ops/s
~1 PiB HBM3 + ~1.4 GiB LPDDR5	~48 PiB/s memory BW	~2M full wikipedias/s (24 GiB)
200 Gbps Slingshot interconnect	~250 TiB/s network bandwidth	~2x the total Internet bandwidth

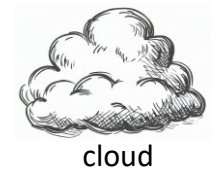



If we can't do it with this machine – who else could?

Climate prediction is extremely demanding (“impossible” – decades long)

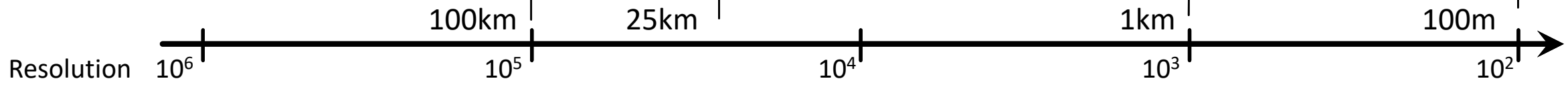


resolved
processes



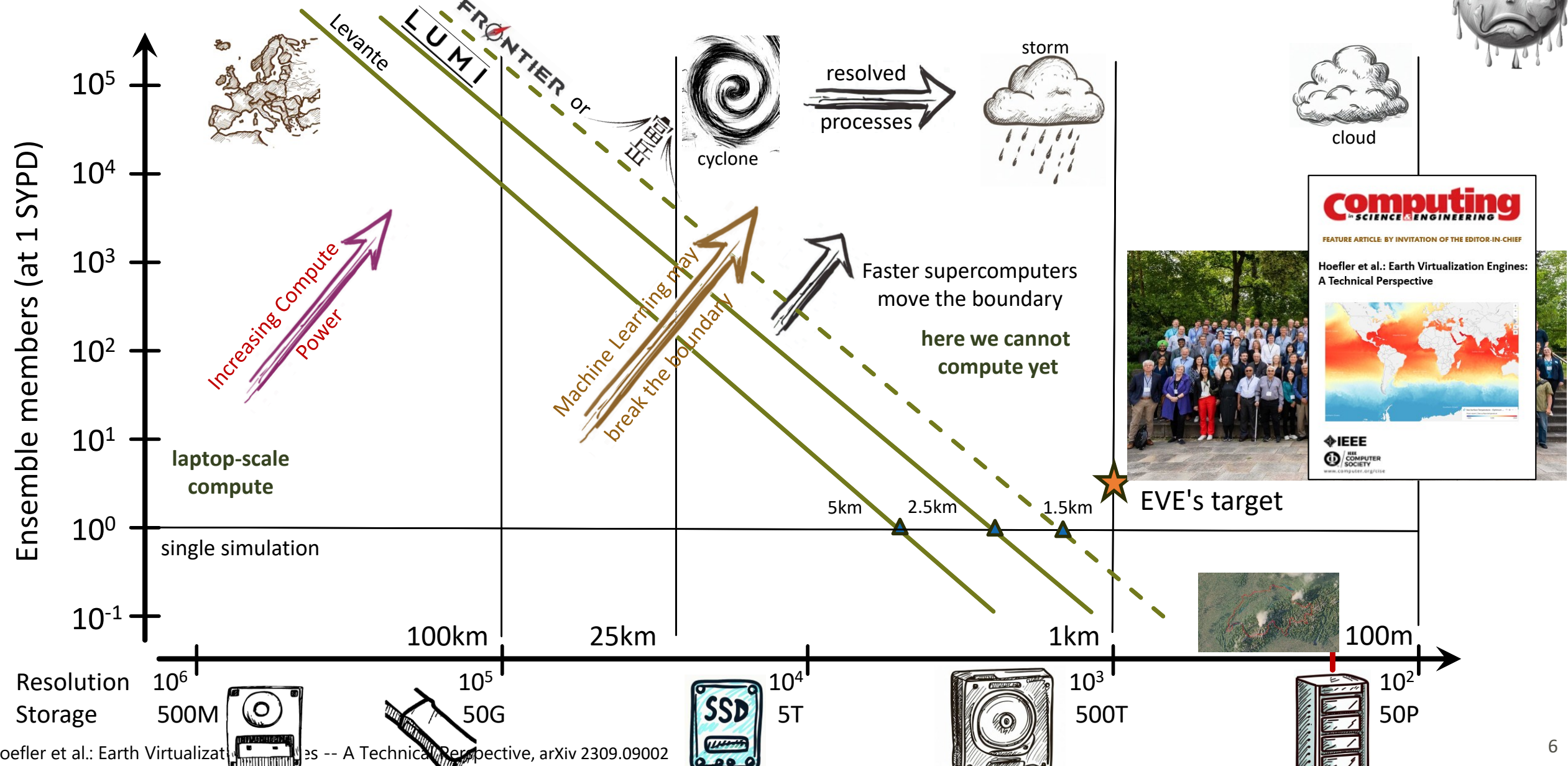

 Schweizerische Eidgenossenschaft
 Confédération suisse
 Confederazione Svizzera
 Confederaziun svizra

Federal Office of Meteorology and
 Climatology MeteoSwiss





Climate prediction is extremely demanding ("impossible" – decades long)



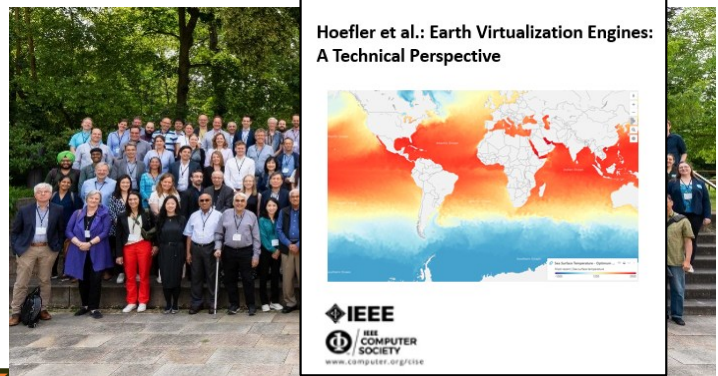
Computing
 IN SCIENCE & ENGINEERING

FEATURE ARTICLE BY INVITATION OF THE EDITOR-IN-CHIEF

Hoeffler et al.: Earth Virtualization Engines: A Technical Perspective



IEEE
 IEEE COMPUTER SOCIETY
 www.computer.org/ise



The three pillars of AI in Climate Sciences

Data

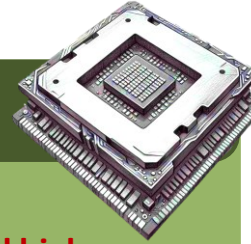


- Unstructured **observation data**
- Structured **simulation data**

Combine both to train models

- Learn physics and data-driven prediction

Compute



- AI models require **accelerated high-performance computing** for training

Accelerate AI computations

- Re-use infrastructure from LLMs and related generative AI methods (GNN, CNN)

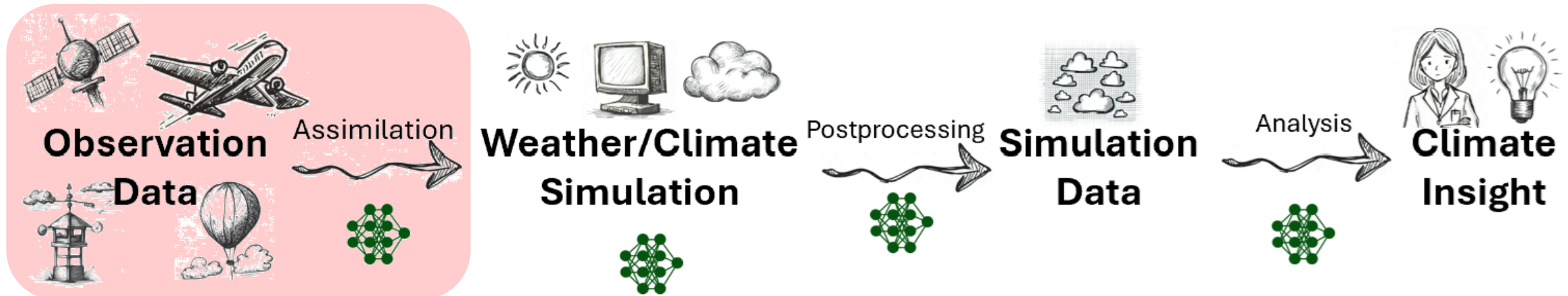
Models



- Models need to provide the right structural bias/prior

Develop better AI methods

- Step 1: use generative AI models: tformer, CNN, GNN, Diffusion, etc.
- Step 2: use **automatically parameterized physics-based models** encoding equations

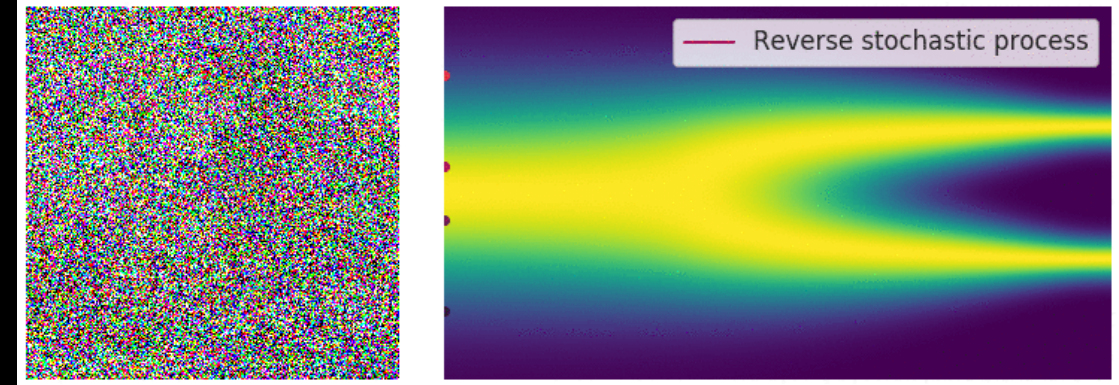
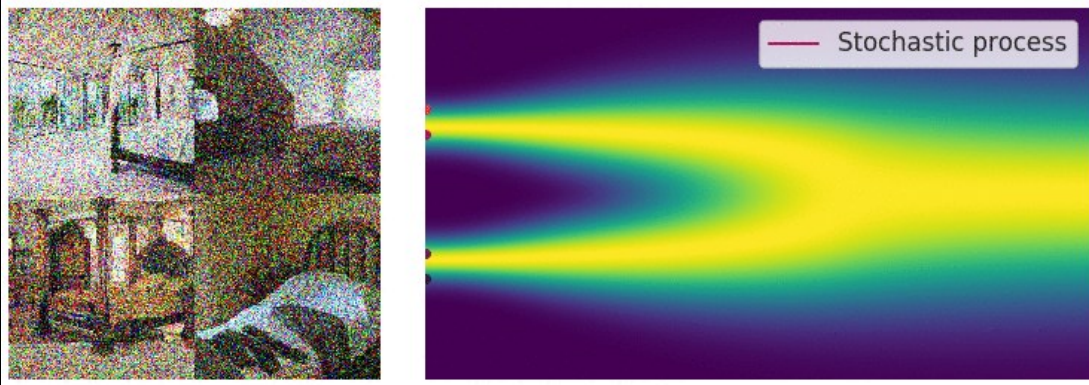


Diffusion-based Data Assimilation





How do diffusion models work?



source: medium.com – Vadim Titko



DiffDA: A Diffusion Model for Weather-scale Data Assimilation

DiffDA: A Diffusion Model for Weather-scale Data Assimilation

Langwen Huang¹ Lukas Gianinazzi¹ Yuejiang Yu¹ Peter D. Dueben² Torsten Hoefler¹

Abstract

The generation of initial conditions via accurate data assimilation is crucial for weather forecasting and climate modeling. We propose DiffDA as a denoising diffusion model capable of assimilating atmospheric variables using predicted states and sparse observations. Exploiting the similarity between a weather forecasting model and a denoising diffusion model dedicated to weather applications, we adapt the pretrained GraphCast neural network as the backbone of the diffusion model. Through experiments based on simulated observations from the ERA5 reanalysis dataset, our method can produce assimilated global atmospheric data consistent with observations at 0.25° (≈30km) resolution globally. This marks the highest resolution achieved by ML data assimilation models. The experiments also show that the initial conditions assimilated from sparse observations (less than 0.96% of gridded data) and 48-hour forecast can be used for forecast models with a loss of lead time of at most 24 hours compared

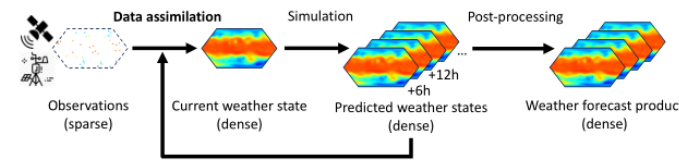
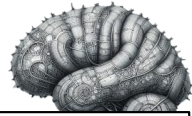


Figure 1. Diagram of a numerical weather forecasting pipeline. It consists of data assimilation, simulation and post-processing. Data assimilation produces gridded values from sparse observations and predicted gridded values from previous time steps. Simulation takes in gridded values and produces predictions in gridded values at future time steps. Post-processing improves prediction so that it is closer to future observations.

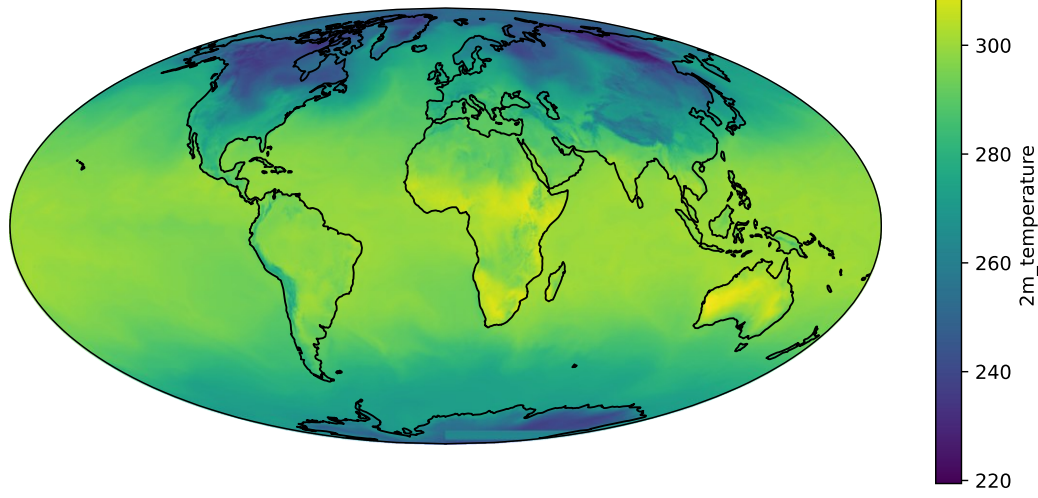
observations from various locations. The quality of these weather simulation models depends heavily on data assimilation, as errors in initial conditions are one of the main sources of forecast error (Bonavita et al., 2016). Additionally, data assimilation is employed in creating reanalysis datasets, which contain reconstructed historical weather variables as gridded fields. These reanalysis datasets play

32v3 [cs.CE] 10 Jun 2024

Case study: Assimilated 2m temperature at 2022-01-03 06z

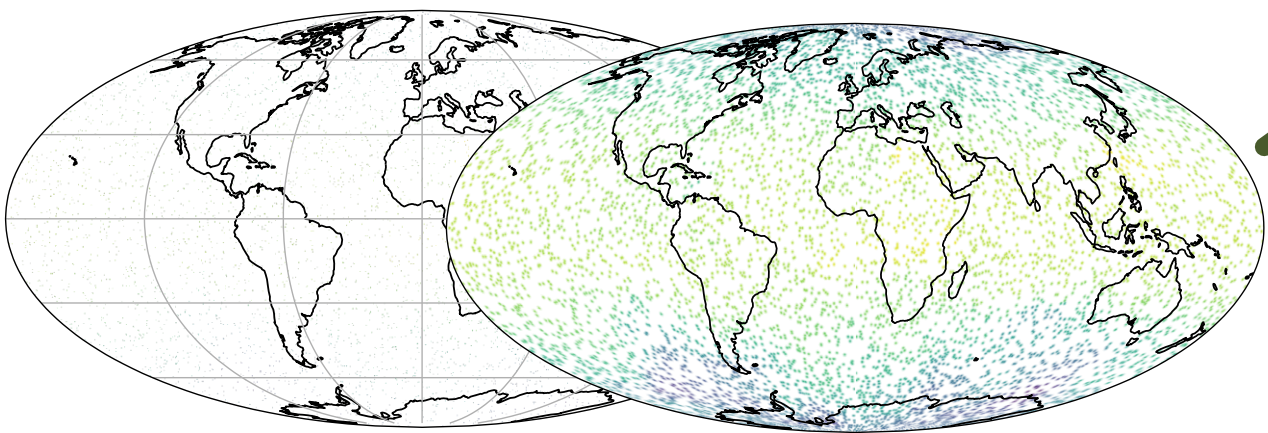


+48h GraphCast Forecast

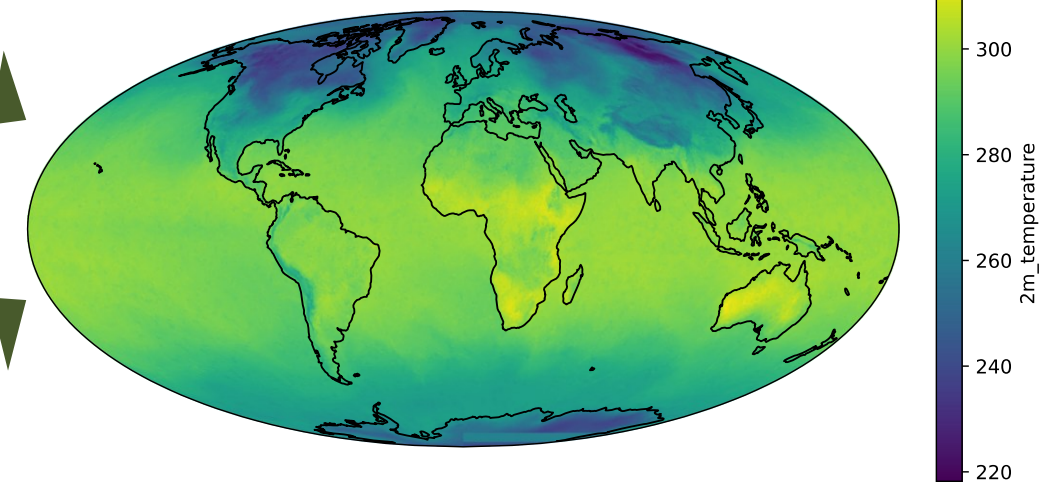


+48h Sparse Observations

+softmask



DiffDA: Diffusive Assimilation



**How good is this really?
 Let's look at Errors!**

DiffDA: A Diffusion Model for Weather-scale Data Assimilation

Langwen Huang¹ Lukas Gianinazzi¹ Yuejiang Yu¹ Peter D. Dueben² Torsten Hoefler¹

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 The generation of initial conditions via accurate data assimilation is crucial for weather forecasting and climate modeling. We propose DiffDA, as a denoising diffusion model capable of assimilating atmospheric variables using predicted states and sparse observations. Exploiting the similarity between a weather forecasting model and a denoising diffusion model dedicated to weather applications, we adapt the pretrained GraphCast neural network as the backbone of the diffusion model. Through experiments based on simulated observations from the ERA5 reanalysis dataset, our method can produce assimilated global atmospheric data consistent with observations at 0.25° (≈20km) resolution globally. This marks the highest resolution achieved by ML data assimilation models. The experiments also show that the initial conditions assimilated from sparse observations (less than 0.06% of gridded data) and 48-hour forecast can be used for forecast models with a loss of lead time of at most 24 hours compared

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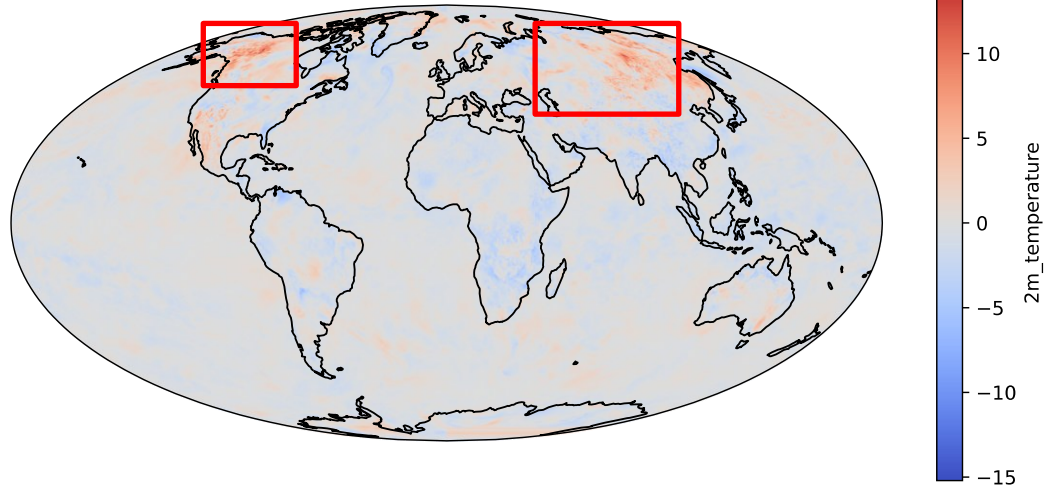
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32v3 [cs,CE] 10 Jun 2024

