Technological challenges in Brazil for the advancement of numerical forecasts

Pedro Leite da Silva Dias
Institute of Astronomy, Geophysics and Atmospheric Sciences
University of São Paulo

Numerical predictions for strategic sectoral applications:
Modeling and verification approaches and challenges

30 Nov to 01 Dec 2023 São José dos Campos, SP, Brazil

WORLD METEOROLOGICAL ORGANIZATION
WCRP World Climate Research Programme
WWRP World Weather Research Programme

Typical dimension 10^{10} - 10^{12}

Modeling the Earth Atmosphere System – <u>based on conservation principles</u>

$$\frac{\partial X_a}{\partial t} + L_a X_a = N_a(X_a, X_o, X_v, X_c, X_s) + F_a(X_a, X_o, X_v, X_c, X_s)$$

atmosphere

$$\frac{\partial X_o}{\partial t} + L_o X_o = N_o(X_a, X_o, X_v, X_c, X_s) + F_o(X_a, X_o, X_v, X_c, X_s)$$

ocean+hydrology + ice

$$\frac{\partial X_s}{\partial t} + L_s X_s = N_s(X_a, X_o, X_v, X_c, X_s) + F_s(X_a, X_o, X_v, X_c, X_s)$$

soil

$$\frac{\partial X_v}{\partial t} + L_v X_v = N_v(X_a, X_o, X_v, X_c, X_s) + F_v(X_a, X_o, X_v, X_c, X_s)$$

vegetation

$$\frac{\partial X_c}{\partial t} + L_c X_c = N_c(X_a, X_o, X_v, X_c, X_s) + F_c(X_a, X_o, X_v, X_c, X_s)$$

chemical species

$$X_a = (u, v, w, T, q_v, q_l, q_r, q_i, ...)$$

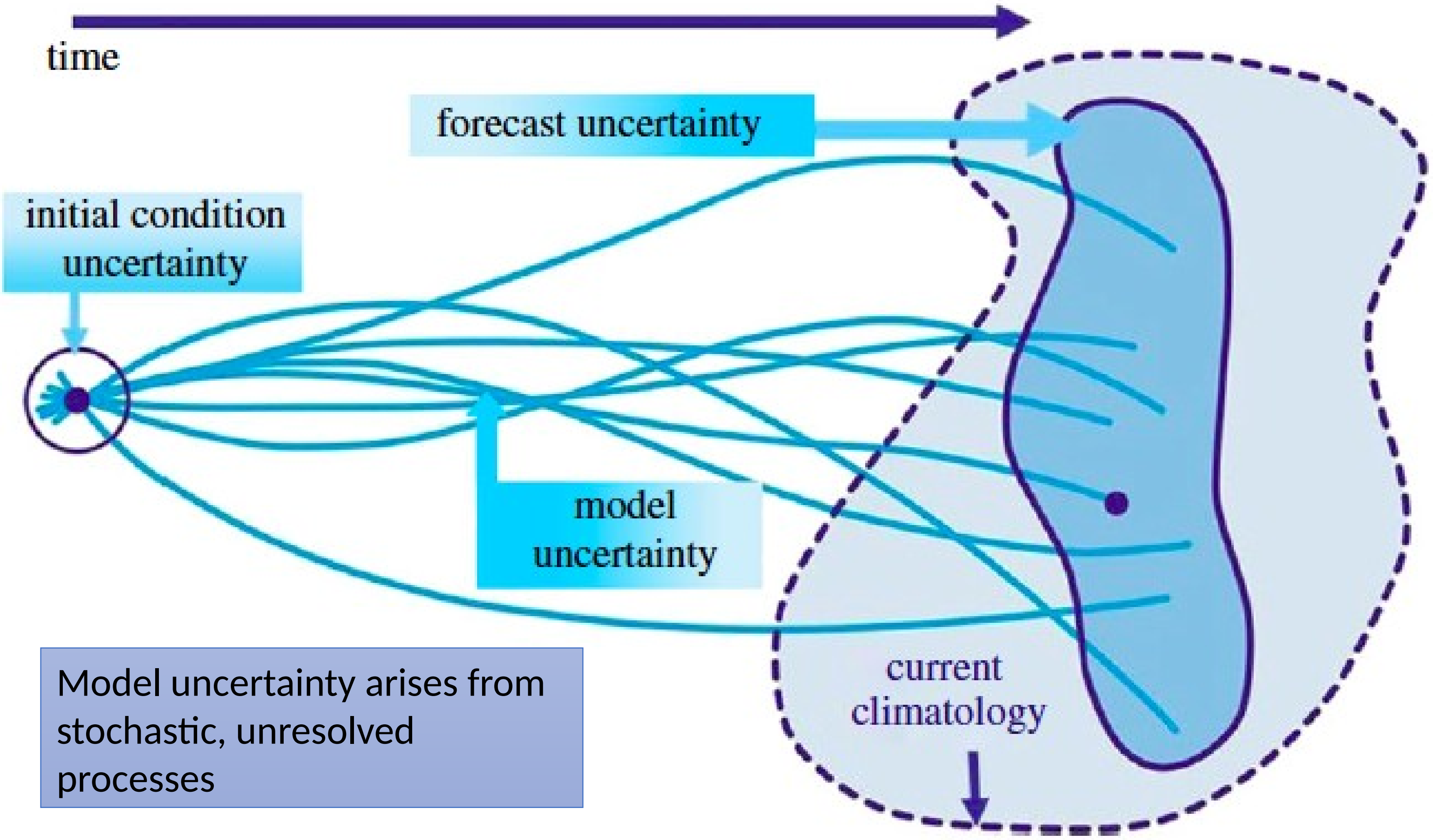
$$X_o = (u, v, w, T, s_v, ...)$$

$$X_s = (T^{is}, W^{is}, N^{in}, ...)$$

$$X_v = (lai^{i}, sig^{iv}, root^{id}, stom^{ic}, VOC^{i}, C^{i}, N_{i}, ...)$$

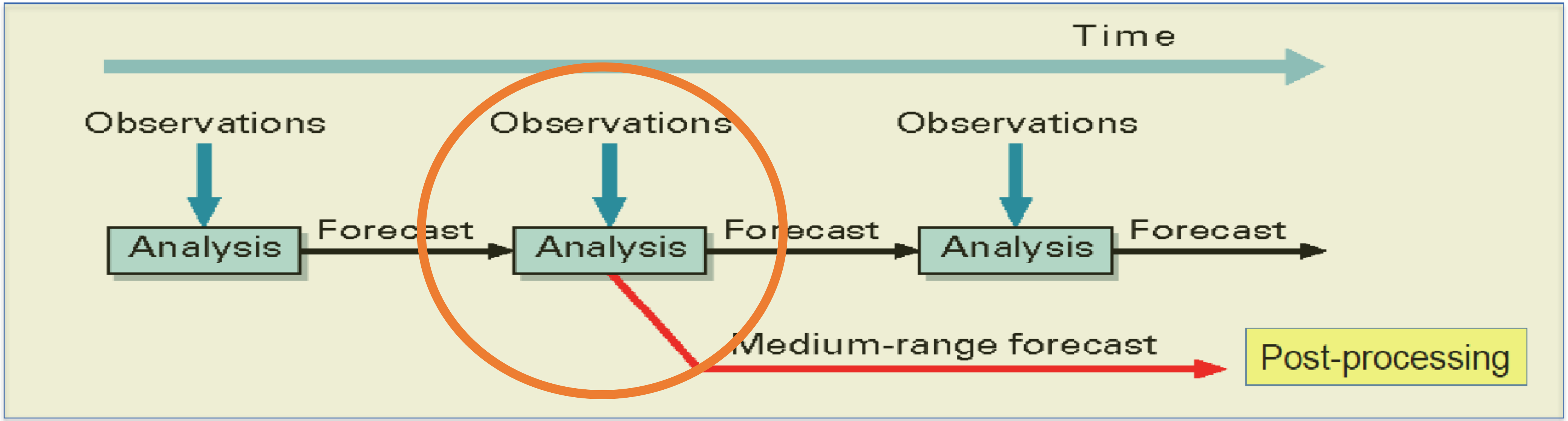
$$X_c = (CO_2, CH_4, O_3, NO_x, VOC's, SO_2, ...)$$

