

Responses to Reviewer(s)

I. Response to Reviewer #1

5 The paper presents implementation of LICOM3 using HIP framework targeting an HPC cluster with AMD GPUs. Atmospheric modeling in not my area of expertise, therefore I will not comment on this aspect of the paper; I will only comment on the model implementation and parallelization efforts. Here are some specific comments about individual sections.

Response: Thanks for your insightful comments. We were planning to document the final version and test at first. Therefore, we only present the final version and the results from a large-scale test in the manuscript. Another paper shows details of the model porting and results of the small-scale test are preparing. Based on your suggestions, we have done some additional tests, added much more information of the system's software and hardware, and further polished this manuscript's English. Also, we have modified the format of the references. The point-to-point responses are listed below.

15 Section 2.3: "The nodes of both partitions are interconnected through the high performance InfiniBand (IB) networks." Which partitions? Prior system description does not mention any partitions, instead it states that the system consists of 7000 nodes with 4 GPUs per node.

Response: Thanks for your questions. In fact, the implementation of the network is a 3-level fat-tree architecture using Mellanox 200Gb/s HDR InfiniBand, whose measured point-to-point communication performance is about 23GB/s. The supercomputer consists of 6 partitions (or rings, each has 1200 nodes, and the job system schedules about 7200 nodes). We have modified the descriptions in the revised manuscript in Section 2.3.

25 Section 3.1: There is some repetition here, e.g., the authors state several times that HIP supports both AMD and NVIDIA GPUs.

Response: Thanks. We have revised the repetition in Section 3.1.

30 Section 3.2: Good work on converting the original Fortran code to C and verifying the results to be identical between the two implementations. However, the authors do not say much about this ported code in terms of the optimizations applied to it, if the code is purely executed as a single thread on each node, if any 3rd party libraries have been used, etc. Also, how the execution time of this newly ported C version of the code compares to the execution time of the original Fortran code? It is important to have a well-performing CPU code as a starting point.

Response: Thanks for your comments. First, we would like to correct the statement of this porting. Actually, we have only ported the main computation part of LICOM3 from Fortran code to C, which includes the seven kernels listed in Figure 2 (readyt, readyc, barotr, belinc, tracer, icesnow, and convadj). All seven kernels account for about 25% of the code and about 99% of the computation and communication time (Table R1). Other parts, mainly the initialization, the time integration control, and the IO parts, still use Fortran code. Therefore, the so-called C version of LICOM3 is a Fortran and C mixed code, not a pure C code. In this way, we can replace F90 subroutines one by one and easily check the correctness of ported C codes. The C code is purely executed as a single thread on each node.

The Fortran and C mixed code is the starting point of following CUDA-C or HIP programming. To guarantee the correctness of the porting, we did NOT optimize the model in this step, and there were not any additional 3rd party libraries used. We simply translated the Fortran code to C code sentence by sentence. The translations include converting array index from Fortran (start from 1) to C (start from 0), changing the array subscript sequence, etc. Since the code is the same for 100km and 5km, we only test the Fortran and C mixed version for lower resolution cases.

We have tested the byte-to-byte correctness of the Fortran and C mixed code and tested the execution time. The Fortran and C hybrid version's speed is slightly faster than the original Fortran code, less than 10%. Figure R1 shows a speed benchmark by the LICOM3 for 100km and 10km running on an Intel platform. The results are the time running one model month for a low-resolution test and one model day for a high-resolution test. The details of the platform are in the caption of Figure R1. This indicates that we have successfully ported these kernels from Fortran to C.

We have added more descriptions of the porting and added a figure (Figure R1) in the revised manuscript in Section 3.2, Lines 187-195.

Section 3.3: From section 3.2, I understood that the entire code was ported to C. However, section 3.3 states that a mixed Fortran/C code was used here. Please clarify to resolve this inconsistency. Also, I do not quite follow the discussion in lines 222-227 about array size. I understand that the original Fortran code uses static arrays and these arrays need to be changed to be dynamically allocated in order to move them to the GPU global memory. Is this what you are implying here? I also have a hard time following the discussion about halo data packing and Fig. 4.

Response: Thanks for your questions. Sorry for the confusing statements. As our response to the previous section, the code of LICOM3 is not a pure C code but a Fortran and C mixed one. We have modified the vague statement in the manuscript to avoid this inconsistency in Section 3.2, Lines 187-189.

65 The “lines 222-227” problem is not really what you understand. It occurs for the 5km resolution version when the static data array beyond 2GB. We met this problem in both the HIP hipcc and CUDA nvcc compiler. It is perhaps due to the compiler limitation of the GPU compilation tool. We have revised this part to state the problem clearly in Section 3.2, Lines 228-230.

70 To optimize the heavy halo in the kernel “barotr”, we have tried to reduce the amount of data using the halo data packing method. Only the necessary data are transferred. The test indicates that the method can decrease by about 30% of the total wall clock time of “barotr” when 384 GPUs used. But we have not optimized other kernels so far because its performance not as good as 384GPUs’ when GPUs scale beyond 10000. This optimization is not turn on in the following experiments, and we just keep it here as an option to improve the performance of ‘barotr’. Other methods, such as NCCL (NVIDIA Collective Communication Library), are also implemented and tested, but not presented here. We have revised this part to state the problem clearly in Section 3.2, Lines 252-255.

75 Section 3.4: What storage and file system do you use? These I/O performance numbers are not very meaningful without specifying the underlying storage architecture. It is possible that the low original performance of the I/O operations was solely due to a low-performing storage system and would not be an issue on a higher-performing storage. Also, how exactly is data loaded/stored to disk? The size of data transfers would play a huge role on the overall performance.

80 **Response:** Thanks. The storage file system of the supercomputer is ParaStor300S with a ‘parastor’ file system, whose measured write and read performance is about 520GB/s and 540 GB/s. We have added this information in the revised manuscript in Section 2.3, Lines 138-139.

85 We agree with you that the I/O time depends on system I/O performance. When the large scale LICOM3 tests are performing, the system is forced to be one user mode by the administrator. It means no other users' job and heavy I/O tasks are running at the same time. Hence, the I/O of storage is enough to hold all LICOM3’s I/O tasks. The improvement of I/O performance has been depicted in Figure 5 of the manuscript. The ratio of I/O in the total calculation time is less than 50% for 9216 cards, which is almost 90% before the I/O processes have been optimized.

90 After optimization, the forcing data, about 3GB total, are read from disk every model year, while the daily mean predicted variables, about 60GB total, are stored to disk every model day. Therefore, the performance of output dominated the I/O performance. We have added the above statements in the revised manuscript in Section 3.4, Lines 256-257.

Section 4.1: I think the correct way to quantify the speedup is to use all CPU cores vs. the GPUs, not just a single CPU core.
95 Also, it is not clear from the text how the GPUs are managed. For example, is each GPU managed by a single CPU thread, or is the same thread is used to manage all 4 GPUs?

Response: Thanks. We agree with you and have already computed the speedup using the one CPU, but not shown in the manuscript. Since each node has 32 CPU cores and 4 GPUs, each GPU is managed by one CPU thread in the present cases. We can also quantify GPUs' speedup vs. all CPU cores' on the same number of nodes. For example, the 384 (768) GPUs correspond to 96 (192) nodes, which have 3072 (6144) CPU cores. Therefore, the overall speedup is about 6.375 (0.51/0.08) for 384 GPUs and 4.15 (0.83/0.2) for 768 GPUs (Figure 6). The speedups are comparable with our previous work porting LICOM2 to GPU using OpenACC (Jiang et al., 2019), which is about 1.8-4.6 times speedup using one GPU card vs. two 8-core Intel GPU in small-scale experiments for specific kernels. Our results are also slightly better than Xu et al. (2015), which has ported another ocean model to GPU using Cuda C. But due to the limitation of the number of intel CPUs (maximal 9216 cores), we didn't obtain the overall speedup for 1536 and more GPUs. We have added discussions about this issue in the revised manuscript in Section 4.1, Lines 300-307.

Section 5.1: Interesting discussion about failure rates. However, I wonder how realistic your assumptions are with regards to existing studies such as <https://www.christianengelmann.info/publications/gupta17failures.pdf>.

Response: Thanks for your suggestion and the interesting paper. We have read this manuscript and have cited it in the revised version. Unlike Gupta's study (23 types of failures), only three types of failures we have mostly met are discussed in Section 5.1. We only do simple analysis by predefined hypothesis (failure occur rate 10^{-5} , which means 1 failure in 100000 hours.) to illustrate the difficulty of submitting jobs beyond 10000 GPUs. The realistic failures are essential, but not the critical problem of this study, so we did not discuss it more. We have added discussions about this issue in the revised manuscript in Section 5.1, Lines 360-364.

Overall, the presented implementation is rather straightforward and not well-thought. The authors ported to GPU several time-consuming kernels within the existing HPC application. Such approach is typically not very productive as it limits the design choices and does not give enough flexibility to optimize the overall application. Before proceeding with such an effort, the authors should have analyzed the amount of time spent in each of the subroutines on the CPU with regards to all other aspects of the code, such as I/O and network communication. Figure 8 shows such kernel time distribution after porting, but I could not find much about the amount of time spent on cross-node communication. It is important to understand the potential benefits of one or another approach before starting the actual implementation effort.

Response: Thanks for your comments and suggestions. Before the implementation, we actually have tested the performances of all seven Fortran subroutines on a supercomputer system using Intel CPUs. Figure R2 shows our test results, including the seven subroutines' time cost percentage for 384 and 9216 CPU cores and the subroutines' time cost at six scales. Here, we used the 1/20° resolution LICOM3. Although the two experiments have been conducted on different platforms, the two model versions' configurations are identical, particularly using the same time steps, 1s for the barotropic part, the 60s for both baroclinic and tracer parts. That will grantee the same numbers of halo for two versions. Because the code of I/O in Fortran and the Fortran-C mixed version is the same, we will not discuss more I/O for the original Fortran code.

We found that the “tracer” is the most time-consuming subroutine for the CPU version. With the increase of CPU cores from 384 to 9216, the ratio of cost time for “tracer” is also increasing from 38% to 49%. “readyt” and “readyc” are computing intensive subroutines. “tracer” is both computing intensive and communication intensive subroutine. “barotr” is communication intensive subroutine and the communication of “barotr” is 45 times than that of “tracer”. The computing intensive subroutines can achieve good speedup by GPU, but the communication intensive subroutine will achieve poor performance.

We have done a set of experiments to measure the time cost of both halo update and memory copy in the HIP version. These two processes in the time integration are conducted in three subroutines: “barotr”, “bclinc,” and “tracer”. The figure shows that “barotr” is the most time-consuming subroutine, and the memory copy dominates, which takes about 40% of the total time cost. These results can also be treated as a reference for the CPU experiments because the Halo update codes in the HIP version are the same as the CPU version.

We have added discussions about the above issues in the revised manuscript in Section 3.3, Lines 235-244.

Next, there is no discussion about dominant computations in each of the kernels and how to best implement them on the GPU. There is no information in the paper that would indicate anything about the quality of implementation of these GPU kernels, e.g., how well they use GPU resources. I would like to see achieved FLOPS and memory bandwidth of these kernels with respect to the roofline model for this particular GPU to be convinced that the authors did a good job porting these kernels. The discussion about performance improvements is very convoluted by the fact that the authors start comparing performance at some rather large scale of 384 GPUs. What about performance of a single GPU on a much smaller model vs. performance of a single CPU socket, or a 4-GPU node vs. all CPU cores in that node? There is no discussion about what happens inside a single node, for example, how well are all 4 GPUs are utilized and if there is anything that one could benefit from the fact that these 4 GPUs have access to the same host memory.

Response: Thank you very much for your suggestion. This paper's critical point is developing a high-resolution heterogeneous version of the ocean circulation model, so we just give out some brief introduction of GPU implementation and optimization methods in section 3. Follow the Reviewer's suggestions; we append more discussions about floating-point operations performance of the subroutines in section 4.1. The addition roofline test is archived by a 100km version.

Figure R4 shows the roof-line model using the Stream-GPU and LICOM program's measured behavioral data on a single computation node bound to one GPU Card depicting the relationship between arithmetic intensity and performance floating points operations.