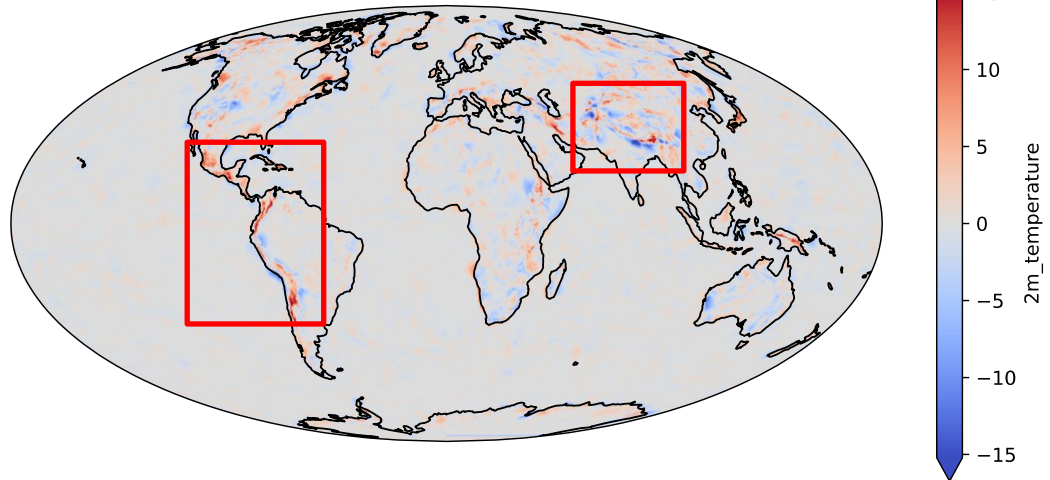
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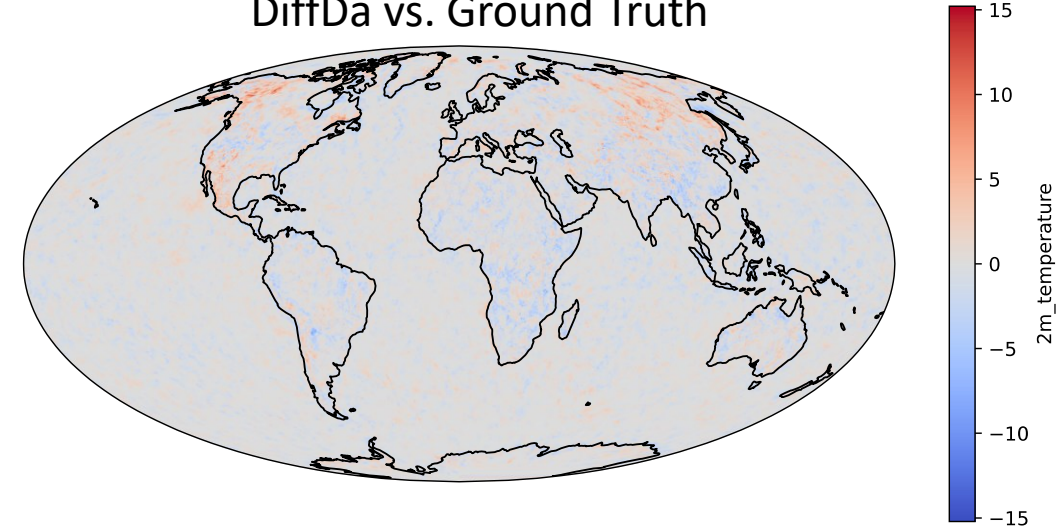
+48h GraphCast Forecast vs. Ground Truth



+48h Interpolation vs. Ground Truth



DiffDa vs. Ground Truth



DiffDa-Assimilated data is better than both, forecast and interpolated observations

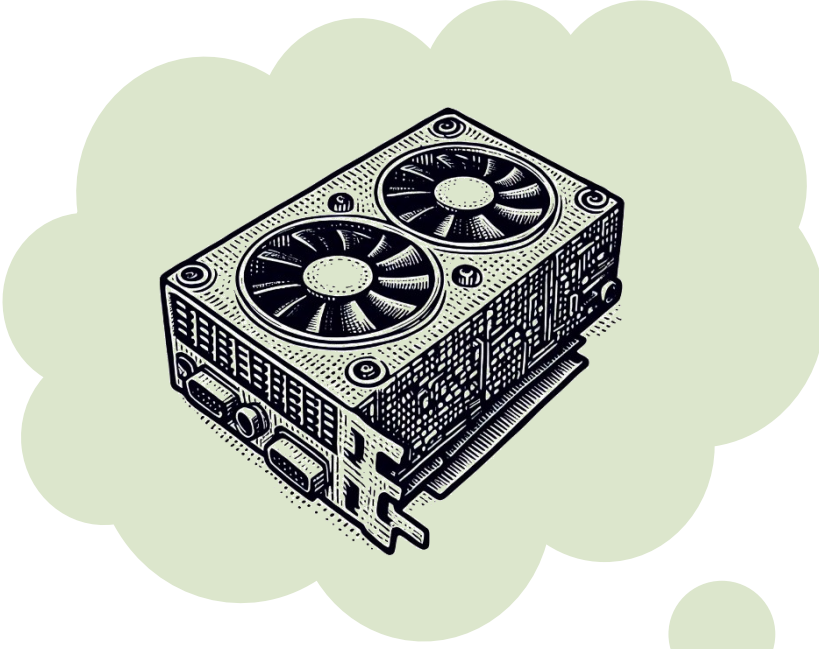
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32v3 [cs,CE] 10 Jun 2024



```

!$ACC DATA &
!$ACC PRESENT(density1,energy1) &
!$ACC PRESENT(vol_flux_x,vol_flux_y,volume,mass_flux_x,mass_flux_y,vertexdx,vertexdy) &
!$ACC PRESENT(pre_vol,post_vol,ener_flux)

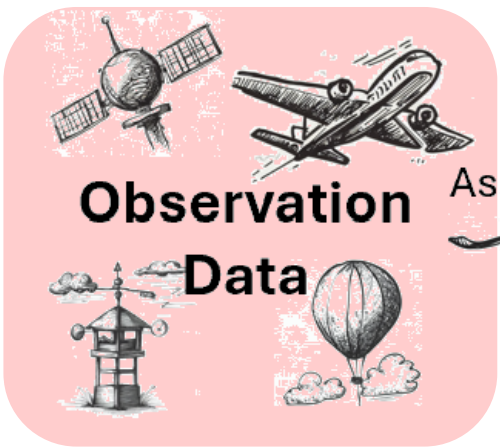
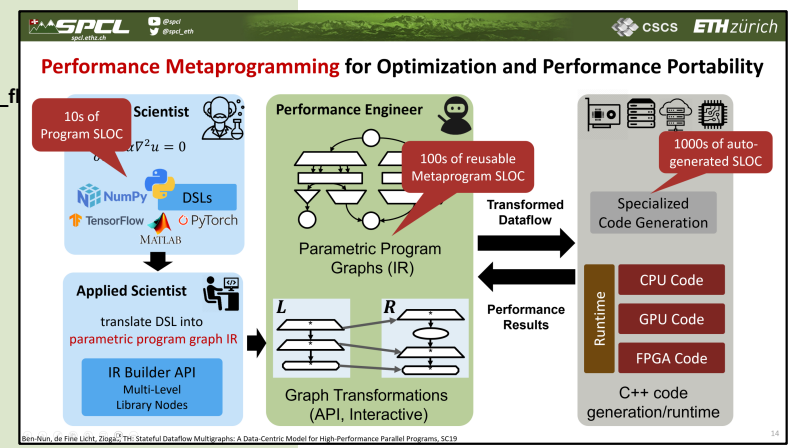
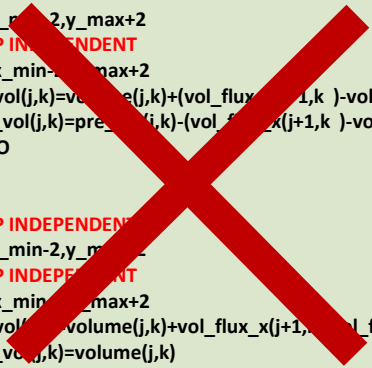
!$ACC KERNELS

IF(dir.EQ.g_xdir) THEN

IF(sweep_number.EQ.1)THEN

!$ACC LOOP INDEPENDENT
DO k=y_min-2,y_max+2
!$ACC LOOP INDEPENDENT
DO j=x_min-2,x_max+2
pre_vol(j,k)=volume(j,k)+(vol_flux_x(j+1,k)-vol_flux_x(j,k)+vol_flux_x(j,k)-vol_flux_x(j-1,k))
post_vol(j,k)=pre_vol(j,k)-(vol_flux_x(j+1,k)-vol_flux_x(j,k))
ENDDO
ENDDO
ELSE
!$ACC LOOP INDEPENDENT
DO k=y_min-2,y_max+2
!$ACC LOOP INDEPENDENT
DO j=x_min-2,x_max+2
pre_vol(j,k)=volume(j,k)+vol_flux_x(j+1,k)-vol_flux_x(j,k)
post_vol(j,k)=volume(j,k)
ENDDO
ENDDO
ENDIF
  
```

AI?



Assimilation



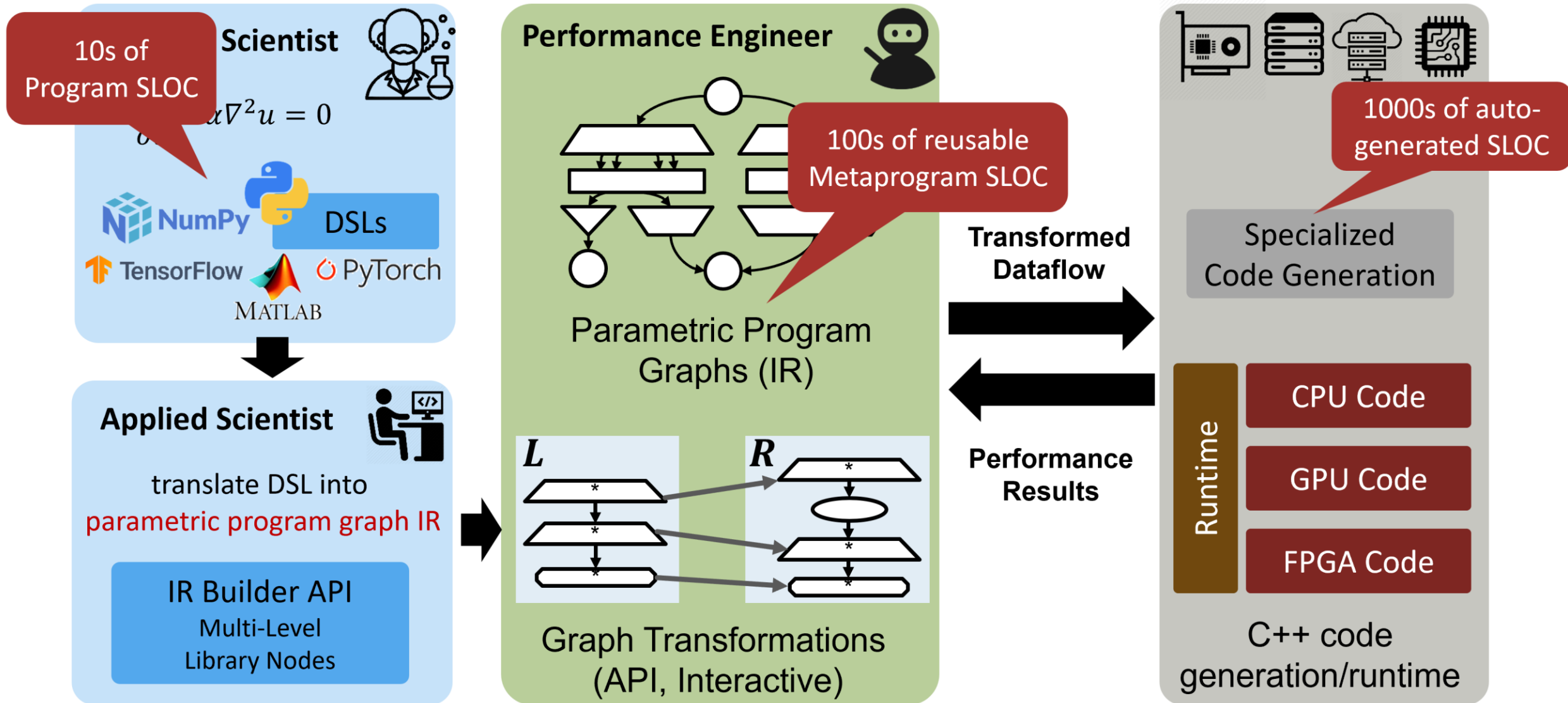
Postprocessing



Analysis



Performance Metaprogramming for Optimization and Performance Portability



Pace in DaCe for **Performance Metaprogramming** – 12k SLOC Python

AI-based Transfer Tuning to the Rescue!



Another real production code ... ECMWF's CLOUDSC

```

9
10 SUBROUTINE CLOUDSC &
11 !---input
12 & (KIDIA, KFDIA, KLON, KLEV, &
13 & PTSPHY,&
14 & PT, PQ, tendency_cml,tendency_tmp,tendency_loc, &
15 & PVFA, PVFL, PVFI, PDYNA, PDYNL, PDYNI, &
16 & PHRSW, PHRLW,&
17 & PVERVEL, PAP, PAPH,&
18 & PLSM, LDCUM, KTYPE, &
19 & PLU, PLUDE, PSNDE, PMFU, PMFD,&
20 !---prognostic fields
21 & PA,&
22 & PCLV, &
23 & PSUPSAT,&
24 !-- arrays for aerosol-cloud interactions
25 !!! & PQAER, KAER, &
26 & PLCRIT_AER,PICRIT_AER,&
27 & PRE_ICE,&
28 & PCCN, PNICE,&
29 !---diagnostic output
30 & PCOVPTOT, PRAINFRAC_TOPRFZ,&
31 !---resulting fluxes
32 & PFSQLF, PFSQIF, PFCQNG, PFCQLNG,&
33 & PFSQRF, PFSQSF, PFCQRNG, PFCQSNG,&
34 & PFSQLTUR, PFSQITUR, &
35 & PFPLSL, PFPLSN, PFHPSL, PFHPSN, KFLDX, &
36 & YDCST, YDTHF, YDECLDP)
  
```

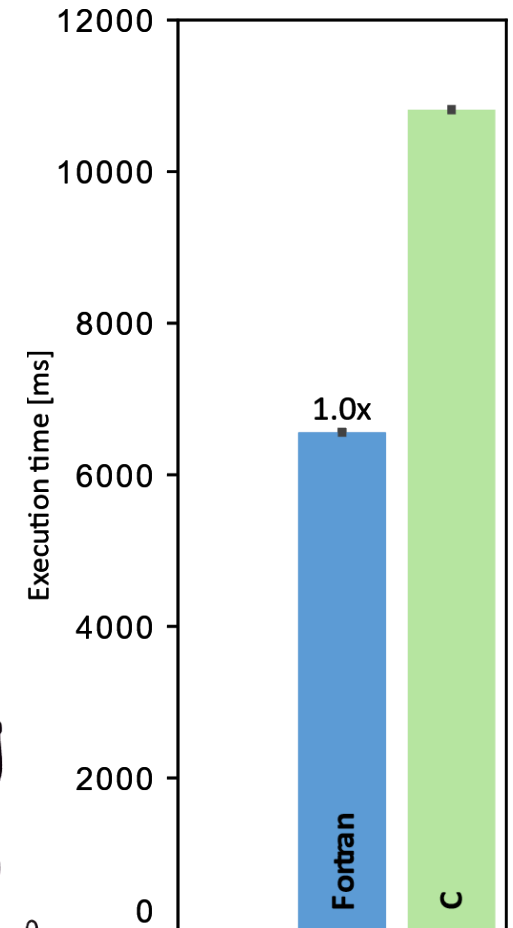
... variable setup/initialization until line 500 ;-)

- **Cloud Microphysics of IFS**
 - Resolve sub-grid features
 - Original 2,525 SLOC of **Fortran 95**

- **Rewritten for performance portability benchmarking (optimization took months!)**
 - 2,635 SLOC C
 - 2,610 SLOC C++/CUDA

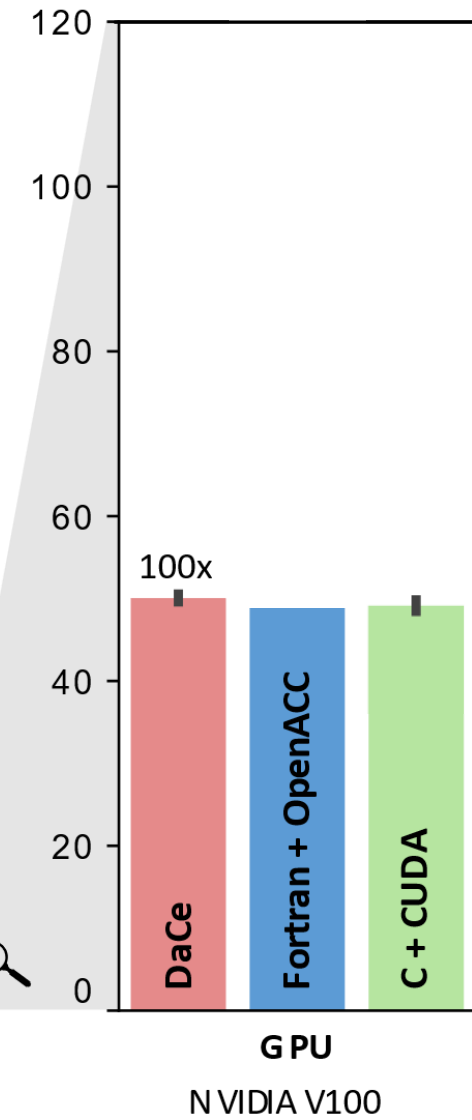
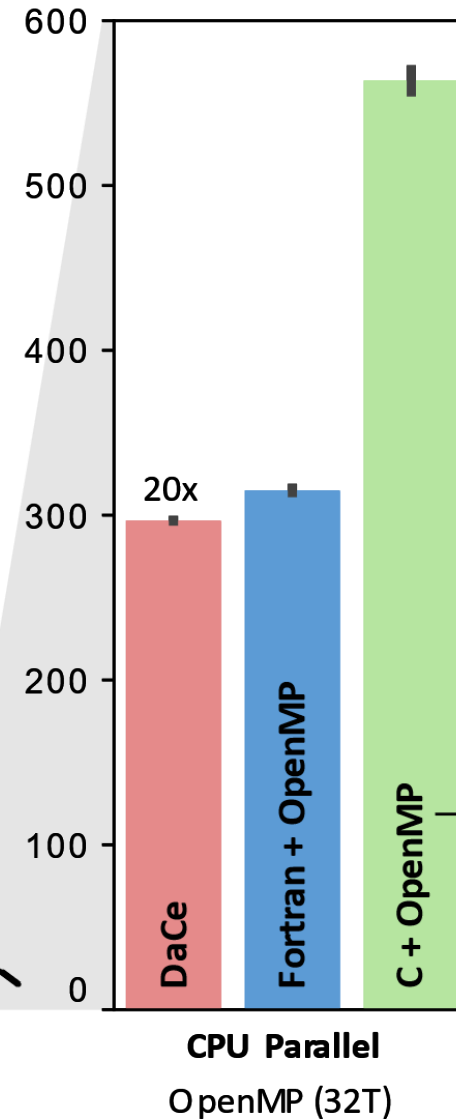
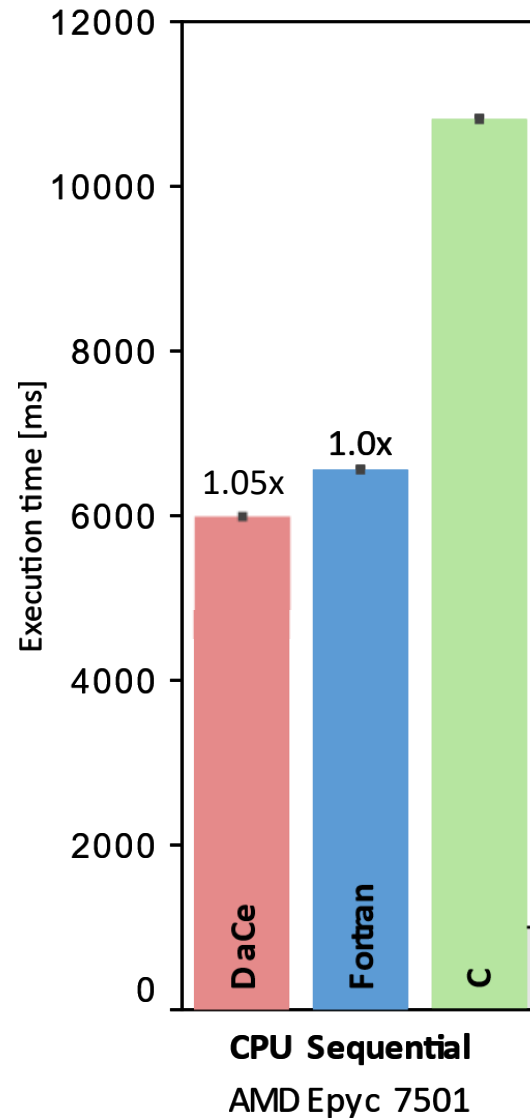
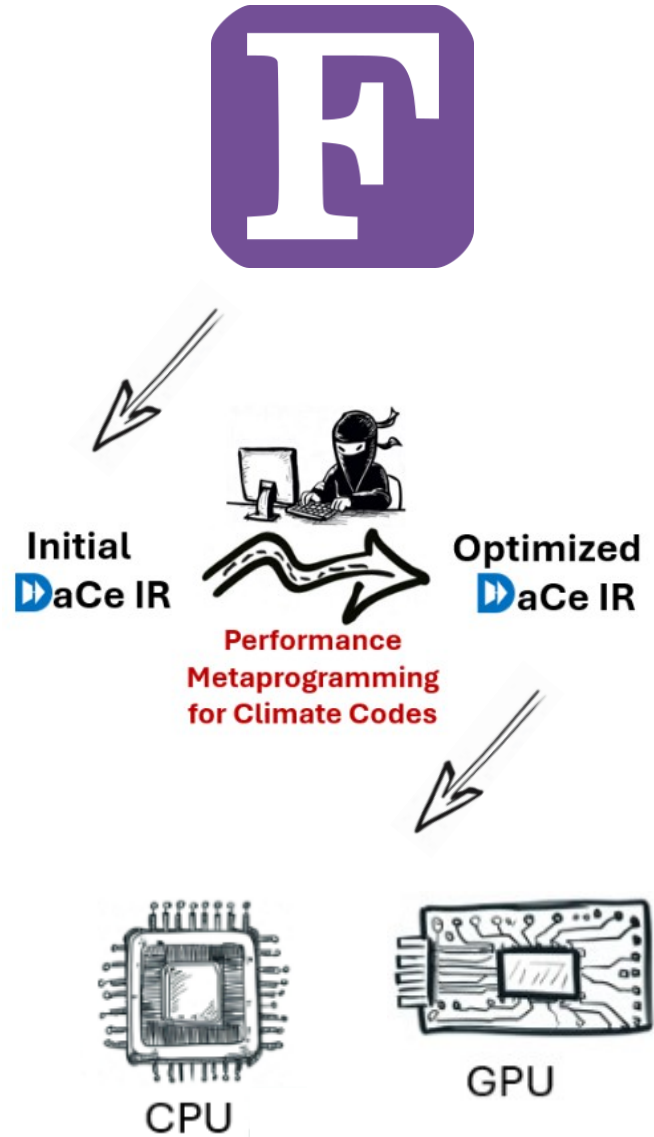


<https://github.com/ecmwf-ifs/dwarf-p-cloudsc>



CPU Sequential
AMD Epyc 7501

Performance Metaprogramming – from the **unchanged** CLOUDSC Fortran code!



