# **High-Performance Computing in Meteorology**

Subjects: Environmental Sciences Contributor: Tosiyuki Nakaegawa

High-performance computing (HPC) enables atmospheric scientists to better predict weather and climate because it allows them to develop numerical atmospheric models with higher spatial resolutions and more detailed physical processes.

Keywords: meteorology ; graphical processing unit (GPU) ; high-performance computing (HPC) ; heterogeneous computing ; floating point ; spectral transform ; co-design ; data-driven ; physical-based ; weather forecast model

# 1. Introduction

Numerical weather predictions were one of the first operational applications of scientific computations <sup>[1]</sup> since Richardson's dream in 1922, which attempted to predict changes in the weather by a numerical method <sup>[2]</sup>. The current year of 2022 is the hundred year anniversary. After so-called programable and electronic digital computers were developed, computers such as ENIAC have been used for weather predictions. High-performance computing (HPC) enables atmospheric scientists to better predict weather and climate because it allows them to develop numerical atmospheric models with higher spatial resolutions and more detailed physical processes. Therefore, they develop numerical weather/climate models (hereafter referred to as weather models) so that the models can be run on any HPC system available to them.

In the 1980s, supercomputers composed of vector processors such as CRAY-1 and -2 dominated computing fields because computing was primarily used in the business and scientific fields [3]. These computations focused on floating point operations per second (FLOPS); the supercomputers had central processing units (CPU) that implemented an instruction set where its instructions were designed to operate efficiently and effectively on large one-dimensional arrays of data called vectors (https://en.wikipedia.org/wiki/Vector\_processor, accessed on 3 May 2022). Since the middle of the 1980s, CPUs for personal computers (PCs) such as the Intel x86 CPU became popular and the cost performance became higher for CPUs for PCs because of the economics of scale and lower CPUs with vector processors (Figure 1). In the late 1990s, many vendors built low supercomputers with the free operating system Linux with many CPUs for PCs as a cluster. This concept is called the Beowulf approach; it faded out the supercomputer and faded in HPC clusters. Multi- and many-core CPUs were released in the late 2000s. This concept was designed to break the technological limitation of a higher operating frequency and a higher density of large integrated circuits to align with Moore's Law. Since the late 2000s, HPC clusters have usually been composed of multi- and multi/many-core CPUs. In parallel to the dawn of multi/many-core CPUs, graphical processing units (GPU) have become faster with more generalized computing devices or general purpose GPUs (GPGPUs; GPGPU is hereafter referred to as GPU)<sup>[4]</sup>. Deep learning has also attracted people to the emerging technology because deep learning behaves similar to human intelligence. Capable GPUs play an important role in deep learning. A few HPC machines have been composed of multi/many-core clusters and GPU clusters since the late 2010s because a GPU is fast and cost-effective in HPC businesses and science. However, the two components do not always work with each other and often work independently. Exascale computing of 1018FLOPS has been a hot topic in HPC technology and science since the late 2010s; heterogeneous computers composed of different CPUs and GPUs are essential for exascale computing and broad users with different computing purposes. Since the late 2010s, processing units for deep learning or artificial intelligence (AI-PU, often referred to as an AI accelerator) have been developed because of the high demand for AI applications in many industrial sectors. An AI-PU has similar features to a GPU, but only has special matrix processing chips with a high volume of low-precision computation, which is considered to have an important role in the near future.



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

The current status surrounding HPC is distinctly complicated in both hardware and software terms, and flows similar to fast cascades. It can be difficult to understand and follow the status for beginners. A short review is required to overcome the obstacles to be fully aware of the information on HPC and to connect it to studies. This short entry shows how innovative processing units—including GPUs—are used in HPC computers in meteorology, introduces the current scientific studies relevant to HPC, and discusses the latest topics in meteorology accelerated by HPC computers.