How to deal with uncertainties in weather and climate forecasting: multiple forecasts with disturbances in the initial state and forecast models



Model uncertainty arises from stochastic, unresolved processes

Slingo & Palmer (Phil. Trans. R. Soc. A **(2011)**



All components of the NWP workflow can potentially be improved by ML technologies:

a) **Observations**: Quality Control decisions, Bias correction, Observation operator

b) **Forecast**: Model error correction, Model identification, model development

c) **Analysis**: Model error estimation and correction, Model parameter estimation, linearised/adjoint models

d) **Post-processing**: Ensemble/Determ. post-processing, Sig. Weather ident.,

(adapted from slides by Massimo Bonavita, ECMWF-ESA Workshop, Oct. 2020)

Modeling based on data

Increasing role of Artificial Intelligence /Machine Learning applications

Enhancing Satellite Observation with Machine Learning

Hybrid Data Assimilation - Machine Learning Approaches

Enhancing the representation of small-scale processes

Forecasting with Machine Learning and Hybrid Models

Machine Learning for Post-Processing and Dissemination

Much of this is related to pattern recognition and downscaling

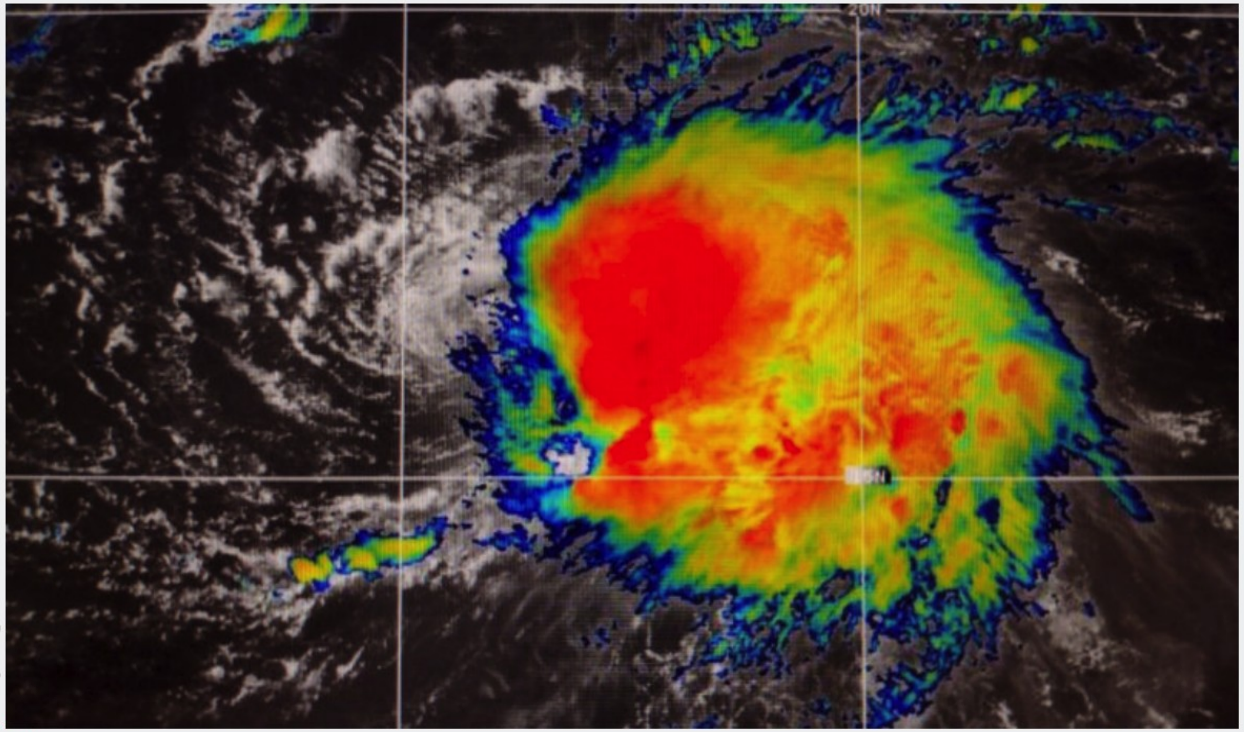
(See also ECMWF-ESA Workshops on Machine Learning for Earth System Observation and Prediction, held online 5-8 October 2020 and upcoming 15-18 November, 2021)

ADVENTURES IN MOVING AIR —

AI outperforms conventional weather forecasting for the first time: Google study

AI models may soon enable more accurate forecasts with higher speed and lower cost.

BENJ EDWARDS - 11/14/2023, 4:53 PM

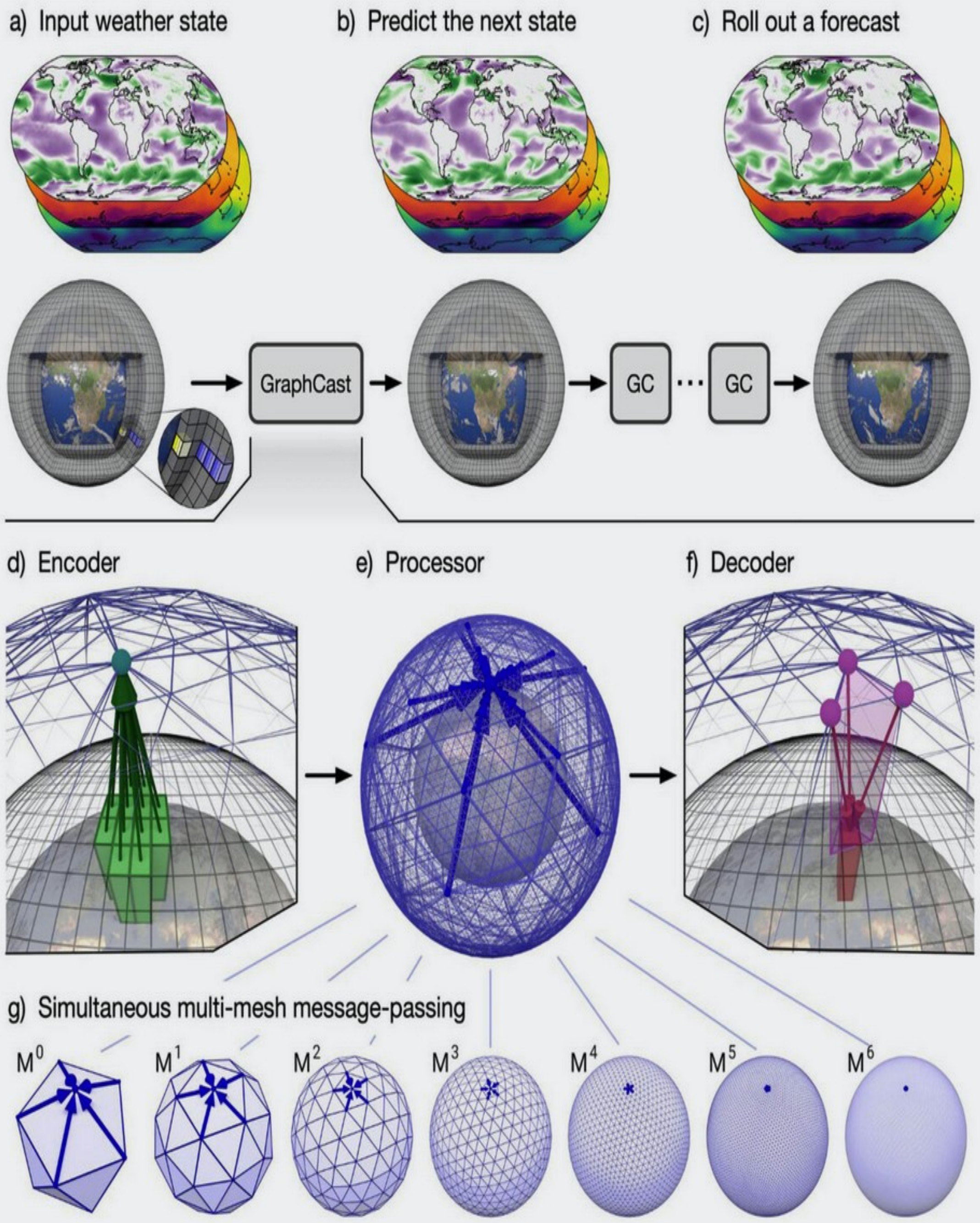


Getty Images

Enlarge / A file photo of Tropical Storm Fiona as seen in a satellite image from 2022.