The three pillars of AI in Climate Sciences

Data



- Unstructured **observation data**
- Structured **simulation data**

Combine both to train models

- Learn physics and data-driven prediction

Compute



- AI models require **accelerated high-performance computing** for training

Accelerate AI computations

- Re-use infrastructure from LLMs and related generative AI methods (GNN, CNN)

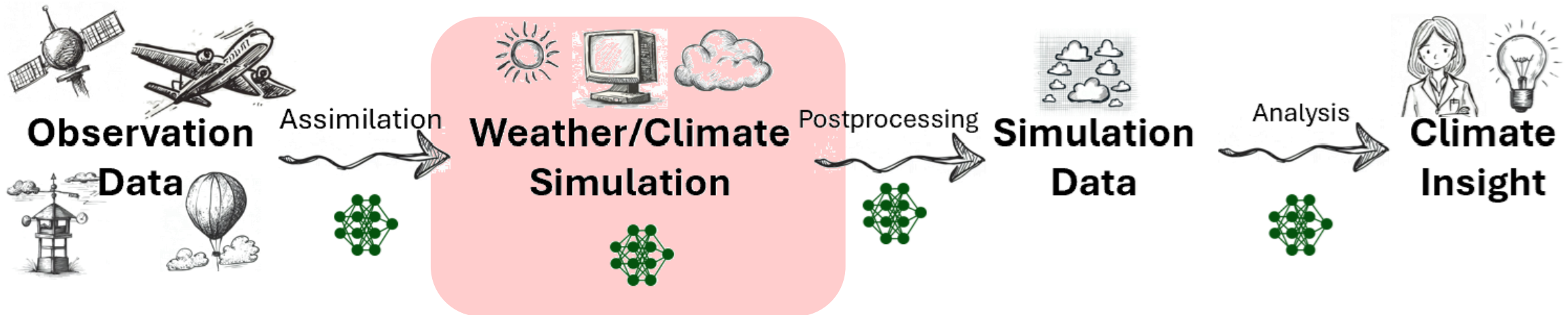
Models



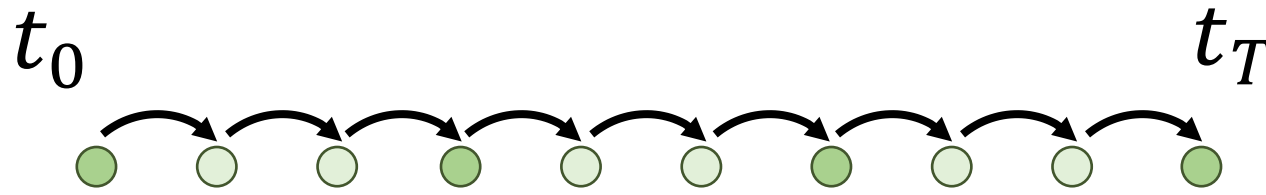
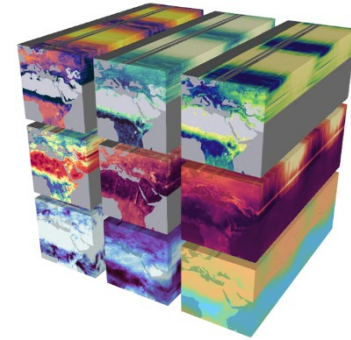
- Models need to provide the right structural bias/prior

Develop better AI methods

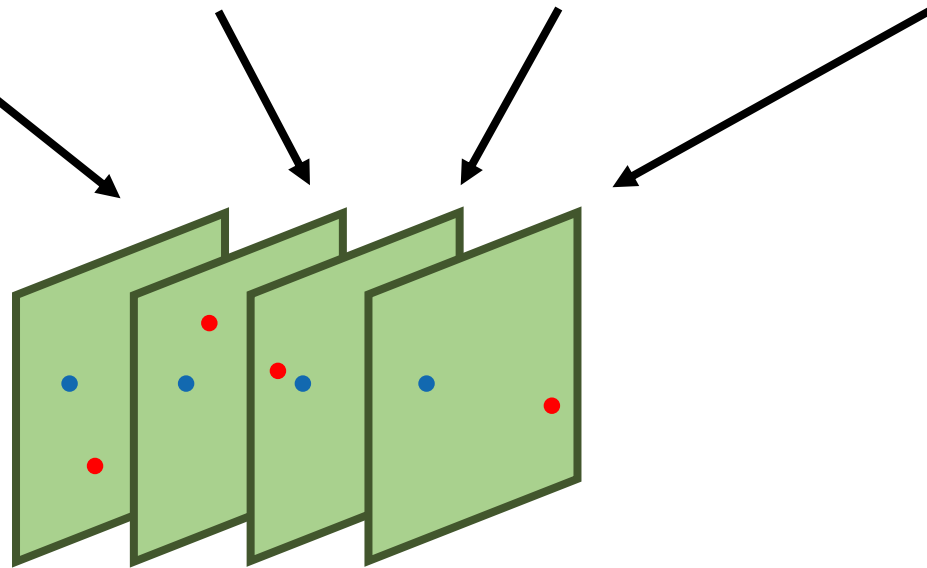
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- Step 2: use **automatically parameterized physics-based models** encoding equations



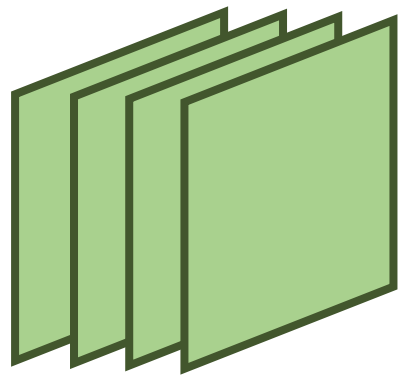
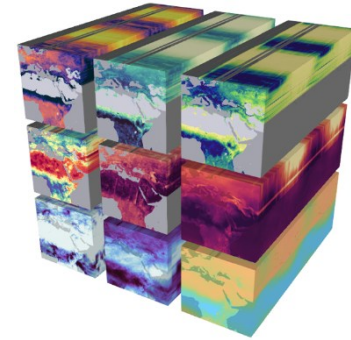
Simulation runs time-stepping forward



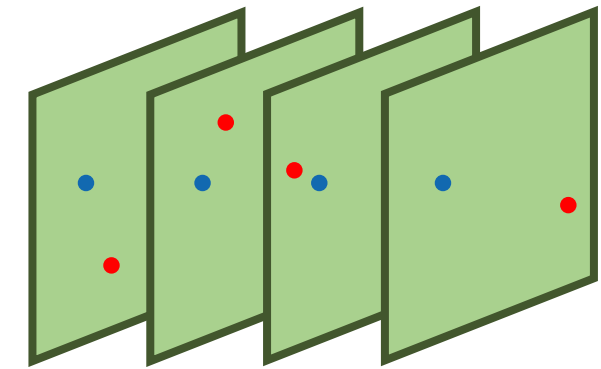
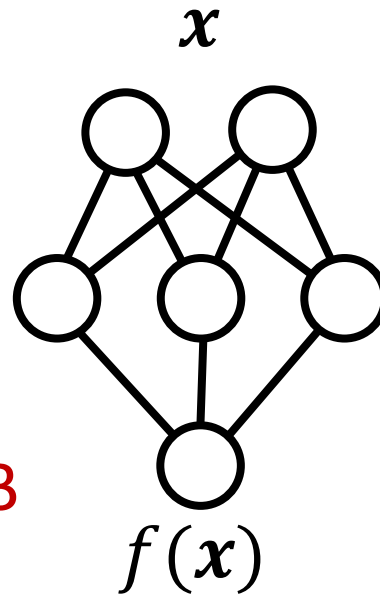
Store some timesteps!



Analysis access pattern is often **strided** or even **random**



Compress/Train
300 x – 3,000 x
15.6GB → 13.8MB

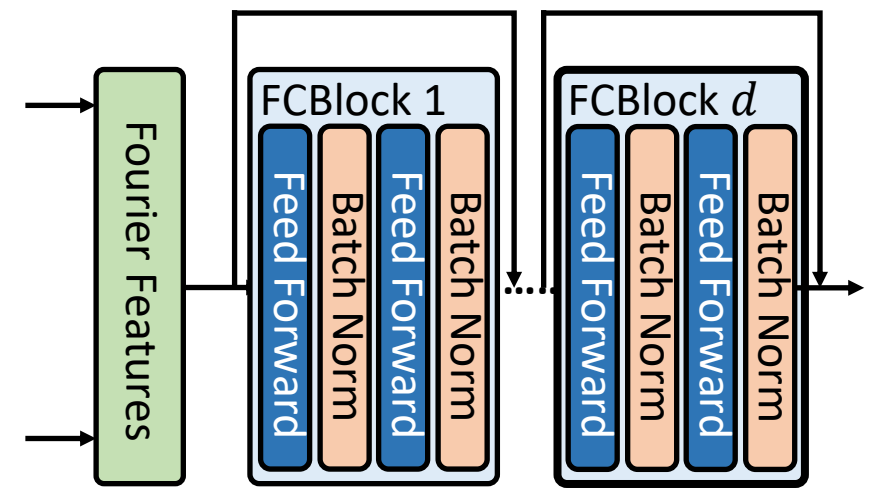
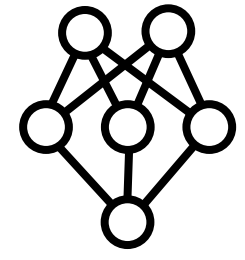


Multidimensional Data

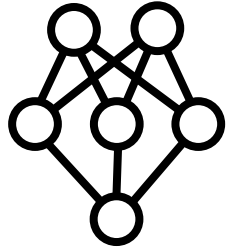
Neural Representation

Analysis Queries

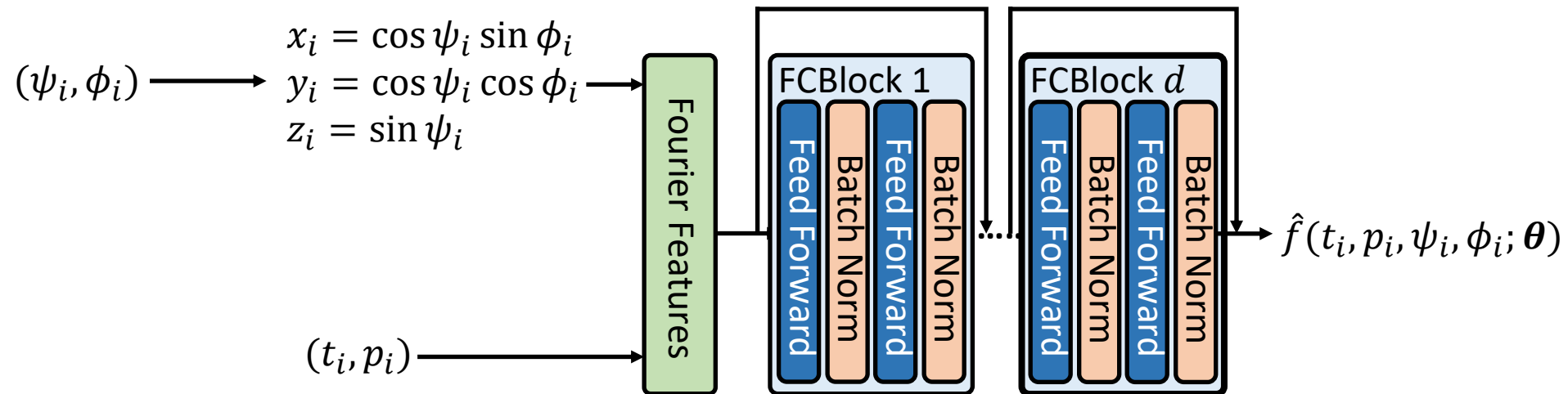
Neural Network Structure



Neural Network Structure

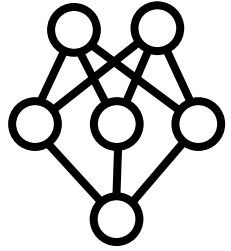


Decompression / Inference

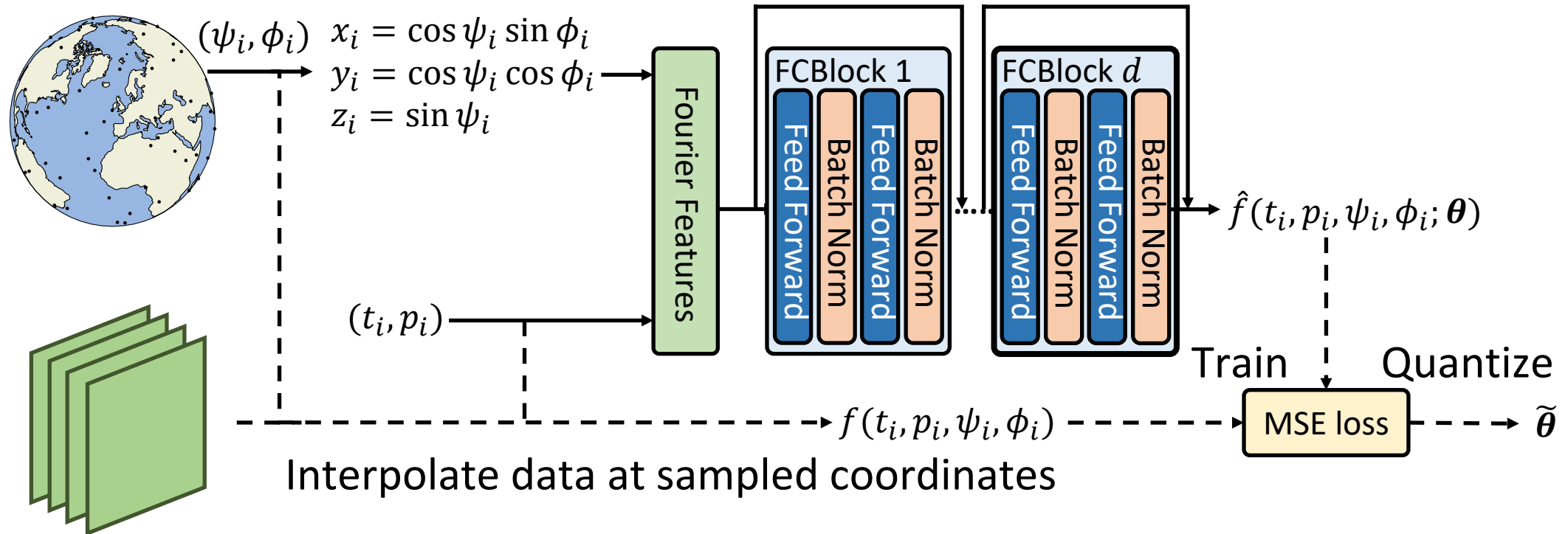


- On-demand decompression
- Fully utilize GPUs

Neural Network Structure

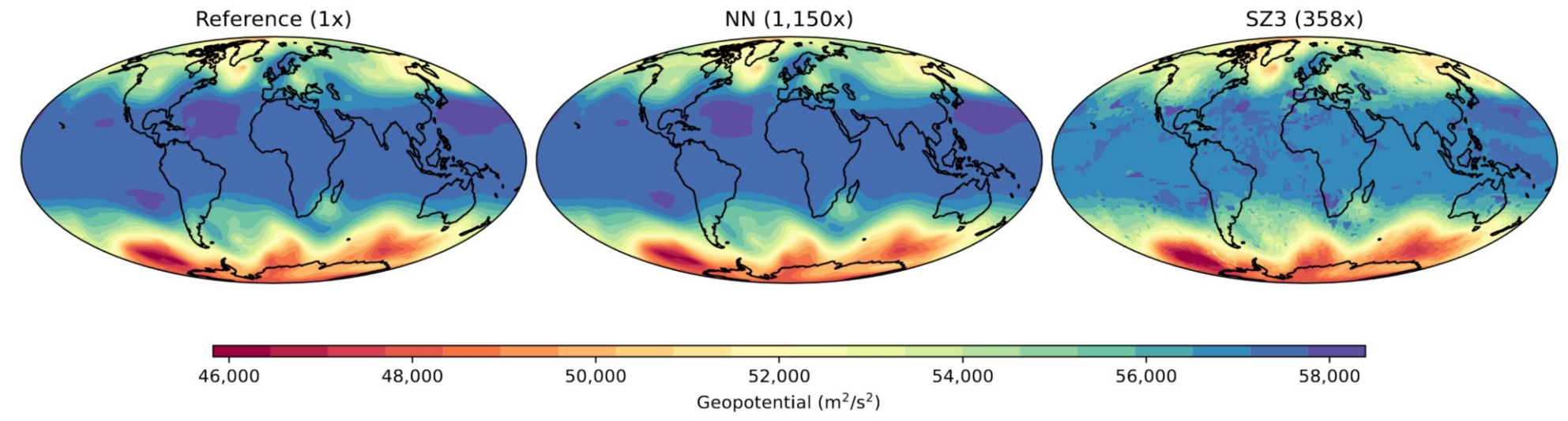


Compression / Training



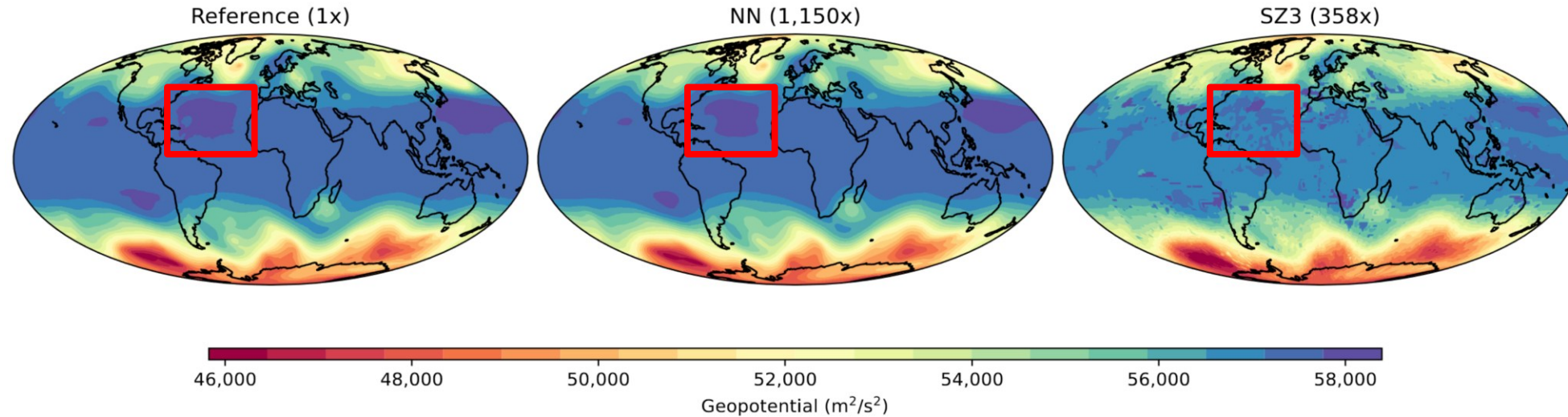
Evaluation: Case Study

Geopotential at 500hPa, 2016 Oct 5th



Evaluation: Case Study

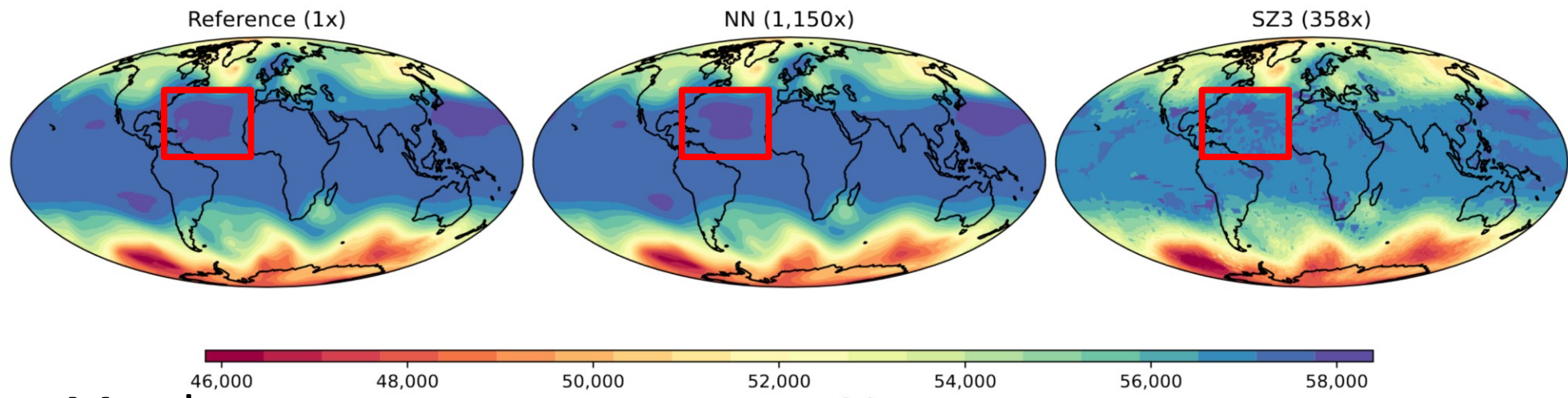
Geopotential at 500hPa, 2016 Oct 5th



Preserves general shapes of important events and average values without introducing significant artifacts