# 2. Utilization of GPUs in Weather Predictions

There are two approaches to the usage of GPUs in meteorology as well as general science: the data-driven approach, and the physical-based approach (**Figure 2**). Deep learning is most popular in the data-driven approach. Deep learning can provide weather forecasts even with large ensemble members in a short computing time once a deep learning model has been trained with a large amount of data <sup>[5][6][7]</sup>. So-called big data or a large amount of data are required to train the deep learning model. Many deep learning models have open-source frameworks and several of them are freely available (e.g., TensorFlow and Keras). The deep learning model can be developed with less effort than a physical-based model. A few of the physical-based models introduced below are freely available from downloads, but it is difficult to understand all codes from the top to the bottom. GPUs can effectively accelerate the training and are always used in deep learning studies. This approach prohibits areas without data to develop a deep learning model in most cases, and contributes little to the progress of the science of meteorology because one cannot tell how input data are mapped to output data through physical processes in the atmosphere.



Figure 2. Schematics for the usage of GPUs in a weather forecast.

The physical-based numerical weather model has been the traditional approach for predicting future weather since Richardson's dream <sup>[2]</sup>. The model is described in discretized mathematical formulas of the physical processes and can implement progress in science in a relatively easy manner. The usage of GPUs brings fast predictions and high cost-performance to weather predictions. However, the original codes of the model are written for CPU-based computers and need to be rewritten or converted to run on GPUs. Software for exporting codes to GPUs (e.g., Hybrid Fortran) <sup>[8]</sup> has

been developed to lower these obstacles. In the following sections, HPC computers for physical-based weather models are discussed.

# 3. HPC in Meteorological Institutes and Centers

### 3.1. European Centre for Medium-Range Weather Forecasts

The European Centre for Medium-Range Weather Forecasts (ECMWF) is the leading center of weather forecasts and research in the world. ECMWF predicts global numerical weather and other data for the members and co-operating states of the European Union as well as the rest of the world. ECMWF has one of the fastest supercomputers and largest meteorological data storage facilities in the world. The fifth generation of the ECMWF re-analysis, ERA5 <sup>[9]</sup>, is one of their distinguished products. Climate re-analyses such as ERA5 combine past observations with models to generate a consistent time series of multiple climate variables. ERA5 is used for quasi-observations in climate predictions and sciences, especially in regions where no observation data are available <sup>[10]</sup>.

ECMWF is scheduled to install a new HPC computer in 2022. It has a total of 1,015,808 AMD EPYC Rome cores (computer processor microarchitecture, Zen2) without GPUs and has a total memory of 2050 TB <sup>[11]</sup>. Its maximal LINPACK performance (Rmax) is 30.0 PFLOS. This HPC computer was ranked 14th on the Top 500 Supercomputer List as of June 2022 (https://www.top500.org/lists/top500/list/2022/06/, accessed on 3 May 2022). The choice of an HPC computer without GPUs was probably because stable operational forecasts are prioritized. Similar choices have been seen at the United Kingdom Meteorological Office (UKMO), Japan Meteorological Agency (JMA), and others. ECMWF is, however, working on a weather model on GPUs with hardware companies such as NVIDIA under a project called ESCAPE <sup>[12]</sup> (http://www.hpc-escape.eu/home, accessed on 3 May 2022) and ESCAPE2 (https://www.hpc-escape2.eu/, accessed on 3 May 2022).

### 3.2. Deutscher Wetterdienst

Deutscher Wetterdienst (DWD) is responsible for meeting the meteorological requirements arising from all areas of the economy and society in Germany. The operational weather model, ICON <sup>[13]</sup>, has an icosahedral grid system to avoid the so-called pole problem, which produces too small grids in polar regions to set long time steps in numerical integrations due to the Courant–Friedrichs–Lewy Condition <sup>[14]</sup>.