75

On Tuesday, the peer-reviewed journal Science published a study that shows how an AI meteorology model from Google DeepMind called GraphCast has significantly outperformed conventional weather forecasting methods in predicting global weather conditions up to 10 days in advance. The achievement suggests that future weather forecasting may become far more accurate, reports The Washington Post and Financial Times.



Google DeepMind

Science RESEARCH ARTICLES

Cite as: R. Lam *et al.*, *Science* 10.1126/science.adi2336 (2023).

Learning skillful medium-range global weather forecasting

Remi Lam[1*†], Alvaro Sanchez-Gonzalez[1*†], Matthew Willson[1*†], Peter Wirnsberger[1†], Meire Fortunato[1†], Ferran Alet[1†], Suman Ravuri[1†], Timo Ewalds[1], Zach Eaton-Rosen[1], Weihua Hu[1], Alexander Merose[2], Stephan Hoyer[2], George Holland[1], Oriol Vinyals[1], Jacklynn Stott[1], Alexander Pritzel[1], Shakir Mohamed[1*], Peter Battaglia[1*]

[1]Google DeepMind, London, UK. [2]Google Research, Mountain View, CA, USA.

*Corresponding author. Email: remilam@google.com (R.L.); alvarosg@google.com (A.S.); matthjw@google.com (M.W.); shakir@google.com (S.M.); peterbattaglia@google.com (P.B.)

†These authors contributed equally to this work.

Global medium-range weather forecasting is critical to decision-making across many social and economic domains. Traditional numerical weather prediction uses increased compute resources to improve forecast accuracy, but does not directly use historical weather data to improve the underlying model. Here, we introduce "GraphCast," a machine learning-based method trained directly from reanalysis data. It predicts hundreds of weather variables, over 10 days at 0.25° resolution globally, in under one minute. GraphCast significantly outperforms the most accurate operational deterministic systems on 90% of 1380 verification targets, and its forecasts support better severe event prediction, including tropical cyclones tracking, atmospheric rivers, and extreme temperatures. GraphCast is a key advance in accurate and efficient weather forecasting, and helps realize the promise of machine learning for modeling complex dynamical systems.

How about computer technologies and weather/climate prediction with physics based and data driven models?

Operational Suite of Global Forecasting Centers

14 global centers

Forecast Centre (Country)
ECMWF (Europe)
Met Office (UK)
Météo France (France)
DWD (Germany)
HMC (Russia)
NCEP (USA)
Navy/FNMOC/NRL (USA)
CMC (Canada)
CPTEC/INPE (Brazil)
JMA (Japan)
CMA (China)
KMA (Korea)
IMD (India)
BoM (Australia)

- Global Modelling:
  - Deterministic Model (-> 10km)
  - Global Ensemble Prediction System
  - Global Data Assimilation Scheme (most 4dVAR)
- Regional Modelling
  - Regional deterministic model (few km)
  - Regional Ensemble Prediction System. (order of 10km)
  - Regional Data Assimilation Scheme. (3DdVar✉ 4dVAR)
- Atmospheric composition
  - Global atmospheric composition modelling
  - Regional atmospheric composition modelling

computers

Review

High-Performance Computing in Meteorology under a Context of an Era of Graphical Processing Units

Tosiyuki Nakaegawa

Nakaegawa, T. High-Performance Computing in Meteorology under a Context of an Era of Graphical Processing Units. Computers 2022, 11, 114. https://doi.org/10.3390/computers11070114

- one of the first operational applications of scientific computations since Richardson's dream in 1922

- Late 70's /80s - major developments related to introduction of vector CPU's - CRAY1/2, CYBER 205, IBM360…. => changes in algorithm development.

https://www.mdpi.com/2073-431X/11/7/114

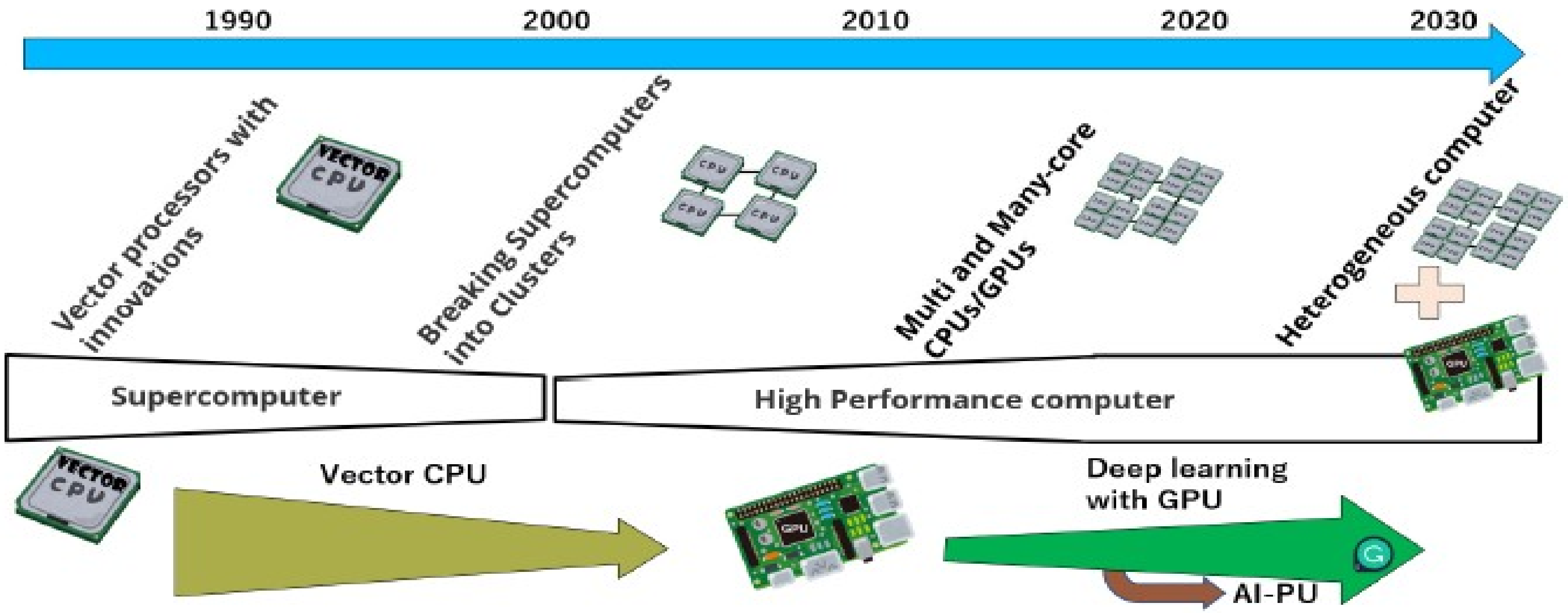
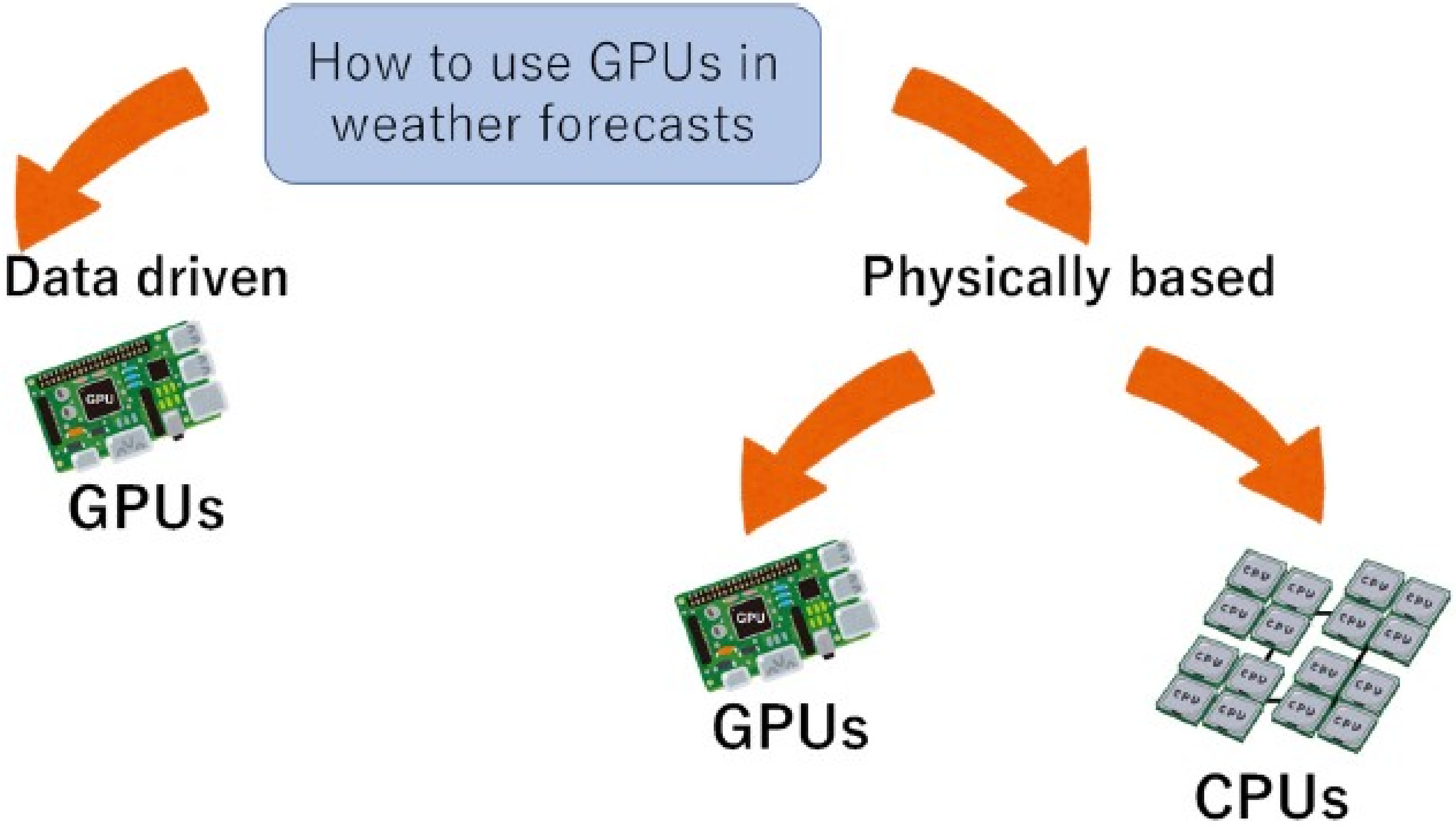