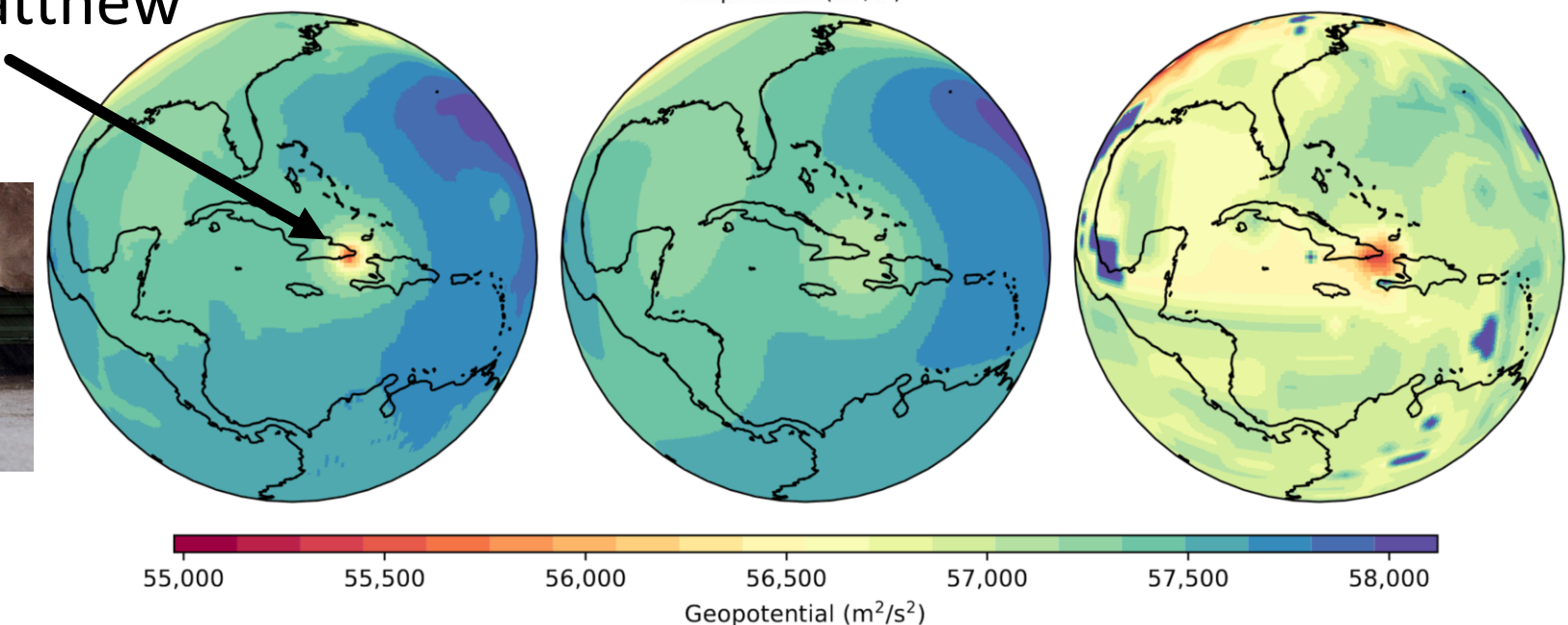
Evaluation: Case Study

Geopotential at 500hPa, 2016 Oct 5th



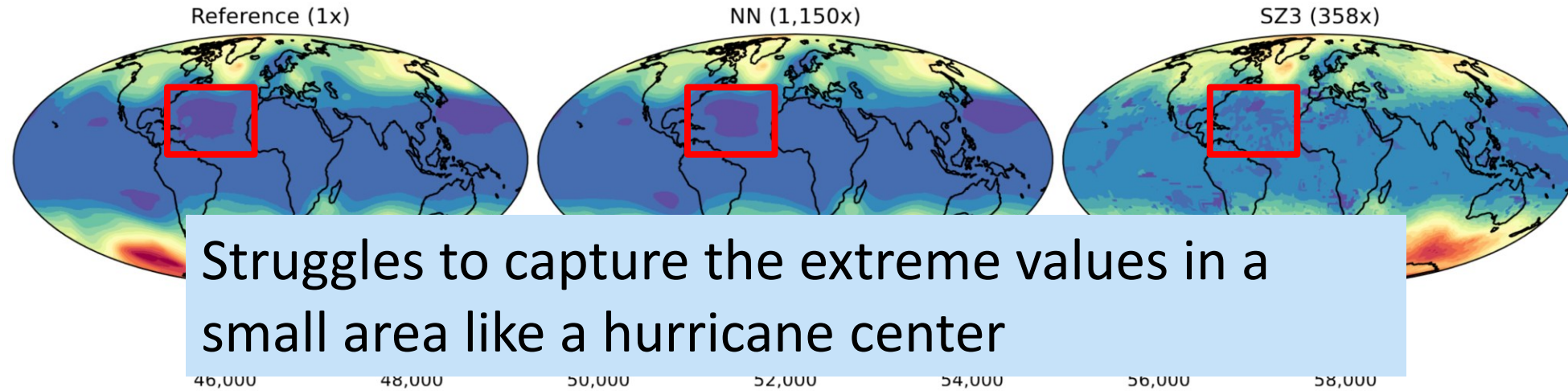
Hurricane Matthew

16.5bn damage
603 fatalities



Evaluation: Case Study

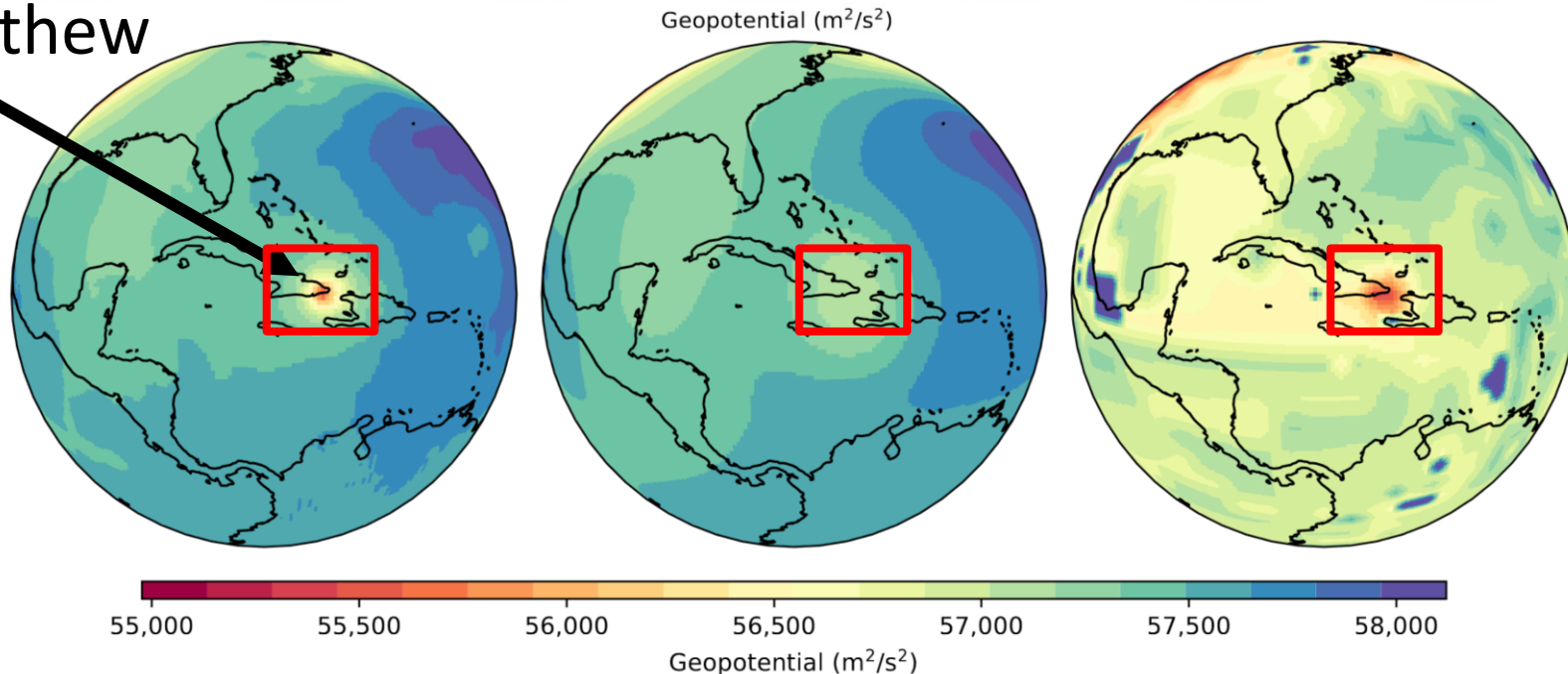
Geopotential at 500hPa, 2016 Oct 5th



Struggles to capture the extreme values in a small area like a hurricane center

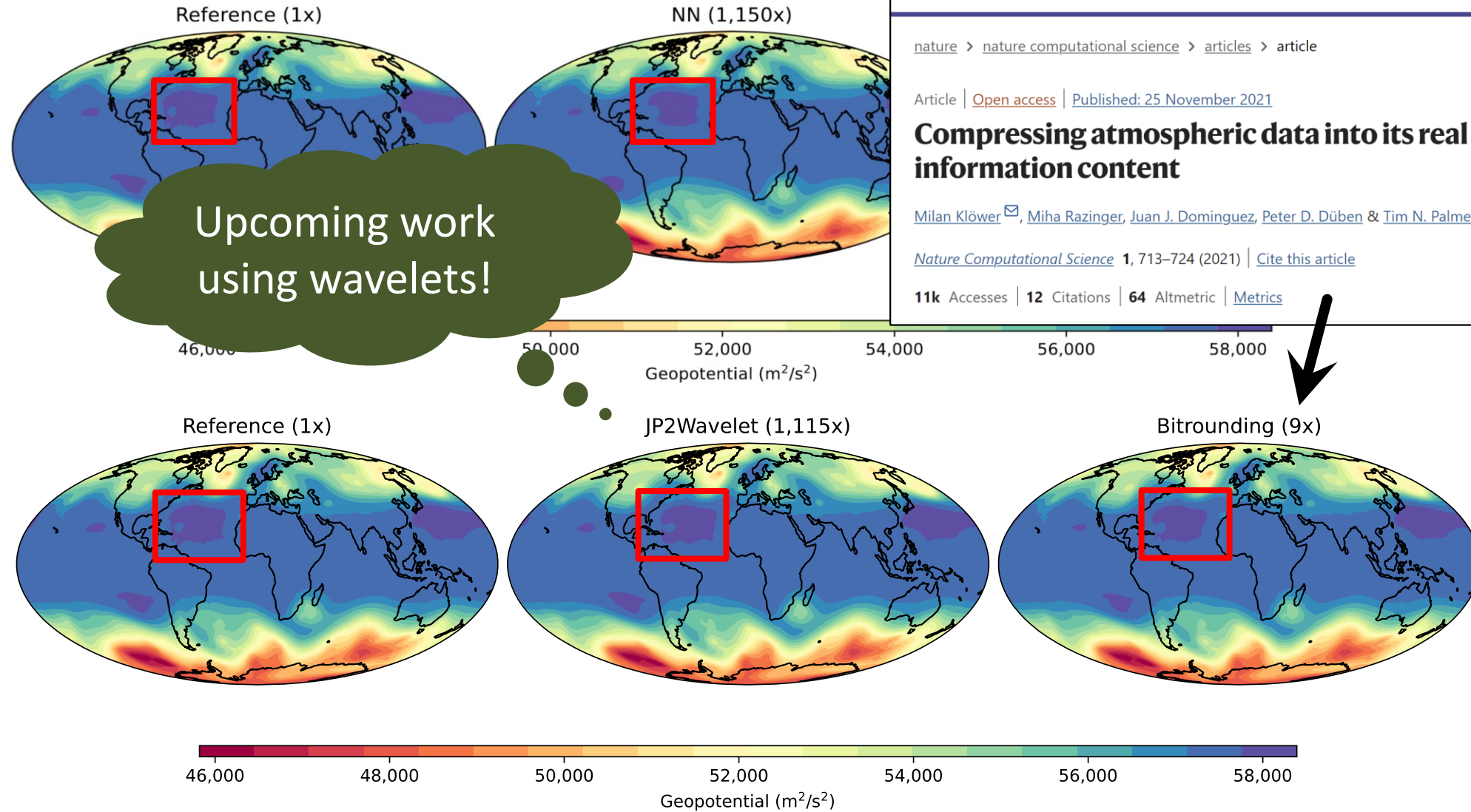
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603 fatalities



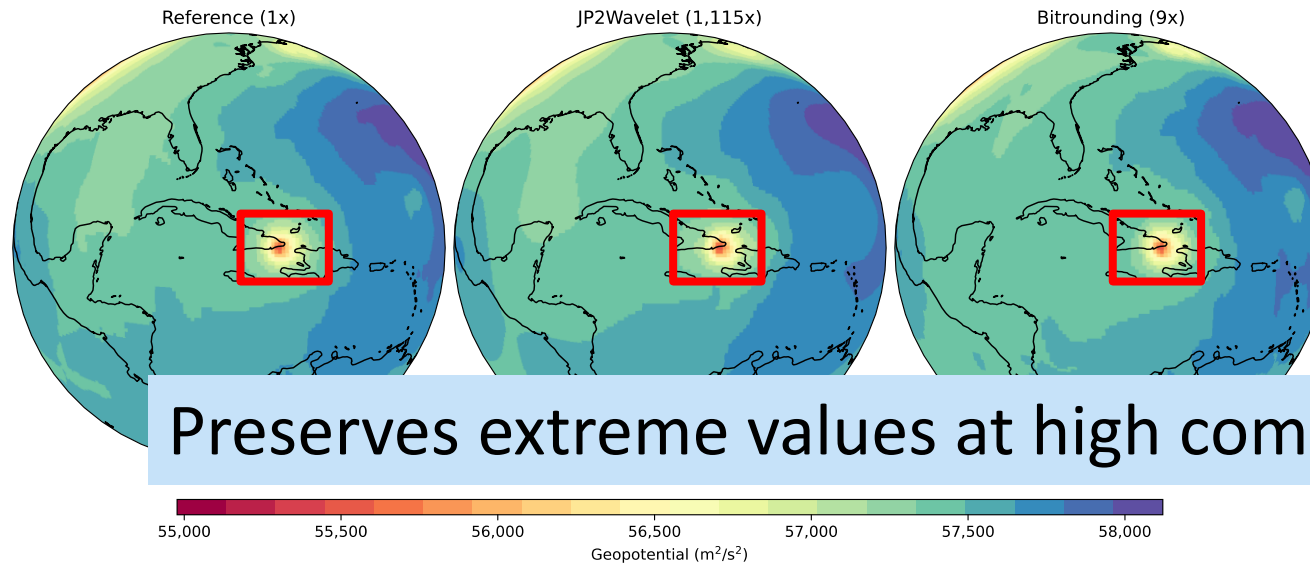
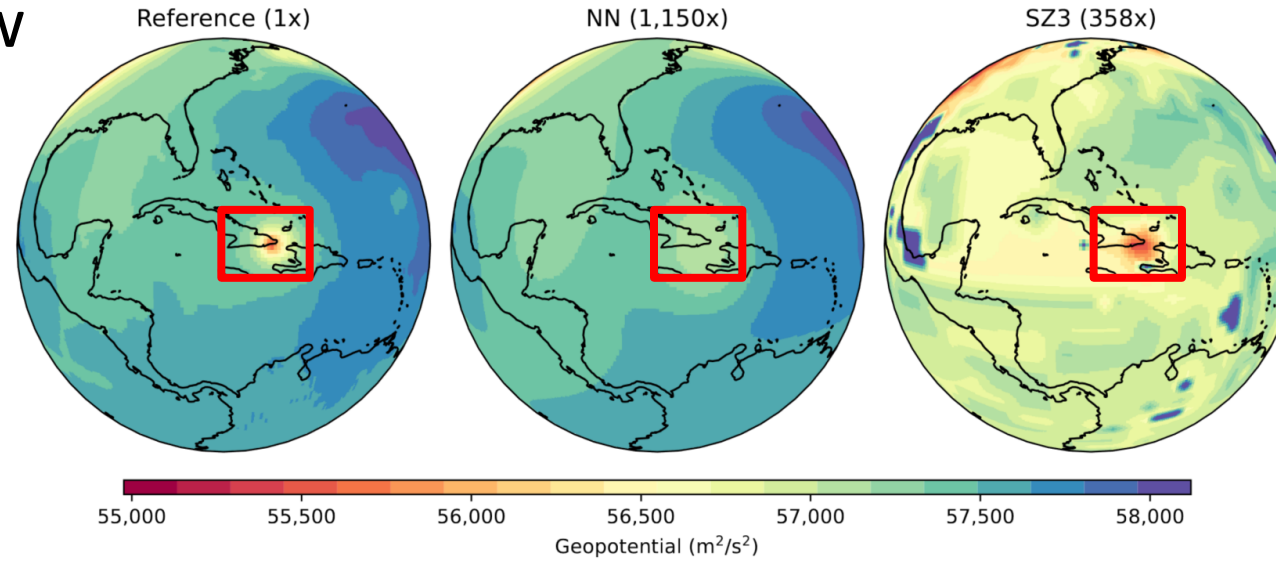
Evaluation: Case Study

Geopotential at 500hPa, 2016



Evaluation: Case Study

Hurricane Matthew



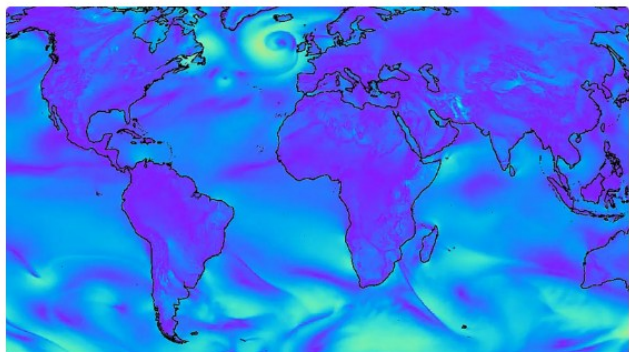
Preserves extreme values at high compression ratio

Is AI based weather and climate prediction a solved problem?

Google DeepMind's AI Weather Forecaster Handily Beats a Global Standard

Machine learning algorithms that digested decades of weather data were able to forecast atmospheric measures more accurately than Europe's top weather center.

Wired, Nov. 23 **GraphCastNet**



Google DeepMind's GraphCast AI software produces weather forecasts for weather variables like wind speed much faster than traditional simulations. COURTESY OF GOOGLE

NVIDIA's New AI Model Revolutionizes Extreme Weather Forecasting with Unprecedented Accuracy FourCastNet

August 20, 2024 by Ali Azhar

Pangu Weather Model

AI Weather Prediction More Accurate, in Just Seconds

Pangu Weather

Huawei Cloud's Pangu-Weather Model is the first AI model that can predict weather more accurately (NWP) methods, and at a speed that is 10,000 times faster. In the past, predicting the path of a typhoon on a high-performance cluster of 3,000 servers took 10 minutes. Now, Pangu-Weather can do that in 10 seconds on a global weather forecast within seconds, with all factors taken into consideration, such as geopotential pressure. Besides typhoon paths, it can also accurately predict precipitation, cold and heat waves, and

Introducing Prithvi WxC, a new general-purpose AI model for weather and climate

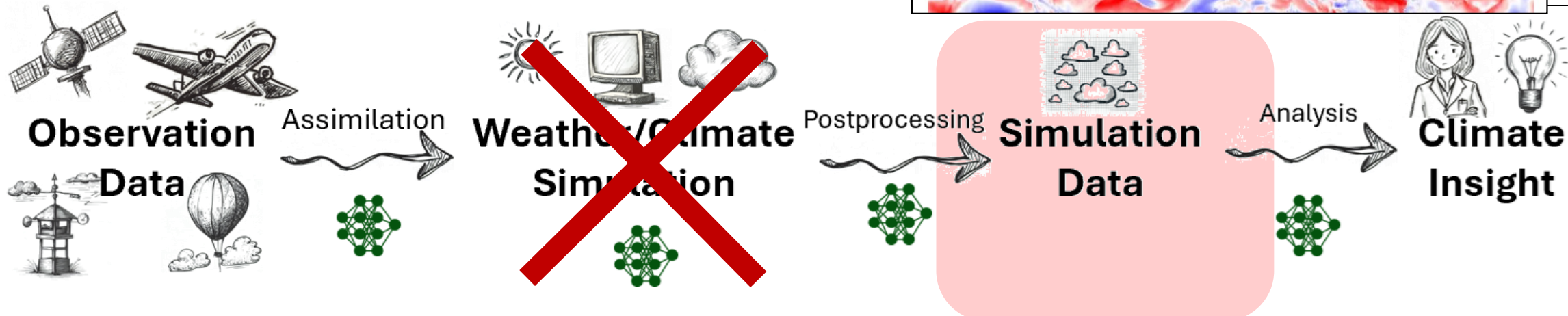
Sept. 2024

In collaboration with NASA, IBM is releasing an open-source foundation model that can be customized for a variety of weather and climate-related applications — and run on a desktop computer.



Record-breaking heat units and precipitation annually in the

AI?



Out of Distribution (Future) Case Study: Storm Ciarán (Nov. 2023)

npj | climate and atmospheric science

Article

Published in partnership with CECCR at King Abdulaziz University



<https://doi.org/10.1038/s41612-024-00638-w>

Do AI models produce better weather forecasts than physics-based models? A quantitative evaluation case study of Storm Ciarán



Andrew J. Charlton-Perez¹✉, Helen F. Dacre¹, Simon Driscoll^{1,2}, Suzanne L. Gray¹,
Ben Harvey^{1,3}, Natalie J. Harvey¹, Kieran M. R. Hunt^{1,3}, Robert W. Lee¹, Ranjini Swaminathan^{1,2},
Remy Vandaele^{1,2} & Ambrogio Volonté^{1,3}

There has been huge recent interest in the potential of making operational weather forecasts using machine learning techniques. As they become a part of the weather forecasting toolbox, there is a

GraphCastNet

Pangu Weather

FourCastNet

VS.

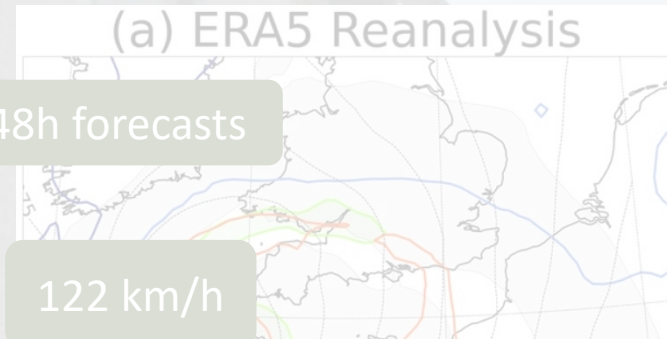


16 dead, gusts over 185 km/h
likely strongest since 1954
1.2m households w/o power
1m residents cut off phone
airports closed (e.g., AMS)

...

