GPU-HADVPPM4HIP V1.0: using the heterogeneous interface for portability (HIP) to speed up the piecewise parabolic method in the CAMx (v6.10) air quality model on China's domestic GPU-like accelerator

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Abstract. The graphics processing units (GPUs) are becoming a compelling acceleration strategy for geoscience numerical model due to their powerful computing performance. In this study, AMD's heterogeneous compute interface for portability (HIP) was implemented to port the GPU acceleration version of the Piecewise Parabolic Method (PPM) solver (GPU-HADVPPM) from the NVIDIA GPUs to China' s domestically GPU-like accelerators as GPU-HADVPPM4HIP, and further introduced the multi-level hybrid parallelism scheme to improve the total computational performance of the HIP version of CAMx (CAMx-HIP) model on the China' s domestically heterogeneous cluster. The experimental results show that the acceleration effect of GPU-HADVPPM on the different GPU accelerator is more obvious when the computing scale is larger, and the maximum speedup of GPU-HADVPPM on the domestic GPU-like accelerator is 28.9 times. The hybrid parallelism with a message passing interface (MPI) and HIP enables achieve up to 17.2 times speedup when configure 32 CPU cores and GPU-like accelerators on the domestic heterogeneous cluster. And the OpenMP technology is introduced to further reduce the computation time of CAMx-HIP model by 1.9 times. More importantly, by comparing the simulation results of GPU-HADVPPM on NVIDIA GPUs and domestic GPU-like accelerators, it is found that the simulation results of GPU-HADVPPM on domestic GPU-like accelerators have less difference than the NVIDIA GPUs, and the reason for this difference may be related to the fact that the NVIDIA GPU loss part of the accuracy for improved computing performance. Furthermore, we also exhibit that the data transfer efficiency between CPU and GPU has an important impact on heterogeneous computing, and point out that optimizing the data transfer efficiency between CPU and GPU is one of the important directions to improve the computing efficiency of geoscience numerical models in heterogeneous clusters in the future.

1. Introduction

Over the recent years, GPUs have become an essential part of providing processing power for high performance computing (HPC) application, and heterogeneous supercomputing based on CPU processors and GPU accelerators has become the trend of global advanced supercomputing development. The 61st edition of the top 10 list, released in June 2023, reveals that 80% of advanced supercomputers adopt the heterogeneous architectures (Top500, 2023), and the Frontier system equipped with AMD Instinct MI250X GPU at the Oak Ridge National Laboratory remains the only true exascale machine with the High-Performance Linpack benchmark (HPL) score of 1.194 Exaflop/s (News, 2023). How to realize the large-scale parallel computing and improve the computational performance of geoscience numerical models on the GPU has become one of the significant directions for the future development of numerical models.

In terms of the heterogeneous porting for air quality model, most scholars select the chemical module, one of the hotspots, to implement heterogeneous porting, and porting the computational process originally on the CPU processes to the GPU accelerator, in order to improve the computing efficiency. For example, Sun et al. (2018) used CUDA technology to port the second-order Rosenbrock solver of chemistry module of CAM4-Chem to NVIDIA Tesla K20X GPU, and achieved up 11.7x speedup compared to the AMD Opteron™ 6274 (Interlagos) CPU (16 cores) using one CPU core. Alvanos and Christoudias (2017) developed a software that automatically generates CUDA kernels to solve chemical kinetics equation in the chemistry module for the global climate model ECHAM/MESSy Atmospheric Chemistry (EMAC) and performance evaluation shows a 20.4x speedup for the kernel execution. Linford et al. (2011) presented the Kinetic PreProcessor (KPP) to generate the chemical mechanism code in CUDA language which can be implemented on NVIDIA Tesla C1060 GPU. The KPP-generated SAPRC'99 mechanism from CMAQ model achieved a maximum speedup of 13.7x and KPP-generated RADM2 mechanism from WRF-chem model achieved an 8.5x speedup both compared to the Intel Quad-Core Xeon 5400 series CPU. Similarly, the advection module is also one of the hotspot modules in the air quality model, Cao et al. (2023) adopted the Fortran-C-CUDA C scheme and implemented a series of optimizations, including reduction the CPU–GPU communication frequency, optimize the GPU memory access, and thread and block co-indexing, to increase the computational efficiency of the HADVPPM advection solver. It can achieve up to the 18.8x speedup on the NVIDIA Tesla V100 GPU compared to the Intel Xeon Platinum 8168 CPU.

The CUDA technology was implemented to carry out heterogeneous porting for the atmospheric chemical models from the CPU processors to different NVIDIA GPU accelerators. In this study, the Heterogeneous-computing Interface for Portability (HIP) interface was introduced to implement the porting of GPU-HADVPPM from the NVIDIA GPU to the China' s domestically GPU-like accelerators based on the research of Cao et al. (2023). The domestic GPU-like accelerator plays the same role as the NVIDIA GPU, which is also used to accelerate the advection module in the CAMx model, so we refer to it as a GPU-like accelerator. First, we compared the simulation results of the Fortran version CAMx model with the CAMx-CUDA and CAMx-HIP model which were coupled with the CUDA and HIP versions of GPU-HADVPPM program, respectively. And then, the computing performance of GPU-HADVPPM programs on different GPUs were compared. Finally, we tested total coupling performance of CAMx-HIP model with multi-level hybrid parallelization on the China' s domestically heterogeneous cluster.

2. Model and experimental platform

2.1. The CAMx model description and configuration

The Comprehensive Air Quality Model with Extensions version 6.10 (CAMx v6.10; ENVIRON, 2014) is a state-of-the-art air quality model which simulates the emission, dispersion, chemical reaction, and removal of the air pollutants on a system of nested three-dimensional grid boxes (CAMx, 2023). The Eulerian continuity equation is expressed as shown Cao et al. (2023), the first term on the right-hand side represents horizontal advection, the second term represents net resolved vertical transport across an arbitrary space and time varying height grid, and the third term represents turbulent diffusion on the sub-grid scale. Pollutant emission represents both point source emissions and grided source emissions. Chemistry is treated by solving a set of reaction equations defined by specific chemical mechanisms. Pollutant removal includes both dry deposition and wet scavenging by precipitation.

In terms of the horizontal advection term on the right-hand side, this equation is solved using either the Bott (1989) scheme or the Piecewise Parabolic Method (PPM) (Colella and Woodward, 1984; Odman and Ingram, 1996) scheme. The PPM horizontal advection scheme (HADVPPM) was selected in this study because it provides higher accuracy with minimal numerical diffusion (ENVIRON, 2014). The other numerical schemes selected during the CAMx model testing are listed in Table S1. As described by Cao et al. (2023), the -fp-model precise compile flag which can force the compiler to use the vectorization of some computation under value safety is 41.4% faster than -mieee-fp compile flag which comes from the Makefile of the official CAMx version with the absolute errors of the simulation results are less than ± 0.05 ppbV. Therefore, the -fp-model precise compile flag was selected when compiling the CAMx model in this research.

2.2. CUDA and ROCm introduction

Compute Unified Device Architecture (CUDA; NVIDIA, 2020) is a parallel programming paradigm which was released in 2007 by NVIDIA. CUDA is a proprietary application programming interface (API) and as such is only supported on NVIDIA's GPUs. For the CUDA programming, it uses a programming language similar to standard C, which achieves efficient parallel computing of programs on NVIDIA GPUs by adding some keywords. In the previous study, CUDA technology was implemented to port the HADVPPM program from CPU to NVIDIA GPU (Cao et al., 2023).