165 The blue and gray oblique line is the fitting line related to the Stream-GPU program's behavioral data using 5.12×10^8 and 1×10^6 threads, respectively, both with blocksize of 256, which attain the best configuration. For details, the former is approximately the maximum threads number restricted by GPU card memory achieving the bandwidth limit to 696.52 GB/s. In comparison, the latter is close to the average number of threads in GPU parallel calculations used by LICOM, reaching the bandwidth of 344.87 GB/s on average. Here we use the oblique gray line as a benchmark to verify the rationality of LICOM's performance,
170 accomplishing the bandwidth of 313.95 GB/s averagely.

Due to the large calculation scale of the whole LICOM program, the divided calculation grid bound to a single GPU card is limited by video memory; most kernel functions actually issue no more than 1.2×10^6 threads. As a result, the floating-point operations performance is a little far from the oblique roof-line shown in Figure R3. In particular, the subroutine bcline
175 apparently stray off the whole trend for the reason of including frequent 3d-array Halo MPI communications as well as a lot of data transmission between CPU and GPU.

We have added discussions about the above issues in the revised manuscript in Section 4.1, Lines 281-293.

180 There is no discussion about how the halo exchanges are implemented at the MPI level, how much overlapping is happening for computation, communication, and I/O.

Response: Thanks for your suggestion. The halo exchange in the MPI level is similar to POP have (see Jiang, et.al. 2019). We did not change these codes in the HIP version. We call an F90 subroutine to do halo from GPU space. The overlapping between communication data packing/unpacking and point-to-point communication was implemented. We did not apply the
185 overlapping of computation, communications, and I/O in this version because the calculation time was much less than communication time and I/O time. There have no existing solutions to increase these halo performances; we hope it can be improved in the future LICOM3 version. This work's core contribution is to develop a 10000+ GPUs runnable ocean model, which still has sped up in 26200 scales. The seven core computation process put into GPUs space by the HIP framework is the critical solution. All other are not important issues because they cost 99%+ computation time in the model 'stepon' procedure.
190 The brief hardware and software environments are presented in the manuscript. Since all supercomputer has their unique settings, this model may have different performance in other computers than we have.

The paper is short on many technical details, ranging from characteristics of the underlying hardware, to software/compiler environment, to implementation details, making it very difficult for others to put the results obtained by the authors compared
195 to other work.

Response: Thanks. We have revised our manuscript following your suggestions, and we have tried to provide much more information as we can.

Above all, the paper is hard to read due to a very poor use of language; almost every sentence needs corrections.

200 **Response:** Thanks for your suggestion. We have revised the manuscript as possible and will invite a 3rd part English editor to improve the revised manuscript.

If the authors want their paper to be printed with the existing implementation, they must provide a much better description and analysis of this implementation. Interactive comment on Geosci. Model Dev. Discuss., <https://doi.org/10.5194/gmd-2020-323>,

205 2020.

Response: Thanks. We have revised our manuscript following your suggestions, and we have tried to provide much more information as we can.

Reference

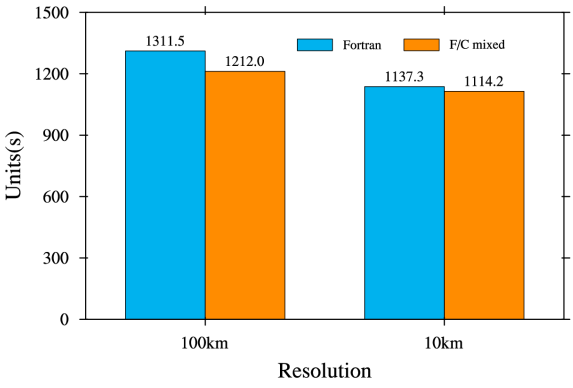
210 Jiang, J. R., P. F. Lin, J. Wang, H. L. Liu, X. B. Chi, H. Q. Hao, Y. Z. Wang, W. Wang, and L. H. Zhang, 2019: Porting LASG/IAP Climate system Ocean Model to GPUs using OpenACC. *IEEE Access*, 7(1), 154490-154501. doi:10.1109/ACCESS.2019.2932443

Xu, S., Huang, X., Oey, L. Y., Xu, F., Fu, H., Zhang, Y., and Yang, G. (2015). POM. gpu-v1. 0: a GPU-based Princeton Ocean Model. *Geoscientific Model Development*, 8(9), 2815-2827. <https://doi.org/10.5194/gmd-8-2815-2015>

215

Table R1 The seven major subroutines’ time cost for one model day at different scales for LICOM3 (1/20°). The time cost of I/O and total time are also listed. These tests were conducted on a platform of Intel Xeon CPU (E5-2697A v4, 2.60GHz). Unit: second.

	384 cores	768 cores	1536 cores	3072 cores	6144 cores	9216 cores
readyt	1678.93	784.14	454.38	278.18	142.23	95.28
readyc	4751.21	2244.72	939.51	463.71	228.88	146.45
barotr	3449.31	1628.74	642.58	396.34	143.41	91.86
bclinc	1431.89	696.73	363.93	234.59	137.11	101.76
tracer	7439.98	3147.73	1822.47	1467.40	614.94	445.63
icesnow	31.54	17.17	8.61	4.80	2.85	2.37
convadj	620.61	370.03	193.95	90.87	42.50	29.56
I/O	150.52	128.62	134.42	132.80	152.85	157.15
Total	19553.98	9017.89	4559.86	3068.69	1464.76	1070.06



225

Figure R1. The wall clock time of a model day for the 10km version and a model month for the 100km version. The blue and orange bars are for the Fortran and the Fortran and C mixed version. These tests were conducted on a platform of Intel Xeon CPU (E5-2697A v4, 2.60GHz). We used 28 and 280 cores for the low and high resolution, respectively.

230

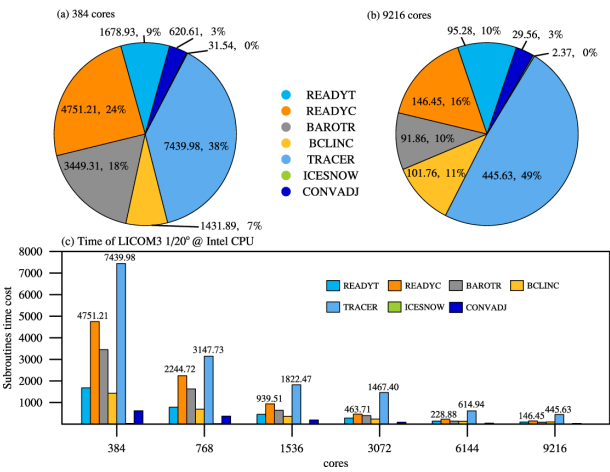


Figure R2 The seven core subroutines' time cost percentage for (a) 384 and (b) 9216 CPU cores. (c) the subroutines' time cost at different scales of LICOM3 (1/20°). These tests were conducted on a platform of Intel Xeon CPU (E5-2697A v4, 2.60GHz).

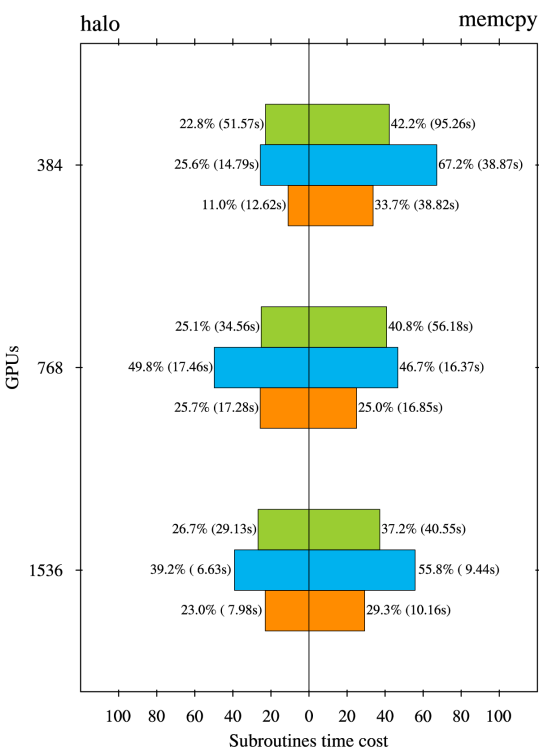


Figure R3 The ratio of the time cost of halo update and memory copy to the total time cost for three subroutines, “barotr” (green), “bclinc” (blue), and “tracer” (orange) in the HIP version LICOM for three scales (Unit: %). The numbers in the blankets are the time cost of the two processes (Unit: second).

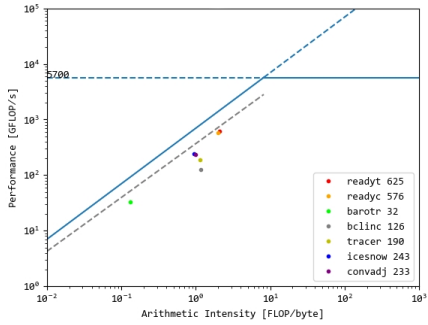


Figure R4 Roofline model for AMD GPU and the performance of LICOM's main subroutines.

II. Response to Reviewer #2

Numerical climate modeling is a key method for scientists and researchers to better understand our planet, and one of the most popular applications that greatly challenges the most state-of-the-art high performance computing (HPC) systems. In this work, LICOM3, a standard ocean model is selected and scaled onto the GPU-based heterogeneous supercomputing system. The authors have done lots of porting and optimizing work to put almost all of the time-consuming computation processes into the GPU side, and greatly reduce the communication overhead. As a result, both the dynamic core and the physics part are ported and parallelized on GPUs. A speedup of 42x is achieved when using 284 AMD GPUs VS 384 CPU cores. Excellent scalability is also achieved. A test of 1/20 degree LICOM3-HIP is reached using 6550 nodes and 26200 GPUs, 2.72 SYPD in time-to-solution.

As a computer scientist who also focuses on porting and tuning climate models onto different HPC platforms, dealing with a complete model with lots of code legacies using a new accelerator is obviously not an easy work. Sometimes rewriting and redesigning are necessary to obtain a satisfactory performance. In this work, the optimizing techniques provided are sound and solid, and can be used as a good guidance for corresponding work. AMD GPU and HIP, though not as popular as Nvidia GPU and CUDA for now, are still very promising GPU accelerators for current generation supercomputers. Moreover, it is likely that some of the forthcoming Exa-scale supercomputers, will also be adopting AMD GPUs. So this work is also a good trials ahead of time. More specifically to the strategies: only the most time-consuming parts (seven subroutines) are translated into HIP C, deeply re-coded, ported onto the GPUs, and fully optimized (such as the usage of temporary arrays to avoid data dependency, the change of data structure of original Fortran arrays, etc.). Halos that contain partial communications are handled by CPU part. Therefore, a hybrid computing model is performed, to further improve the overall performance. This is also a very popular strategy when dealing with numerical problems with inter-node or inter-process communications. Besides, The IO part is also considered and tuned by rewriting the data reading strategies and doing parallel scattering.

Overall, the paper is well-structured, with sufficient figures and tables to help better illustrate the ideas where necessary. But there are grammar errors and misleading descriptions here and there. So I suggest the authors ask help from native speakers for further proofreading.

Response: Thank you very much for your comments and suggestions. We have revised the English of the manuscript as possible and will find a professional English editor to further improve the final manuscript.

Here are some other suggestions,

The authors mentioned the dynamic and physics parts, but lacks further explanations to what they are. I understand that most communications exist within the dynamic part, but could the authors be more specific in pointing out the optimizing strategies for the dynamic part and the physics part, respectively? Are there any differences?

Response: Thanks. To explicitly separate the dynamic core and the physical package is an excellent ideal for further optimization. But so far, the optimizing strategies are mostly at the program level, not treat the dynamic or physics parts separately. We only ported all seven core subroutines within the time integration loops to GPU, including both the dynamic and physics parts.

Unlike the atmospheric models, there are no many time-consuming physical processes in the ocean model, such as the radiative transportation, cloud, precipitation, and convection processes. Therefore, the two kinds of parts are usually not clearly separated in the ocean model, particular in the early stage of model development. This is also the case of LICOM. We have added the discussion of this issue in the revised version in Section 6, Lines 424-429.