Out of Distribution (Future) Case Study: Storm Ciarán (Nov. 2023)

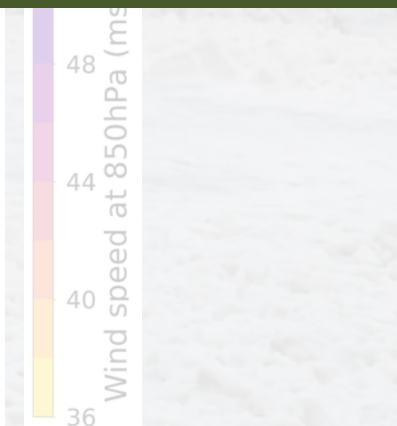
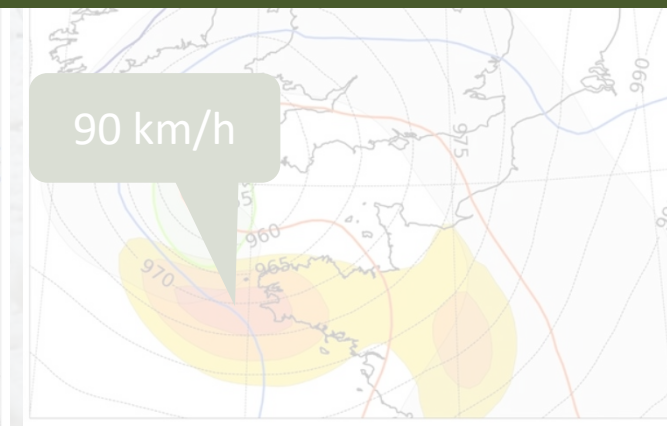
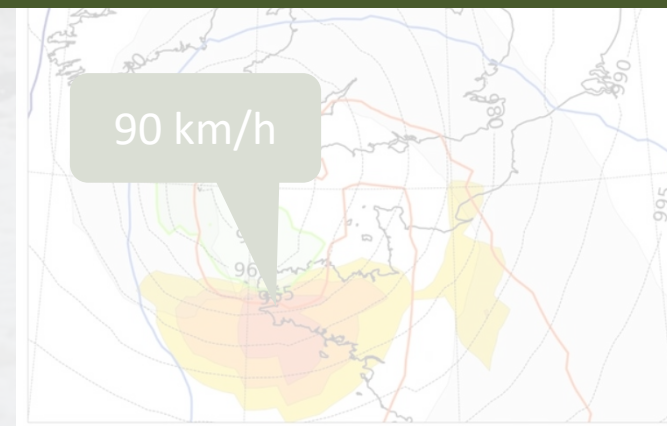
npj climate and atmospheric science
 Article
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 Andrew J. Charlton-Peay, Helen F. Diers, Simon Driscoll, Suzanne L. Gray, Ben Harvey, Natalie J. Harvey, Kieran M. R. Hart, Robert W. Lee, Raghav Srinivasan, Pooja Venkatesh & Rodrigo Velasco



Germany would issue

“more than 48 h before Storm Ciarán [...], forecasts of the rapid MSLP deepening and track of the storms produced by the ML models were essentially indistinguishable”

“when considering the damaging winds associated with Storm Ciarán in detail, forecasts from the ML models had significant errors and poorer performance than conventional NWP models”



Why? A deeper look inside some physics in ML-based Weather Prediction

Physics Case Study: Typhoon Doksuri, July 2023 (SE Asia, 137 dead, \$28.4bn damage – strongest in region in 2023)

 **AGU** ADVANCING
EARTH AND
SPACE SCIENCES

Geophysical Research Letters®


RESEARCH LETTER

10.1029/2023GL107377

Key Points:

- Forecasts from Machine Learning (ML) models have energy spectra notably different from those of their training reanalysis fields and Numerical Weather Prediction models
- This results in overly smooth predictions and weather phenomena at spatial scales shorter than 300–400 km are not properly represented
- Fundamental physical balances and derived quantities are not realistically represented in the forecasts of the ML models

On Some Limitations of Current Machine Learning Weather Prediction Models


Massimo Bonavita¹ 

¹ECMWF, Reading, UK

Abstract Machine Learning (ML) is having a profound impact in the domain of Weather and Climate Prediction. A recent development in this area has been the emergence of fully data-driven ML prediction models which routinely claim superior performance to that of traditional physics-based models. We examine some aspects of the forecasts produced by three of the leading current ML models, Pangu-Weather, FourCastNet and GraphCast, with a focus on their fidelity and physical consistency. The main conclusion is that these ML models are not able to properly reproduce sub-synoptic and mesoscale weather phenomena and lack the fidelity and physical consistency of physics-based models and this has impacts on the interpretation of their forecasts and

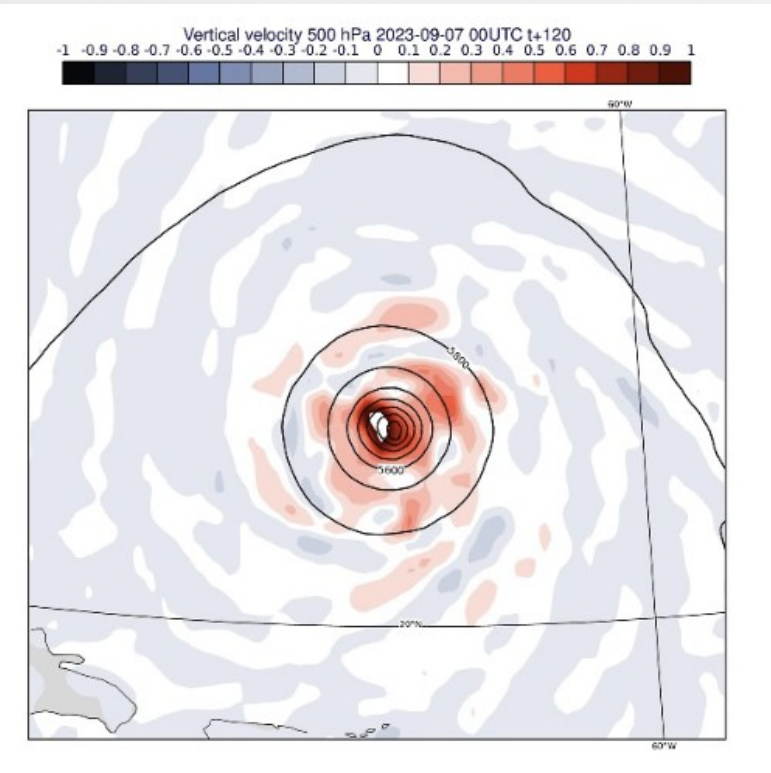
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Physics Case Study: Typhoon Doksuri, July 2023 (SE Asia, 137 dead, \$28.4bn damage – strongest in

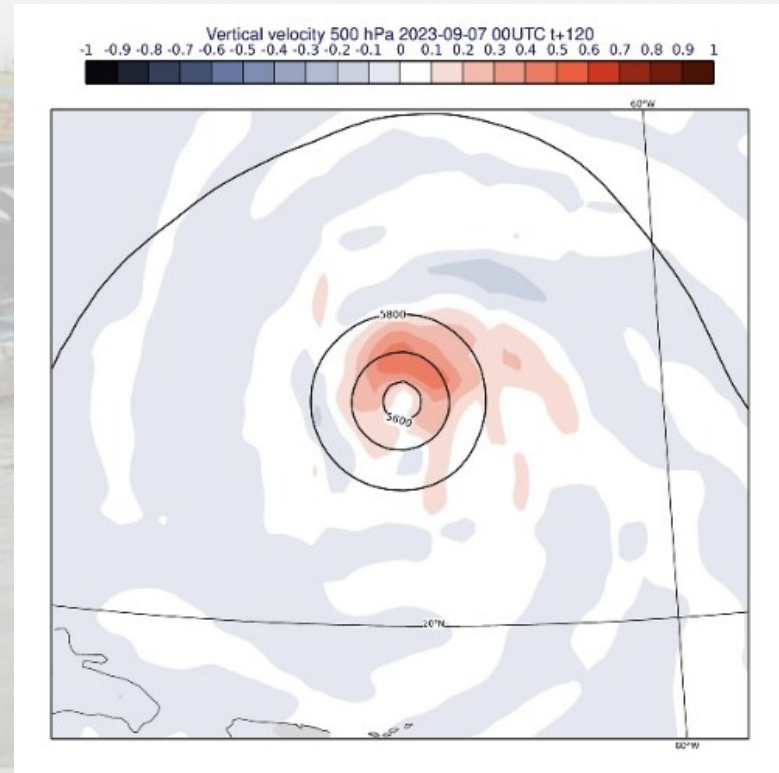

 Geophysical Research Letters
 RESEARCH LETTER
 10.1029/2023GL107377
On Some Limitations of Current Machine Learning Weather Prediction Models
 Massimo Bonavita*
 *ECMWF, Reading, UK
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Vertical wind from continuity (mass conservation)

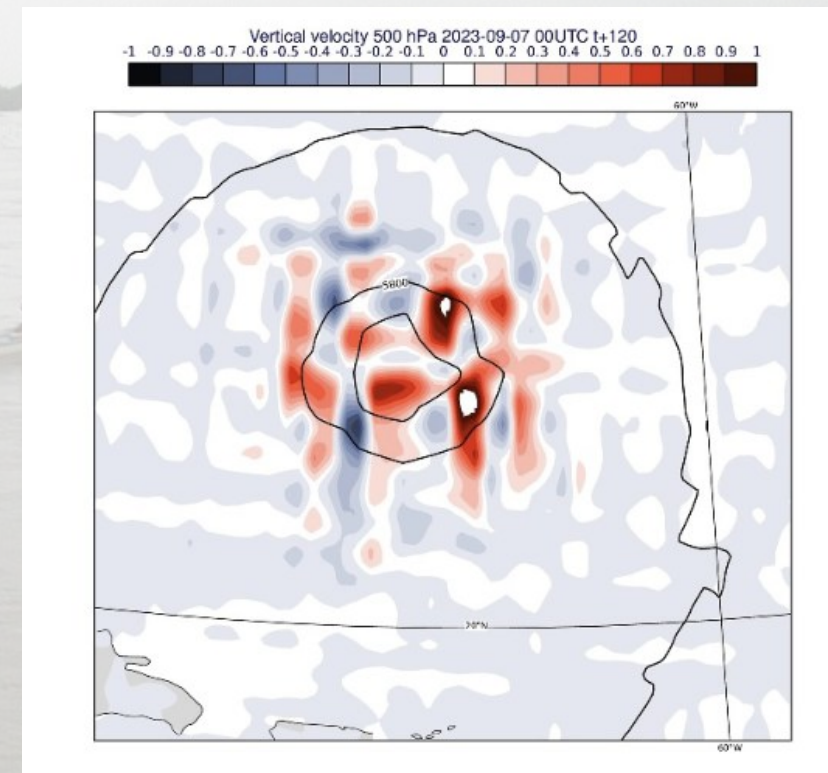
$$\omega(p) = \omega(p_s) - \int_{p_s}^p \text{div}(u)_p dp$$



ERA-5 data
(ground truth)



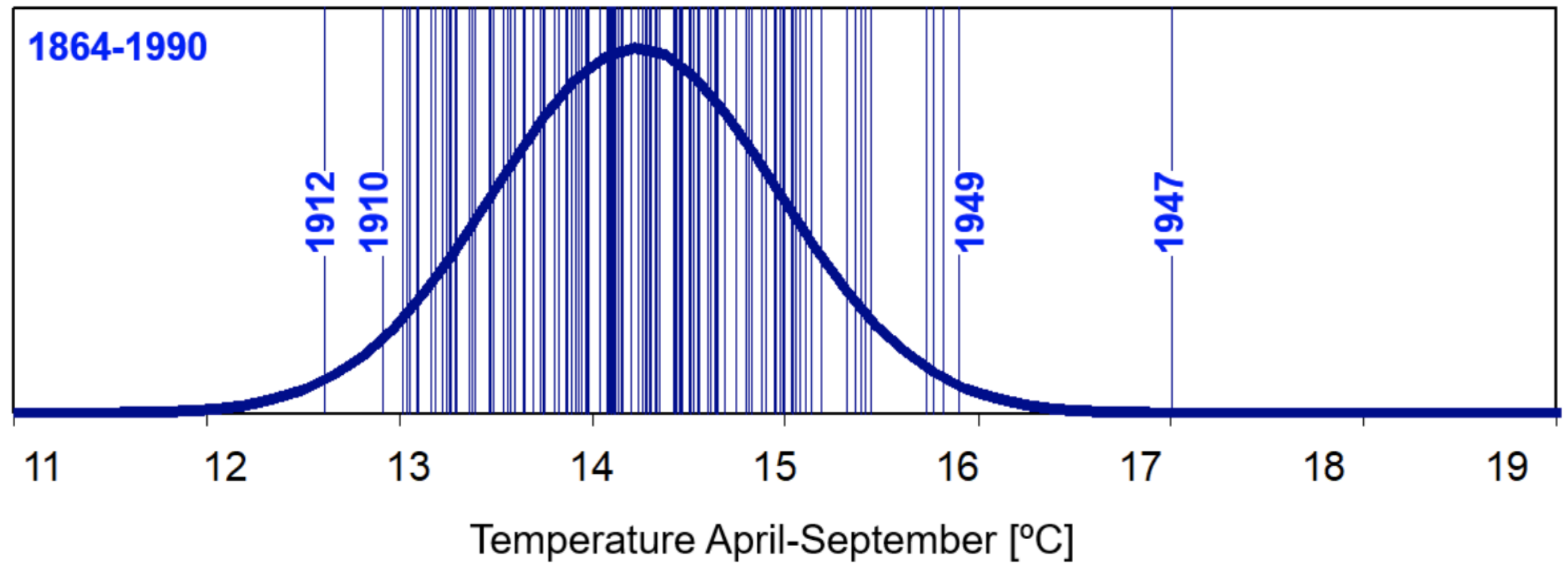
ECMWF's IFS
(simulation forecast)



Pangu Weather
(AI based forecast)

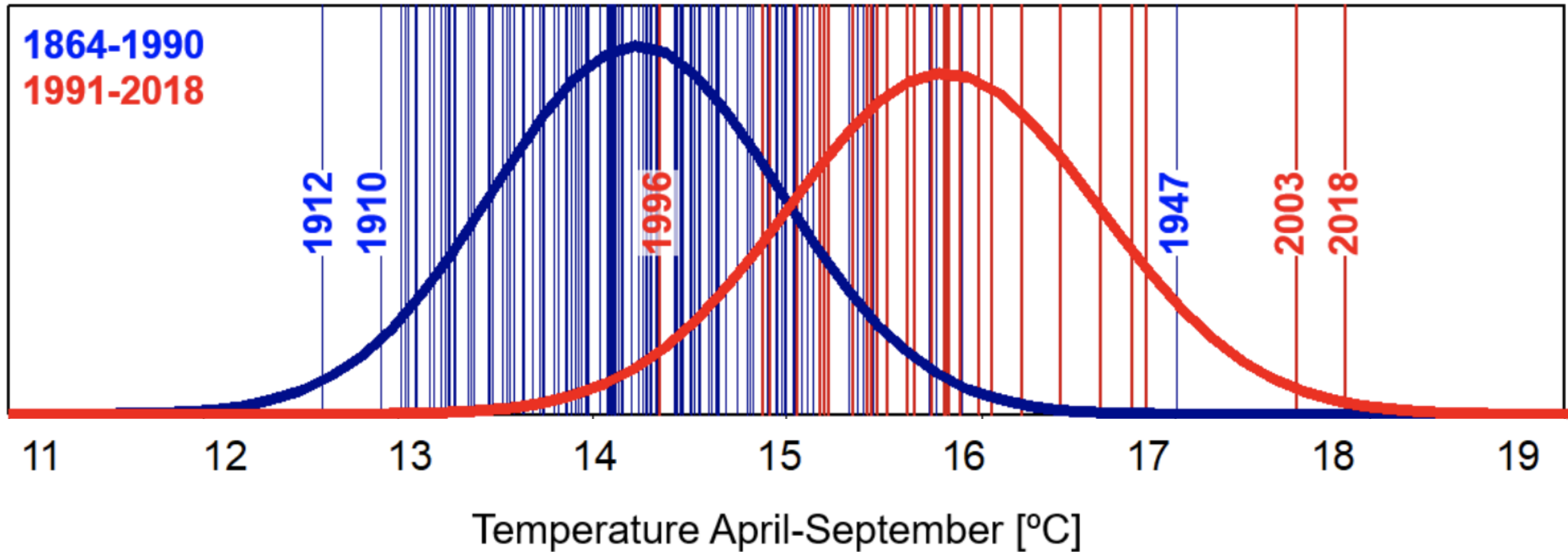
What about **global warming**? Can data-driven methods **predict the future**?

Observed temperatures April-September (credit: C. Schaer)



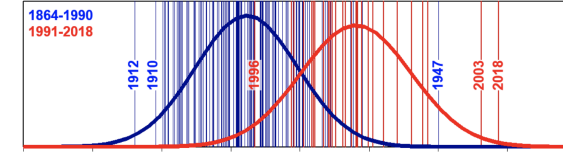
What about **global warming**? Can data-driven methods **predict the future**?

Observed temperatures April-September (credit: C. Schaer)

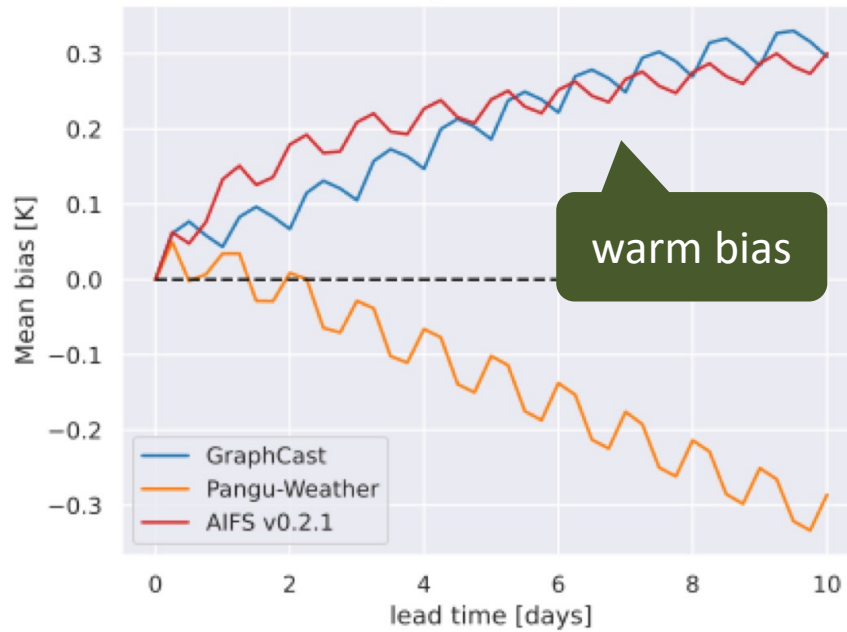


What about **global warming**? Can data-driven methods **predict the future**?

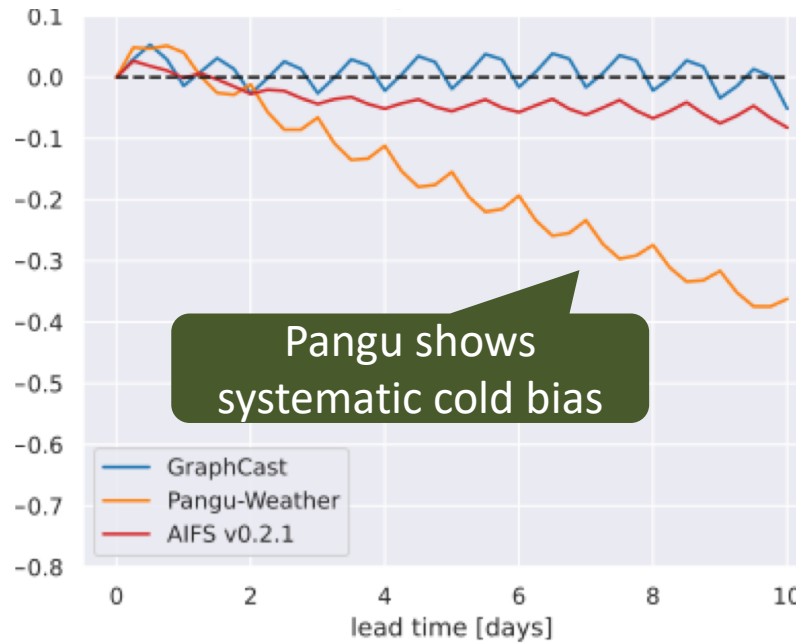
forecast bias for 2m temperature with different starting conditions



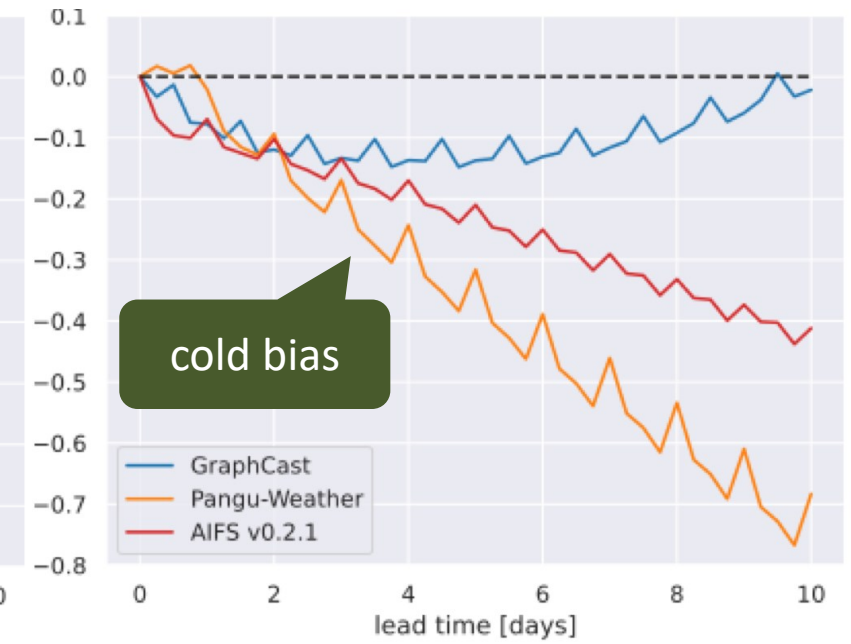
starting in 1955



starting in 2023

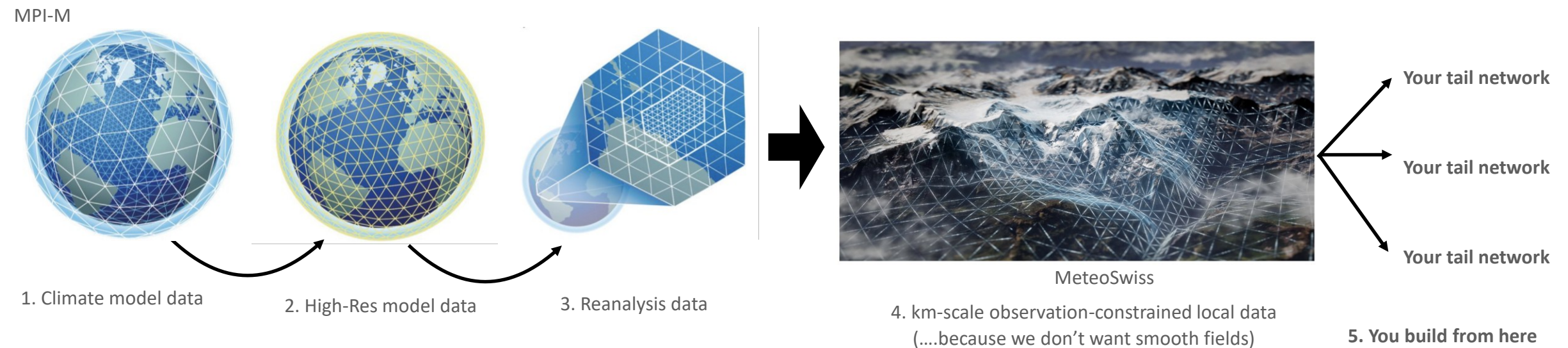


starting in 2049



Swiss AI Climate Approach: More and Better Data and Computation

- **More data, more climate models, more variables at more vertical levels and higher resolution**
 - Data from 19 different climate models at 1.0° (~1000 simulated years): ~2.9B equivalent images
 - Potentially early 1km-resolution data (TBD)
 - Fine tuning with ERA-5 0.25° reanalysis data (~40 years of reanalysis): ~ 1.0B equivalent images
 - **>4T tokens for pre-training a 160B parameter model**
 - Fine tuning with km-scale regional data at 1-10 km resolution: data still under production at MeteoSwiss