Radeon Open Compute platform (ROCm; AMD, 2023) is an open-source software platform developed by AMD for HPC and hyperscale GPU computing. In general, ROCm for the AMD GPU is equivalent to CUDA for NVIDIA GPU. On the ROCm software platform, it uses the AMD's HIP interface which is a C++ runtime API allowing developers to run programs on AMD GPUs. In general, they are very similar and their code can be converted directly by replacing the string "cuda" with "hip" in the most cases. More information about HIP API is available on the AMD ROCm website (ROCm, 2023). Similar to AMD GPU, developers can also use ROCM-HIP programming interface to implement programs running on the China' s domestically GPU-like accelerator. The CUDA code cannot run directly on domestic GPU-like accelerators, and it needs to be transcoded into HIP code.

2.3. Hardware components and software environment of the testing system

Table 1 lists four GPU clusters where we conducted the experiments, two NVIDIA heterogeneous clusters which have the same hardware configuration as Cao et al. (2023) and two China' s domestically heterogeneous clusters newly used in this research, namely "Songshan" supercomputer and "Taiyuan" computing platform. Two NVIDIA heterogeneous clusters are equipped with NVIDIA Tesla K40m and V100 GPU accelerators, respectively. Both two domestic clusters include thousands of computing nodes and each containing one China' s domestically CPU processor, four China' s domestically GPU-like accelerators, and 128 GB of DDR4 2666 memory. The domestic CPU has four NUMA nodes, each NUMA node has eight X86 based processors. The accelerator adopts a GPU-like architecture consisting of a 16 GB HBM2 device memory and many compute units. The GPU-like accelerators connected to CPU with PCI-E, the peak bandwidth of the data transfer between main memory and device memory is 16 GB/s.

It is worth noting that the "Taiyuan" computing platform, which has been updated in three main aspects compared to the "Songshan" supercomputer. The CPU clock speed has been increased from 2.0 GHz to 2.5 GHz, the number of GPU-like computing units has been increased from 3,840 to 8,192, and the peak bandwidth between main memory and video memory has been increased from 16 GB/s to 32 GB/s. In terms of the software environment, the NVIDA GPU is programmed using the CUDA toolkit, and the domestic GPU-like is programmed using the ROCm-HIP toolkit developed by AMD (ROCm, 2023). More details about the hardware composition and software environment of the four heterogeneous clusters are presented in Table 1.

Table 1. Configurations of the NVIDIA K40m cluster, NVIDIA V100 cluster, "Songshan" supercomputer, and "Taiyuan" computing platform.

	Hardware components	
	CPU	GPU
NVIDIA K40m cluster	Intel Xeon E5-2682 v4 CPU @2.5 GHz, 16 cores	NVIDIA Tesla K40m GPU, 2880 CUDA cores, 12 GB video memory
NVIDIA V100 cluster	Intel Xeon Platinum 8168 CPU @2.7 GHz, 24 cores	NVIDIA Tesla V100 GPU, 5120 CUDA cores, 16 GB video memory
Songshan supercomputer	China' s domestically CPU processor A, 2.0GHz, 32 cores	China' s domestically GPU-like accelerator A, 3840 computing units, 16 GB memory
Taiyuan computing platform	China' s domestically CPU processor B, 2.5GHz, 32 cores	China' s domestically GPU-like accelerator B, 8192 computing units, 16 GB memory

	Software environment	
	Compiler and MPI	Programming model
NVIDIA K40m cluster	Intel Toolkit 2021.4.0	CUDA-10.2
NVIDIA V100 cluster	Intel Toolkit 2019.1.144	CUDA-10.0
Songshan supercomputer	Intel Toolkit 2021.3.0	ROCm-4.0.1/ DTK-23.04
Taiyuan computing platform	Intel Toolkit 2021.3.0	DTK-23.04

3. Implementation details

This section mainly introduced the strategy of porting HADVPPM program from CPU to NVIDIA GPU and domestic GPU-like accelerator, as well as the proposed multi-level hybrid parallelism technology to make full use of computing resources.

3.1. Porting the HADVPPM program from CPU to NVIDIA GPU and domestic GPU-like accelerator

Fig. 1 shows the heterogeneous porting process of HADVPPM from CPU to NVIDIA GPU and domestic GPU-like accelerator. First, the original Fortran code was refactored using standard C language. Then the CUDA and ROCm HIP technology were used to convert the standard C code into CUDA C and HIP C code to make it computable on the NIVIDA GPU and domestic GPU-like accelerator. Similar to CUDA technology, the HIP technology is implemented to convert the standard C code to HIP C code by adding related built-in functions (such as hipMalloc, hipMemcpy, hipFree, etc.). To facilitate the portability of applications across different GPU platforms, ROCm provides hipify toolkits to help transcode. The hipify toolkit is essentially a simple script written in the Perl language, and its function is text replacement, which replaces the function name in CUDA C code with the corresponding name in HIP C code according to certain rules. For example, for the memory allocation function cudaMalloc in CUDA, the hipify toolkit can automatically recognize and replace it with hipMalloc. Therefore, the thread and block configuration of GPU remain unchanged due to the simple text substitution during the transcoding. In this study, the ROCm HIP technology was used to implement the operation of GPU-HADVPPM on domestic GPU-like accelerator based on the CUDA version of GPU-HADVPPM which was developed by Cao et al. (2023). The HIP code was compiled using the "hipcc" compiler driver with the library flag "-lamdhip64".

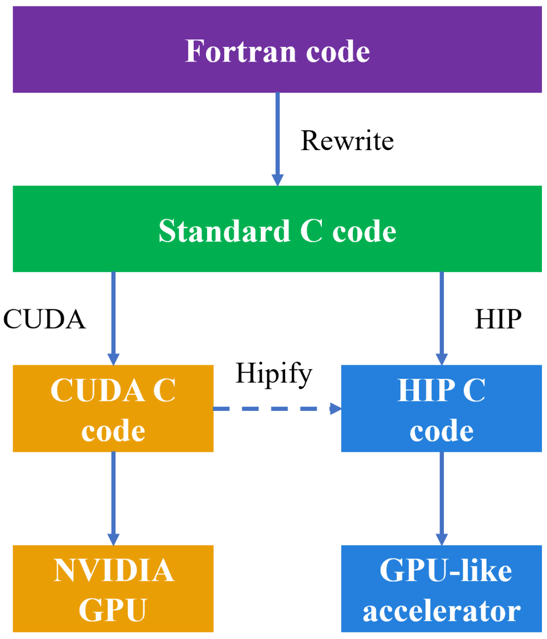

Figure 1. The heterogeneous porting process of HADVPPM Fortran code from CPU to NVIDIA GPU and domestic GPU-like accelerator.

3.2. Multi-level hybrid parallelization of CAMx model on heterogeneous platform

The original CAMx model running on the CPUs supports two types of parallelization (ENVIRON, 2014): (1) OpenMP (OMP), which supports multi-platform (e.g., multi-core) shared-memory programming in C/C++ and Fortran; (2) Message Passing Interface (MPI), which is a message passing interface standard for developing and running parallel applications on the distributed-memory computer cluster. During the process of CAMx model simulation, MPI and OMP hybrid parallelism can be used, several CPU processes can be launched, and each process can spawn several threads. This hybrid parallelism can significantly improve the computational efficiency of CAMx model.

As mentioned above, the original CAMx model supports message passing interface (MPI) parallel technology running on the general-purpose CPU. The simulation domain is divided into several sub-regions by MPI, and each CPU process is responsible for computation of its sub-region, which includes the computation tasks of advection module and other modules such as photolysis module, deposition module, chemical module, etc. In the previous studying, Cao et al. (2023) adopt a parallel architecture with an MPI and CUDA (MPI+CUDA) hybrid paradigm to configure one GPU accelerator for each CPU process. For the advection module, the simulation originally implemented by the CPU is handed over to the GPU. Other module computing tasks continue to be completed on the CPU.