In the end, the authors claimed that the 1/20_ LICOM3-HIP version can not only reproduce the observations, but also produce much smaller scale activities, such as submesoscale eddies and frontal scales structures. Could the authors explain how they obtain the observation version?

Response: Thanks. This is kind of misleading. So far, the horizontal resolution of most global-scale observation is commonly no more than 25km from merged remote sensing products, which cannot resolve the submesoscale eddies in most places of the ocean. Some products, such as sea surface temperature, indeed have higher resolution at several kilometers. But these products usually have either short period or limited region, and not suitable for the global-scale, long-term climate research. Here, we only would like to say that much finer scale processes can be captured in this 1/20 model and didn't intend to compare with the fine scale observation.

We have revised the sentences and tied to avoid misunderstanding in Section 6, Lines 409-411.

Porting a complete model is not an easy work. In this work, approximately 12000 lines Fortran code were rewrote from fortran to C. Could the authors estimate the cost? For example, the number and time cost of persons in the whole project.

Response: Thanks. This is a good question. To port the Fortran code to C costs us about five months (2018.11-2019.3), and five Ph.D. students and five part-time staff participated in this programming work. Then, it took about ten months to port these C codes to GPU in CUDA (2019.4-2020.1) and further four months (2020.2-2020.5) to optimize them on the HIP framework, such as introducing IO parallel and doing the large-scale test. Therefore, it totally took nineteen months, and five Ph.D. students and five part-time staff to finish this kind of porting work. We have added the discussion of this issue in the revised version in Section 6, Lines 392-393.

The following work is suggested to be cited and comment as well, to enrich the related work part. Optimizing high-resolution Community Earth System Model on a heterogeneous many-core supercomputing platform.

Response: Thanks for your suggestion and for providing a new reference. We have cited it in the revised paper in Section 1,
315 Lines 55-57.

Line 45, I suggest to update the TOP 500 list using the latest one (Nov. 2020);

Response: Thanks. We updated the list in the revised manuscript, Lines 45-47.

320 Line 49, I don't think the energy result is provided in the work of Xu et al. (2015). Please double check.

Response: Thanks. We have checked the work of Xu et al. (2015). They did provide the energy result in Sub-section 5.3.4 of their paper, shown in the following image (Figure R1).

325 Line 71, and the conclusions is in Section 6 -> and the conclusions are in Section 6

Line 74: which started to develop -> which has been developed

Line 83: That makes the coupler is suitable to apply to high resolution modelling. -> It makes the coupler suitable to be applied to high resolution modeling.

330 Line 85: improve -> improves

Line 103: remove totally

Response: Thanks for your careful reading. We have corrected all five typos in the revised manuscript.

335 Part 2.3: add some citations or links with more detailed introductions to the supercomputer used in this work.

Response: Thanks. Because there is no publication about this supercomputer, we have added some information about this machine, including InfiniBand network speed and structure, the speed of the storage file system, etc. We have added this information in the revised manuscript, please see Section 2.3.

340 Line 140: place -> replacing

Line 143: Some... the others... -> Some... some...

Response: Thanks for your careful reading. We have corrected these two typos in the revised manuscript.

Lots of professional words are used in this article, such as theses syntax and macros used in HIP or CUDA. Please use a different syntax (e.g. *italic*) for these professional word, to help better identify them. For example, I suspect that 'for tracer', 'baroclinic' and 'barotropic' may refer to professional processes or subroutines in LICOM3, and 'including', 'cuda_', 'hip_', may refer to professional designations of CUDA or HIP framework.

350

Response: Thanks for your suggestion. We have revised the manuscript to avoid misunderstanding. Now “barotr”, “HipMemcpy” and etc., which inside “” are the function name in .cpp source file. The “cuda” and “hip” in Lines 154 is the prefix for the conversion of function call (or header files) from CUDA style to HIP style. For example “CudaMemcpy” need to be changed to “HipMemcpy”, and "cuda_runtime.h" to "hip_runtime.h".

355

Line 244, an → a

Response: Thanks. Corrected.

360 Figure 5, I suspect the IO time is the result after the IO optimization (part 3.4) being applied. Is that right?

Response: Thanks. Yes, it is correct.

Line 263, times → time

365

Response: Thanks. Corrected.

Please provide more details about the hardware configurations, e.g., the version of CPU and GPUs, the version of compilers, OS, etc.

370 **Response:** Thanks. We have added all the information in the revised manuscript following your suggestions in Section 2.3.

Please replace Flops/s with Flops.

Response: Thanks. Replaced.

375

Figure

two GPUs and 92% on four GPUs. When more GPUs are used, the size of each subdomain becomes smaller. This decreases the performance of POM.gpu in two aspects. First, the communication overhead may exceed the computation time of the inner region as the size of each subdomain decreases. As a result, the overlapping methods in Sect. 4.2 are not effective. Second, there are many “small” kernels in the POM.gpu code, in which the calculation is simple and less time-consuming. With fewer inner region computations, the overhead of kernel launching and implicit synchronization with kernel execution must be counted.

Geosci. Model Dev., 8, 2815–2827, 2015

5.3.4 Comparison with a cluster

In the last test, we compare the performance of POM.gpu on a workstation containing four GPUs with that on the *Tansuo100* cluster. Three different high-resolution grids (Grid-1: $962 \times 722 \times 51$; Grid-2: $1922 \times 722 \times 51$; Grid-3: $1922 \times 1442 \times 51$) are used. Figure 13 shows that our workstation with four GPUs is comparable to 408 standard CPU cores ($= 34 \text{ nodes} \times 12 \text{ cores/node}$) in the simulation. Because the thermal design power of one X5670 CPU is 95 W and that of one K20X GPU is 235 W, we reduce the energy consumption by a factor of 6.8. Theoretically, as the subdo-

www.geosci-model-dev.net/8/2815/2015/

Figure R1. Image from Xu et al. (2015).

385 **The GPU version of LICOM3 under the HIP framework and its**
large-scale application

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Abstract. A high-resolution (1/20°) global ocean general circulation model with Graphics processing units (GPUs) code implementations is developed based on the LASG/IAP Climate system Ocean Model version 3 (LICOM3) under Heterogeneous-compute Interface for Portability (HIP) framework. The dynamic core and physics package of LICOM3 are both ported to the GPU, and 3-dimensional parallelization is applied. The HIP version of the LICOM3 (LICOM3-HIP) is 42 times faster than the same number of CPU cores when 384 AMD GPUs and CPU cores are used. The LICOM3-HIP has excellent scalability; it can still obtain a speedup of more than four on 9216 GPUs comparing to 384 GPUs. In this phase, we successfully performed a test of 1/20° LICOM3-HIP using 6550 nodes and 26200 GPUs, and at the grand scale, the model's time to solution can still obtain an increasing, about 2.72 simulated years per day (SYPD). The high performance was due to putting almost all of the computation processes inside GPUs, reducing the time cost of data transfer between CPUs and GPUs. Simultaneously, a 14-year spin-up integration following phase 2 of the Ocean Model Intercomparison Project (OMIP-2) protocol of surface forcing has been conducted, and the preliminary results have been evaluated. We found that the model results have little difference from the CPU version. Further comparison with observations and lower-resolution LICOM3 results suggests that the 1/20° LICOM3-HIP can reproduce the observations and produce many smaller scale activities, such as submesoscale eddies and frontal scales structures.

405 **1 Introduction**

Numerical models are a powerful tool for weather forecasts and climate prediction and projection. High-resolution atmospheric, ocean and climate models remain significant scientific and engineering challenges because of the enormous computing, communication, and input/output (IO) involved. Kilometer-scale weather and climate simulation start to emerge recently (Schär et al., 2020). Due to the tremendous increase in computation cost, such models will only work with extreme-scale high-performance computers and new technologies.

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The global ocean general circulation models (OGCMs) are a fundamental tool for oceanography research, ocean forecast, and climate change research (Chassignet et al., 2019). Such models' performance is determined mainly by model resolution and sub-grid parameterization, and surface forcing. The horizontal resolution of global OGCMs has increased to about 5-10 km, which is also called eddy-resolving models. The increasing resolution will significantly improve the simulation of the western boundary currents, mesoscale eddies, fronts and jets, and the currents in narrow passages (Hewitt et al., 2017). Meanwhile, the ability of an ocean model in simulating the energy cascade (Wang et al., 2019), the air-sea interaction (Hewitt et al., 2017), and the ocean heat uptake (Griffies et al., 2015) will be improved with the increasing resolution. All these will effectively improve ocean models' performance in simulation and prediction of the ocean circulation. Additionally, the latest numerical and observational results show that the much smaller eddies (sub-mesoscale eddies with a spatial scale of about 5-10 km) are crucial to the vertical heat transport in the upper-ocean mixed layer, and also significant to biological processes (Su et al., 2018). To resolve the smaller-scale processes raises a new challenge for the horizontal resolution of OGCMs, which also demands much more computing resources.

Heterogeneous computing has become a development trend of high-performance computers. In the latest TOP500 supercomputer list released in Nov. 2020, Central Processing Unit (CPU) and Graphics Processing Unit (GPU) heterogeneous machines account for six of the top 10. After the NVIDIA Corporation provided the supercomputing technics on GPU, more and more ocean models applied these high-performance acceleration ways to conduct weather or climate simulations. Xu et al. (2015) developed POM.gpu, a full GPU solution based on the mpiPOM on a cluster, and gained 6.8 times energy reduction. Yashiro et al. (2016) deployed the NICAM model on the TSUBAME supercomputer, and the model sustained a double-precision performance of 60T Flops on 2560 GPUs. Yuan et al. (2020) developed a GPU version of a wave model with 2 V100 cards, and obtained 10-12 times speedup than the 36 cores of CPU. Yang et al. (2016) implemented a fully implicit β -plane dynamic model with 488m grid spacing on the TaihuLight system and achieving 7.95P Flops. Fuhrer et al. (2018) reported a 2-km regional Atmospheric General Circulation Model (AGCM) test using 4888 GPU cards, and obtained simulation performance for 0.043 simulated years per wall clock day (SYPD). Zhang et al. (2020) successfully ported a high-resolution (25 km atmosphere and 10 km ocean) Community Earth System Model in TaihuLight supercomputer, and obtained 1-3.4 SYPD.

At the same time, the AMD company also provides its GPU solutions. In general, AMD GPU uses Heterogeneous Compute Compiler (HCC) tools to compile codes; and they cannot use the Compute Unified Device Architecture (CUDA) development environments, which is supported by the NVIDIA GPU only. Therefore, due to the wildly used and numerous CUDA learning resources, AMD developers have to study two kinds of GPU programming skills. AMD's Heterogeneous-compute Interface for Portability (HIP) is an open-source solution to deal with this problem. It provides a higher-level framework to contain these two types of lower-level development environments, i.e., CUDA and HCC, simultaneously. The HIP code's grammar is like that of the CUDA code, and with a simple convert tool, the code can be compiled and run at CUDA and AMD architectures, respectively. The HCC/OpenACC is convenient for AMD GPU developers before the HIP is popular from the coding

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490 **viewpoint**. Another reason is that CUDA GPU has more market share in the present. It is believed that more and more codes will be ported to the HIP in the future. However, almost no ocean models use the HIP framework so far.

The study **aims** to develop a high-performance OGCM based on the LICOM3, which can be run on AMD GPU architecture using **the** HIP framework. Here, we will **focus** on the **model's** best computing performance **and** its practical usage for research and operation purposes. Section 2 is the introduction of the LICOM3 model. Section 3 contains the main optimizing of the LICOM3 under the HIP. Section 4 covers performance analysis and model verification. Section 5 is for discussion, and the conclusions **are** in Section 6.

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2 LICOM3 model and experiments

2.1 LICOM3 model

In this study, the targeting model is LASG/IAP Climate system Ocean Model version 3 (LICOM3), which **has been developed** in the late 1980s (Zhang and Liang, 1989). Now the LICOM3 is the ocean model for two air-sea coupled models of the CMIP6, the Flexible Global Ocean-Atmosphere-Land System model version 3 with **a** finite-volume atmospheric model (FGOALS-f3; He et al., 2020) and Flexible Global Ocean-Atmosphere-Land System model version 3 with **a** grid-point atmospheric model (CAS FGOALS-g3; Li et al., 2020). The LICOM version 2 (LICOM2.0, Liu et al., 2012) is also the ocean model of the CAS Earth System Model (CAS-ESM, Zhang, et al., 2020). The paper to fully describe the new features and baseline performances of LICOM3 **are** preparing.