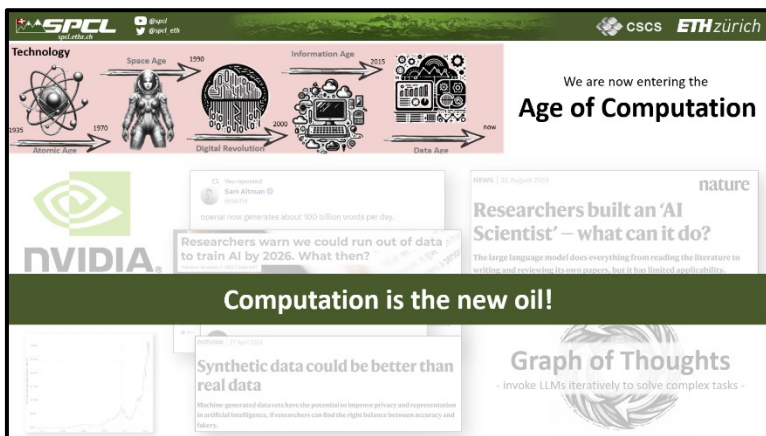
Summary and Key Points

More of SPCL's research:

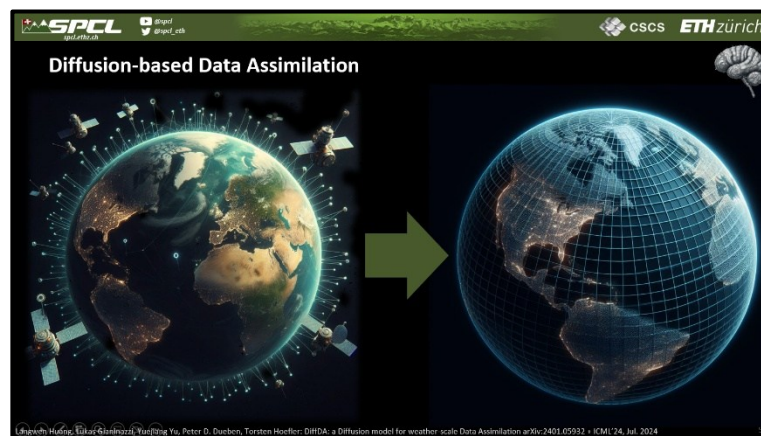
 youtube.com/@spcl  150+ Talks

 twitter.com/spcl_eth  1.2K+ Followers

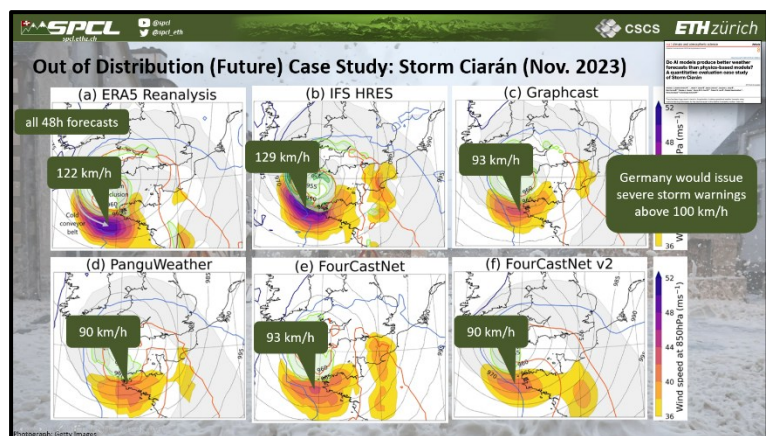
 github.com/spcl  2K+ Stars



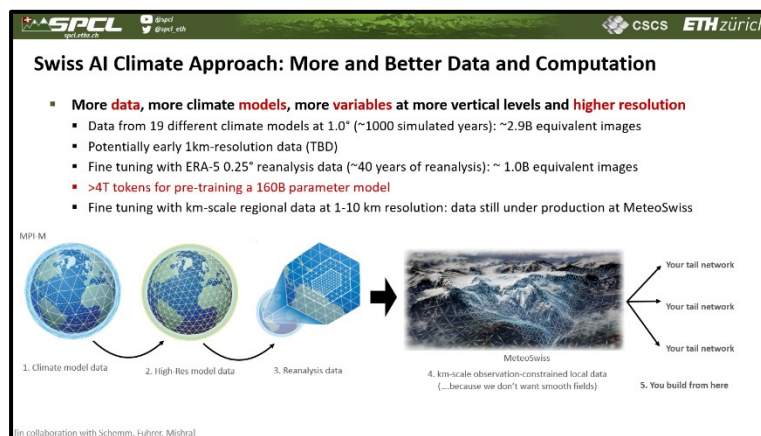
Technology: Atomic Age (1915), Space Age (1950), Information Age (2011), Data Age (2024).
 We are now entering the **Age of Computation**.
 Researchers warn we could run out of data to train AI by 2026. What then?
Computation is the new oil!
 Synthetic data could be better than real data.
 Graph of Thoughts - invoke LLMs iteratively to solve complex tasks.



Diffusion-based Data Assimilation
 (In collaboration with Scheinin, Luhrer, Mishra)



Out of Distribution (Future) Case Study: Storm Ciarán (Nov. 2023)
 all 48h forecasts
 (a) ERA5 Reanalysis: 122 km/h
 (b) IFS HRES: 129 km/h
 (c) Graphcast: 93 km/h
 (d) PanguWeather: 90 km/h
 (e) FourCastNet: 93 km/h
 (f) FourCastNet v2: 90 km/h
 Germany would issue severe storm warnings above 100 km/h



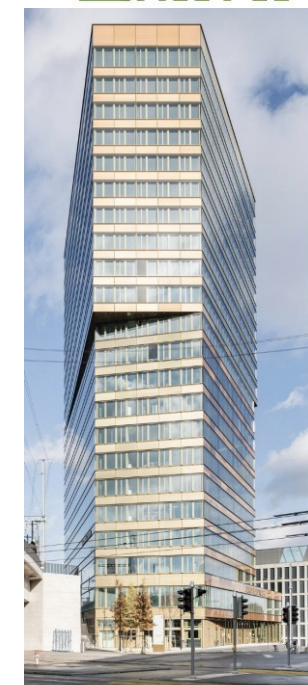
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 Fine tuning with km-scale regional data at 1-10 km resolution: data still under production at MeteoSwiss
 1. Climate model data → 2. High Res model data → 3. Reanalysis data → 4. km-scale observation-constrained local data → 5. You build from here

... or spcl.ethz.ch

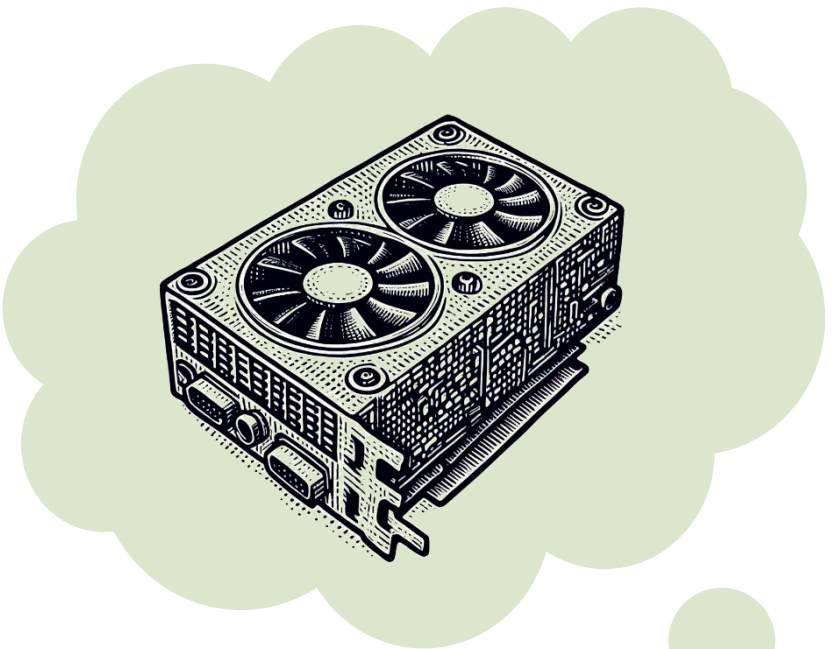


We are looking forward to a fruitful exchange!

<http://spcl.ethz.ch/Jobs/>
<http://spcl.ethz.ch/Visit/>



All of ERA-5 (Earth's 40-year history) on a USB-drive! Run your own analyses on your laptop!



```

!$ACC DATA &
!$ACC PRESENT(density1,energy1) &
!$ACC PRESENT(vol_flux_x,vol_flux_y,volume,mass_flux_x,mass_flux_y,vertexdx,vertexdy) &
!$ACC PRESENT(pre_vol,post_vol,ener_flux)

!$ACC KERNELS

IF(dir.EQ.g_xdir) THEN

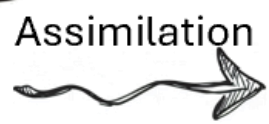
IF(sweep_number.EQ.1)THEN




!$ACC LOOP INDEPENDENT
DO k=y_min-2,y_max+2
!$ACC LOOP INDEPENDENT
DO j=x_min-2,x_max+2
pre_vol(j,k)=volume(j,k)+(vol_flux_x(j+1,k )-vol_flux_x(j,k)+vol_flux_y(j ,k+1)-vol_flux_y(j,k))
post_vol(j,k)=pre_vol(j,k)-(vol_flux_x(j+1,k )-vol_flux_x(j,k))
ENDDO
ENDDO
ELSE
!$ACC LOOP INDEPENDENT
DO k=y_min-2,y_max+2
!$ACC LOOP INDEPENDENT
DO j=x_min-2,x_max+2
pre_vol(j,k)=volume(j,k)+vol_flux_x(j+1,k)-vol_flux_x(j,k)
post_vol(j,k)=volume(j,k)
ENDDO
ENDDO

ENDIF
  
```




Observation Data



Weather/Climate Simulation





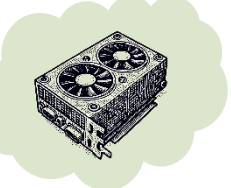

Simulation Data







Climate Insight



!\$ACC DATA &

```
!$ACC COPY(chunk%tiles(1)%field%density0) &
!$ACC COPY(chunk%tiles(1)%field%density1) &
!$ACC COPY(chunk%tiles(1)%field%energy0) &
!$ACC COPY(chunk%tiles(1)%field%energy1) &
!$ACC COPY(chunk%tiles(1)%field%pressure) &
!$ACC COPY(chunk%tiles(1)%field%soundspeed) &
!$ACC COPY(chunk%tiles(1)%field%viscosity) &
!$ACC COPY(chunk%tiles(1)%field%xvel0) &
!$ACC COPY(chunk%tiles(1)%field%yvel0) &
!$ACC COPY(chunk%tiles(1)%field%xvel1) &
!$ACC COPY(chunk%tiles(1)%field%yvel1) &
!$ACC COPY(chunk%tiles(1)%field%vol_flux_x) &
!$ACC COPY(chunk%tiles(1)%field%vol_flux_y) &
!$ACC COPY(chunk%tiles(1)%field%mass_flux_x)&
!$ACC COPY(chunk%tiles(1)%field%mass_flux_y)&
!$ACC COPY(chunk%tiles(1)%field%volume) &
!$ACC COPY(chunk%tiles(1)%field%work_array1)&
!$ACC COPY(chunk%tiles(1)%field%work_array2)&
!$ACC COPY(chunk%tiles(1)%field%work_array3)&
!$ACC COPY(chunk%tiles(1)%field%work_array4)&
!$ACC COPY(chunk%tiles(1)%field%work_array5)&
!$ACC COPY(chunk%tiles(1)%field%work_array6)&
!$ACC COPY(chunk%tiles(1)%field%work_array7)&
!$ACC COPY(chunk%tiles(1)%field%cellx) &
!$ACC COPY(chunk%tiles(1)%field%celly) &
!$ACC COPY(chunk%tiles(1)%field%celldx) &
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!$ACC COPY(chunk%bottom_snd_buffer) &
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!$ACC COPY(chunk%top_rcv_buffer)
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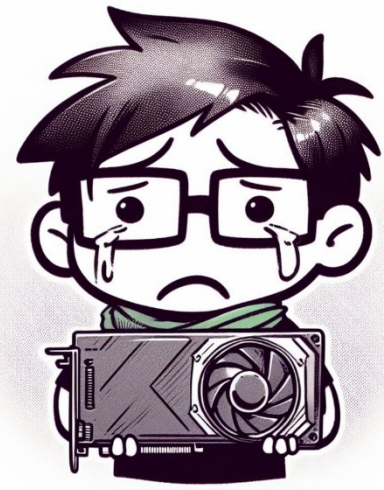
Sloccount *f90: 6,440
 ,mass_flux_x,mass_flux_y,vertexdx,vertexdy) &

!\$ACC: 833 (13%)



1,k
r,1,

l,k)



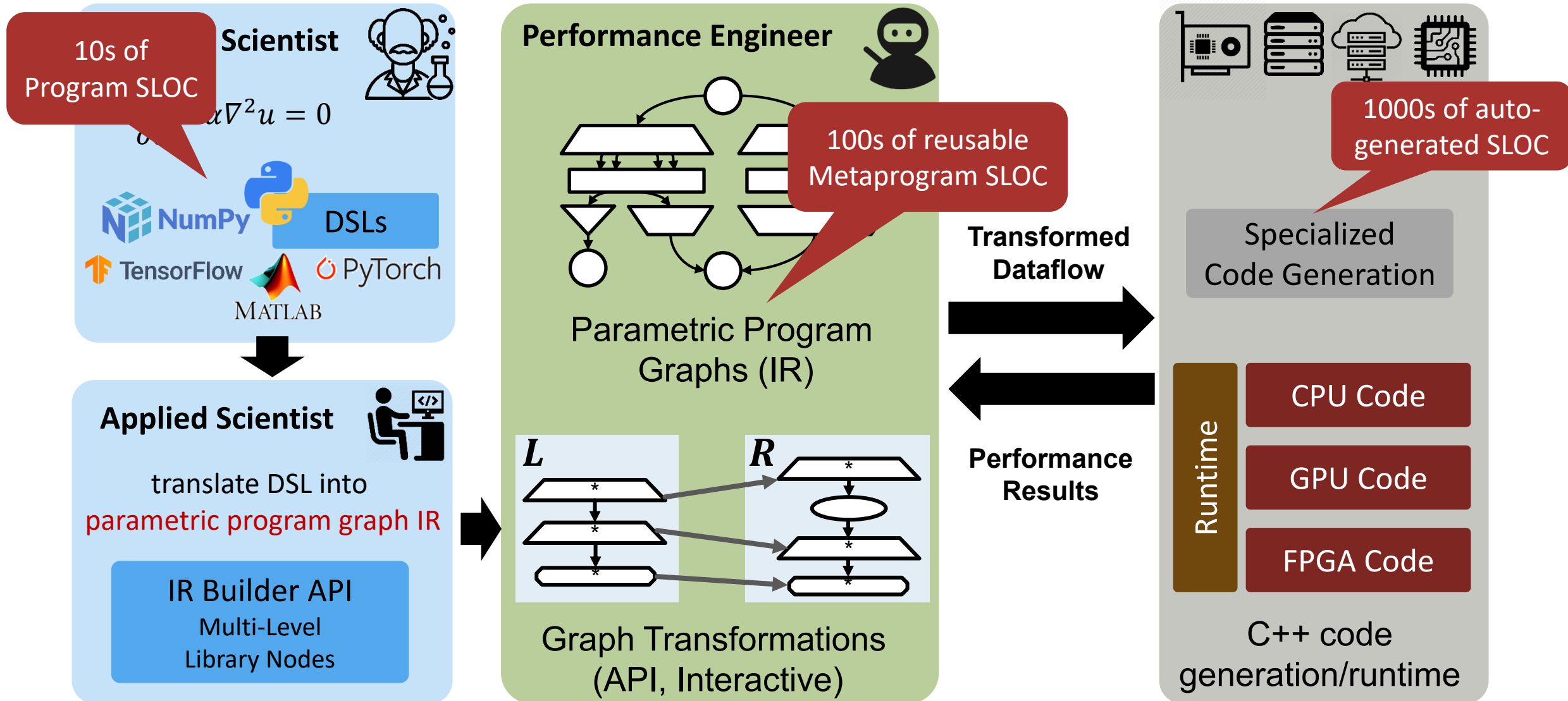
Heitlager et al.: A Practical Model for Measuring Maintainability

source code properties

	volume	complexity per unit	duplication	unit size	unit testing
analysability	X		X	X	X
changeability		X	X		
stability					X
testability		X		X	X

ISO 9126 maintainability

Performance Metaprogramming for Optimization and Performance Portability



Pace in DaCe for Performance Metaprogramming – 12k SLOC Python

AI-based Transfer Tuning to the Rescue!



T. HOEFLER

AI-Driven Performance Metaprogramming

with contributions by the whole SPCL deep learning team (T. Ben-Nun, S. Jakobovits, L. Truemper, A. Calotoiu, and many others) and collaborators (C. Cummins and others)

Keynote talk at the AI for Developers Workshop @ Supercomputing 2023, Denver, CO, 2023





Another real production code ... ECMWF's CLOUDSC

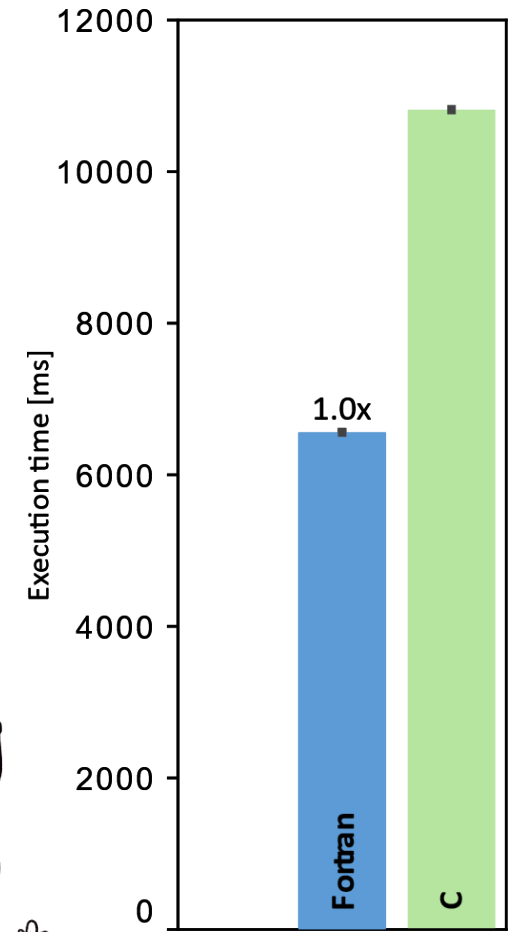
```