In this study, when the CUDA C code of GPU-HADVPPM is converted to HIP C code, GPU-HADVPPM with an MPI and HIP (MPI+HIP) heterogeneous hybrid programming technology can also run on multiple domestic GPU-like accelerators. However, the number of GPU-like accelerators in a single compute node is usually much smaller than the number of CPU cores in the heterogeneous HPC systems. Therefore, in order to make full use of the remaining CPU computing resources, the OMP API of CAMx model is further introduced to realize the MPI+OMP hybrid parallelism of other modules on CPU. A schematic of the multi-level hybrid parallel framework is shown in Figure 2. For example, in a computing node, four CPU processes and four GPU-like accelerators are launched, and each CPU process spawns four threads. Then the advection module is simulated by 4 GPU-like accelerators, and the other modules are done by 4*4 threads spawned by CPU processes.

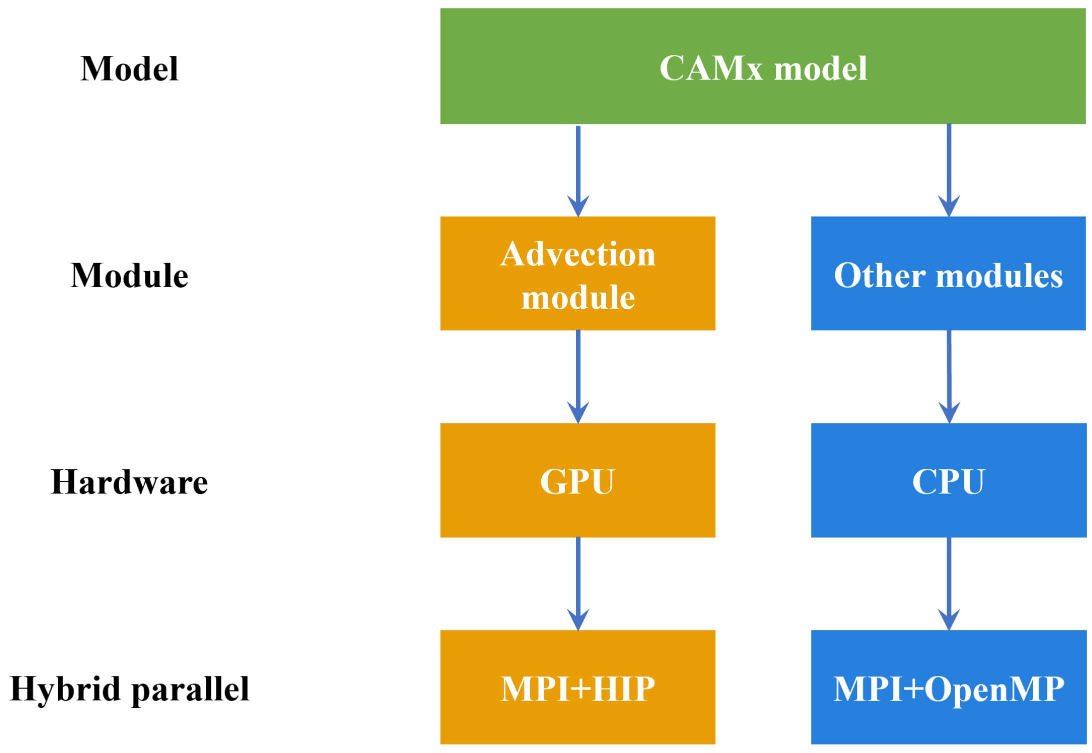

Figure 2. A schematic of the multi-level hybrid parallel framework.

4. Results and evaluation

The computational performance experiments of CUDA and HIP version GPU-HADVPPM are reported in this section. First, we compared the simulation result of the Fortran version CAMx model with CAMx-CUDA and CAMx-HIP model which were coupled with CUDA and HIP version of GPU-HADVPPM program, respectively. Then, the computational performance of GPU-HADVPPM programs on the NVIDIA GPU and domestic GPU-like accelerator are compared. Finally, we tested total performance of CAMx-HIP model with multi-level hybrid parallelization on the the "Songshan" supercomputer. For ease of description, the CAMx versions of the HADVPPM program written in Fortran, CUDA C and HIP C code are named Fortran, CUDA and HIP, respectively.

4.1. Experimental setup

There are three test cases were used to evaluate the performance of CUDA and HIP version

GPU-HADVPPM. The experimental setup for the three test cases is shown in Table 2. In the previous study of Cao et al. (2023), the BJ case was used to carry out the performance tests, HN case and ZY case are the newly constructed test cases in this study. The Beijing case (BJ) covers Beijing, Tianjin, and part of the Hebei Province with 145 × 157 grid boxes, and simulation of BJ case starts on 1 November, 2020. The Henan case (HN) mainly covers the Henan Province with 209 × 209 grid boxes. The starting date of simulation in HN case is 1 October, 2022. The Zhongyuan case (ZY) has the widest coverage of the three cases, with Henan Province as the center, covering the Beijing-Tianjin-Hebei region, Shanxi Province, Shaanxi Province, Hubei Province, Anhui Province, Jiangsu Province, and Shandong Province, with 531 × 513 grid boxes. ZY case started simulation on 4 January, 2023. All of the three performance test cases are 3km horizontal resolution, 48 hours of simulation, and 14 vertical model layers. The number of three-dimensional grid boxes in BJ, HN, and ZY cases are totally 318,710, 611,534 and 3,813,642, respectively. The meteorological fields inputting the different versions of the CAMx model in the three cases were provided by the Weather Research and Forecasting Model (WRF). In terms of emission inventories, the emission for BJ case is consistent with the Cao et al. (2023), HN case uses the Multi-resolution Emission Inventory for China (MEIC) and ZY case uses the emission constructed by Sparse Matrix Operator Kernel Emission (SMOKE) model in this study.

Table 2. The experimental setup for the BJ, HN, and ZY case.

	BJ	**HN**	**ZY**
Start date	November 1, 2020	October 1, 2022	1 January, 2023
Horizontal resolution	3km	3km	3km
Grid boxes	145 × 157 × 14	209 × 209 × 14	531 × 513 × 14
Meteorological fields	WRF	WRF	WRF
Emission	Cao et al. (2023)	MEIC	SMOKE

4.2. Error analysis

The hourly concentrations of four major species, i.e. O_3, PSO_4, CO, and NO_2, outputted by the Fortran, CUDA, and HIP versions of CAMx for the BJ case are compared to verify the results correctness before testing the computational performance. Fig. 3 shows the four major species simulation results of the three CAMx version, including Fortran version on the Intel E5-2682 v4 CPU, CUDA version on the NVIDIA K40m cluster and HIP version on the "Songshan" supercomputer, after 48 hours integration, as well as the absolute errors (AEs) of their concentrations. As described by Cao et al. (2023), the parallel design of the CAMx model adopts the primary/secondary mode, and P0 process is responsible for inputting and outputting the data and calling the MPI_Barrier function to synchronize the process, and the other processes are responsible for simulation. When comparing the simulation results, we only launched 2 CPU processes on the CPU platform, and launched 2 CPU processes and configure 2 GPU accelerators on the NVIDIA K40m cluster and "Songshan" supercomputer, respectively.

The species' spatial pattern of three CAMx versions on different platform are visually very consistent, and the AEs between the HIP and Fortran version is much smaller than the CUDA and Fortran version. For example, the AEs between the CUDA and Fortran version for O_3, PSO_4, and NO_2 are in the range of ± 0.04 ppbV, ± 0.02 $\mu g \cdot m^{-3}$, and ± 0.04 ppbV. And the AEs between the HIP and Fortran version for above the three species are fall into the range of ± 0.01 ppbV, ± 0.005 $\mu g \cdot m^{-3}$, and ± 0.01 ppbV. For CO, AEs is relatively large due to its high background concentration. However, the AEs between the HIP and Fortran versions is also less than that between the CUDA and Fortran versions where were in the range of ± 0.4 ppbV and ± 0.1 ppbV, respectively.