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In recent years, the LICOM model was substantially improved based on the LICOM2.0 (Liu et al., 2012). There are three main aspects: First, the coupling interface of LICOM has been upgraded. Now the NCAR flux coupler version 7 is employed (Lin et al., 2016), in which the memory usage has been **dramatically** reduced (Craig et al., 2012). **It** makes the coupler **suitable** to **be applied** to high-resolution **modeling**.

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Second, both the orthogonal curvilinear coordinate (Murray, 1996; Madec & Imbard, 1996) and the tripolar grid have been introduced in the LICOM. Now, the two poles are at (65°E, 60.8°N) and (115°W, 60.8°N) for the 1° model, at (65°E, 65°N) and (115°W, 65°N) for the 0.1° model, and at (65°E, 60.4°N) and (115°W, 60.4°N) for the 1/20° model of the LICOM. After that, the zonal filter in the high latitude, particularly in the northern hemisphere, has been **eliminated**, which **significantly improves** the scalability and efficiency of the parallel algorithm of **the** LICOM3 model. In addition, the dynamic core of the model **has also been** updated accordingly (Yu et al., 2018), including applying a new advection scheme for the tracer formulation (Xiao, 2006) and a vertical viscosity for the momentum formulation (Yu et al., 2018).

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Third, the physical package has been updated, including introducing an isopycnal and thickness diffusivity scheme (Ferreira et al., 2005) and the vertical mixing due to internal tides breaking at **the** bottom (St. Laurent et al., 2002). The coefficient of both isopycnal and thickness diffusivity **is** set to 300 **m**² s⁻¹ as the depth is within the mixed layer or the water depth is shallower than 60 m. The upper and lower boundary values of the coefficient are 2000 and 300 m² s⁻¹, respectively. Additionally, the

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chlorophyll-dependent solar shortwave radiation penetration scheme of Ohlmann (2003), the isopycnal mixing scheme (Redi, 1982; Gent & McWilliams, 1990), and the vertical viscosity and diffusivity schemes (Canuto et al. 2001; 2002) are employed in LICOM3.

Both the low-resolution (1°) (Lin et al., 2020) and high-resolution (1/10°) (Li Y. et al., 2020) stand-alone LICOM3 are also involved in the OMIP-1 and OMIP-2; their outputs can be downloaded from websites. The two versions of LICOM3's performances compared with other CMIP6 ocean models are shown in Tsujino et al. (2020) and Chassignet et al. (2020), respectively. The 1/10° version has also been applied to do short-term ocean forecasts (Liu et al., 2020, under review).

2.2 Configurations of models

To investigate the GPU version, we have employed three configurations in the present study. They are 1°, 0.1°, and 1/20°. Details of these models are listed in Table 1. The numbers of horizontal grid points for the three configurations are 360×218, 3600×2302, and 7200×3920, respectively. The vertical levels for the low-resolution are 30, while they are 55 for the other two high-resolution models. From 1° to 1/20°, it increases the computational effort by about 8000 (20³) times (considering the 20 times for decreasing the time step), plus the vertical resolution increase from 30 to 55, totally approximately 15000 times. The original CPU version of 1/20° with MPI parallel on Tianhe-1A only reached 0.31 SYPD using 9216 CPU cores. This speed will slow down the 10-year spin-up simulation of LICOM3 to more than one month, not practical for climate research. Therefore, such simulations are suitable for extreme-scale high-performance computers by applying the GPU version. Besides the different grid points, three main aspects are different among the three experiments, particularly between 1° version and the other two versions. First, the horizontal viscosity schemes are different: using Laplacian for 1° and biharmonic for 1/10° and 1/20°. The viscosity coefficient is one order smaller for the 1/20° version than for the 1/10° version, namely, -1.0×10⁹ m⁴/s for 1/10° vs -1.0×10⁸ m⁴/s for 1/20°. Second, although the forcing including dataset (JRA55-do; Tsujino et al., 2018) and the bulk formula for the three experiments are all standard of the OMIP-2, the periods and temporal resolutions of the forcing fields are different: 6-hour data from 1958 to 2018 for the 1° version, and daily mean data in 2016 only for both the 1/10° and 1/20° versions. Third, the 1° version is coupled with a sea ice model of the CICE4, via NCAR's flux coupler version 7, while the two higher-resolution models are stand-alone, without a coupler or sea ice model. Additionally, the two higher-resolution experiments employ the new HIP version of LICOM3 (i.e., LICOM3-HIP). The low-resolution experiment does not, which was the CPU version of LICOM3 and the same as the version submitted to OMIP (Lin et al., 2020). We also listed all the important information in Table 1, such as the bathymetry data and the bulk formula, etc., though these items are similar in the three configurations.

The spin-up experiments for two high-resolution versions are conducted for 14 years, forced by the daily JRA55-do dataset in 2016. The atmospheric variables include the wind vectors at 10-m, air temperature at 10-m, relative humidity at 10-m, total precipitation, the downward shortwave radiation flux, the downward longwave radiation flux, and the river runoff. According

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to the kinetic energy evolution, the models reach a quasi-equilibrium state after more than ten years of spin-up. The daily mean data are output for store and analysis.

2.3 Hardware and software environments of the testing system

590 The two higher-resolution experiments were performed on a heterogeneous Linux cluster supercomputer, located at the Computer Network Information Center (CNIC) of the CAS, China. This supercomputer consists of 7200 nodes, (6 partitions or rings, each partition has 1200 nodes), with a 1.9 GHz X64 CPU of 32 cores on each node. Also, each node is equipped with four gfx906 AMD GPU cards with 16 GB memory. The GPU has 64 cores, total of 2560 threads on each card. The nodes are interconnected through the high-performance InfiniBand (IB) networks, (3-level fat-tree architecture using Mellanox 200Gb/s HDR InfiniBand, whose measured point-to-point communication performance is about 23GB/s). The OpenMPI version 4.02 is employed for compiling, and the AMD GPU driver and libraries are rocm-2.9 integrated with HIP version 2.8. The storage file system of the supercomputer is ParaStor300S with a 'parastor' file system, whose measured write and read performance is about 520GB/s and 540 GB/s.

3 LICOM3 GPU code structure and optimization

600 **3.1 Introduction to HIP on an AMD hardware platform**

AMD's HIP is a C++ runtime API and kernel language. It allows developers to create portable applications that can be run on AMD's accelerators and CUDA devices. The HIP provides an API for an application to leverage GPU acceleration for both AMD and CUDA devices. It is syntactically similar to CUDA, and most CUDA API calls can be converted in placing of the character "cuda" by "hip" (or "Cuda" by "Hip"). The HIP supports a strong subset of CUDA runtime functionality, and its

605 open-source software is currently available on GitHub (https://rocmdocs.amd.com/en/latest/Programming_Guides/HIP-GUIDE.html).

Some supercomputers install NVIDIA GPU cards, such as P100 and V100, some install AMD GPU cards, like AMD VERG20, etc. Hence, our HIP version LICOM3 can adapt and gain very high performance at different supercomputer centers, such as Tianhe-2 and AMD clusters. Our coding experience on AMD GPU indicates that the HIP is a good choice for high-performance

610 model development. Meanwhile, the model version is easy to keep consistent in these two commonly used platforms. In the following, the successful simulation of LICOM3-HIP is confirmed to be adequate to employ HIP.

Figure 1 demonstrates the HIP implementations to support different types of GPUs. Besides the differences in naming and including libraries, there are other differences between HIP and CUDA: 1) AMD Graphics Core Next (GCN) hardware "warp" size = 64; 2) device and host pointers allocated by HIP API use flat addressing (unified virtual addressing is enabled by default);

615 3) dynamic parallelism not currently supported; 4) some CUDA library functions do not have AMD equivalents, and 5) shared memory and registers per thread may differ between AMD and NVIDIA hardware. Despite these differences, most of the CUDA codes in applications can be easily translated to the HIP, and vice versa.

Technical supports of CUDA and HIP also have some differences. For example, CUDA applications have some CUDA-aware MPI to direct MPI communication between different GPU space nodes, but HIP applications have no such functions so far. We have to transfer data from GPU memory to CPU memory for exchanging data with other nodes, and then transfer them back to the GPU memory.

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3.2. Core computation process of LICOM3 and C transitional version

We tried to apply the LICOM on a heterogeneous computer about five years earlier, cooperating with the NVIDIA Corporation. The LICOM2 was adapted to NVIDIA P80 by OpenACC technical (Jiang et al., 2019). That was a convenient implementation of LICOM2-gpu using 4 NVIDIA GPUs to achieve a 6.6 speedup compared to 4 Intel CPUs, but its speedup was not so good when further increasing the GPU number.

This time we started from the CPU version of LICOM3. The code structure of LICOM3 includes four steps. The first step is the model setup; it involves MPI partition and ocean block distribution. The second stage is model initialization, which includes reading the input data and initialize the variables. The third stage is integration loops, the core computation of the model. Three explicit time loops, which are for tracer, baroclinic and barotropic steps, are in one model day. The outputs and final processes are included in the fourth step.

Figure 2 shows the flowchart of LICOM3. The major processes within the model time integration include baroclinic, barotropic, and thermohaline equations, which are solved by the leapfrog or Euler forward scheme. There are seven individual subroutines, such as “readyt”, “readyc”, “barotr”, “belinc”, “tracer”, “icesnow”, and “convadj”. When the model finishes one day’s computation, the diagnostics and output subroutine will write out the predicted variables to files. The output files contain all the necessary variables to restart the model and for analysis.

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To obtain high performance, using the native GPU development language is more efficient. In the CUDA development forum, both CUDA-C and CUDA-Fortran are provided; however, Fortran’s support is not as good as that for C++. We plan to push all the core process codes into GPUs; hence, the seven significant subroutines’ Fortran codes must be converted to HIP/C++. Due to the complexity and many lines in these subroutines (approximately 12000 lines Fortran code) and making sure the converted C/C++ codes be correct, we rewrote them to C before finally converting them to HIP codes.

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A bit-reproducible climate model produces the same numerical results for a given precision, regardless of the choice of domain decomposition, the type of simulation (continuous or restart), compilers, and the architectures executing the model (i.e., the same hardware and software conduct the same result). The C transitional version (not fully C code, but the seven cores subroutine) is bit-reproducible with the F90 version of the LICOM3 (the binary output data are the same under Linux with the “diff” command). We have also tested the execution time. The Fortran and C hybrid version’s speed is slightly faster than the original Fortran code, less than 10%. Figure 3 shows a speed benchmark by the LICOM3 for 100km and 10km running on an Intel platform. The results are the time running one model month for a low-resolution test and one model day for a high-resolution test. The details of the platform are in the caption of Figure 3. The results indicate that we have successfully ported these kernels from Fortran to C.

695 This C transitional version becomes the starting point of HIP/C++ codes, and reduces the complexity of developing the HIP version of the LICOM3.

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3.3. Optimization and tuning methods in LICOM3-HIP

The unit of computation in LICOM3-HIP is a horizontal grid point. For example, $1/20^\circ$ corresponds to 7200×3920 grids. For the convenience of MPI parallelism, the grids were united as blocks, that is, if $\text{Proc}_x \times \text{Proc}_y$ MPI processes are used in x and y directions, then each block has $B_x \times B_y$ grids, where $\text{Proc}_x \times B_x = 7200$ and $\text{Proc}_y \times B_y = 3920$. Each GPU process does 2-D or 3-D computation in these $B_x \times B_y$ grids as the MPI process does. In practice, four lateral columns are added to B_x and B_y (two on each side, $\text{imt} = B_x + 4$, $\text{jmt} = B_y + 4$) for halo. Table 2 lists the frequently used block definitions of LICOM3.