9
10 SUBROUTINE CLOUDSC &
11 !---input
12 & (KIDIA, KFDIA, KLON, KLEV, &
13 & PTSPHY,&
14 & PT, PQ, tendency_cml,tendency_tmp,tendency_loc, &
15 & PVFA, PVFL, PVFI, PDYNA, PDYNL, PDYNI, &
16 & PHRSW, PHRLW,&
17 & PVERVEL, PAP, PAPH,&
18 & PLSM, LDCUM, KTYPE, &
19 & PLU, PLUDE, PSNDE, PMFU, PMFD,&
20 !---prognostic fields
21 & PA,&
22 & PCLV, &
23 & PSUPSAT,&
24 !-- arrays for aerosol-cloud interactions
25 !!! & PQAER, KAER, &
26 & PLCRIT_AER,PICRIT_AER,&
27 & PRE_ICE,&
28 & PCCN, PNICE,&
29 !---diagnostic output
30 & PCOVPTOT, PRAINFRAC_TOPRFZ,&
31 !---resulting fluxes
32 & PFSQLF, PFSQIF, PFCQNG, PFCQLNG,&
33 & PFSQRF, PFSQSF, PFCQRNG, PFCQSNG,&
34 & PFSQLTUR, PFSQITUR, &
35 & PFPLSL, PFPLSN, PFHPSL, PFHPSN, KFLDX, &
36 & YDCST, YDTHF, YDECLDP)
  
```

... variable setup/initialization until line 500 ;-)

- **Cloud Microphysics of IFS**
 - Resolve sub-grid features
 - Original 2,525 SLOC of **Fortran 95**

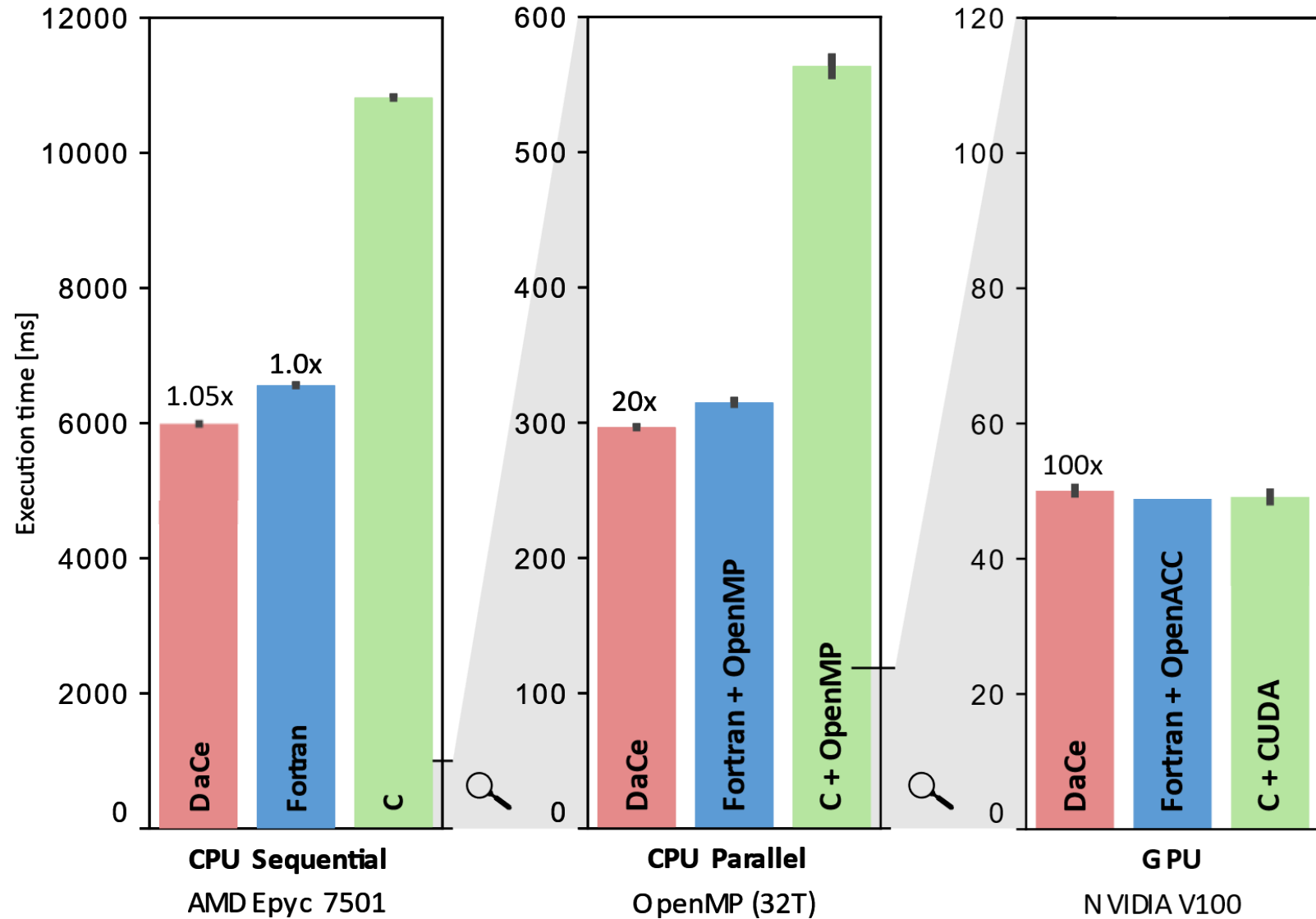
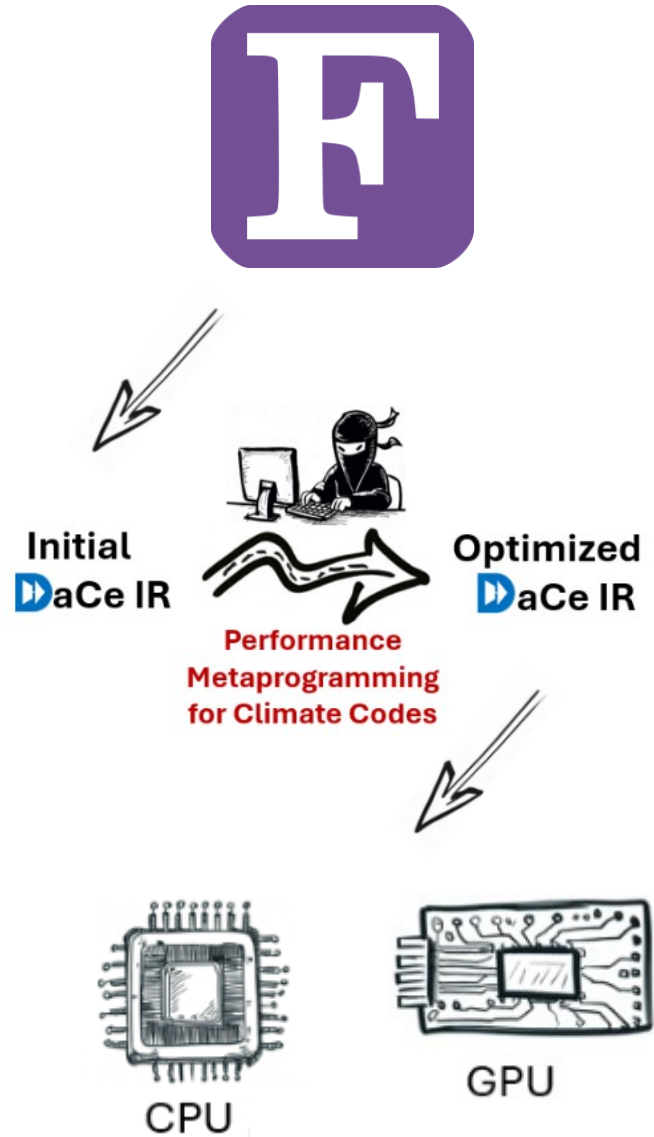
- **Rewritten for performance portability benchmarking (optimization took months!)**
 - 2,635 SLOC C
 - 2,610 SLOC C++/CUDA



CPU Sequential
AMD Epyc 7501

<https://github.com/ecmwf-ifs/dwarf-p-cloudsc>

Performance Metaprogramming – from the **unchanged** CLOUDSC Fortran code!



The three pillars of AI in Climate Sciences

Data

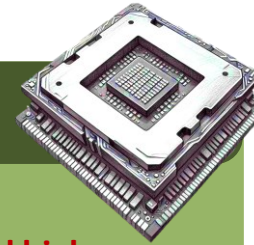


- Unstructured **observation data**
- Structured **simulation data**

Combine both to train models

- Learn physics and data-driven prediction

Compute



- AI models require **accelerated high-performance computing** for training

Accelerate AI computations

- Re-use infrastructure from LLMs and related generative AI methods (GNN, CNN)

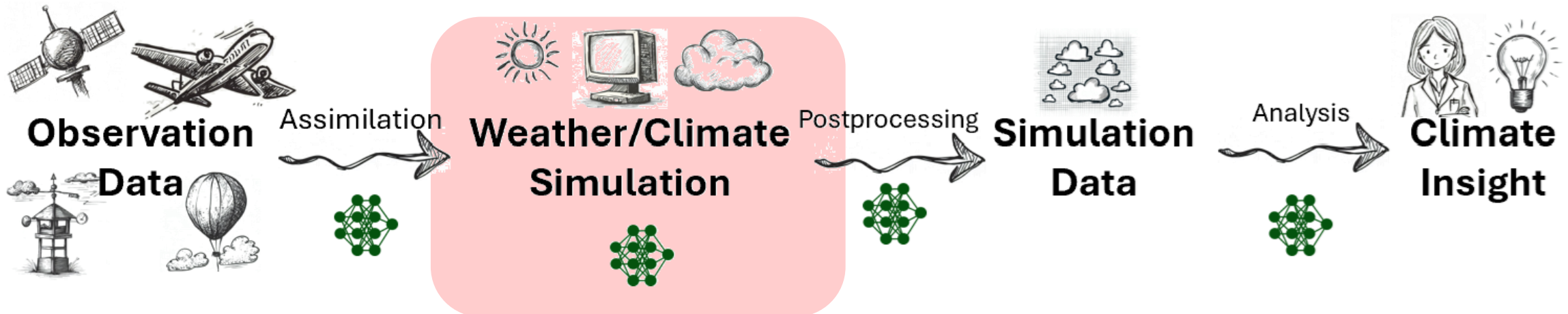
Models



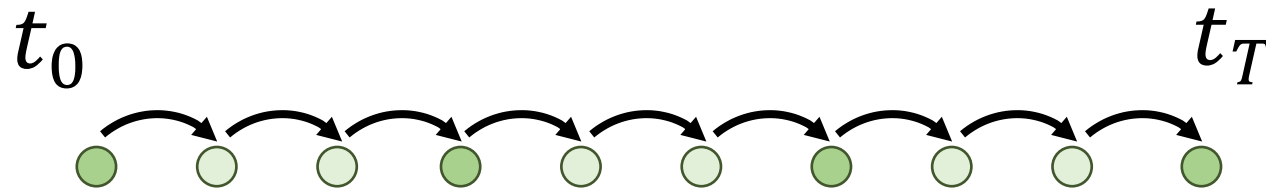
- Models need to provide the right structural bias/prior

Develop better AI methods

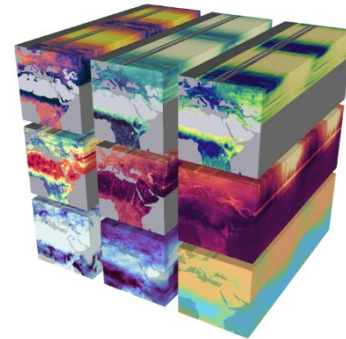
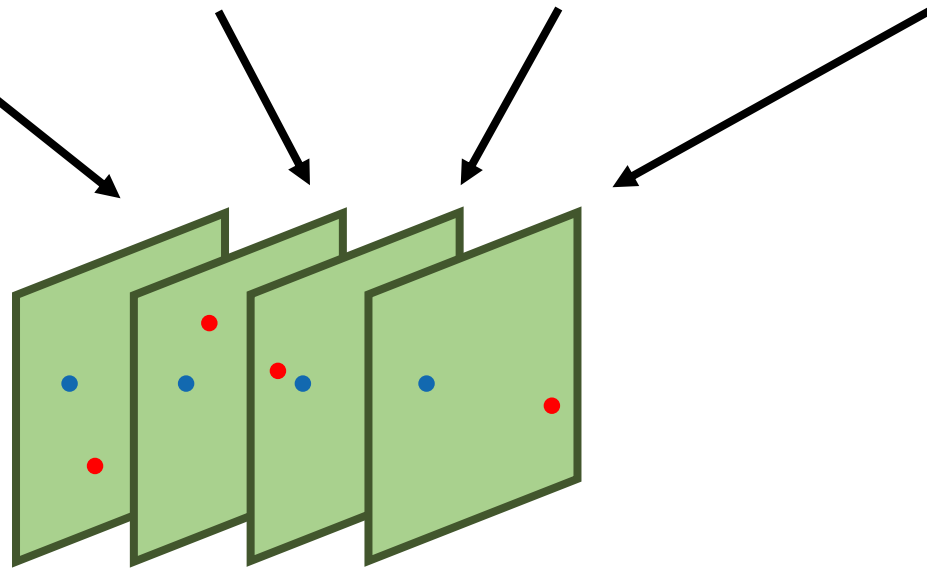
- Step 1: use generative AI models: tformer, CNN, GNN, Diffusion, etc.