Considering the situation of AEs accumulate and grow, Fig. 4 highlights the time series of AEs between Fortran and CUDA versions and between Fortran and HIP versions after grid averaging. As is shown in Fig. 4, the AEs of O_3, PSO_4, CO, and NO_2 between the Fortran version and the CUDA version are -0.0002 to 0.0001 ppbV, -0.00003 to 0.00001 $\mu g \cdot m^{-3}$, -0.0004 to 0.0004 ppbV, and -0.0002 to 0.0002 ppbV, respectively, and fluctuate. Although the AEs of the above four species between the Fortran and the HIP version also fluctuates, the fluctuation range is much smaller than that of the CUDA version. Importantly, the AEs between Fortran and CUDA versions and between Fortran and HIP versions both do not accumulate and grow over prolonged simulation periods.

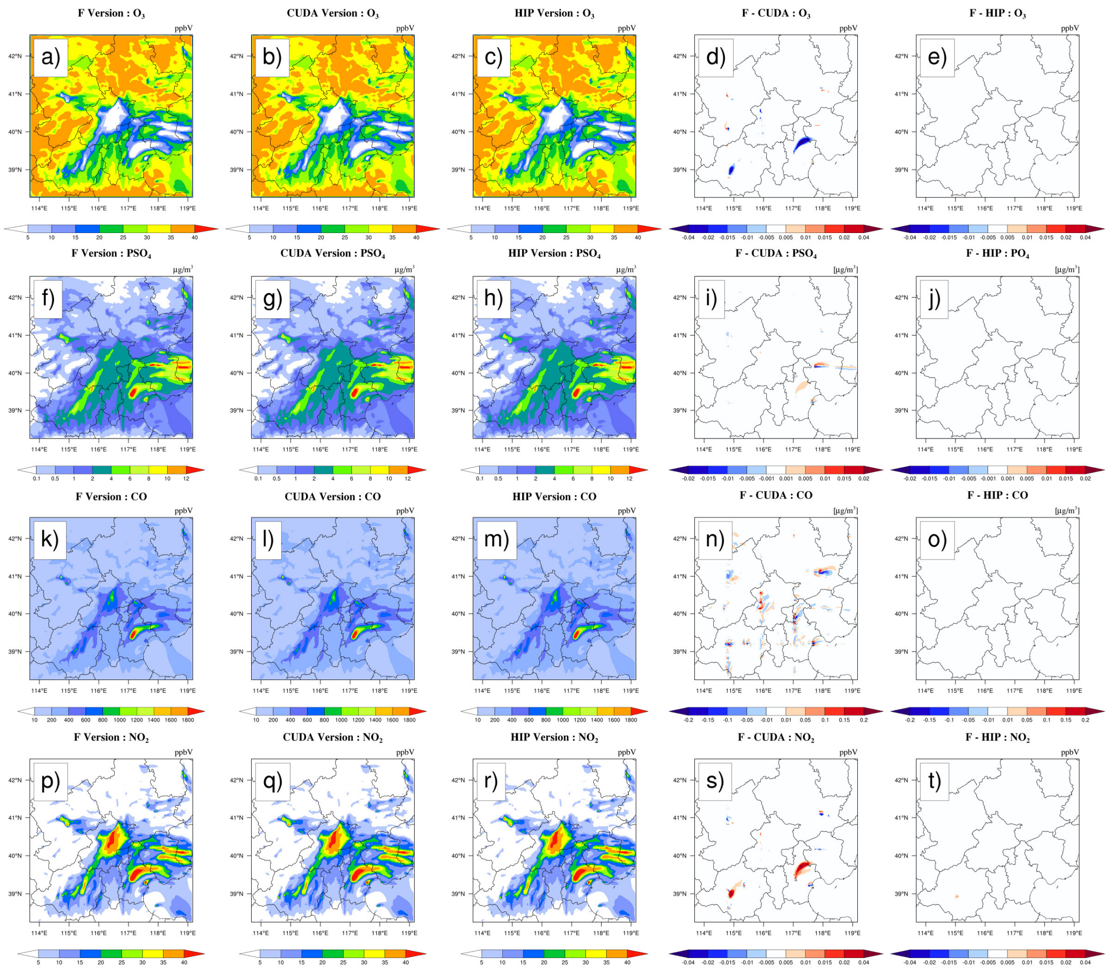

Figure 3. O_3, PSO_4, CO, and NO_2 concentrations outputted by the CAMx Fortran version on the Intel E5-2682 v4 CPU, CUDA version on the NVIDIA K40m cluster and HIP version on the "Songshan" supercomputer under the BJ case. Panels (a), (f), (k), and (p) are from the Fortran version of simulation results for four species. Panels (b), (g), (l), and (q) are from the CUDA version of simulation results for four species. Panels (c), (h), (m), and (r) are from the HIP version of simulation results for four species. Panels (d), (i), (n), and (s) are the AEs between the Fortran and CUDA versions. Panels (e), (j), (o), and (t) are the AEs between the Fortran and HIP versions.

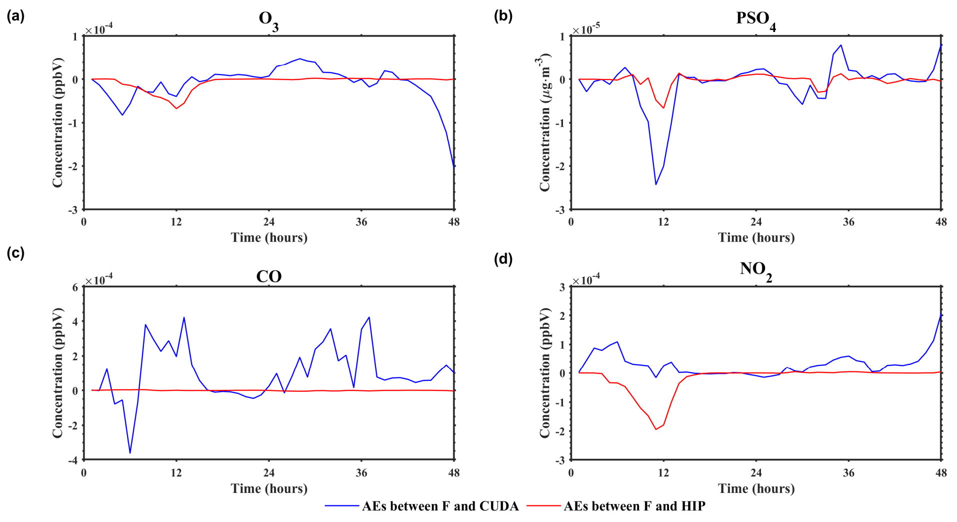

Figure 4. The time series of AEs between Fortran and CUDA versions (solid blue line) and between Fortran and HIP versions (solid red line) after grid averaging. Panel (a)~(d) represent the AEs of O_3, PSO_4, CO, and NO_2, respectively.

Fig. 5 presents the boxplot of the relative errors (REs) in all grid boxes for the PSO_4, PNO_3, PNH_4, O_3, CO, and NO_2 during the 48 hours simulation under the BJ case. Statistically, the REs between the CUDA version on the NVIDIA K40m cluster and Fortran version on the Intel E5-2682 v4 CPU for the above six species are in the range of $\pm$0.006%, $\pm$0.01%, $\pm$0.008%, $\pm$0.002%, $\pm$0.002%, and $\pm$0.002%. In terms of REs between the HIP version on the "Songshan" supercomputer and Fortran version on the Intel E5-2682 v4 CPU, the values are much smaller than REs between CUDA and Fortran versions which are fall into the range of $\pm$0.0005%, $\pm$0.004%, $\pm$0.004%, $\pm$0.00006%, $\pm$0.00004%, and $\pm$0.00008%, respectively. In the air quality model, the secondary particulate matter, such as PNH_4, PNO_3, and PSO_4, have a common characteristic: their initial concentration is very low and they are mainly generated through complex chemical reactions. Therefore, when calculating the relative error on different hardware platforms, because the value in the denominator is very small, it is very sensitive to a small difference in the numerator, resulting in a large relative error. But from the absolute error in Fig.3, the absolute error of PSO_4 on different hardware platforms is smaller than that of other species. For gaseous pollutants such as CO, O_3, and NO_2, the initial concentration is large due to emission, and the denominator value is large when calculating the relative error, which is insensitive to small differences in the numerator.