Figure 1. History of high-performance computing with the evolution of hardware since the 1980s.

GPU's in Atmospheric Models

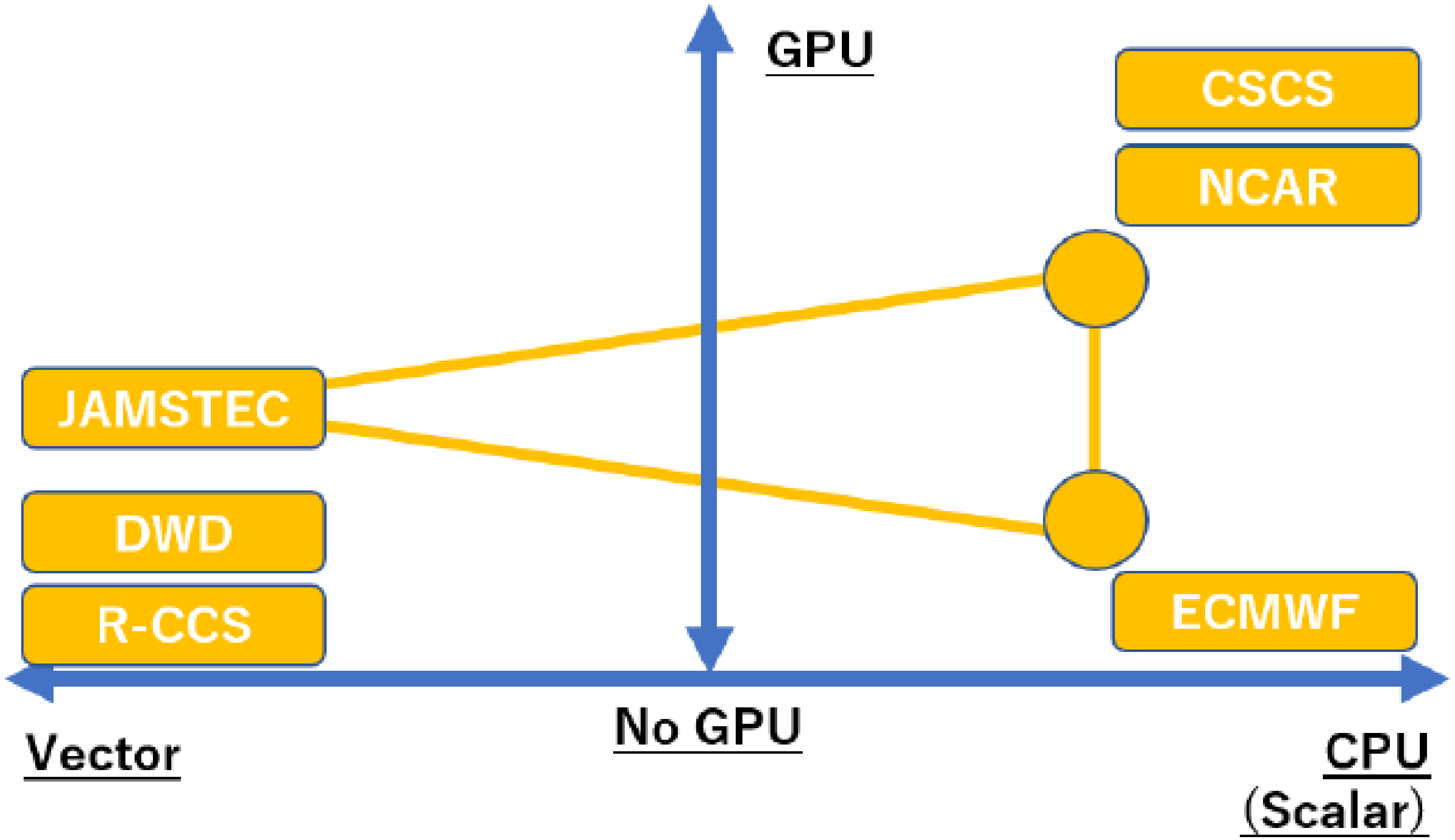
- The data-driven approach: e.g deep learning (DP) is popular => large amount of data required to train DP

- Physically based models: Navier Stokes Equations – multiscaling – multiphysics (physical processes)



- Codes for using GPU's in traditional CPU's had to be re-written :
- Concern with numerical efficiency and operational stability in weather forecasting facilities.
    - Some of my personal experience with GPU's – early 2000's:

What was the decision of the Global Weather Forecasting Centers concerning CPU, vector facilities, GPU's....????



Schematics for positions of each type of HPC in main global forecasting centers on a simplified field expressed as with/without CPUs and/or GPUs.

What was the decision of the Global Weather Forecasting Centers concerning CPU, vector facilities, GPU's....????

European Centre for Medium-Range Weather Forecasts ECMWF

- Always has one of the fastest and largest meteorological data storage system (forecasts, reanalysis...)
    - Spectral model, nonhydrostatic – operational

- Since the beginning with vector CPU's and up to now, no GPU's in operational mode for physically based models

- **Current computer system:**

    - **1,015,808 AMD EPYC Rome cores (Zen2) without GPUs and has a total memory of 2050 TB**
    - **RMAX LINPACK : 30.0 PFLOS**
    - **Ranked 14 on the Top500 June 2022**

- Choice of an HPC computer without GPUs ✉ stable operational forecasts are prioritized.

Deutscher Wetterdienst (DWD)

- ICON model: Finite volume – icosahedral

- Current computer system:
  - **40,200 AMD EPYC Rome cores (Zen2) without GPUs and has a total memory of 429 TB (256 GB X 1675 CPUs);**
  - **With vector engines**
    - Vector engines and GPUs share a similar design from the ground-up to handle large vectors, but a vector engine has a wider memory bandwidth
  - **3.3 PFLOS**
  - **2 systems: one ranked 130th and the other 150th June 2022 Top500.**

- This choice also prioritizes a stable operational HPC system for weather forecasts.