- Step 2: use **automatically parameterized physics-based models** encoding equations



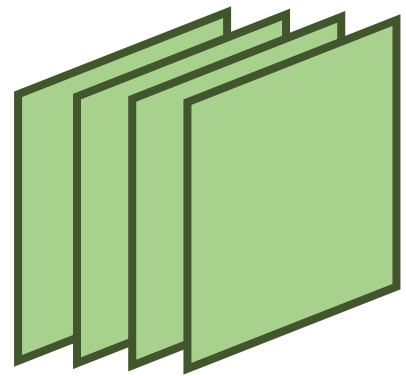
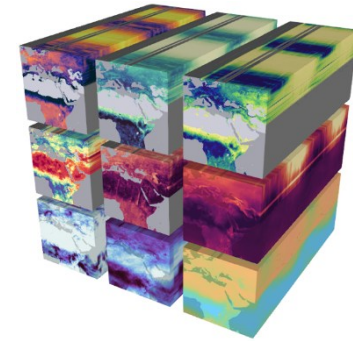
Simulation runs time-stepping forward



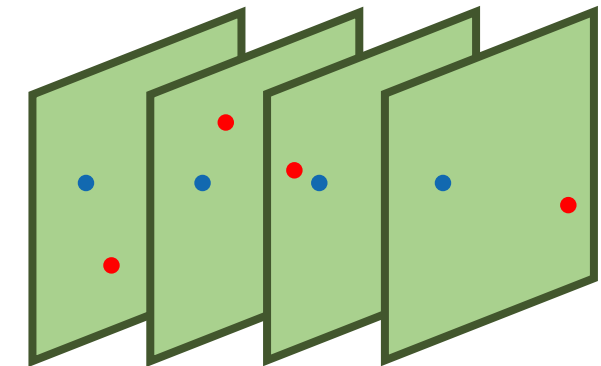
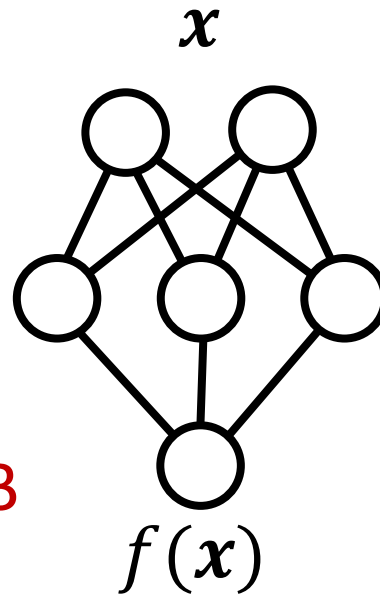
Store some timesteps!



Analysis access pattern is often **strided** or even **random**



Compress/Train
300 x – 3,000 x
15.6GB → 13.8MB

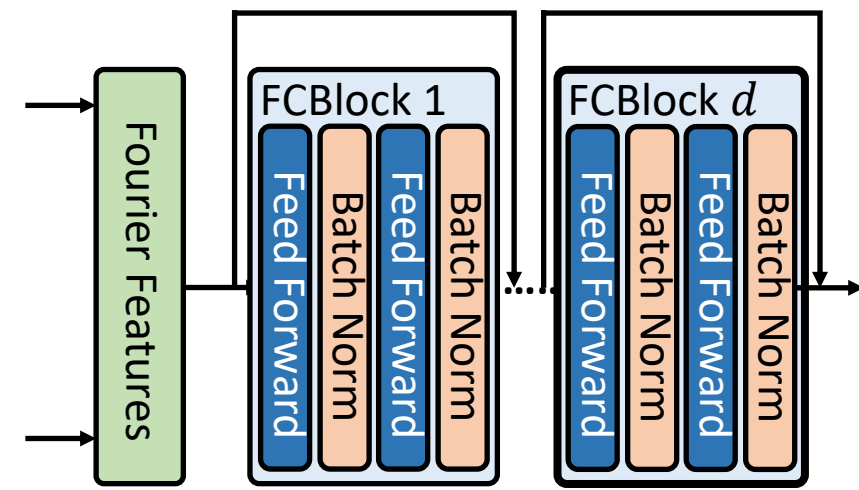
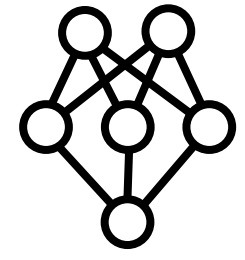


Multidimensional Data

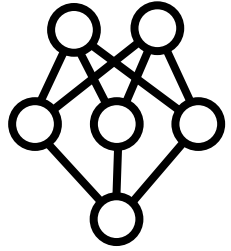
Neural Representation

Analysis Queries

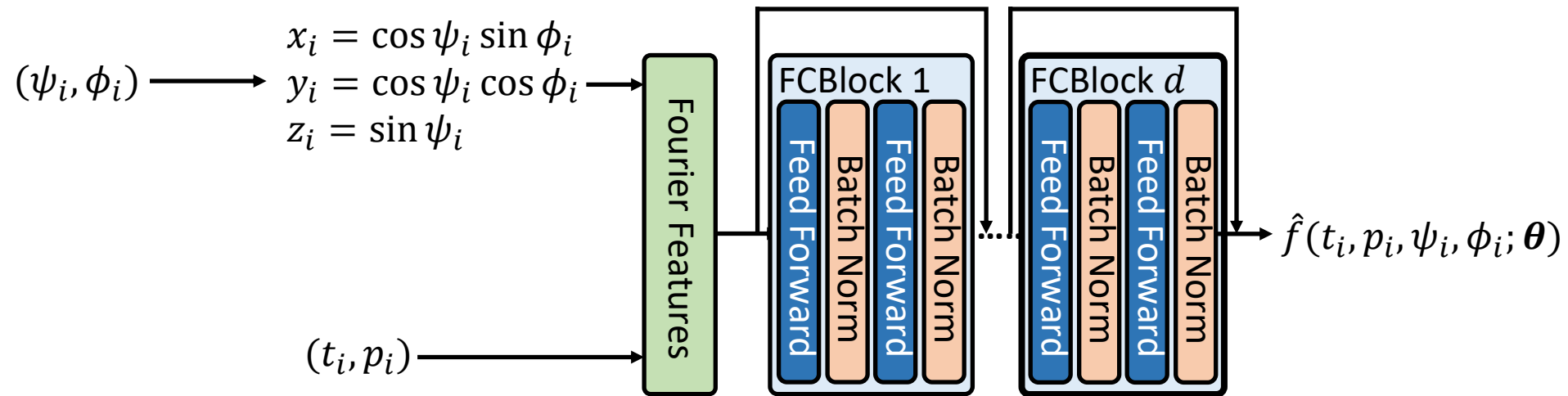
Neural Network Structure



Neural Network Structure

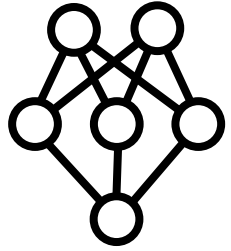


Decompression / Inference

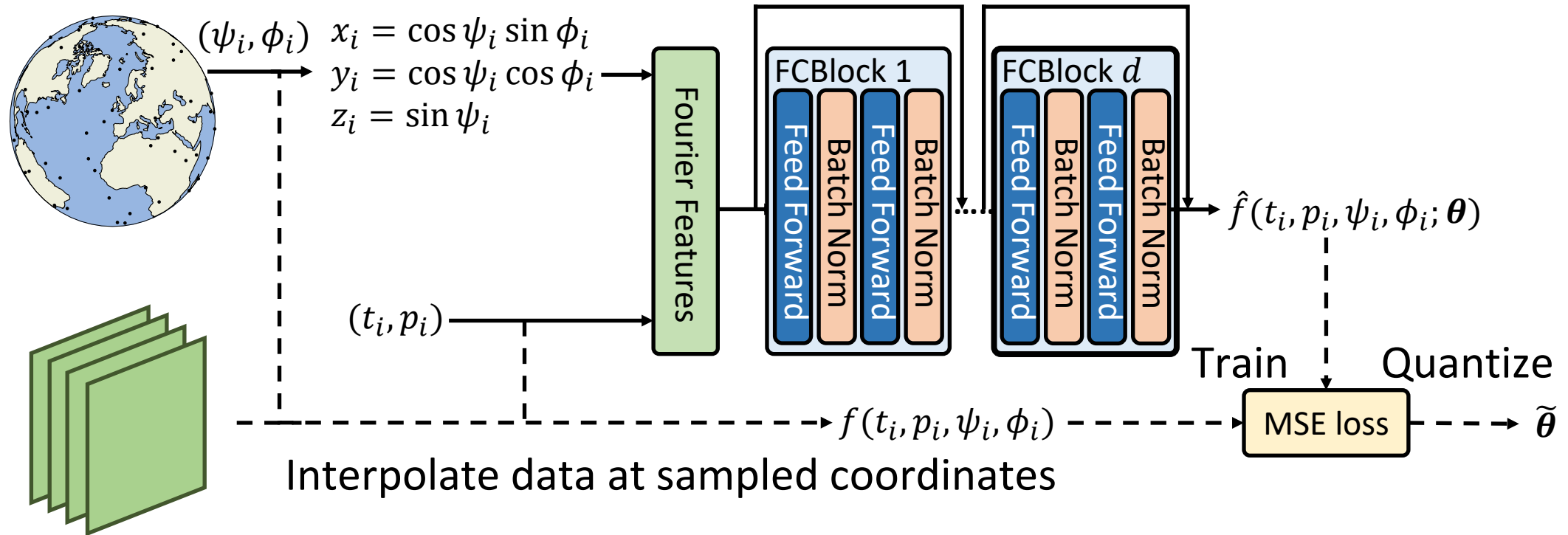


- On-demand decompression
- Fully utilize GPUs

Neural Network Structure

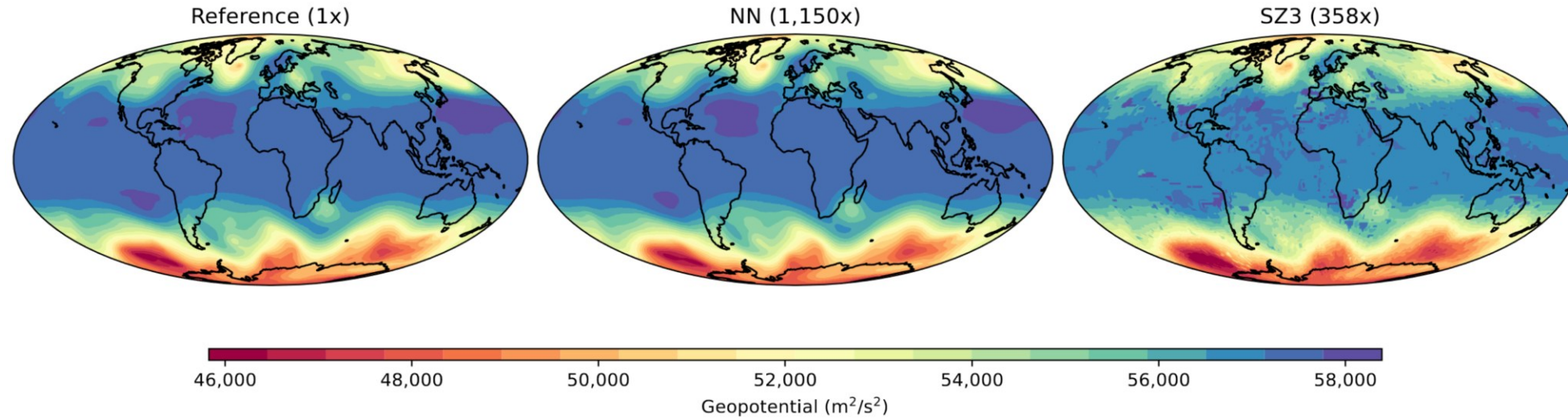


Compression / Training



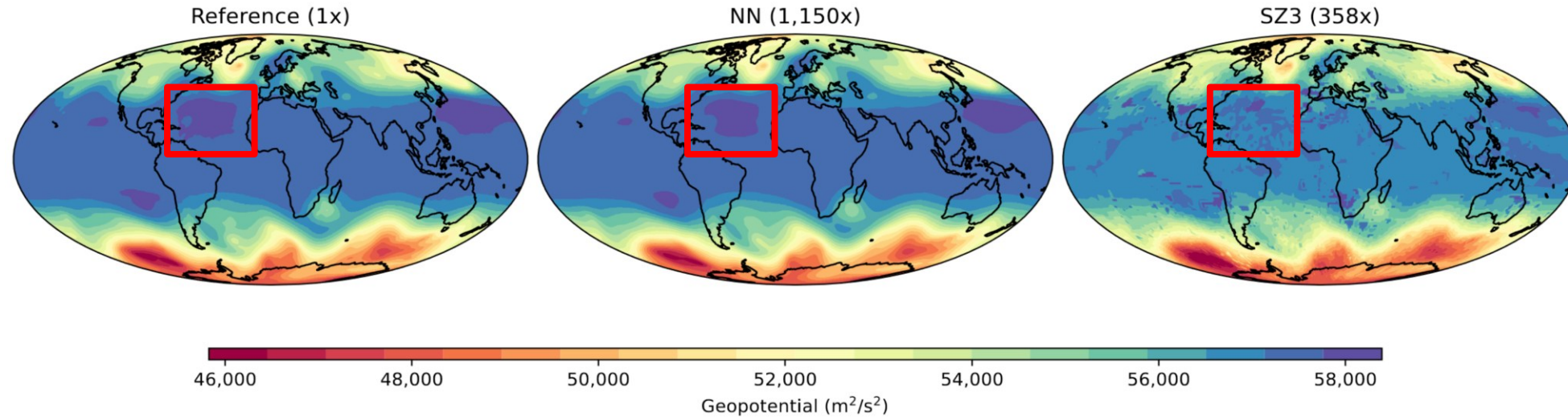
Evaluation: Case Study

Geopotential at 500hPa, 2016 Oct 5th



Evaluation: Case Study

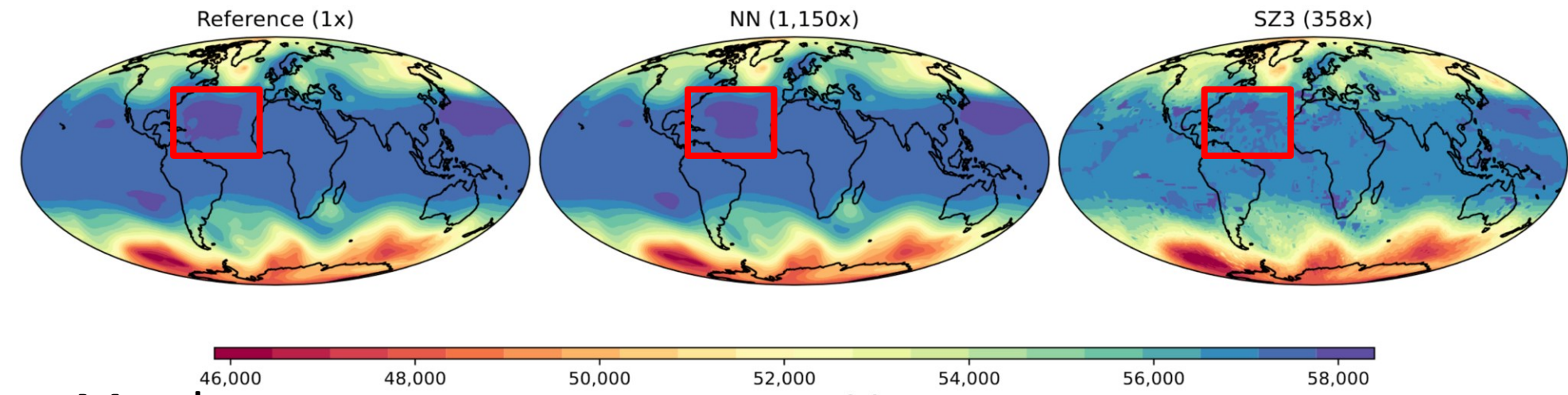
Geopotential at 500hPa, 2016 Oct 5th



Preserves general shapes of important events and average values without introducing significant artifacts

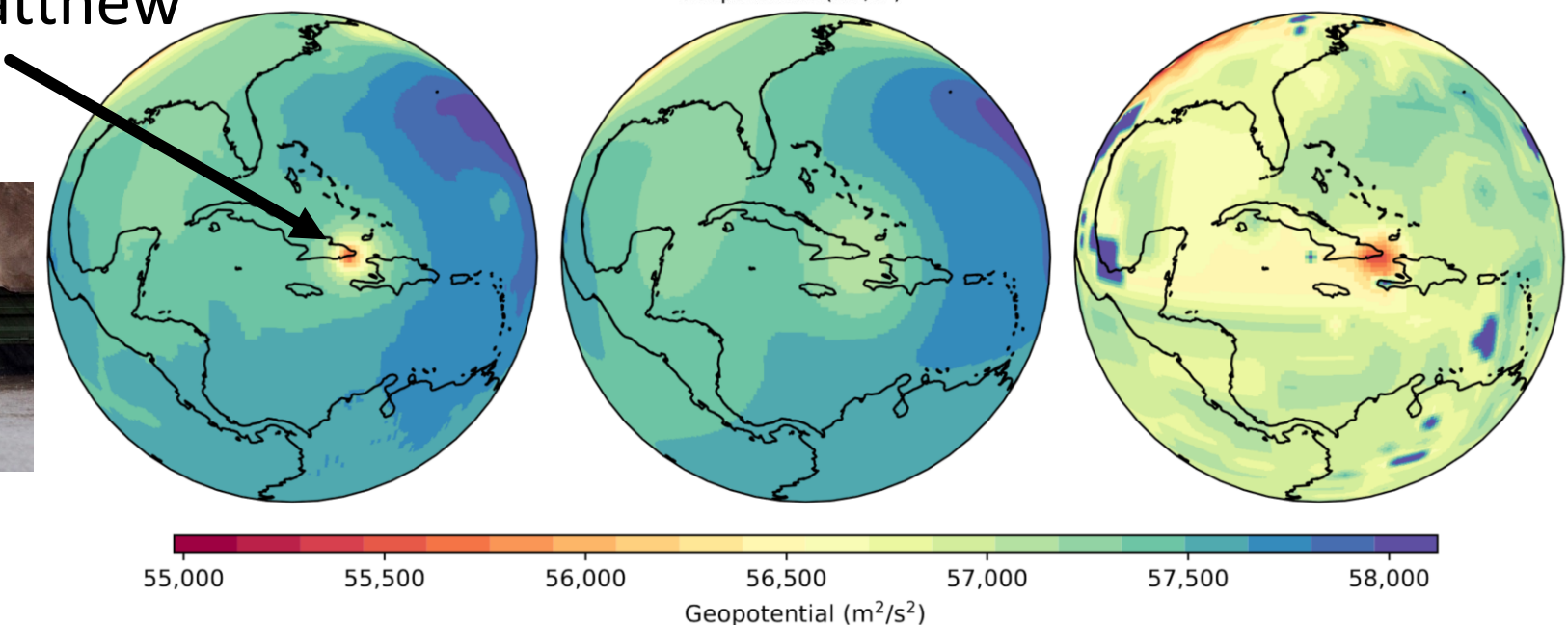
Evaluation: Case Study

Geopotential at 500hPa, 2016 Oct 5th



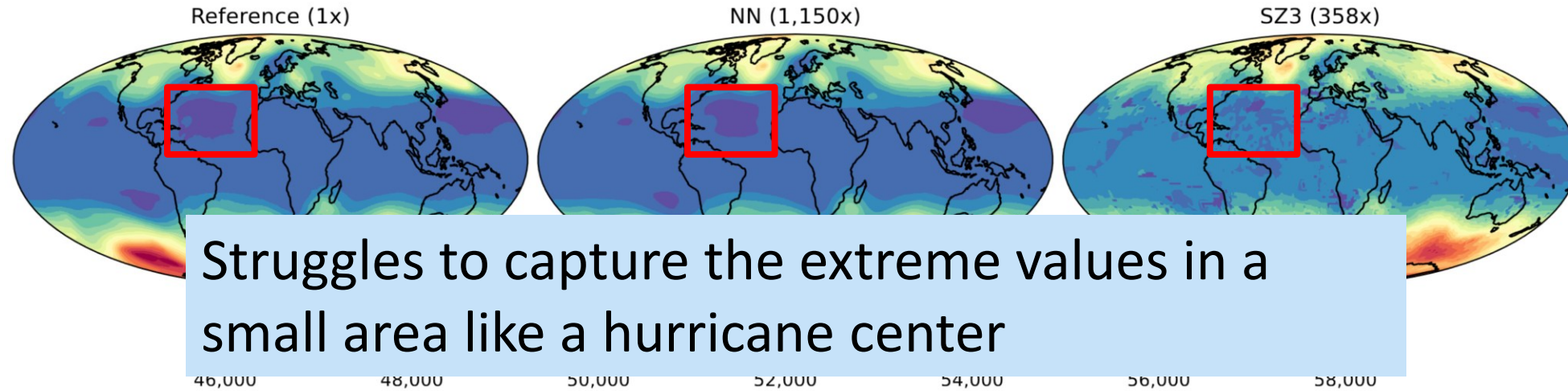
Hurricane Matthew

16.5bn damage
603 fatalities



Evaluation: Case Study

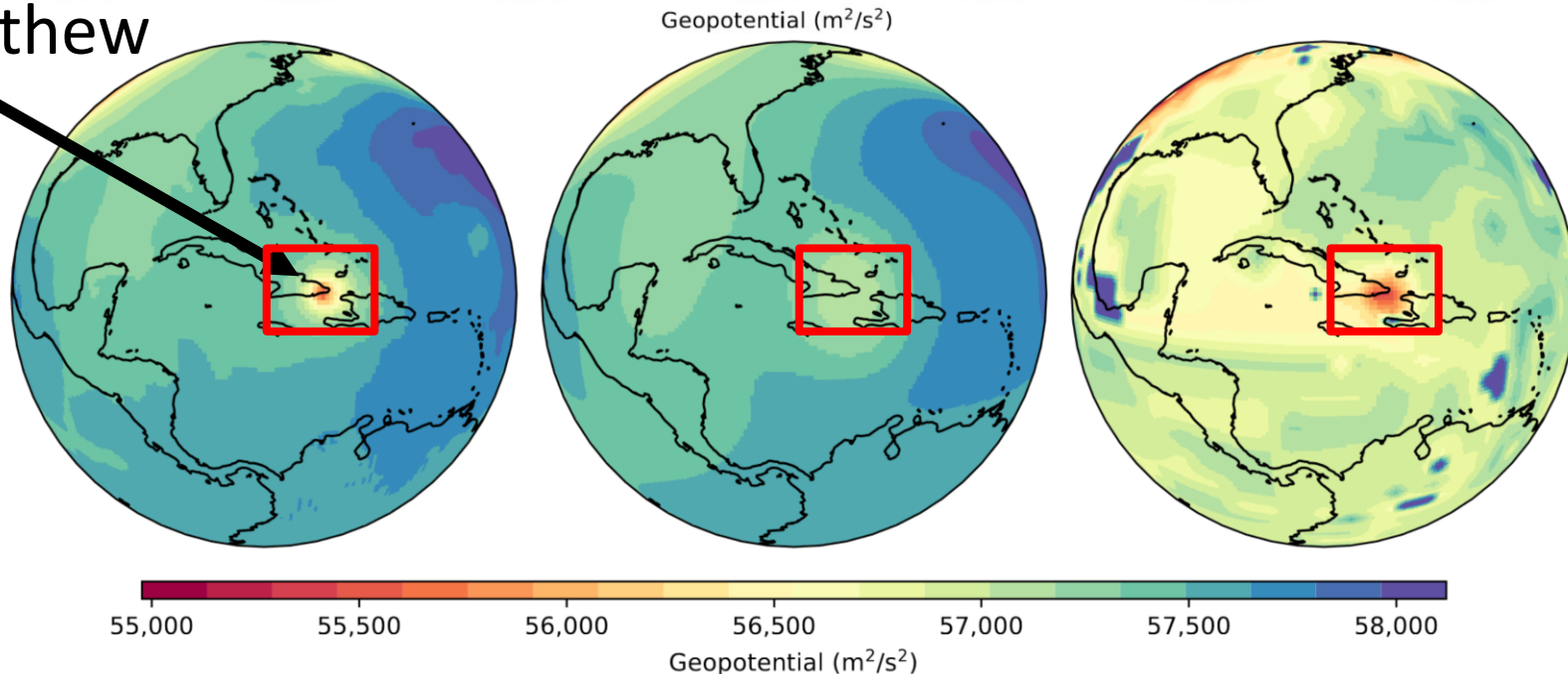
Geopotential at 500hPa, 2016 Oct 5th



Struggles to capture the extreme values in a small area like a hurricane center

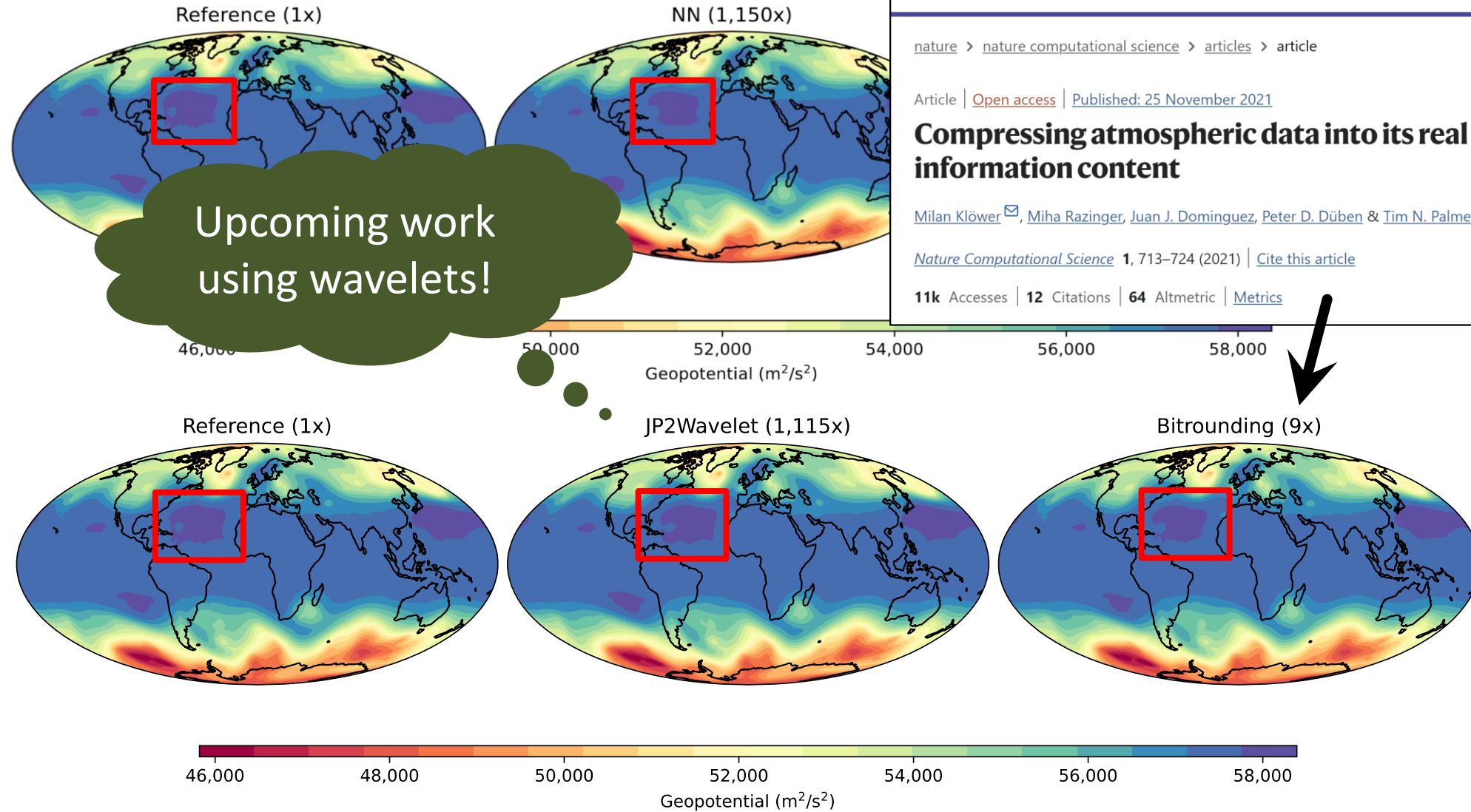
Hurricane Matthew

16.5bn damage
603 fatalities



Evaluation: Case Study

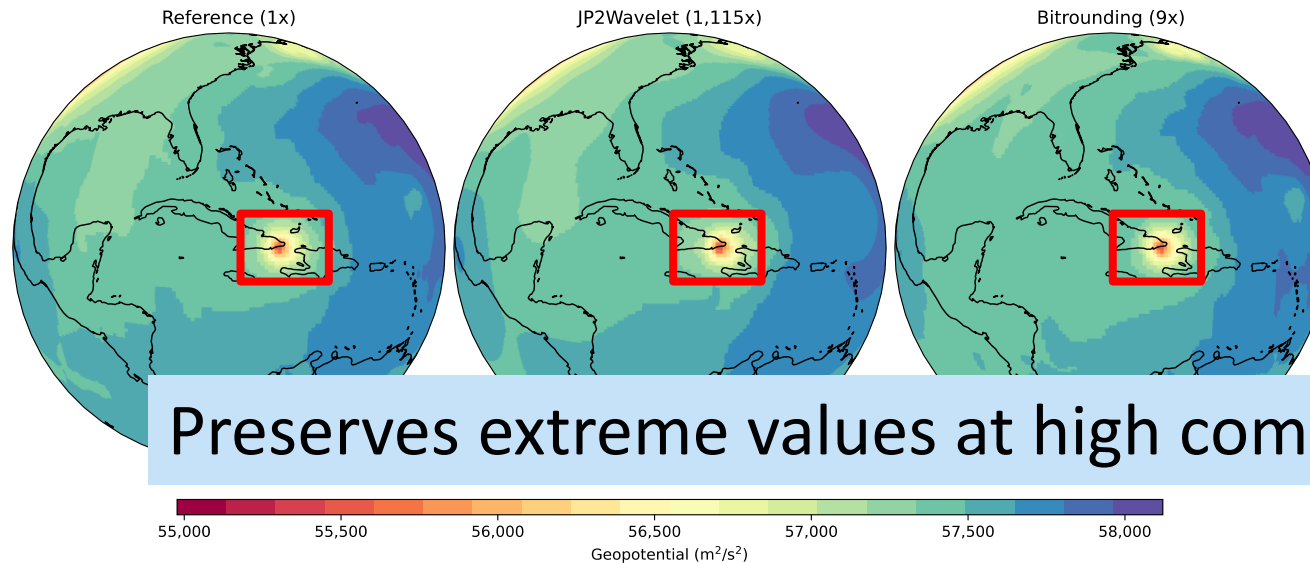
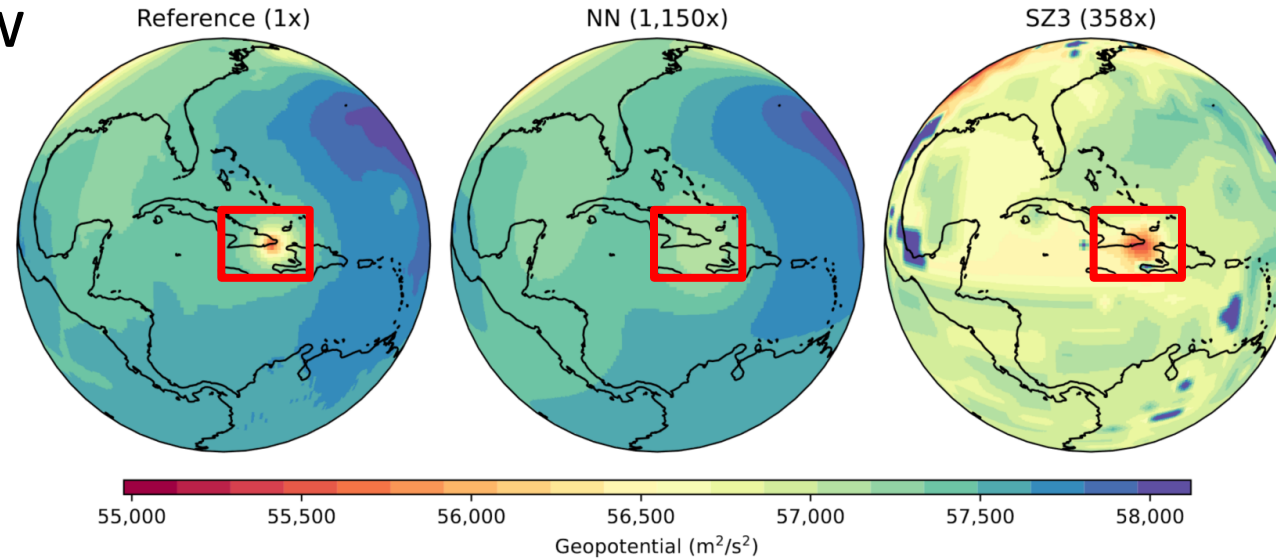
Geopotential at 500hPa, 2016



Upcoming work using wavelets!

Evaluation: Case Study

Hurricane Matthew



Preserves extreme values at high compression ratio