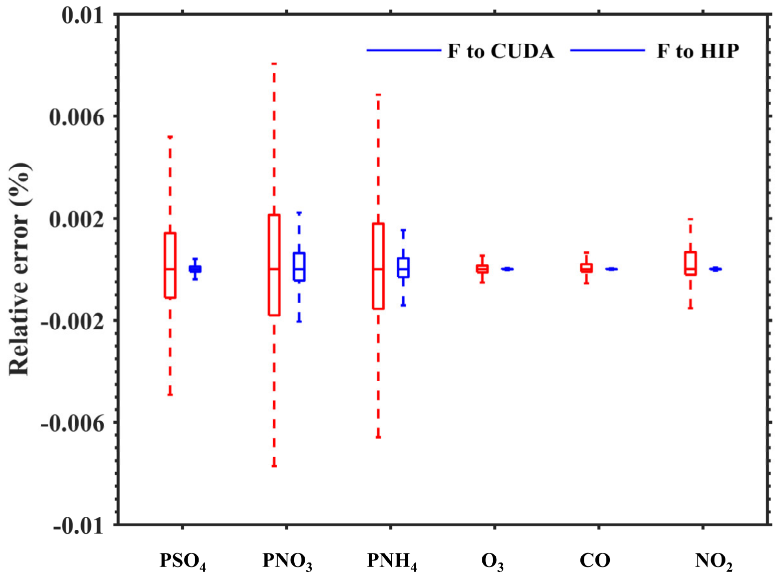

Figure 5. The distribution of REs in all grid boxes for the PSO_4, PNO_3, PNH_4, O_3, CO, and NO_2 under the BJ case. The red boxplot represents the REs between the CUDA version on the NVIDIA K40m cluster and Fortran version on the Intel E5-2682 v4 CPU, and blue boxplot represents the REs between the HIP version on the "Songshan" supercomputer and Fortran version on the Intel E5-2682 v4 CPU.

Wang et al. (2021) verified the applicability of the numerical model in scientific research by computing the ratio of root mean square error (RMSE) between two different model versions to system spatial variation (standard deviation, std). If the ratio is smaller, it is indicated that the difference in the simulation results of the model on the GPU is minimal compared with the spatial variation of the system, that is to say, the simulation results of the model on the GPU are accepted for scientific research. Here, we calculate the standard deviation of O_3, PSO_4, CO and NO_2 on the Intel Xeon E5-2682 v4 CPU, and their RMSE between the NVIDIA V100 cluster, NVIDIA K40m cluster and "Songshan" supercomputer and the Intel Xeon E5-2682 v4 CPU, which are presented in Table 3. The std for the above four species on the Intel Xeon E5-2682 v4 CPU are 9.6 ppbV, 1.7 $\mu g \cdot m^{-3}$, 141.9 ppbV, and 7.4 ppbV, respectively, and their ratios of RMSE and std on the "Songshan" supercomputer are 5.8×10^{-5}%, 4.8×10^{-6}%, 5.7×10^{-8}%, and 2.1×10^{-4}%, which are smaller than two NVIDIA clusters, especially much smaller than the NVIDIA V100 cluster. For example, the ratio on the NVIDIA K40m cluster for four species are 1.2×10^{-4}%, 6.6×10^{-5}%, 7.0×10^{-5}%, and 4.1×10^{-4}%, and ratio on the NVIDIA V100 cluster are 1.5×10^{-2}%, 2.5×10^{-3}%, 6.4×10^{-3}%, and 1.3×10^{-3}%, respectively.

Table 3. The standard deviation (std) of O_3, PSO_4, CO and NO_2 on the Intel Xeon E5-2682 v4 CPU, root mean

square error (RMSE) and its ratio on the NVIDIA V100 cluster, NVIDIA K40m cluster and "Songshan" supercomputer

		NIVIDA V100 cluster		**NIVIDA K40m cluster**		**"Songshan" supercomputer**	
	std	RMSE	RMSE/std	RMSE	RMSE/std	RMSE	RMSE/std
O_3 (ppbV)	9.6	1.5×10^{-3}	1.5×10^{-2}	1.1×10^{-5}	1.2×10^{-4}	7.4×10^{-6}	7.7×10^{-5}
PSO_4 ($\mu g \cdot m^{-3}$)	1.7	4.3×10^{-5}	2.5×10^{-3}	1.1×10^{-6}	6.6×10^{-5}	2.5×10^{-7}	1.5×10^{-5}
CO (ppbV)	141.9	9.0×10^{-3}	6.4×10^{-3}	1.0×10^{-4}	7.0×10^{-5}	4.4×10^{-7}	3.1×10^{-7}
NO_2 (ppbV)	7.4	9.3×10^{-5}	1.3×10^{-3}	3.0×10^{-5}	4.1×10^{-4}	2.0×10^{-5}	2.7×10^{-4}

From AEs, REs, and ratio of RMSE and std between different CAMx versions, it is less difference that the GPU-HADVPPM4HIP program runs on the “Songshan” supercomputer. Because the simulation accuracy of geoscience numerical model is closely related to the model efficiency, and many model optimization works improve the computational performance by reducing the precision of the data, such as Váňa et al. (2017) changed some variables precision in the atmospheric model from double precision to single precision, which increased the overall computational efficiency by 40%, and Wang et al. (2019) improved the computational efficiency of the gas-phase chemistry module in the air quality mode by 25%~28% by modifying the floating-point precision compile flag. Therefore, we speculate that this may be related to the manufacturing process of NVIDIA GPUs and domestic GPU-like accelerators, especially NIVIDA Tesla V100 series GPUs, which may use unknown optimizations to improve GPU performance efficiency by losing part of the accuracy. In this study, we mainly focus on numerical simulation. Of course, we also want to know the specific reasons for this, but we are not professional GPU research and development designers after all and do not know the underlying design logic of the hardware, so we can only present our experimental results in the air pollution model to you, and discuss with each other to jointly promote the application of GPU in the field of geoscience numerical models.

4.3. Application performance

4.3.1. GPU-HADVPPM on a single GPU accelerator

As described in Sect. 4.2, we validate the 48 hours simulation results outputted by the Fortran, CUDA, and HIP versions of CAMx. Next, computational performance was compared for the

Fortran version of HADVPPM on the Intel Xeon E5-2682 v4 CPU and domestic CPU processor A, the CUDA version of GPU-HADVPPM on the NVIDIA Tesla K40m and V100 GPU, and the HIP version of GPU-HADVPPM on the domestic GPU-like accelerator A, under the BJ, HN and ZY case. The simulation time in this section is 1 hour unless otherwise specified.

Similarity, since the CAMx model adopts the primary/secondary mode, two CPU processes P0 and P1 are launched on the CPU, and the system_clock functions in the Fortran language are used to test the elapsed time of the advection module in P1 process. When testing the computation performance of the advection module on the GPU-like accelerator, we also only launch 2 CPU processes and 2 GPU-like accelerators. When a P1 process runs to the advection module, the original computation process is migrated from the CPU to the GPU, and the hipEvent_t function in HIP programming is used to test the running time of the advection module on the GPU-like accelerator. When comparing the speedup on different GPU accelerators, the elapsed time of advection module launched one CPU process (P1) on the domestic CPU processor A is taken as the benchmark, that is, the speedup is 1.0x. The runtime of the advection module on Intel CPU processor and different GPU accelerators is compared with the baseline to obtain the speedup.