Swiss National Supercomputing Centre (CSCS)

- CSCS operates cutting edge high-performance computing systems as an essential service facility for Swiss researchers.
- MeteoSwiss operates the Consortium for Small-Scale Modelling (COSMO) with a 1.1 km grid on a GPU-based supercomputer.

- **First fully capable weather and climate model to become operational on a GPU-accelerated supercomputer:** codes rewritten from FORTRAN C++ near global area

- Computer system installed in 2016:
  - 387,872 Intel E5-2969 v3 cores with 4888 NVIDIA P100 GPUs and has a total memory of 512 TB
  - Rmax is 21.23 PFLOS
  - **Ranked 23rd** on the Top500 June 20922

National Center for Atmospheric Research - NCAR

- Global models – spectral, finite volume, spectral elements, finite difference
  - MPAS – finite volume has been designed for global weather and climate prediction with GPU accelerator.
- Limited area model WRF widely used for operational forecasting in several countries and regional officesGPU-accelerated version of WRF was developed by TQI

- **Computer facilities:**

  - **GPU-accelerated total of 323,712 AMD EPYC Milan 7763 cores (Zen3) with a total of 328 GPUs of NVIDIA A100 and a total memory of 692 TB**
  - **Rmax is 19.87 PFLOS**
  - **Ranked 25th on the Top 500 Supercomputer List in June 2022**

- Choice of an HPC computer with GPUs was because NCAR is the leading atmospheric science institution in the world, seeking the potential of GPU acceleration in weather models such as WRF and GPU-enabled MPAS

Institute of Physical and Chemical Research (RIKEN)

- One of the main research fields by computers is atmospheric science such as large ensemble atmospheric predictions.
  - One thousand ensemble members of a short-range regional-scale prediction were investigated for disaster prevention and evacuation.
  - Reliable probabilistic prediction of a heavy rain event was achieved with mega-ensemble members of 1000.

- **Computer system: HPC computer, Fugaku (2021)**
  - **Total of 7,630,848 Fujitsu A64FX cores without GPUs and has a total memory of 4850 TB**
  - **LINPACK performance (Rmax) is 997 PFLOS**
  - **Ranked 2nd on the Top 500 in June 2022**

- The choice of an HPC computer without GPUs was probably because A64FX is a fast processor with a scalable vector extension, which allows for a variable vector length and retains its speed for actual versatile programs.

Japan Agency for Marine–Earth Science and Technology (JAMSTEC)

- JAMSTEC : weather/climate prediction, climate change
- Future climate projections with 20 km resolution
- High Resolution Model Intercomparison Project (HighResoMIP)

- **Computer System: 3 computers installed in 2021**

- **first one has a total of 43,776 AMD EPYC Rome cores (Zen2) without GPUs and has a total memory of 2050 TB; with vector engines similar to DWD**
- **Its Rmax is 9.99 PFLOS**
- **51st on the Top500 June 2022**

- Choice of a heterogeneous HPC system was probably because JAMSTEC promotes studies on artificial intelligence in Earth system science as well as the conventional ones.

China Meteorological Administration - CMA

- 2 Computer Systems:
  - one has a total of 50,816 Xeon Gold cores with an NVIDIA Tesla P100
  - Rmax of 2.55 PFOPS;
  - the other has a total of 48,128 Xeon Gold cores without GPUs
  - Rmax of 2.44 PFOPS.

National Oceanic and Atmospheric Administration (NOAA)

- Twin computer system installed in 2018:
- 327,680 AMD EPYC 7742 cores (Zen2) and 48,128 without GPUs
- New system installed in 2022……
    - **twin supercomputers, located in Manassas, Virginia, and Phoenix, Arizona, now operate at a speed of 14.5 petaflops**
    - **Coupled with NOAA's research and development supercomputers in West Virginia, Tennessee, Mississippi and Colorado, which have a combined capacity of 20 petaflops, the supercomputing capacity supporting NOAA's new operational prediction and research is now 49 petaflops.**

https://wgne.net/nwp-systems-wgne-table/wgne-table/

WORLD METEOROLOGICAL ORGANIZATION
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Working Group on Numerical Experimentation

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WGNE Overview of Plans at NWP Centres with Global Forecasting Systems — 2023
(the information marked yellow has not been updated)

WGNE Overview of Plans at NWP Centres with Global Forecasting Systems — 2022
(the information marked yellow has not been updated)

WGNE Overview of Plans at NWP Centres with Global Forecasting Systems — 2021
(the information marked yellow has not been updated)

WGNE Overview of Plans at NWP Centres with Global Forecasting Systems — 2020
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WGNE Overview of Plans at NWP Centres with Global Forecasting Systems — 2019
(the information marked yellow has not been updated)

WGNE Overview of Plans at NWP Centres with Global Forecasting Systems — 2018
(the information marked yellow has not been updated)

LATEST NEWS

- AGU Fall Meeting 2023 (11-15 December 2023)
- EWGLAM 2023, 25-28 September 2023, Reykjavík
- WCRP Open Science Conference: Registrations open!
- DKRZ selected to host the ESMO Project Office
- WCRP Open Science Conference (23-27 October 2023, Rwanda): deadline extended to 14 March 2023

How about Brazil’s position in HPC – TOP500?

2 Brazilian entries in the November 1994 TOP500

	Rank	System	Cores	Rmax (GFlop/s)	Rpeak (GFlop/s)	Power (kW)
INPE – Operational Weather//Climate	199	SX-3/12R, NEC INPE (National Institute for Space Research) Brazil	1	2.90	3.20	
Marine Research – Military	426	POWER CHALLENGE, HPE Instituto de Estudos do Mar Brazil	6	1.47	1.80	

2 Brazilian entries in the November 2011 TOP500

	Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
INPE – Operational Weather//Climate	29	**Tup** - Cray XT6 12-core 2.1 GHz, Cray/HPE INPE (National Institute for Space Research) Brazil	30,720	205.10	258.05	
University – Engineering – COPPE/UFRJ	117	**Galileu** - Sun Blade x6048, Xeon X5560 2.8 Ghz, Infiniband QDR, Oracle NACAD/COPPE/UFRJ Brazil	6,464	64.63	72.40	430

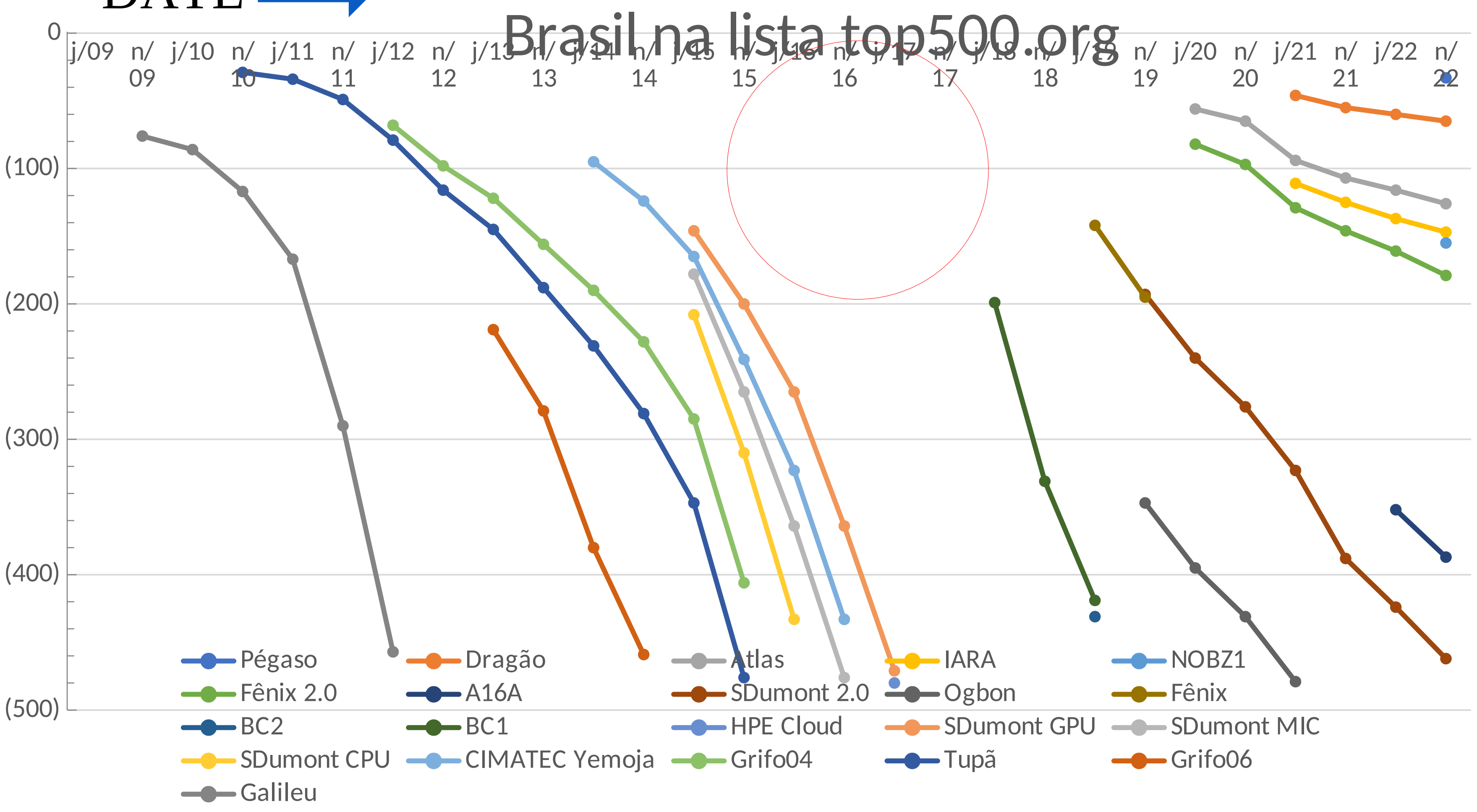
6 Brazilian entries in the June 2015 TOP500

	Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
National Laboratory for Scientific Computing	146	**Santos Dumont GPU** - Bullx B710, Intel Xeon E5-2695v2 12C 2.4GHz, Infiniband FDR, Nvidia K40, Atos Laboratório Nacional de Computação Científica Brazil	10,692	456.80	657.52	371
CIMATEC – Industrial Research	165	**CIMATEC Yemoja** - SGI ICE X, Intel Xeon E5-2690v2 10C 3GHz, Infiniband FDR, HPE SENAI CIMATEC Brazil	17,200	405.37	412.80	2,580
National Laboratory for Scientific Computing	178	**Santos Dumont Hybrid** - Bullx B710, Intel Xeon E5-2695v2 12C 2.4GHz, Infiniband FDR, Intel Xeon Phi 7120P, Atos Laboratório Nacional de Computação Científica Brazil	24,732	363.23	478.83	859
National Laboratory for Scientific Computing	208	**Santos Dumont CPU** - Bullx B71x, Intel Xeon E5-2695v2 12C 2.4GHz, Infiniband FDR, Atos Laboratório Nacional de Computação Científica Brazil	18,144	321.18	348.37	630
Petrobras	285	**Grifo04** - Itautec Cluster, Xeon X5670 6C 2.930GHz, Infiniband QDR, NVIDIA 2050, Itautec Petróleo Brasileiro S.A Brazil	17,408	251.50	563.36	366
INPE – Operational Weather//Climate	347	**Tup** - Cray XE6, Opteron 6172 12C 2.10GHz, Cray Gemini interconnect, Cray/HPE INPE (National Institute for Space Research) Brazil	31,104	214.20	261.27	

With GPU

DATE

Ranking in TOP500



From Antonio Tadeu Gomes/LNCC

Hardware upgrade interval in major weather/climate forecasting centers

Center	Time between grades
	yr
ECMWF	2-4
KMA	4-5
METEO	4-6
UKMO	3-4
NCEP	3-6
CMA	4-9
DWD	2-8
JMA	5-6
BOM	5-6
NCMRWF	4
CPTEC	> 8

Summary expected upgrades in computer systems in Brazil **2024**

- Upgrade of CPTEC computer system – R$60 mi (+ R$140mi next 3 years)
- Upgrade LNCC - Santos Dumont Computer - 100 mi
- Upgrade LNCC- SINAPAD system R$50mi (3 regional centers)
- New "Scientific SuperComputing Center of the State of São Paulo"- R$50 mi

Main challenges in HPC application in Meteorology

1. Floating Point

- double-precision floating point and numerical integration scheme have been prerequisites in weather prediction.

- However, single (and half) precision have been investigated for two reasons:
  - 1^{st}: the volume of variables is reduced -> cache and memory -> fast access to memory
  - 2^{nd} : several GPUs have a fast processing unit for single- and half-precision floating
    - several GPUs have a fast processing unit for single- and half-precision floating
    - NVIDIA introduced mixed-precision (TensorFloat-32) running on the A100 GPU, reaching 156 TFLOPS

Main challenges in HPC application in Meteorology

2. Spectral Transform in Global Weather Models

- Fourier along latitude: FFT is very efficient
- Legendre in the meridional direction (not so efficient as FFT's)

Versus

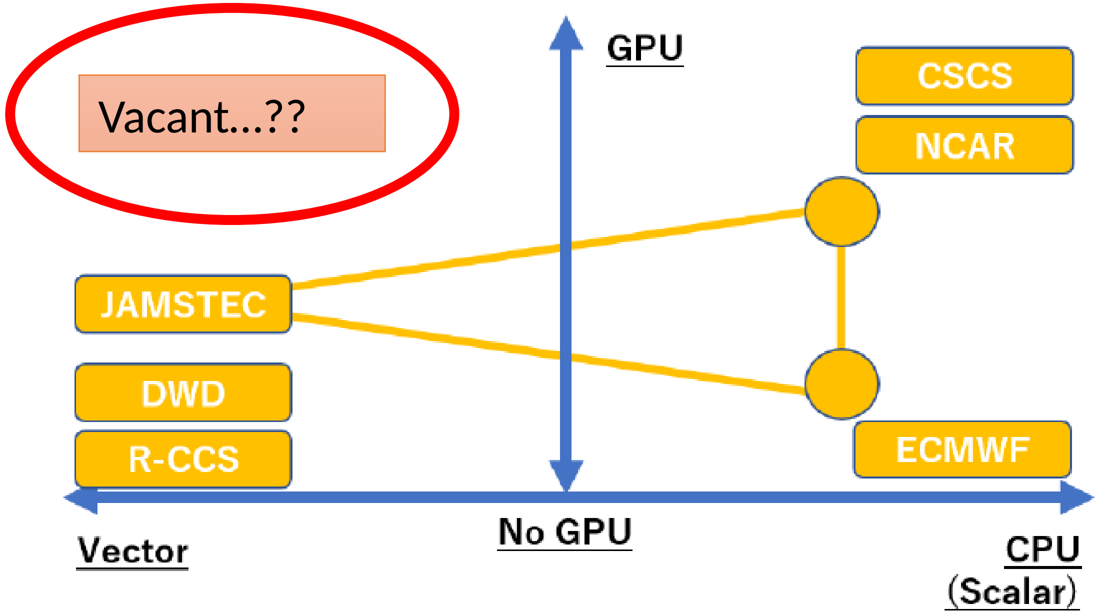
- Double Fourier transform (lat x lon)

(need more research!)

Main challenges in HPC application in Meteorology

3. Heterogeneous Computing

- CPUs, GPUs, and AI-PUs each have strong features
- Typical heteogeneous system: CPU + single type of GPU
- Another heterogeneous system is composed of multi-type CPUs and multi-type GPUs by a natural extension
- Growth of AI applications => more heterogeneous system composed of a mix of processor architectures across CPUs, GPUs, FPGAs, AI-PUs, DLPs (deep learning processors), and others such as vector engines, collectively described as XPUs.