The original LICOM3 was written in F90. To adapt it to GPU, we applied the Fortran/C hybrid programming. As shown in Figure 2, the codes are kept using the F90 language before entering device-step on and after step on-out. The core computation processes within the steps are rewritten by using HIP/C. Data structures in the CPU space remain the same as the original Fortran structures. The data commonly used by F90 and C are then defined by extra C, including files and defined by “extern” type pointers in C syntax to refer to them. In the GPU space, newly allocated GPU global memories hold the arrives correspondence to those in the CPU space, and the HipMemcpy is called to copy them in and out.

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Seven major subroutines (including their sub-recurrent calls) are converted from Fortran to HIP. The seven subroutine calls sequences are maintained, but each subroutine is deeply re-coded in the HIP to obtain the best performance. The CPU space data are 2-D or 3-D arrays; in the GPU space, we change them to 1-D arrays, improving the data transfer speed between different GPU subroutines.

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The LICOM3-HIP is two-level parallelism, each MPI process corresponding to an ocean block. The computation within one MPI process is then pushed into GPU. The latency of data copy between GPU and CPU is one of the bottlenecks for daily computation loops. All read-only GPU variables are allocated and copied at the initial stage, to reduce the data copy time. Some data copy is still needed in the stepping loop, e.g., MPI call in barotr.cpp.

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The computation block in MPI (corresponding to 1 GPU) is a 3-D grid; in HIP revision, the 3-D parallelism is implemented. This change adds extra parallel inside one block than the MPI solo parallelism (only 2-D). Some optimizations are needed to adapt to this change, such as increasing the global arrays to avoid data dependency. A demo of using a temporary array to parallel the computation inside a block can be found in Figure 4. Figure 4a represents a loop of the original code in the k direction. Since the variable $v(i,j,k)$ has a dependence on $v(i,j,k+1)$, it will cause an error when the GPU threads are paralleled in the k direction. We then separate the variable into two HIP kernel computations. In the upper of Figure 4b, a temporary array vt is used to hold the result of $f1()$, and it can be GPU threads parallel in the k direction. Then, at the bottom of Figure 4b, we use vt to do the computations of $f2()$ and $f3()$; it can still be GPU threads parallel in the k direction. Finally, this loop of codes is parallelized.

750 The parallel in GPU is more like a shared-memory program; the memory write conflicts occur in the subroutine “tracer” advection computation. We change the if-else tree in this subroutine; hence, the data conflicts between neighboring grids are avoided, making the 3-D parallelism successful. Moreover, in this subroutine, we use more operations to alternate the data movement to reduce the cache usage. Since the operation can be GPU threads parallelized and will not increase the total computation time, reducing the memory cache improves this subroutine’s final performance.

755 A notable problem when the resolution is increased to $1/20^\circ$ is that the total size of Fortran common blocks will be bigger beyond 2 GB. This change will not cause abnormal for C in the GPU space. But if the GPU process references the data, the system call in HipMemcpy will occur compilation errors. (It is perhaps due to the compiler limitation of the GPU compilation tool). We should change the original Fortran arrays’ data structure from “static” to “allocatable” type in this situation. Since a GPU is limited to 16 GB GPU memory, the ocean block size in one block should not be too large. In practice, the $1/20^\circ$ version starts from 384 GPUs (and it is regarded as the baseline for speedup here); if the partition is smaller than that value, sometimes the GPU memory insufficient errors will occur.

We found that the “tracer” is the most time-consuming subroutine for the CPU version (Figure 5). With the increase of CPU cores from 384 to 9216, the ratio of cost time for “tracer” is also increasing from 38% to 49%. “readyt” and “readyc” are computing-intensive subroutines. “tracer” is both computing-intensive and communication-intensive subroutine. “barotr” is a communication-intensive subroutine. The communication of “barotr” is 45 times more than that of “tracer” (Table 3). The computing-intensive subroutines can achieve good GPU speed, but the communication-intensive subroutine will achieve poor performance.

765 We have done a set of experiments to measure the time cost of both halo update and memory copy in the HIP version (Figure 6). These two processes in the time integration are conducted in three subroutines: “barotr”, “belinc,” and “tracer”. The figure shows that “barotr” is the most time-consuming subroutine, and the memory copy dominates, which takes about 40% of the total time cost.

770 Variable operations in CPU and GPU memory are at least one magnitude faster than the data transfer between GPU and CPU through 16X PCI-e. The halo exchange in the MPI level is similar to POP have (Jiang et al. 2019). We did not change these codes in the HIP version. The four blue rows and columns in Figure.7 demonstrate the data that need to be exchanged with the neighbors. As shown in Figure 7, in GPU space, we pack the necessary lateral data for halo operation from $imt \times jmt$ to $4(imt+jmt)$. This change reduces the HipMemcpy data size to $(4(imt+4jmt))$ of the original one. The larger imt and jmt are, the less the transferred data is. At 384 GPUs, this change saves about 10% of the total computation time. The change is valuable for the HIP since the platform has no CUDA-aware MPI installed; otherwise, the halo operation can be done in the GPU space directly as POM.gpu does (Xu et al., 2015). The test indicates that the method can decrease by about 30% of the total wall clock time of “barotr” when 384 GPUs are used. But we have not optimized other kernels so far because their performance not as good as 384GPUs’ when GPUs scale beyond 10000. We just keep it here as an option to improve the performance of ‘barotr’ at operational scales (i.e., GPU scales under 1536).

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3.4. Model I/O optimization

Approximately 3GB forcing data are read from disk every model year, while about 60GB daily mean predicted variables are stored to disk every model day. The time cost for reading daily forcing data from the disk is increased to 200 s in one model day after the model resolution is updated from 1° to 1/20°. This time is equivalent to one step when 1536 GPUs are applied; hence, we must optimize it for total speedup. The cause of low performance is daily data reading and scattering to all nodes every model day; we then rewrite the data reading strategy and do parallel scattering for ten different forcing variables. Finally, the time cost of input is reduced to about 20 s, 1/10 of the original one (shown below).

As indicated, the core-process time cost is about 200s using 1536 GPUs. One model day's output needs about 250 s; it is also beyond the GPU computation time for one step. We modify the subroutine to a parallel version, and it decreases the data write time to 70 s on the test platform (this also depends on system I/O performance).

4 Model performance

4.1. Model performance in computing

Performing kilometer-scale and global climatic simulation are challenging (Palmer, 2014; Schär et al., 2020). As Fuhrer et al. (2018) pointed out, the SYPD is a useful metric to evaluate model performance for a parallel model (Balaji et al., 2017). Because a climate model often needs to be run at least 30-50 years for each simulation, 0.2-0.3 SYPD will require too much time to finish the experiment. The common view is that at least 1-2 SYPD is an adequate entrance for a realistic climate study. It also depends on the time scale in a climate study. For example, for 10-20-year simulation, 1-2 SYPD seems acceptable, and for 50-100 year simulation, 5-10 SYPD is better. NCEP weather prediction system's throughput standard is 8 minutes to finish one model day, equivalent to 0.5 SYPD.

Figure 8 illustrates the I/O performance of LICOM3-HIP, comparing the performances of computation processes. When the model applies 384 GPUs, the I/O costs 1/10 of the total simulation time (Figure 8a). While the scale increases to 9216 GPUs, the I/O time increases, but is still smaller than the GPU's step time (Figure 8b). The improved LICOM3 I/O totally costs about 50-90 s (depends on scales), especially the input remains stable (Figure 8c) while scaling increases. This optimization of I/O maintains that the LICOM3-HIP 1/20° runs well at all practice scales for a realistic climate study. The I/O time has been cut off from the total simulation time in the follow-up test results to analyze the purely parallel performance.

Figure 9 shows the roof-line model using the Stream-GPU and LICOM program's measured behavioral data on a single computation node bound to one GPU card depicting the relationship between arithmetic intensity and performance floating points operations. The 100km resolution case is employed for the test. The blue and grey oblique line is the fitting line related to the Stream-GPU program's behavioral data using 5.12e8 and 1e6 threads, respectively, both with a blocksize of 256, which attain the best configuration. For details, the former is approximately the maximum threads number restricted by GPU card memory achieving the bandwidth limit to 696.52 GB/s. In comparison, the latter is close to the average number of threads in

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GPU parallel calculations used by LICOM, reaching the bandwidth of 344.87 GB/s on average. Here we use the oblique grey line as a benchmark to verify the rationality of LICOM's performance, accomplishing the bandwidth of 313.95 GB/s averagely. Due to the large calculation scale of the whole LICOM program, the divided calculation grid bound to a single GPU card is limited by video memory; most kernel functions issue no more than $1.2e6$ threads. As a result, the floating-point operations performance is a little far from the oblique roof-line shown in Figure 9. In particular, the subroutine bcline apparently stray off the whole trend for including frequent 3d-array Halo MPI communications and a lot of data transmission between CPU and GPU.

Figure 10 shows the SYPD at various parallel scales. The baseline (384) of GPUs could achieve 42 times speedup than that of the same number of CPU cores. Sometimes, we also count the overall speedup, 384 GPUs in 96 nodes versus the total 3072 CPU cores in 96 nodes. We can get the overall performance speedup of 384 ~~is~~ about 6-7 times. The figure also indicates that for all scales, the SYPD keeps increasing. ~~On~~ the scale of 9216 GPUs, the SYPD first goes beyond 2, ~~seven times the same~~ CPUs result. A quasi-whole machine (26200 GPUs, $26200 \times 65 = 1703000$ cores totally, one process corresponds to one CPU core plus 64 GPU cores) result indicates it can still obtain an increasing SYPD to 2.72.

Since each node has 32 CPU cores and 4 GPUs, each GPU is managed by one CPU thread in the present cases. We can also quantify GPUs' speedup vs. all CPU cores' on the same number of nodes. For example, the 384 (768) GPUs correspond to 96 (192) nodes, which have 3072 (6144) CPU cores. Therefore, the overall speedup is about 6.375 (0.51/0.08) for 384 GPUs and 4.15 (0.83/0.2) for 768 GPUs (Figure 10). The speedups are comparable with our previous work porting LICOM2 to GPU using OpenACC (Jiang et al., 2019), which is about 1.8-4.6 times speedup using one GPU card vs. two 8-core Intel GPU in small-scale experiments for specific kernels. Our results are also slightly better than Xu et al. (2015), which has ported another ocean model to GPU using Cuda C. But due to the limitation of the number of intel CPUs (maximal 9216 cores), we didn't obtain the overall speedup for 1536 and more GPUs.

Figure 11 depicts the actual times and speedups of different GPUs computation. The green line in Figure 11a is the function of stepon time cost; it decreases while the GPU number increases. The blue curve of Figure ~~1~~ 1a shows the ~~increase~~ of speedup with the ~~rise~~ of the GPU scale. Despite the speedup increase, the efficiency of the model decreases. At 9216 GPUs, the model efficiency starts under 20%; and for more GPUs (19600 and 26200), the efficiency is flattened to about 10%. The efficiency decreasing is mainly caused by the latency of data copy in and out to the GPU memory. For economical consideration, the 384-1536 scale is a better choice for realistic modeling studies.

Figure ~~1~~ 2 depicts the time cost of seven core subroutines of LICOM3-HIP. We find that the top four most time cost subroutines are "barotr," "tracer," "bcline," and "readyc"; and the other subroutines cost only about 1% of the whole computation time. When 384 GPUs are applied, the "barotr" costs about 50% of the total time (Figure ~~1~~ 2a), which solves the barotropic equations. When GPUs are increased to 9216, ~~each subroutine's~~ time cost ~~decreases~~, but the percentage of subroutine "barotr" is increased to 62% (Figure ~~1~~ 2b). As mentioned above, the phenomenon can be interpreted by ~~haloing~~ in "barotr" being more than the other subroutines; hence, the memory data copy and communication latency make it slower.

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900 4.2. Model performance in climate research

905 ~~The~~ daily mean sea surface height (SSH) fields of CPU and HIP versions' simulations are compared ~~to test the usefulness of the HIP version of the LICOM for the numerical precision of scientific usage. Here,~~ the results from 1/20° experiments on a particular day, March 1st of the 4th model year, ~~are used~~ (Figures ~~13a~~, b). The general SSH spatial patterns of the two are very similar visually. The significant differences are only found in very limited areas, such as in the eddy rich regions near strong currents or high-latitude ~~regions~~ (Figure ~~13c~~); in most places, the difference values fall into the range -0.1 and 0.1 cm. Because the hardware is different and the ~~HIP codes'~~ mathematical operation sequence ~~is not always the same as that for the Fortran version,~~ the HIP and CPU versions are not identical byte-by-byte. Therefore, it is hard to verify the correctness of the results from the HIP version. Usually, the ensemble method is employed to evaluate the consistency of two model runs (Baker et al., 2015). Considering the unacceptable computing and storage resources, besides the differences between the two versions, we here simply compute Root Mean Square Errors (RMSEs) between the two versions, which is only 0.18 cm, much smaller than the spatial variation of the system, which is 92 cm (about 0.2%). That indicates the results of LICO3-HIP are generally acceptable for research.