DWD installed a new HPC system in 2020. It is supposed to have a total of 40,200 AMD EPYC Rome cores (Zen2) without GPUs 429 ΤВ and has а total memory of (256 GB x 1675 CPUs: [15]; https://www.dwd.de/DE/derdwd/it/\_functions/Teasergroup/datenverarbeitung.html, accessed on 3 May 2022) when all computers are facilitated. Its Rmax is 3.9 and has 3.3 PFLOS. This HPC computer was ranked 130th and 155th on the Top 500 Supercomputer List in June 2022. The unique feature of this system is vector engines, which are exiting in the development of HPC computers because of the small economic scale as mentioned in the Introduction. The vector engines are an excellent accelerator for weather models that were written for CPUs with vector processors. 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. This choice also prioritizes a stable operational HPC system for weather forecasts.

### 3.3. Swiss National Supercomputing Centre

The Swiss National Supercomputing Centre (CSCS) develops and operates cutting-edge high-performance computing systems as an essential service facility for Swiss researchers. These computing systems, Piz Daint, are used by scientists for a diverse range of purposes from high-resolution simulations to the analysis of complex data (https://www.cscs.ch/about/about-cscs/, accessed on 3 May 2022). MeteoSwiss operates the Consortium for Small-Scale Modelling (COSMO) with a 1.1 km grid on a GPU-based supercomputer, which was the first fully capable weather and operational on a GPU-accelerated supercomputer (http://www.cosmoclimate model to become model.org/content/tasks/achievements/default.htm, accessed on 3 May 2022). This required the codes to be rewritten from Fortran to C++ [16]. Fuhrer et al. [17] demonstrated the first production-ready atmospheric model, COSMO, at a 1 km resolution for near-global areas. These simulations were performed on the Piz Daint supercomputer. This simulation opens a door for less than 1 kilometer-scale global simulations.

CSCS installed an HPC system in 2016. It has a total of 387,872 Intel E5-2969 v3 cores with 4888 NVIDIA P100 GPUs and has a total memory of 512 TB (CSCS 2017; <u>https://www.cscs.ch/computers/decommissioned/piz-daint-piz-dora/</u>, accessed on 3 May 2022) <sup>[18]</sup>. Its Rmax is 21.23 PFLOS. This HPC computer was ranked 23rd on the Top 500

Supercomputer List in June 2022. This choice was due to their leading efforts on exporting to GPUs as well as multi-user environments.

# 3.4. National Center for Atmospheric Research

The National Center for Atmospheric Research (NCAR) was established by the National Science Foundation, USA, in 1960 to provide the university community with world-class facilities and services that were beyond the reach of any individual institution. NCAR has developed a weather model, the Weather Research and Forecasting (WRF), which is widely used in the world. WRF is a numerical weather prediction system designed to serve both atmospheric research and operational forecasting needs. WRF is also used for data assimilation and has derivations such as WRF-Solar and WRF-Hydro. A GPU-accelerated version of WRF was developed by TQI (<u>https://wrfg.net/</u>, accessed on 3 May 2022). NCAR is developing a Model for Prediction Across Scales (MPAS) for global simulations. MPAS has a GPU-accelerated version as well as WRF.

The Centre will install a new HPC computer, DERECHO, at the NCAR Wyoming Supercomputing Center (NWSC) in Cheyenne, Wyoming, in 2022 <sup>[19]</sup> (<u>https://arc.ucar.edu/knowledge\_base/74317833</u>, accessed on 3 May 2022). It has a 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 <sup>[20]</sup>. Its Rmax is 19.87 PFLOS. The high-speed interconnection bandwidth in a Dragonfly topography reaches 200 Gb/s. The HPC computer was ranked 25th on the Top 500 Supercomputer List in June 2022. The 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 WRFg and GPU-enabled MPAS.

### 3.5. Riken or Institute of Physical and Chemical Research in Japan

The Institute of Physical and Chemical Research (RIKEN) Center for Computational Science <sup>[20]</sup> is the leading center of computational science, as the name suggests. There are three scientific computing objectives: the science of, by, and for computing. 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. A reliable probabilistic prediction of a heavy rain event was achieved with mega-ensemble members of 1000 <sup>[21]</sup>.