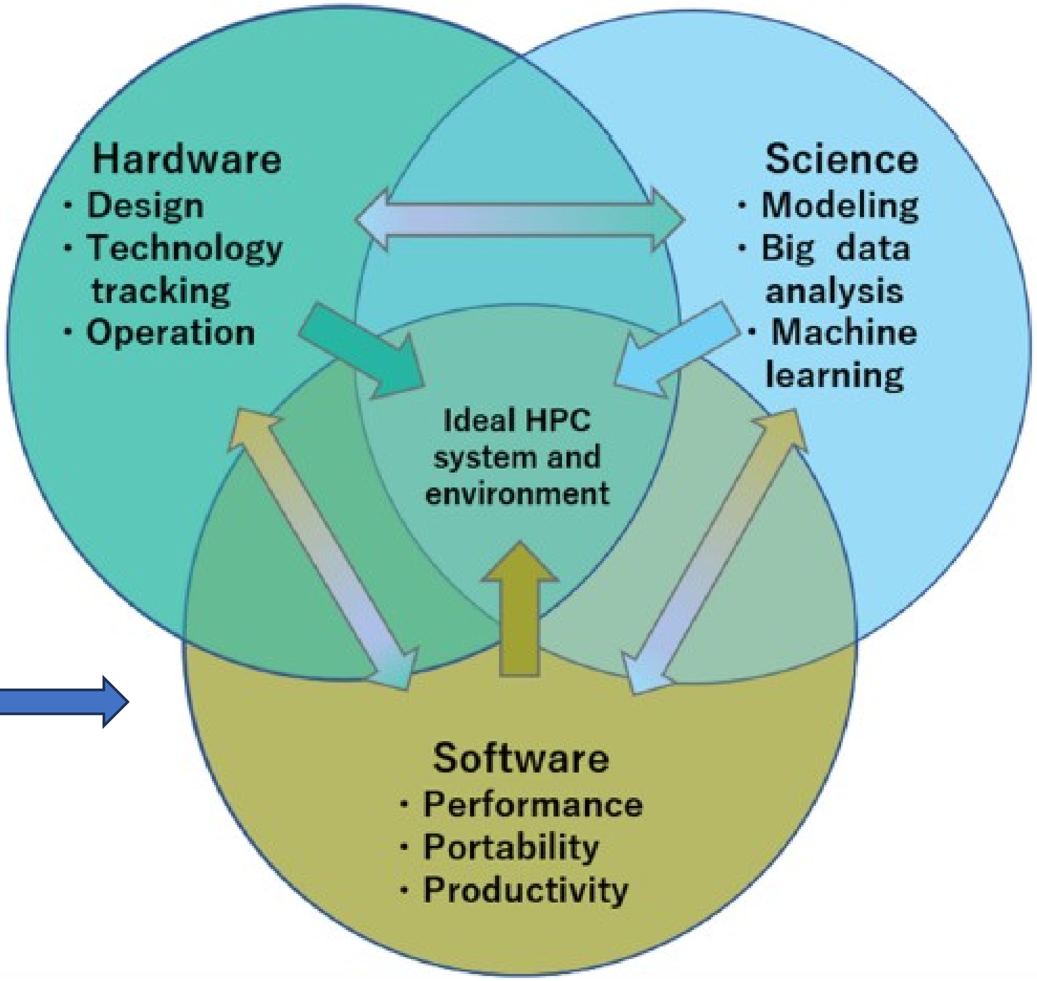
- Programming was more difficult in heterogeneous systems... (personnal experience with Santos Dumont computer)
- New high-level programming SYCL
- ECMWF is leading institution in heterogeneous computing - experience in Brazil

Main challenges in HPC application in Meteorology

4. Co-Design

- Computer science: design of new systems.
  - A "Zoo" of scientists , software developers and hardware developers
  - Need collaborative work including experts in the application .
  - Shared development!!!!

These three communities are essential for a better HPC system and keep the co-design



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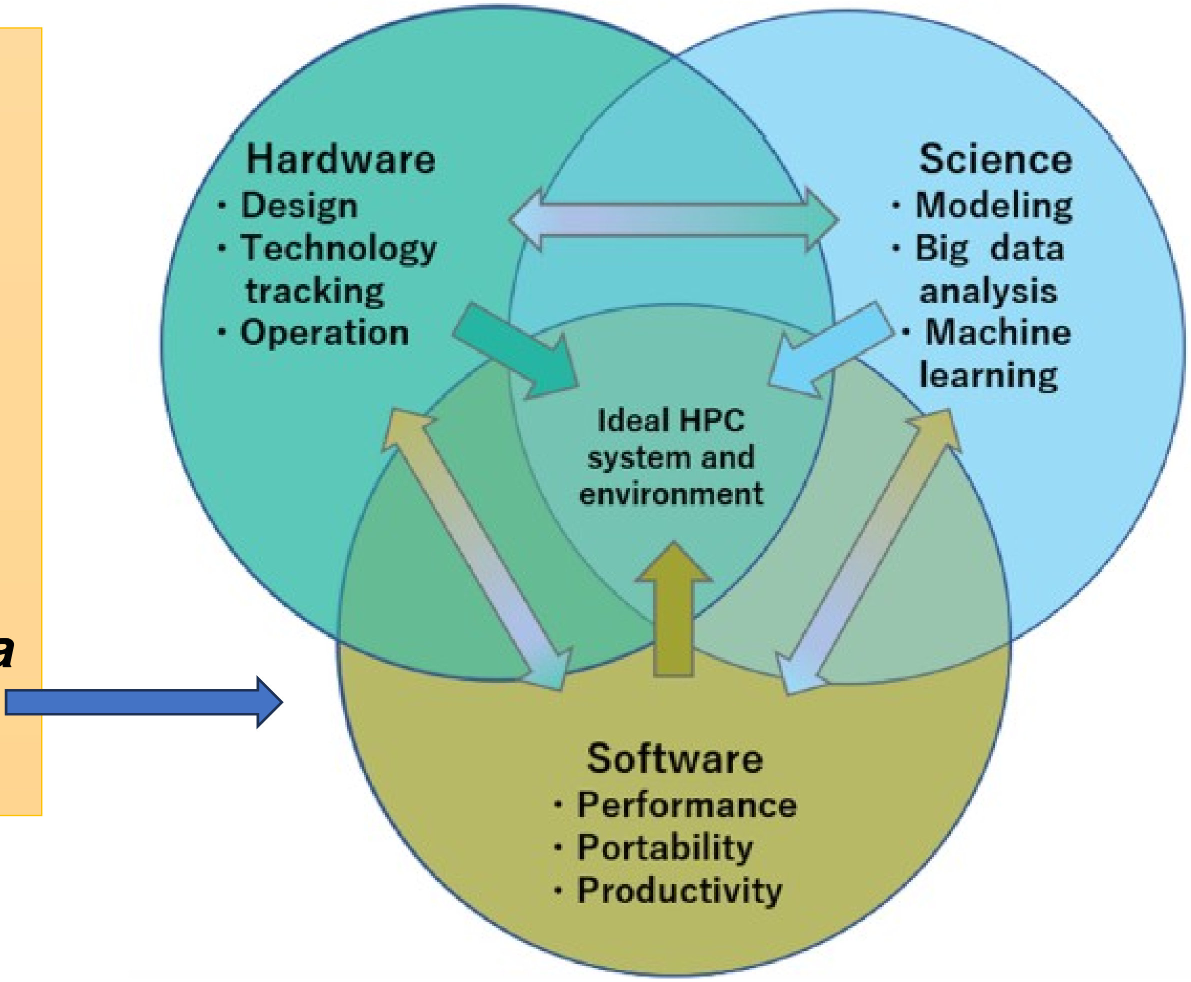

Main challenges in HPC application in Meteorology

5. New technologies

- Photonics - Advancements in photonic computing, particularly in the development of optical interconnects and photonic integrated circuits, are expected to have a significant impact on the next generation of supercomputers.