915 ~~The GPU version's~~ sea surface temperature (SST) ~~is compared with the observed SST to evaluate the global 1/20° simulation's preliminary results from LICOM3-HIP~~ (Figure ~~14~~). Because the LICOM3-HIP experiments are forced by the daily mean atmospheric variables in 2016, we also compare the outputs with the observation data of 2016. Here, the 1/4° Optimum Interpolation Sea Surface Temperature (OISST) is employed for comparison, and the simulated SST is interpolated to the same resolution as the OISST's. We find that the global mean values of SST are close to each other, but with a slight warming bias, 18.49°C for observations vs. 18.96°C for the model. The spatial pattern of SST in 2016 is well reproduced by LICOM3-HIP. The spatial Standard Deviation (STDs) of SST ~~is~~ 11.55°C for OISST and 10.98°C for LICOM3-HIP. The RMSE of LICOM3-HIP against the observation is only 0.84°C.

920 With ~~an~~ increasing horizontal resolution of the observation, we now know that mesoscale eddies are ubiquitous in the ocean with ~~a 100-300 km~~ spatial scale. The rigorous eddies usually occur along ~~significant~~ ocean currents, such as the Kuroshio and its Extension, the Gulf Stream, and the Antarctic Circumpolar Current (Figure ~~15a~~). The eddies also capture more than 80% of the ~~ocean's~~ kinetic energy, estimated using satellite data (e.g., Chelton et al., 2011). Therefore, these mesoscale eddies must be solved in the ocean model. ~~A numerical model's~~ horizontal resolution ~~must be higher than 1/10° to resolve the global ocean's eddies,~~ but that cannot resolve the eddies in the high latitude and shallow waters (Hallberg, 2013). Therefore, ~~a~~ higher resolution is required to ~~determine~~ the eddies globally. ~~The~~ EKE for the 1° version is low, even in the areas with strong currents, while the 1/10° version can reproduce most of the eddy-rich regions in the observation. The EKE is increased when the resolution is further enhanced to 1/20°, indicating much more eddy activities are resolved.

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5 Discussion

5.1. Application of ocean climate model beyond 10000 GPUs

Table 4 summarizes detailed features of some published GPU version models. We can find that various programing methods have been implemented for different models. A near-kilometer atmospheric model using 4888 GPUs was reported as a large-scale example of weather/climate studies. With supercomputing development, the horizontal resolution of ocean circulation models will keep increasing, and more sophisticated physical processes will also be developed. The LICOM3-HIP has a larger scale, not only in terms of grid size but also in final GPU numbers.

We successfully performed a quasi-whole machine (26200 GPUs) test, and the results indicate the model obtained an increasing SYPD (2.72). The application of an ocean climate model beyond 10000 GPUs is not easy because the multi-nodes plus multi-GPUs running requires that the network connection, PCI-e and memory speed, and input/output storage systems all work in their best performances. Gupta (Gupta et al., 2017) have investigated the 23 types of system failures to improve HPC systems' reliability. Unlike Gupta's study, only three types of failures we have mostly met are discussed here. The three most occur errors when running LICOM3-HIP are MPI hardware errors, CPU memory access errors, and GPU hardware errors. Let's suppose that the probability of an individual hardware (or software) error to occur is 10^{-5} (which means 1 failure in 100000 hours). Along with the MPI (GPUs) scale increasing, the total error rate is increased; and once a hardware error occurs, the model simulation will fail.

When 384 GPUs are applied, the success rate within one hour can be expressed as $(1-384 \times 10^{-5})^3 = 98.85\%$, and the failure rate is then $1-(1-384 \times 10^{-5})^3 = 1.15\%$. Applying this formula, we can obtain the failure rate corresponding to 1000, 10000, and 26200 GPUs. The results are listed in Table 5. As shown in Table 5, in the medium-scale (i.e., 1000 GPUs are used), three failures will happen through 100 runs; when the scale increases to 10000 GPUs, 1/4 of them will fail. The 10^{-5} error probability also indicates that 10000 GPUs task cannot run in continuous hours on average. If the success time restriction decreases, the model success rate will increase. For example, within 6 minutes, the 26200 GPUs task success rate is $(1-26200 \times 10^{-6})^3 = 92.34\%$, and its failure rate is $1-(1-26200 \times 10^{-6})^3 = 7.66\%$.

5.2. Energy to solution

We also measured energy to solution here. A simulation normalized energy (E) has been employed here as a metric. The formula is as follows:

$$E = TDP \times N \times 24 / SYPD$$

where TDP is the Thermal Design Power, N is the computer nodes used, and SYPD/24 equals the simulated years per hour. So, the smaller the E value, the better, which means that we can get more simulated years within a limited power supply. To calculate E's value, we estimated the TDP of 1380 W for a node on the present platform (1 AMD CPU and 4 GPUs) and 290 W for a reference node (2 Intel 16-core CPUs). We only include the TDP of CPUs and GPUs here.

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Based on the above power measurements, ~~simulations'~~ energy cost ~~is~~ shown in Table 6 in MWh per Simulation Year (MWh/SY). The energy costs for the 1/20° LICOM3 simulations running on CPUs and GPUs are comparable when the numbers of ~~MPI~~ processors are within 1000. The energy costs of LICOM3 at 1/20° running on 384 (768) GPUs and CPUs are about 6.234 (7.661) MWh/SY and 6.845 (6.280) MWh/SY, respectively. But the simulation speed of LICOM3 on GPU is much faster than that on CPU, about 42 times for 384 processors and 31 times for 768 processors. When the number of MPI processors is beyond 1000, the value of E for GPU becomes much larger than that for CPU. This ~~result~~ indicates the GPU is not fully loaded from this scale.

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6 Conclusions

The GPU version of LICOM3 under ~~the~~ HIP framework has been developed in the present study. The dynamic core and physic packages are both ported to the GPU, and 3-D parallelization is applied. The new model has been implemented and gained ~~an~~ ~~excellent~~ accelerating rate on a Linux cluster with AMD GPU cards. This is also the first time an ocean general circulation model is fully applied on a heterogeneous supercomputer using the HIP framework. ~~It totally took nineteen months, and five Ph.D. students and five part-time staff to finish the porting and testing work.~~

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Based on our test using the 1/20° configuration, the LICOM3-HIP is 42 times fast than the CPU ~~does~~, when 384 AMD GPUs and CPU cores are used. The LICOM3-HIP has good scalability, ~~and~~ it can still obtain ~~a~~ speedup of more than four on 9216 GPUs comparing to 384 GPUs. The SYPD, which is equilibrium to the speedup, keeps ~~increasing as the number of GPUs increases.~~ We successfully performed a quasi-whole machine test, which was 6550 nodes and 26200 GPUs, using 1/20° LICOM3-HIP on the supercomputer, and at the grand scale, the model can still obtain an increasing SYPD of 2.72. The modification or optimization of the model also improves ~~10 and 100 km~~ performances, ~~although we did not analyze their~~ performances in this article.

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The efficiency of ~~the~~ model decreases with the increasing number of GPUs. At 9216 GPUs, the model ~~efficiency~~ starts under 20% against 384 GPUs; and when the number of GPUs reaches or exceeds 20000, the efficiency is only about 10%. Based on our ~~kernel functions~~ ~~test~~, the decreasing efficiency was mainly caused by the latency of data copy in and out to the GPU memory in solving the barotropic equations, ~~particularly~~ for the number of GPUs larger than 10000.

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Using the 1/20° configuration of LICOM3-HIP, ~~we have conducted~~ a 14-year spin-up integration. Because the hardware is different and the ~~GPU codes'~~ mathematical operation sequence ~~is~~ not always the same as that of the Fortran version, the GPU and CPU versions cannot be identical byte by byte. ~~The~~ comparison between GPU and CPU versions of LICOM3 shows that the differences in most places are ~~minimal~~, indicating that the results from LICOM3-HIP can be used for practical research. Further comparison with the observation and the lower-resolution results ~~suggests~~ that the 1/20° configuration of LICOM3-HIP can ~~reproduce the observed large-scale features and produce much more smaller-scale activities than that of lower-resolution results.~~

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The eddy-resolving ocean circulation model, which is a virtual platform for oceanography research, ocean forecast, and climate prediction and projection, can simulate the variations of the circulations, temperature, salinity, and sea level with a spatial scale larger than 15 km and temporal scale from diurnal cycle to decadal variability. As mentioned above, 1-2 SYPD is a good entrance for a realistic climate research model. The more practical GPU scale range for realistic simulation is around 384-1536 GPUs. At these scales, the model still has 0.5-1.22 SYPD. Even if we decrease the loops in “barotr” procedure to 1/3 of the original in the spin-up simulation, the performance will achieve 1-2.5 SYPD for 384-1536 GPUs. This performance will satisfy 10-50-year scale climate studies. Besides, this version can be used for short-term ocean prediction in the future.

Besides, the block size 36×30×55 (1/20° setup, 26200 GPUs) is not an enormous computation task for one GPU. Since one GPU has 64 cores total of 2560 threads, if a subroutine computation is 2-D, each thread's operation is too small. Even for the 3-D loops, it is still not big enough to load the whole GPU. This indicates that it will gain more speedup when the LICOM resolution is increased to the kilometer level. The LICOM3-HIP codes are now written for 1/20°, but they are kilometer-ready GPU codes.

The optimizing strategies here are mostly at the program level, not treat the dynamic or physics parts separately. We only ported all seven core subroutines within the time integration loops to GPU, including both the dynamic and physics parts. Unlike the atmospheric models, there are no many time-consuming physical processes in the ocean model, such as the radiative transportation, cloud, precipitation, and convection processes. Therefore, the two kinds of parts are usually not separated in the ocean model, particular in the early stage of model development. This is also the case of LICOM. Further optimization to explicitly separate the dynamic core and the physical package should be done in the future.

There is still potential to further increase the speedup of LICOM3-HIP. The bottleneck is in the high-frequency data copy in and out to the GPU memory in the barotropic part of the LICOM3. Unless the HIP-aware MPI is supported, data transfer latency between CPU and GPU cannot be overcome. So far, we can only reduce the time consumed by decreasing the frequency or magnitude of the data copy, and even modifying the method to solve the barotropic equations. Additionally, using the single precision within the time integration of LICOM3 might be another solution. The mixing precision method has already been tested using an atmospheric model, and an average gain in computational efficiency by approximately 40% (Vána et al., 2017). We would like to try these methods in the future.

Code availability

The model code (LICOM3-HIP V1.0) along with the dataset and a 100km case can be downloaded from the website <https://zenodo.org/record/4302813#.X8mGWcsvNb8> with the Digital Object Identifier (doi): 10.5281/zenodo.4302813.

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Data availability

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Author contribution

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Pengfei Wang: Software, Visualization, Formal analysis, and writing-original draft

Jinrong Jiang: Software and Writing – review & editing

Pengfei Lin: Software and Writing – review & editing

Mengrong Ding: Visualization and Data curation

Junlin Wei: Software

Zhang Feng: Software

Lian Zhao: Software

Yiwen Li: Software and Visualization

Zipeng Yu: Software and Data curation

Weipeng Zheng: Formal analysis

Yongqiang Yu: Conceptualization

Xuebin Chi: Conceptualization

Hailong Liu: Supervision, Formal analysis, and writing-original draft

Competing interests:

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The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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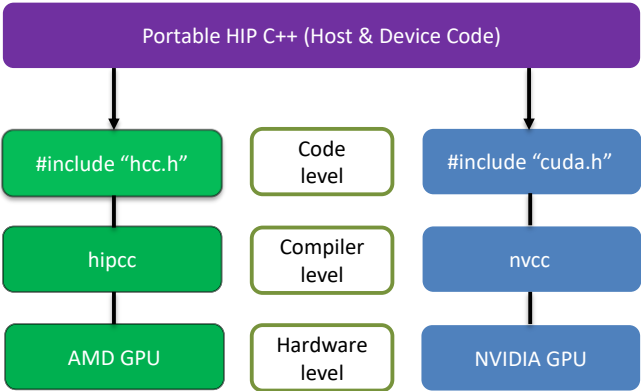
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Figure 1: The schematic diagram of the comparison of coding on AMD and NVIDIA GPU in three levels.