Fig. 6(a) and (b) shows the elapsed time and speedup of the different versions of HADVPPM on the CPU processors and GPU accelerators for BJ, HN, and ZY cases, respectively. The results show that using CUDA and HIP technology to port HADVPPM from CPU to GPU can significantly improve its computational efficiency. For example, the elapsed time of the advection module on the domestic processor A is 609.2 seconds under the ZY case. After it is ported to the domestic GPU accelerator and NVIDIA V100 GPU, it only takes 21.1 seconds and 7.6 seconds to complete the computing, and the speedups are 28.9x and 80.2x, respectively. The ZY case had the largest number of grids in the three cases and exceeded the memory of a single NVIDIA Tesla K40m GPU accelerator, so it was not possible to test its elapsed time on it. Moreover, the optimization of thread and block co-indexing is used to simultaneously compute the grid point in the horizontal direction (Cao et al., 2023). Therefore, it can be seen from Fig. 6(b) that the larger the computing scale, the more obvious the acceleration, which indicates that GPU is more suitable for super-large scale parallel computing, and provides technical support for accurate and fast simulation of ultra-high-resolution air quality at the meter level in the future.

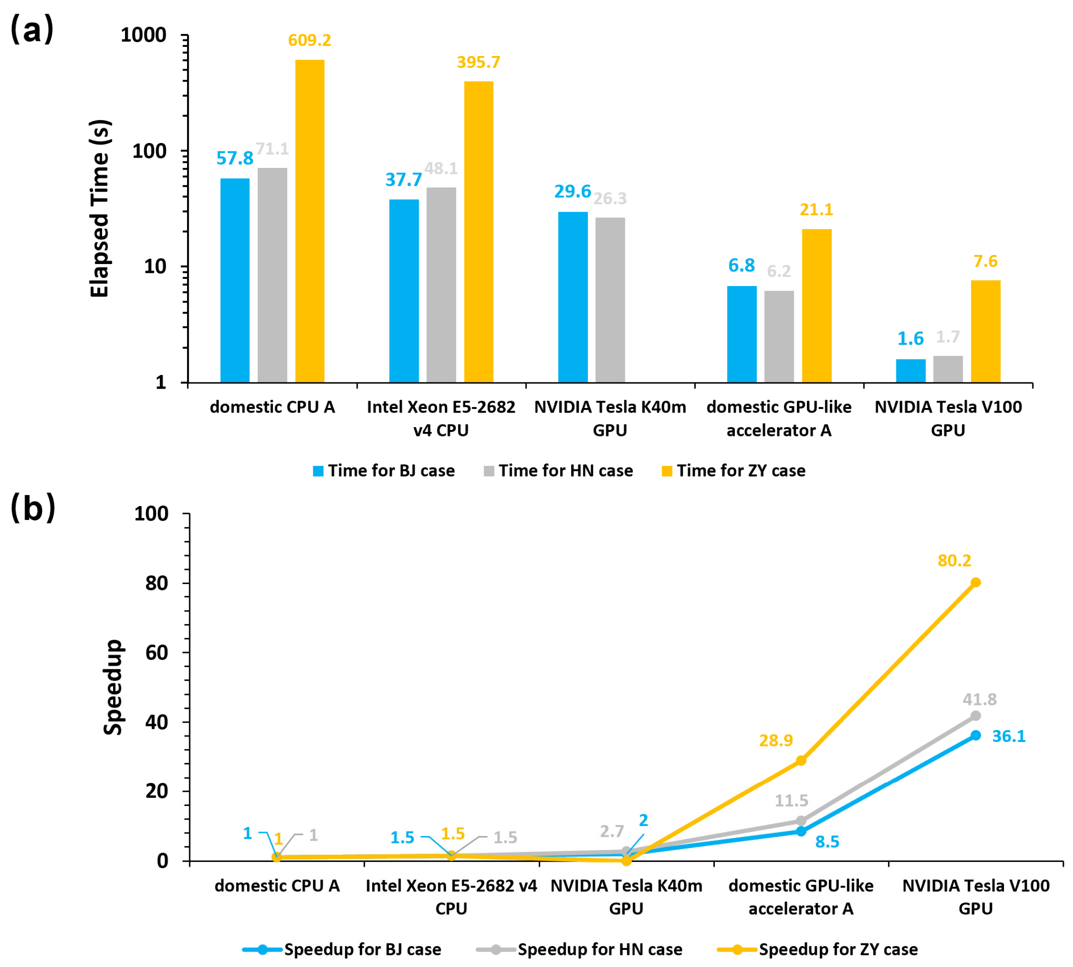

Figure 6. The elapsed time (a) and speedup (b) of the Fortran version of HADVPPM on the Intel Xeon E5-2682 v4 CPU and the domestic CPU processor A, the CUDA version of GPU-HADVPPM on the NVIDIA Tesla K40m GPU, NVIDIA Tesla V100 GPU, and the HIP version of GPU-HADVPPM on the domestic GPU-like accelerator A for BJ, HN, and ZY case. The unit of elapsed time is in seconds (s).

The timestep of BJ, HN and ZY case were 59, 47, and 61, respectively. Fig. 7 shows the GPU-HADVPPM4HIP acceleration in each time step on a single domestic GPU-like accelerator A. It can be seen from the figure that all three cases have the smallest speedup of 8.2x, 11.2x, and 27.8x at the first timestep, which is related to the time required for GPU-like accelerator startup. When the GPU-like is started and operating normally, the speedup of the three cases tend to be stable in the following time steps, and stabilize around 8.5x, 11.5x and 28.0x respectively.

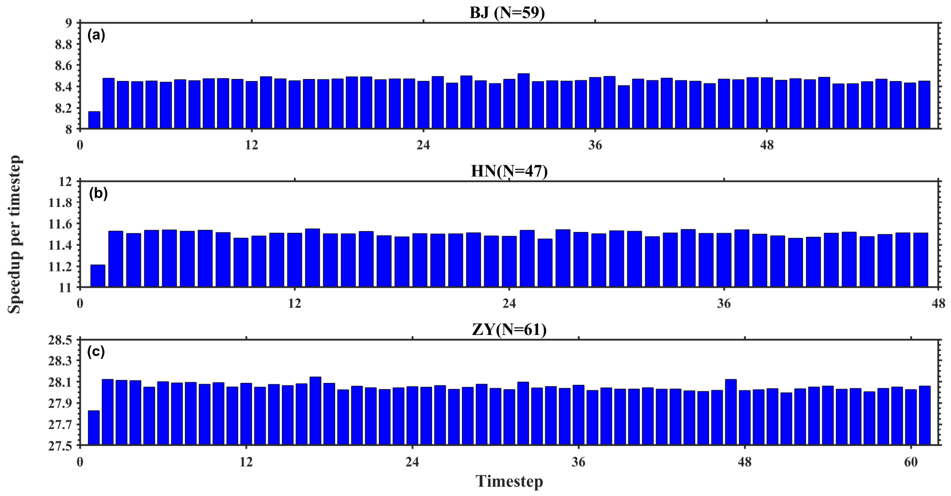

Figure 7. The GPU-HADVPPM4HIP acceleration in each time step on a single GPU-like accelerator for BJ, HN, and ZY case. The timestep of above three cases are 59, 47, and 61, respectively.

Table 4 further lists the total elapsed time of CAMx Fortran and HIP versions for BJ case on the "Songshan" supercomputer and "Taiyuan" computing platform, and the computing time of advection module with or without data transfer. By coupling the GPU-HADVPPM4HIP to CAMx model and adopting a series of optimizations (Cao et al., 2023) such as communication optimization, memory access optimization, and 2D thread optimization, the overall computation time of CAMx-HIP model on a single domestic GPU-like accelerator is faster than that of the original Fortran version on a single domestic CPU core. For example, on the "Songshan" supercomputer, one hour of simulation in CAMx-HIP model takes 469 seconds, and the Fortran version takes 481 seconds. On the "Taiyuan" computing platform, the acceleration effect is more obvious due to the upgrade of hardware and network bandwidth, and the integration time of CAMx-HIP model is 433 seconds when maintaining the same software environment, and the integration time of the Fortran version is 453 seconds.