The Centre installed a new HPC computer, Fugaku—named after Mt. Fuji—in 2021 (<u>https://www.r-ccs.riken.jp/en/fugaku/</u>, accessed on 3 May 2022). It has a total of 7,630,848 Fujitsu A64FX cores without GPUs and has a total memory of 4850 TB <sup>[22]</sup>. Its maximal LINPACK performance (Rmax) is 997 PFLOS, which is almost that of an exascale supercomputer. This HPC computer was ranked second on the Top 500 Supercomputer List in June 2022, having retained the first position for two years. 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.

# 4. Latest Topics in High-Performance Computing in Meteorology

# 4.1. Floating Point

Several topics relevant to GPUs, especially accelerated AI-PUs, are emerging in HCP. The double-precision floating point and numerical integration scheme have been prerequisites in weather prediction. However, the usability of single-precision floating points and even half-precision floating points has been investigated for a few segments of whole computations for two reasons <sup>[23][24]</sup>. First, the volume of variables is reduced by one second and can be stored in the cache and memory, which the CPUs can rapidly access. Second, several GPUs have a fast processing unit for single-and half-precision floating points in comparison with a double one. Moreover, NVIDIA introduced mixed-precision (TensorFloat-32) running on the A100 GPU <sup>[25]</sup>, reaching 156 TFLOPS <sup>[26]</sup>.

# 4.2. Spectral Transform in Global Weather Models

The spectral transform method used in the dynamical core of several global weather models requires large computing resources such as  $O(N^3)$  calculations and  $O(N^3)$  memory, where N is the number of grids in the longitudinal direction representing a horizontal resolution because it usually uses Legendre transformation in the latitudinal direction. There are two reduction methods: fast Legendre transformation  $O(N^2(\log N)^3)$  calculations and  $O(N^3)$  memory <sup>[27]</sup>, and the double Fourier series, which uses fast Fourier transform (FFT) for both longitudinal and latitudinal directions with  $O(N^2\log N)$ 

calculations and O(N) or  $O(N^2)$  memory <sup>[28]</sup>. The latter method is superior in both calculations and memory to the former one, especially for a high horizontal resolution of about 1 km or less.

FFT is widely used in scientific and engineering fields because it rapidly provides the frequency and phase of the data. Hence, several GPU-accelerated libraries are available (<u>https://docs.nvidia.com/cuda/cuda-c-std/index.html</u>, accessed on 3 May 2022) by calling the FFT library application programming interface, cuFFT <sup>[29]</sup>. Hence, the double Fourier series mentioned above has another merit in this availability.

### 4.3. Heterogeneous Computing

Different users utilize computers, including the HPC system, for different purposes. Different hardware such as CPUs, GPUs, and AI-PUs each have strong features. Under these circumstances, a multi-user system may be heterogeneous when it is optimized for different users. A plain heterogeneous system is composed of single-type CPUs and single-type GPUs, which are widely in operation; another heterogeneous system is composed of multi-type CPUs and multi-type GPUs by a natural extension. The recent exponential growth of data and intelligent devices requires a 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 <sup>[30][31]</sup>. The vector-GPU field is vacant in **Figure 3** and will be filled with the institute(s) as heterogeneous computing prevails in HPC.



Figure 3. Schematics for positions of each type of HPC system introduced in Section 3 on a simplified field expressed as with/without CPUs and/or GPUs.

A plain heterogeneous system allows researchers to develop codes/software in single/multiple languages such as C++ and CUDA. However, multiple languages cannot describe the codes/software properly with high optimization for the heterogeneous system. To overcome such an obstacle, a high-level programming model, SYCL, has been developed by the Khronos group (<u>https://www.khronos.org/sycl/</u>, accessed on 3 May 2022), enabling code for heterogeneous processors to be written in a single-source style using completely standard C++. Data Parallel C++ (DPC++) is an Intel open-source implementation <sup>[32]</sup>. DPC++ has additional functions, including unified shared memory and reduction operations (<u>https://www.alcf.anl.gov/support-center/aurora/sycl-and-dpc-aurora</u>, accessed on 3 May 2022).