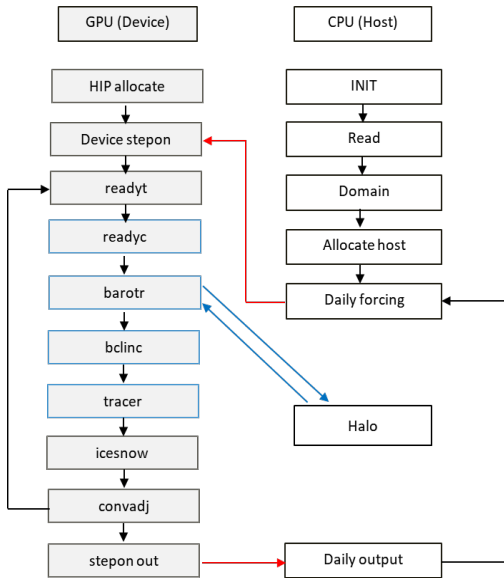


Figure 2: LICOM3 computation flowchart with GPU (HIP device). The red line indicates whole block data transfer between host and GPU, while the blue line means only transferring lateral data of a block.

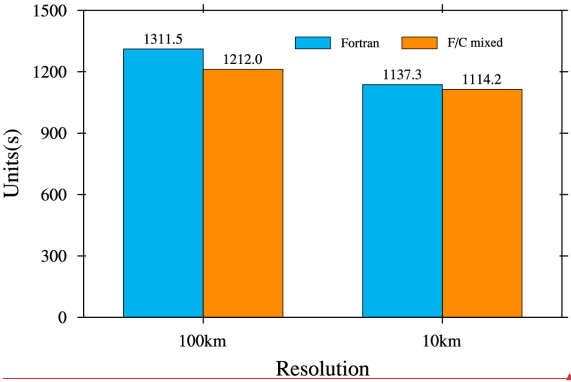


Figure 3: The wall clock time of a model day for the 10km version and a model month for the 100km version. The blue and orange bars are for the Fortran and the Fortran and C mixed version. These tests were conducted on a platform of Intel Xeon CPU (E5-2697A v4, 2.60GHz). We used 28 and 280 cores for the low and high resolution, respectively.

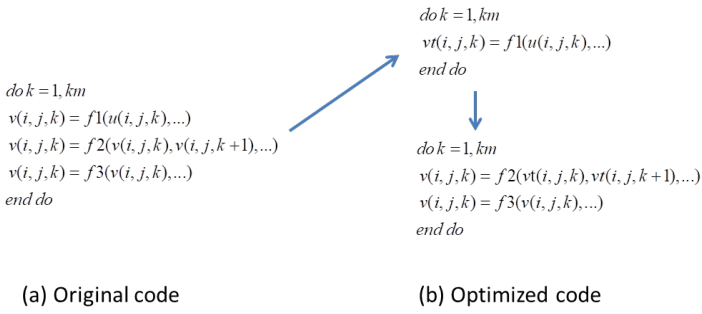
```
do k = 1, km
  v(i, j, k) = f1(u(i, j, k), ...)
  v(i, j, k) = f2(v(i, j, k), v(i, j, k + 1), ...)
  v(i, j, k) = f3(v(i, j, k), ...)
end do
```

(a) Original code

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825 **Figure 4:** The code using temporary arrays to avoid data dependency.

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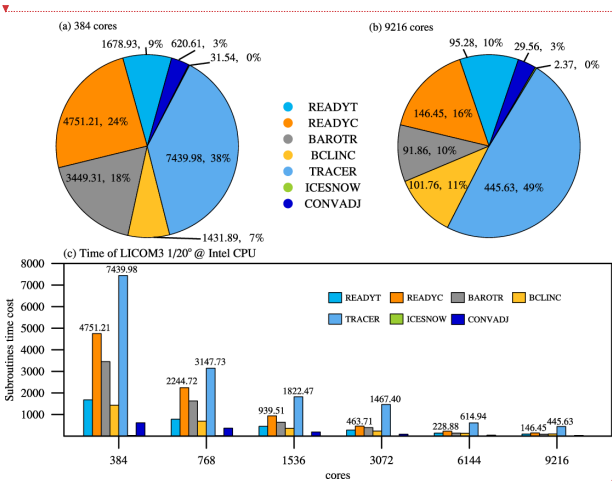
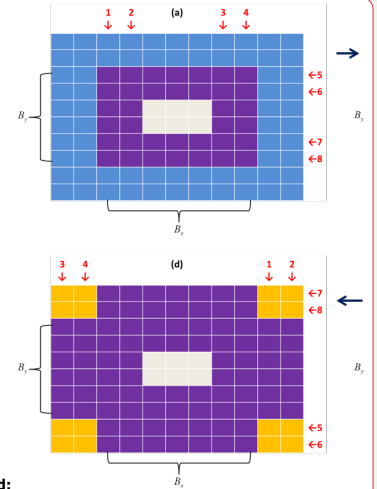


Figure 5: The seven core subroutines' time cost percentage for (a) 384 and (b) 9216 CPU cores. (c) the subroutines' time cost at different scales of LCOM3 (1/20°). These tests were conducted on a platform of Intel Xeon CPU (E5-2697A v4, 2.60GHz).



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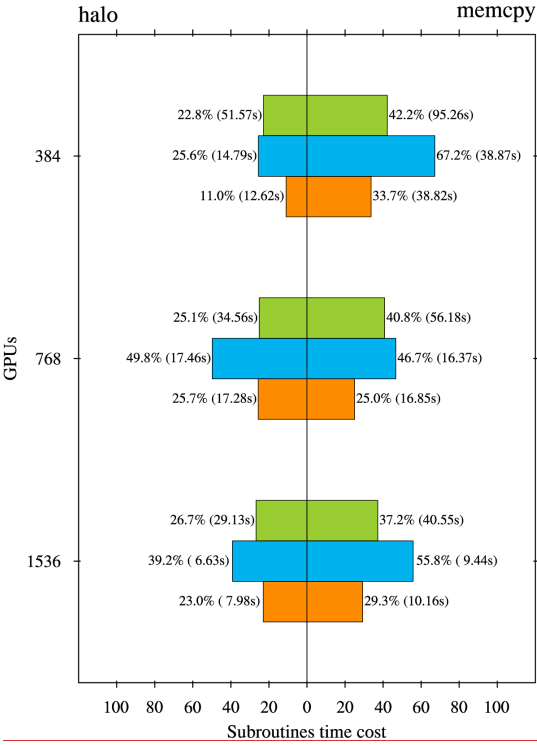
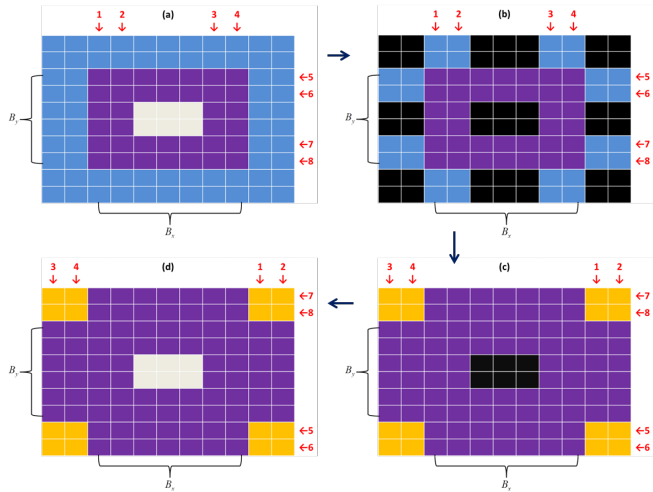


Figure 6: The ratio of the time cost of halo update and memory copy to the total time cost for three subroutines, “halotr” (green), “belinc” (blue), and “tracer” (orange) in the HIP version LICOM for three scales (Unit: %). The numbers in the blankets are the time cost of the two processes (Unit: second).



840 **Figure 7: The lateral packing (only transfer four rows and four columns data between GPU and CPU) method to accelerate halo.** (a) In the GPU space, where central (gray) grids are unchanged; (b) transferred to the CPU space, where black grids mean no data; (c) after halo with neighbors; and (d) transfer back to the GPU space.

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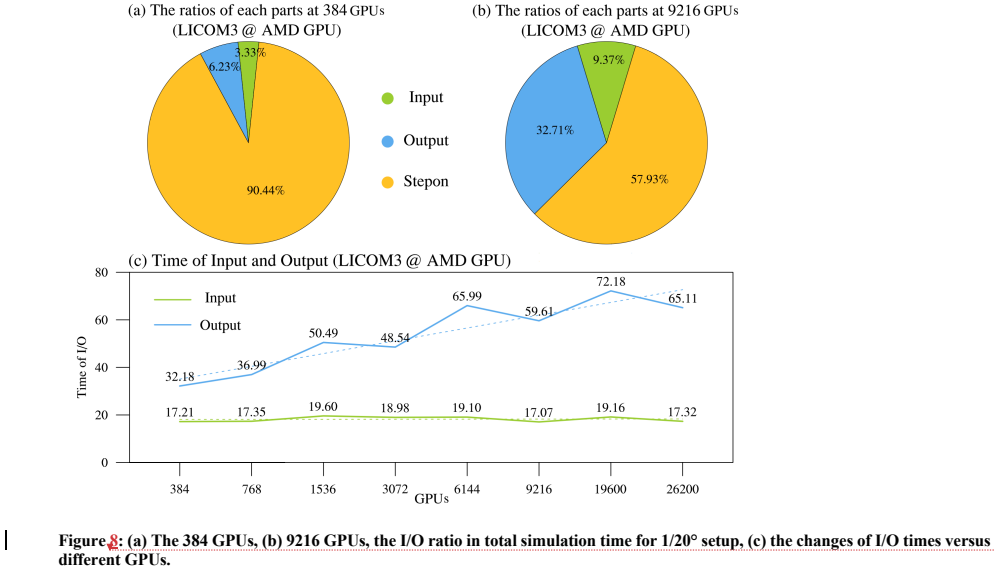


Figure 8: (a) The 384 GPUs, (b) 9216 GPUs, the I/O ratio in total simulation time for 1/20° setup, (c) the changes of I/O times versus different GPUs.

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Figure 6

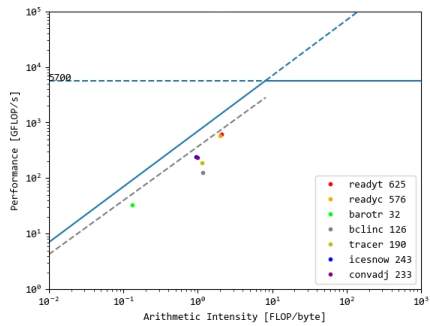
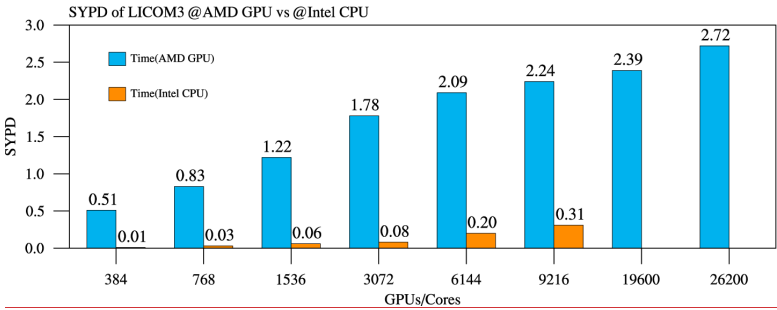


Figure 9: Roofline model for AMD GPU and the performance of LICOM's main subroutines.