- Quantum computing – advencements in algorithms

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Article Type: Research Article

Quantum Computers for Weather and Climate Prediction: The Good, the Bad, and the Noisy

F. Tennie and T. N. Palmer

Online Publication: 27 Feb 2023

Print Publication: 01 Feb 2023

DOI: https://doi.org/10.1175/BAMS-D-22-0031.1

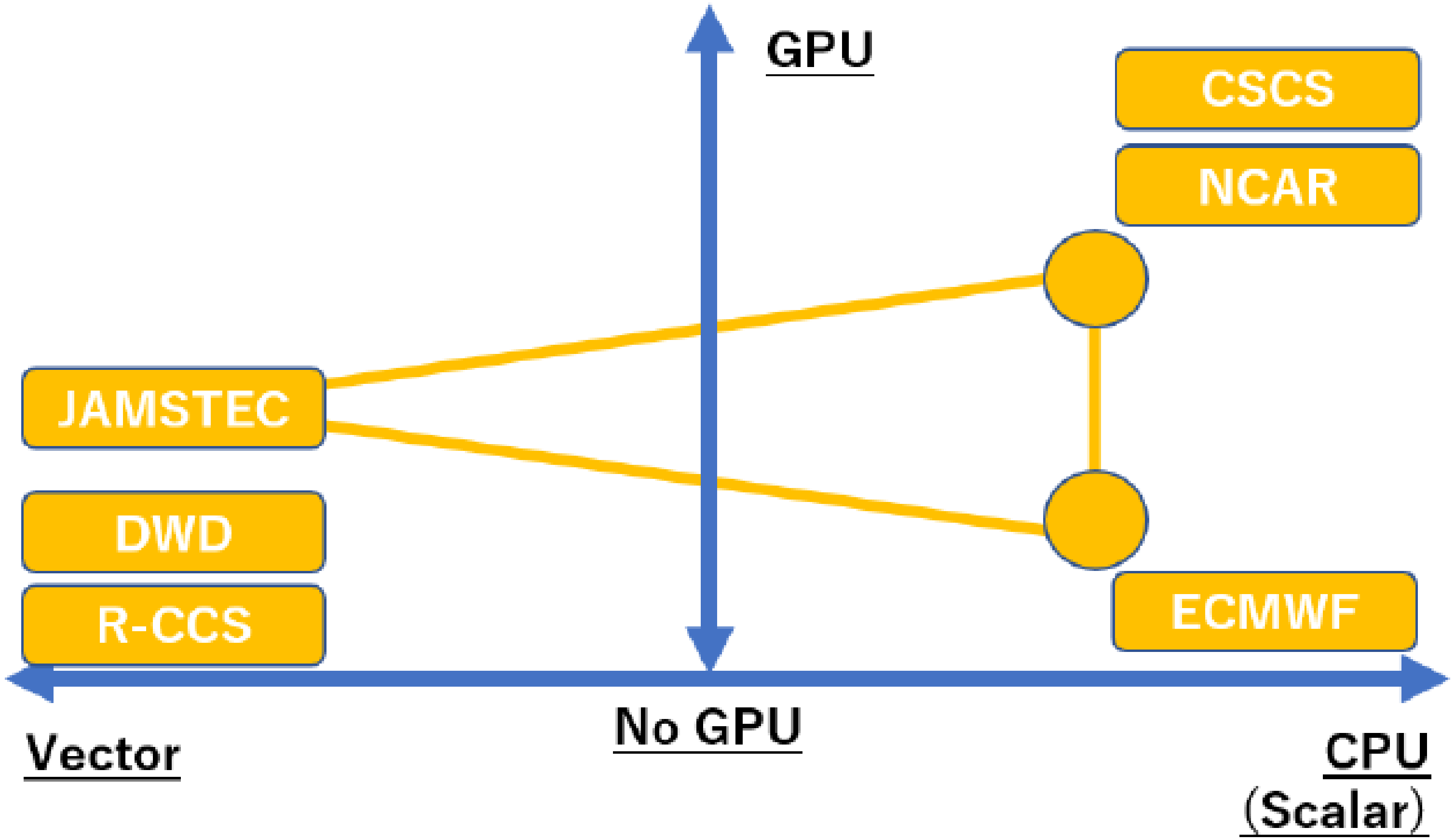
Page(s): E488–E500

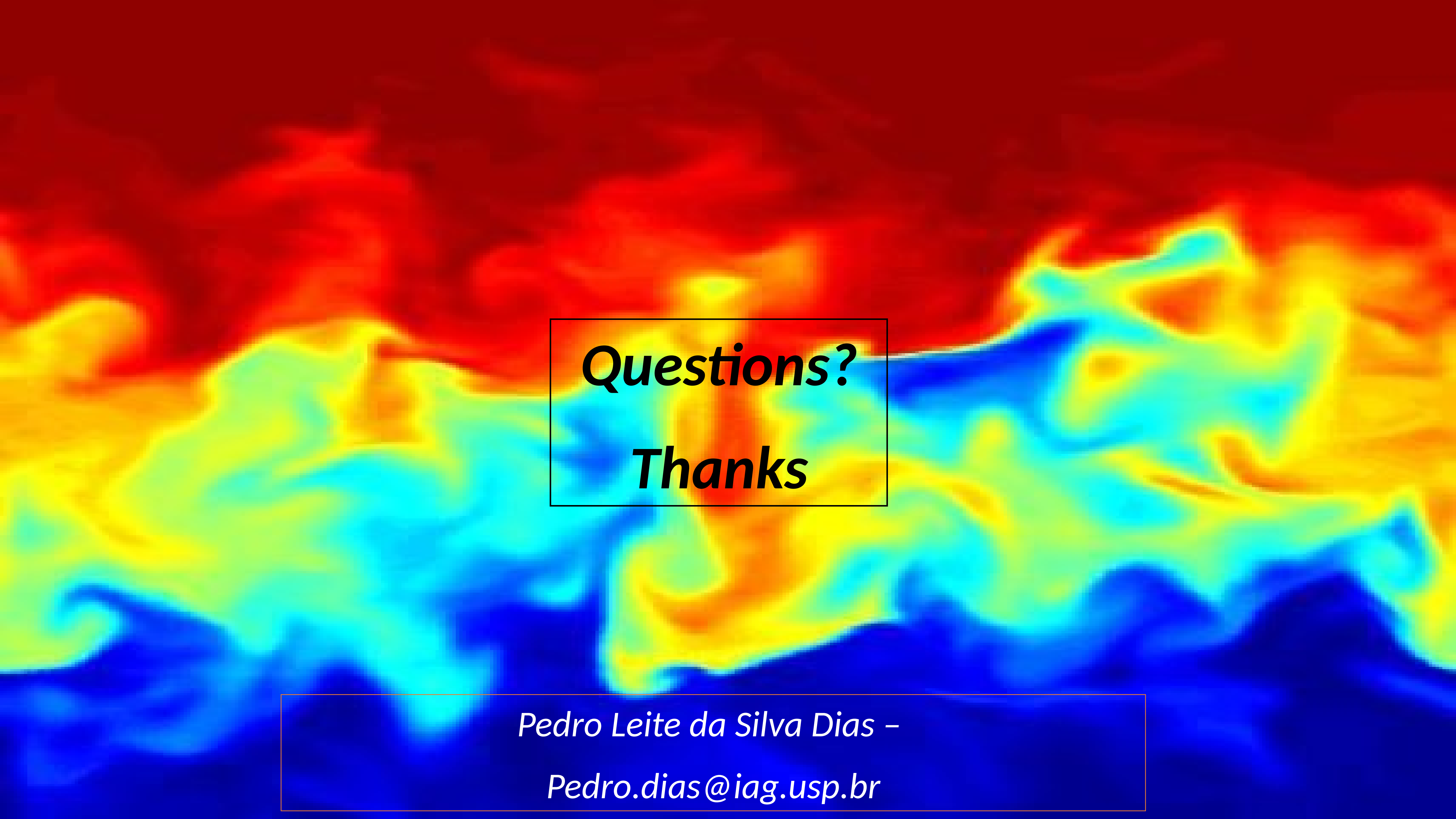
Current status of operational and research activities in earth system modeling in Brazil

- The Weather Forecasting and Climate Studies Center/INPE – one of the big "stars" on the world stage lost experts and funding. CPTEC became outdated in terms of processing capacity during the 2011-2020 decade.

- In 2021, an effort was organized to regain the capacity to predict weather/climate and produce future climate scenarios with the organization of cooperative work involving the university community and MCTI research institutes (led by INPE with the participation of school teachers from north to south of the country).

- The aim is to build a community model that can be used at multiple spatial and temporal scales. The project has support from FINEP (R$200 million over 5 years for now and is led by Dr. Saulo Freitas from INPE and Prof. Pedro Dias from USP).


GPU
CSCS
NCAR
JAMSTEC
DWD
R-CCS
ECMWF
Vector
No GPU
CPU
(Scalar)



Questions?

Thanks

Pedro Leite da Silva Dias –

Pedro.dias@iag.usp.br