ECMWF is leading the research into heterogeneous computing for weather models designed to run on CPU-GPU hardware based on the outcomes of ESCAPE and ESCAPE2 as mentioned above. Weather model developments under literally heterogenous computing composed of three XPUs or more cannot be realized without collaborative efforts among not only model developers, but also semiconductor vendors. Heterogenous computing as HPC is now a preparation stage in meteorology <sup>[33]</sup>.

# 4.4. Co-Design

When researchers design an HPC system and environment, multiple scientists, software developers, and hardware developers need to discuss an optimal system with collaborations; hardware based on existing technology and software running on it as well as new hardware and software not yet emerging result in challenging scientific goals (Cardwell et al.) <sup>[34][35][36]</sup>. The best ideal HPC system requires the shared development of actionable information that engages all communities in charge and the values guiding their engagement. **Figure 4** depicts the co-design of an HPC system, which is drawn from the inspiration of co-producing regional climate information in the Intergovernmental Panel on Climate Change Sixth Assessment Report <sup>[37]</sup>. These three communities are essential for a better HPC system and keep the co-

design process ongoing. Participants in the community represented by the closed circles have different backgrounds and perspectives, meaning a heterogeneous community. Based on the understanding of these conditions, sharing the same concept can inspire trust among all the communities and promote the co-design process. Both co-designed regional climate information and an HPC system share the same idea in terms of collaborations across the three different communities.



**Figure 4.** The co-design of an HPC system. Participants in the community—represented by the closed circles—have different backgrounds and perspectives, meaning a heterogeneous community. The arrows connecting those communities denote the distillation process of providing context and sharing HPC-relevant information. The arrows that point toward the center represent the distillation of the HPC information involving all three communities. This figure is drawn based on Figure 10.17 in the Intergovernmental Panel on Climate Change Sixth Assessment Report <sup>[37]</sup>.

# 4.5. Resource Allocation of an HPC System

A higher horizontal resolution of a physical-based weather model can resolve more detailed atmospheric processes than a lower one <sup>[38][39]</sup>. Operational meteorological institutes/centers do not always allocate their resources to the HPC systems to enhance a horizontal resolution because they have many options to raise their forecast skills such as ensemble forecasts, detailed physical cloud processes, and initial conditions produced by four-dimensional data assimilations. **Figure 5** shows the time evolutions of the theoretical performance of the HPC systems and the horizontal resolutions of the global weather model of JMA <sup>[40]</sup>. As a long trend, the horizontal resolution increases as the HPC system has a higher performance. However, the timing of the operational starts between the improved horizontal resolutions and the HPC systems is different owing to the system optimization (mentioned above), stable operations, and others.



**Figure 5.** Time evolutions of the theoretical performance of the HPC systems and of the horizontal resolutions of the global weather model of JMA. The data were obtained from JMA <sup>[40]</sup>. M, T, and P in this figure represent the unit of Mega, Tera, and Peta, respectively.

#### 4.6. Data-Driven Weather Forecast

This entry focused on physical-based weather models. Data-driven weather forecasts are becoming popular and will be essential components of weather forecasts, enabled by technological advancements in GPUs and DLPs. Here, researchers briefly introduce two studies. Pathak et al. <sup>[Z]</sup> developed a global data-driven weather forecast model, FourCastNet, at 0.25° horizontal resolutions with a lead time from 1 day to 14 days. FourCastNet forecasts large-scale circulations with a similar level to the ECMWF weather forecast model and outperforms small-scale phenomena such as precipitation with the ECMWF weather forecast model. The forecast speed is about 45,000 times faster than the conventional physical-based weather model. Espeholt et al. <sup>[6]</sup> developed a 12 h precipitation model, MetNet-2, and investigated the fundamental shift in forecasts from a physical-based weather model to a deep learning model. This investigation demonstrated how neural networks learn forecasts. This entry may open a door to co-research between the physical-based model and the deep learning model.

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