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860 **Figure 10:** Simulation performances of AMD GPU versus Intel CPU core for LICOM3 (1/20°). Unit: SYPD.

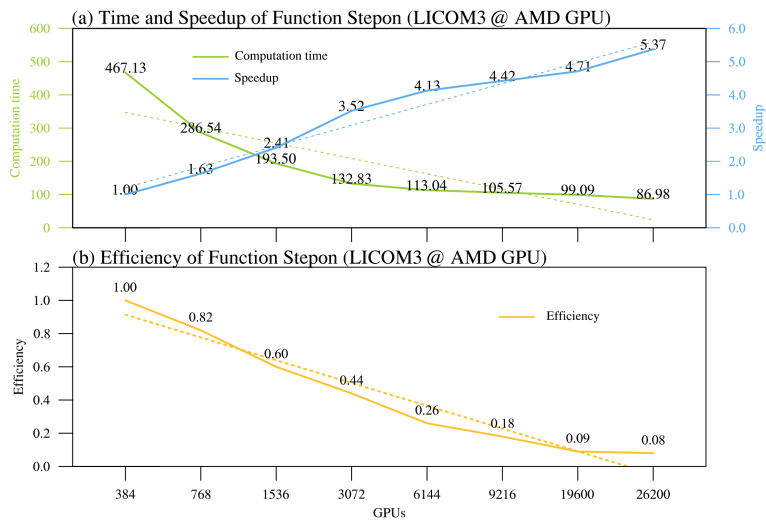


Figure 11: (a) Computation time (green) and speedup (blue), and (b) parallel efficiency (orange) at different scales for stepon of LICOM3-HIP (1/20°).

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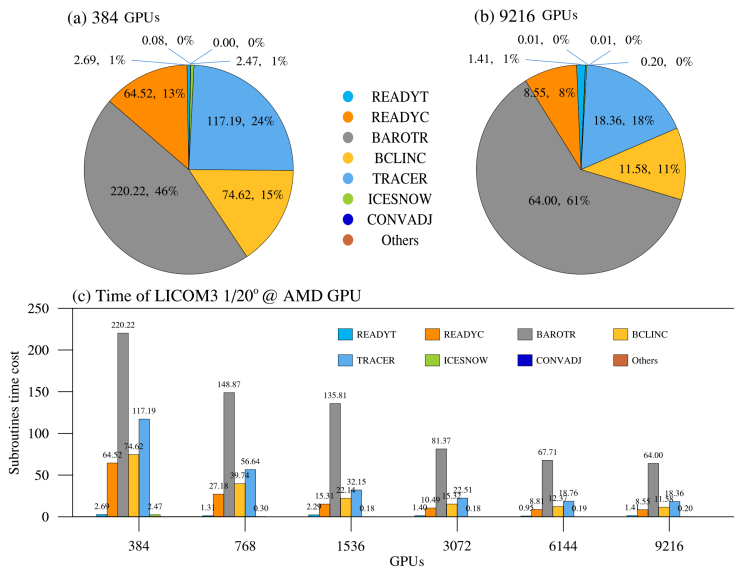


Figure 12: The seven core subroutines' time cost percentage for (a) The 384 GPUs and (b) 9216 GPUs. (c) the subroutines' time cost at different scales of LICOM3-HIP (1/20°).

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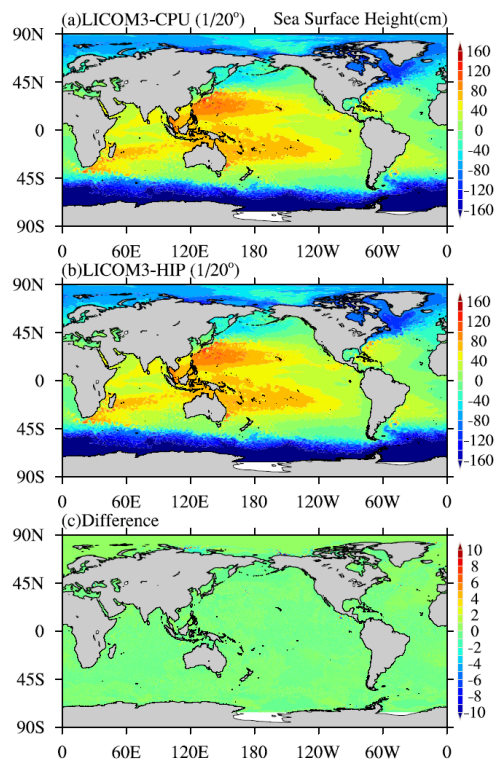


Figure 13: Daily mean simulated sea surface height for (a) CPU and (b) HIP versions of LICOM3 at 1/20° on March 1st of the 4th model year. (c) The difference between the two versions (HIP minus CPU). Units: cm.

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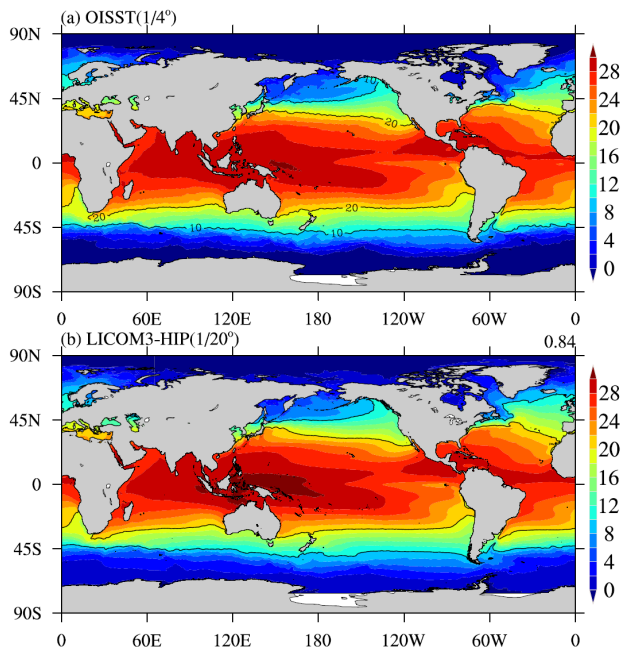


Figure 14: (a) Observed annual mean sea surface temperature in 2016 from Optimum Interpolation Sea Surface Temperature (OISST); (b) simulated annual mean SST for the LICOM3-HIP at 1/20° during the model years 0005-0014. Units: °C.

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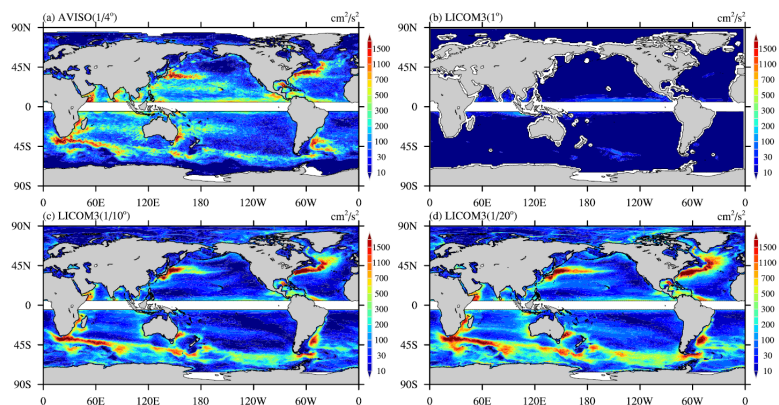


Figure 15: (a) Observed annual mean eddy kinetic energy (EKE) in 2016 from AVISO. Simulated annual mean SST in 2016 for the LICOM3-HIP at (b) 1°, (c) 1/10°, and (d) 1/20°. Units: cm^2/s^2 .

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Table 1: Configurations of **the** LICOM3 model used in the present study.

Experiment	LICOM3-CPU (1°)	LICOM3-HIP (1/10°)	LICOM3-HIP (1/20°)
Horizontal grid spacing	1° (110 km in longitude, about 110 km at the equator, and 70 km at mid-latitude)	1/10° (11 km in longitude, about 11 km at the equator, and 7 km at mid-latitude)	1/20° (5.5 km in longitude, about 5.5 km at the equator, and 3 km at mid-latitude)
Gridpoint	360×218	3600×2302	7200×3920
North Pole	(65°E, 60.8°N) and (115°W, 60.8°N)	(65°E, 65°N) and (115°W, 65°N)	(65°E, 60.4°N) and (115°W, 60.4°N)
Bathymetry data	ETOPO2	Same	Same
Vertical coordinates	30 η levels	55 η levels	55 η levels
Horizontal viscosity	Laplacian $A_2=3000 \text{ m}^2/\text{s}$	Biharmonic (Fox-Kemper & Menemenlis, 2008) $A_4=-1.0 \times 10^9 \text{ m}^4/\text{s}$	Biharmonic (Fox-Kemper & Menemenlis, 2008) $A_4=-1.0 \times 10^8 \text{ m}^4/\text{s}$
Vertical viscosity	Background viscosity of $2 \times 10^{-6} \text{ m}^2/\text{s}$ with the upper limit of $2 \times 10^{-2} \text{ m}^2/\text{s}$	Background viscosity of $2 \times 10^{-6} \text{ m}^2/\text{s}$ with the upper limit of $2 \times 10^{-2} \text{ m}^2/\text{s}$	Background viscosity of $2 \times 10^{-6} \text{ m}^2/\text{s}$ with the upper limit of $2 \times 10^{-2} \text{ m}^2/\text{s}$
Time steps	120/1440/1440 for barotropic/baroclinic/tracer	6s/120s/120s for barotropic/baroclinic/tracer	3s/60s/60s for barotropic/baroclinic/tracer
Bulk Formula	Large & Yeager (2009)	Same	Same
Forcing data	JRA55_do, 1958-2018, 6 hourly	JRA55_do, 2016, daily	JRA55_do, 2016, daily
Integration period	61 years / 6 cycles	14 years	14 years
Mixed layer scheme	Canuto et al. (2001, 2002)	Same	Same
Isopycnal mixing	Redi (1982); Gent & McWilliams (1990)	Laplacian	Laplacian

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Bottom drag	$C_b=2.6\times10^{-3}$	$C_b=2.6\times10^{-3}$	$C_b=2.6\times10^{-3}$
Surface wind-stress	Relative wind stress	Same	Same
SSS restoring	20 m/year; 50 m/30 days for sea ice region	Same	Same
Advection scheme	Leapfrog for momentum; two-step preserved shape advection scheme for tracer	Same	Same
Time stepping scheme	Split-explicit Leapfrog with Asselin filter (0.2 for barotropic; 0.43 for baroclinic; 0.43 for tracer)	Same	Same
Sea ice	Sea ice model of CICE4	Not coupled	Not coupled
Ref.	Lin et al. (2020)	This paper	This paper

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Table 2: Block partition for 1/20° setup.

GPUs	$B_x \times B_y$	$imt \times jmt$
384	600×124	604×128
768	600×62	604×66
1536	300×62	304×66
3072	150×62	154×66
6144	100×62	104×66
9216	75×62	79×66
19600	36×40	40× <u>44</u>
26200	36×30	40×34

Table 3: The number calls of halo in LICOM3 subroutines for each step.

Subroutine	Calls	Calls Percentage
barotr	180	96.7%
bcline	2	1.1%
tracer	4	2.2%

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Table 4: Some GPU versions of weather/climate models.

Model	Language	Max. Grids	Max GPUs	Year and references
POM.gpu	CUDA-C	1922×1442×51	4 (K20X)	2015 (Xu et al., 2015)
LICOM2	OpenACC	360×218×30	4 (K80)	2019 (Jiang et al., 2019)
FUNWAVE	CUDA-Fortran	3200×2400	2 (V100)	2020 (Yuan et al., 2020)
NICAM	OpenACC	56×56km×160	2560 (K20X)	2016 (Yashiro et al., 2016)
COSMO	OpenACC	346×340×60	4888 (P100)	2018 (Fuhrer et al., 2018)
LICOM3	HIP	7200×3920×55	26200 (gfx906)	2020 (This paper)

Table 5: Success and failure rates of different scales for one wall clock hour simulation.

GPUs	Success	Failure
384	98.85%	1.15%
1000	97.02%	2.98%
10000	72.90%	27.10%
26200	40.19%	59.81%

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