The elapsed time of GPU-HADVPPM given in Table 4 on NVIDIA GPU and domestic GPU-like accelerator does not consider the data transfer time between CPU and GPU. However, the communication bandwidth of data transfer between the CPU and GPU is one of the most significant factors that restrict the performance of numerical model on the heterogeneous cluster (Mielikainen et al., 2012; Mielikainen et al., 2013; Huang et al., 2013). To illustrate the significant impact of CPU-GPU data transfer efficiency, the computational performance of GPU-HADVPPM with and without data transfer time for the BJ case is tested on the “Songshan” supercomputer and

“Taiyuan” computing platform with the same DTK version 23.04 software environment and the results are further presented in Table 6. For convenience of description, we refer to the execution time of GPU-HADVPPM program on GPU kernel as kernel execution time, and the time of GPU-HADVPPM running on GPU as total runtime, which contains two parts, namely, kernel execution time and data transfer time between CPU and GPU. After testing, the kernel execution time and total running time of GPU-HADVPPM4HIP program on domestic GPU-like accelerator A are 6.8 and 29.8 seconds, respectively. In other words, it only takes 6.8 seconds to complete the computation on the domestic accelerator, but it takes 23.0 seconds to complete the data transfer between the CPU and the domestic GPU-like accelerator, which is 3.4 times the computation time. The same problem exists in the more advanced the "Taiyuan" computing platform, where the GPU-HADVPPM4HIP takes only 5.7 seconds to complete the computation, while the data transmission takes 18.2 seconds, which is 3.2 times the computation time.

By comparing the kernel execution time and total running time of GPU-HADVPPM4HIP on the domestic accelerator, it can be seen that the data transfer efficiency between CPU and GPU is really inefficient, which seriously restricts the computational performance of numerical models in heterogeneous clusters. On the one hand, improving the data transfer bandwidth between CPU and GPU can improve the computational efficiency of the model in heterogeneous clusters. On the other hand, the optimization measures can be implemented to improve the data transfer efficiency between CPU and GPU. For example, (1) Asynchronous data transfer is used to reduce the communication latency between CPU and GPU. Computation and data transfer are performed simultaneously to hide communication overhead; (2) Currently, some advanced GPU architectures support a unified memory architecture, so that the CPU and GPU can share the same memory space and avoid frequent data transfers. This reduces the overhead of data transfer and improves data transfer efficiency; (3) Cao et al. (2023) adopted communication optimization measures to reduce the communication frequency in one time integration step to one, but there is still the problem of high communication frequency in the whole simulation. In the future, we will consider porting other hotspots of CAMx model, or even the whole integral module except I/O, to GPU-like accelerators for increasing the proportion of code on the GPU and reduce the frequency of CPU-GPU communication.

Video memory and bandwidth are the two most significant factors affecting GPU performance, and high video memory and high bandwidth can better play the powerful computing performance of GPUs. Usually, the memory and bandwidth of the GPU are already given at the factory. In this case, the amount of data transferred to the GPU can be roughly estimated before the data is transferred to the GPU, and the amount of data transferred to the GPU can be adjusted according to the size of the GPU memory to ensure that the amount of data transferred to the GPU each time reaches the maximum GPU video memory, so as to give full play to the GPU performance more efficiently.

Table 4. The total elapsed time of CAMx Fortran and HIP versions for BJ case on the "Songshan" supercomputer and "Taiyuan" computing platform, and the computing time of advection module with or without data transfer. The unit of elapsed time is in seconds (s).

	"Songshan" supercomputer		"Taiyuan" computing platform	
	Fortran version	HIP version	Fortran version	HIP version
Total elapsed time	481.0	469.0	453.0	433.0
Computing time of advection module without data transfer	57.8	6.8	47.8	5.7
Computing time of advection module with data transfer	57.8	29.8	47.8	23.9

4.3.2. CAMx-HIP model on the heterogeneous cluster

Generally, the heterogeneous HPC systems have thousands of compute nodes which are equipped with one or more GPUs on each compute node. To make full use of multiple GPUs, a parallel architecture with an MPI and CUDA hybrid paradigm was implemented to improve the overall computational performance of CAMx-CUDA model (Cao et al., 2023). In this studying, the hybrid parallelism with an MPI and HIP paradigm was used to implement the HIP version of GPU-HADVPPM run on multiple domestic GPU-like accelerators. Fig.8 shows the total elapsed time and speedup of CAMx-HIP model which coupled with the HIP version GPU-HADVPPM on the "Songshan" supercomputer under the BJ, HN, and ZY cases. The simulation of above three cases for one hour took 488 seconds, 1135 seconds and 5691 seconds respectively when launching two domestic CPU processors and two GPU-like accelerators. For the BJ and HN case, the parallel scalability is highest when configured with 24 CPU cores and 24 GPU-like accelerators, with speedup of 8.1x and 11.6x, respectively. In terms of the ZY case, due to its large number of grids, the parallel scalability is the highest when 32 CPU cores and 32 GPU-like accelerators are configured, and the acceleration ratio is 17.2x.

As mentioned above, data transfer between CPU and GPU takes several times more time than computation. Regardless of the CPU-GPU data transfer consumption, GPU-HADVPPM4HIP can achieve up to 28.9x speedup on a single domestic GPU-like accelerator. However, in terms of the total time consumption, the CAMx-HIP model is only 10~20 seconds faster than the original Fortran version when one GPU-like accelerator is configured. And as the number of CPU cores and GPU-like accelerators increases, the overall computing performance of CAMx-HIP model is lower than that of the original Fortran version. The main reason is related to the amount of data transferred to GPU. As the number of MPI processes increases, the number of grids responsible for each process decreases, and the amount of data transmitted by the advection module from CPU to GPU decreases. However, GPUs are suitable for large-scale matrix computing. When the data scale is small, the performance of GPU is low, and the communication efficiency between CPU and GPU is the biggest bottleneck (Cao et al., 2023). Therefore, the computational performance of CAMx-HIP model is not as good as the original Fortran version when MPI processes increase. According to the characteristics of GPUs suitable for large-scale matrix computing, the model domain can be expanded and the model resolution can be increased in the future to ensure that the amount of data transferred to each GPU reaches the maximum video memory occupation, so as to make efficient use of GPU. In addition, the advection module only accounts for about 10% of the total time consumption in CAMx model (Cao et al., 2023), and in the future, it is considered to port the entire integration module except I/O to the GPU to minimize the communication frequency.

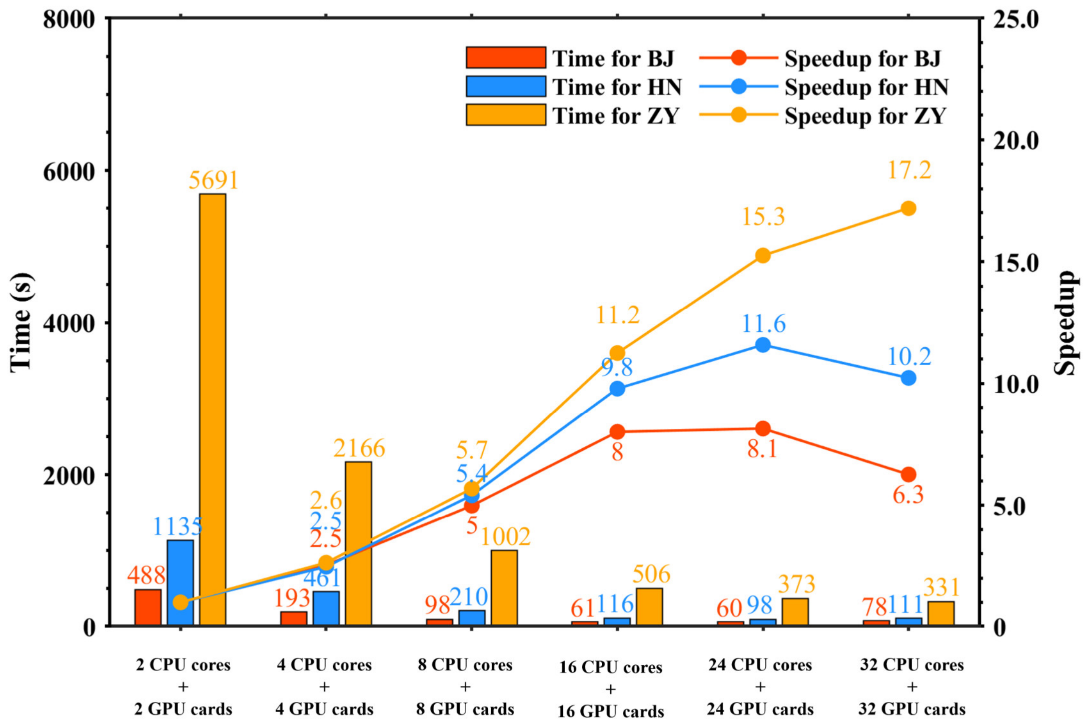

Figure 8. The total elapsed time and speedup of CAMx-HIP model on the "Songshan" supercomputer under the BJ, HN, and ZY cases. The unit is in seconds (s).

The number of GPU accelerators in a single compute node is usually much smaller than the number of CPU cores in the heterogeneous HPC systems. Using the hybrid parallel paradigm with MPI and HIP to configure one GPU accelerator for each CPU process results in idle computing resources for the remaining CPU cores. Therefore, the multi-level hybrid parallelism scheme was introduced to further improve the total computational performance of the CAMx-HIP model. As described in the Sect. 3.2, the horizontal advection module is accelerated by MPI and HIP technology, and the other modules, such as photolysis module, deposition module, chemical module, etc., which runs on the CPU are accelerated by MPI and OMP under the framework of the multi-level hybrid parallelism.

The ZY case achieved the maximum speed-up when launching the 32 domestic CPU processors and GPU-like accelerators. In the same configuration, Fig. 9 shows the total elapsed time and speedup of CAMx-HIP model when further implementing the multi-level hybrid parallelism on the "Songshan" supercomputer. The AEs of the simulation results between the CAMx-HIP model and CAMx-HIP model with the OMP technology is within ±0.04 ppbV, and the specified results are shown in Figure S1. As the number of threads increases, the elapsed time of

CAMx-HIP model is further reduced. When a CPU core launching 8 threads, the one-hour integration time in CAMx-HIP model has been reduced from 338 seconds to 178 seconds, with a maximum acceleration of 1.9x.

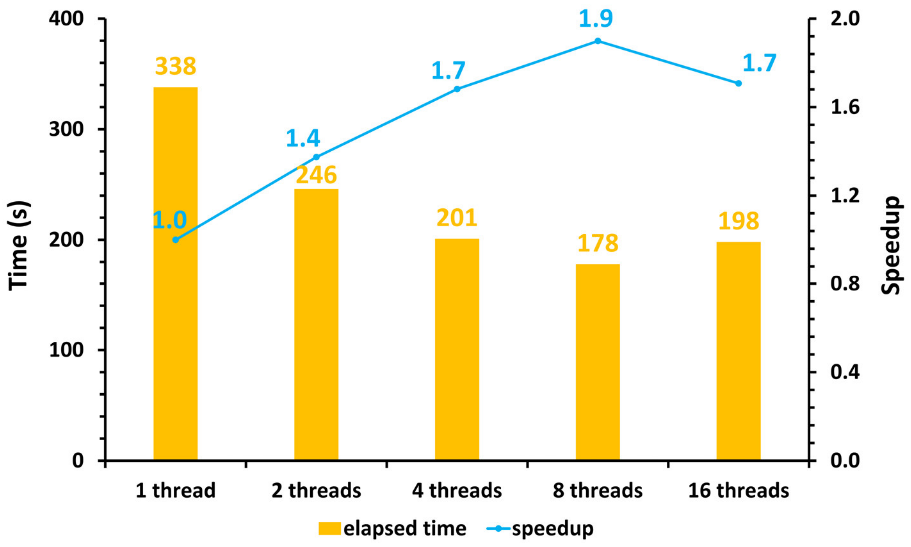

Figure 9. The total elapsed time and speedup of CAMx-HIP model when implementing the multi-level hybrid parallelism in the ZY case. The unit is in seconds (s).

5. Conclusions and discussion

GPUs have become an essential part of providing processing power for high performance computing applications, especially in the field of geoscience numerical models, implementing super-large scale parallel computing of numerical models on GPUs has become one of the significant directions of its future development. In this study, the ROCm HIP technology was implemented to port the GPU-HADVPPM from the NVIDIA GPUs to China’ s domestically GPU-like accelerators, and further introduced the multi-level hybrid parallelism scheme to improve the total computational performance of the CAMx-HIP model on the China’ s domestically heterogeneous cluster.

The consistency of model simulation results is a significant prerequisite for heterogeneous porting, although the experimental results show that the deviation between the CUDA version and the Fortran version of CAMx model, and the deviation between the HIP version and the Fortran version of CAMx model, are within the acceptable rang, the simulation difference between the HIP version of CAMx model and Fortran version of CAMx model is smaller. Moreover, the BJ, HN, and ZY test cases can achieve 8.5x, 11.5x, and 28.9x speedup, respectively, when the HADVPPM program is ported from the domestic CPU processor A to the domestic GPU-like accelerator A. The experimental results of different cases show that the larger the computing scale, the more obvious the acceleration effect of the GPU-HADVPPM program, indicating that GPU is more suitable for super-large scale parallel computing, and provides technical support for accurate and fast simulation of ultra-high-resolution air quality at the meter level in the future. The data transfer bandwidth between CPU and GPU is one of the most important factors affecting the computational efficiency of numerical model in heterogeneous clusters, as shown by the fact that the elapsed time of GPU-HADVPPM program on GPU only accounts for 7.3% and 23.8% when considering the data transfer time between CPU and GPU on the the "Songshan" supercomputer and "Taiyuan" computing platform. Therefore, optimizing the data transfer efficiency between CPU and GPU is one of the important directions for the porting and adaptation of geoscience numerical models on heterogeneous clusters in the future.

There is still potential to further improve the computational efficiency of the CAMx-HIP model in the further. First, improve the data transfer efficiency of GPU-HADVPPM between the CPU and the GPU and reduce the data transfer time. Secondly, increase the proportion of HIP C code in CAMx-HIP model on the domestic GPU-like accelerator, and port other modules of CAMx-HIP model to the domestic GPU-like accelerator for computing. Finally, the data type of some variables could be changed from double precision to single precision, and the mixing-precision method is used to further improve the CAMx-HIP computing performance.

Code and data availability. The source codes of CAMx version 6.10 are available at https://camx-wp.azurewebsites.net/download/source/ (ENVIRON, 2023). The datasets related to this paper and the CAMx-HIP codes are available online via ZENODO (https://doi.org/10.5281/zenodo.10158214), and the CAMx-CUDA code is available online via ZENODO (https://doi.org/10.5281/zenodo.7765218, Cao et al., 2023).

Author contributions. KC and QW conducted the simulation and prepared the materials. QW, LiW and LaW planned and organized the project. KC, QW, HG, HW, XT and LL refactored and optimized the codes. LiW, NW, HC, DXL and DQL collected and prepared the data for the simulation. KC, HW, QW, and HG validated and discussed the model results. KC, QW, LiW, NW, XT, HG, and LaW took part in the discussion.

Competing interests. The authors declare that they have no conflict of interest.

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