

Dear Anonymous Referee #1,

We are extremely grateful for your valuable and fruitful comments that helped improve our manuscript. The referee's comments have been given in blue, whereas our responses have been written in black.

5 1. Page 7, line 20: "Virtualised IT resources are easier to allocate and manage than physical resources, but performance is slower because physical resources are provided through the software layer. Because the N/W resources are provided via virtualisation, the network is slower than the physical N/W environment." There are two unsubstantiated statements here: "Virtualised IT resources are easier to allocate and manage than physical resources." and, in reference to the network: "Because the network resources are provided via virtualisation, the network is slower than the physical network environment." I see no evidence in the paper to support either of the claims. The former is rather subjective, but the latter can surely be objectively measured. On a local system, you could demonstrate that the introduction of a virtualisation layer reduces the performance of the network. Or else, you could cite a study that does this comparison. The analysis of the results is littered with these kind of statements. I would encourage the authors to read this paper on benchmarking scientific codes: InProceedings{HoefflerBelli2015, author = {T. Hoeffler and R. Belli}, title = {ScientificBenchmarking of Parallel Computing Systems}, year = 2015, pages = {73:1-73:12}, month = {Nov.}, publisher = {ACM}, note = {Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC15)}, location= {Austin, TX, USA}, }

Answer:

20 Thank you for recommending the reference on benchmarking scientific codes for our research. We already measured the latency of the N/W layer in a virtualised physical server but did not include this in the manuscript. We will add the result in the revised manuscript according to your suggestion. We found that the introduction of a virtualisation layer reduces the performance of the network. The latency of the physical server is smaller than that of the virtualised server, and the difference is approximately 5~7%.

25 Table R1. Test environment for the N/W latency of the virtualised server and the physical server

	CPU		Memory	Hypervisor	OS	Compiler
Physical server	Intel® CPU E5-2680 v3 at 2.50 GHz	Xeon® v3	128 GB		CentOS 6.9	Intel Compiler 2018 update 1
Virtual server	Intel processor (2.499 GHz)	Core Haswell	120 GB	KVM	CentOS 6.9	Intel Compiler 2018 update 1

The measured network latency of the physical server in the 1G Switch and the value of the network latency are presented below.

30 Table R2. N/W latency and bandwidth of the physical server according to the message size

Message size	1 byte	2 bytes	4 bytes	8 bytes	16 bytes	32 bytes
Latency ( $\mu$ s)	171	172	172	170	172	172
Bandwidth (MB/s)	2.52	4.9	9.8	18.6	36	69

The measured network latency of the virtualised server in the 1G Switch and the value of the network latency are presented below.

35 Table R3. N/W latency and bandwidth of the virtualised server according to the message size

Message size	1 byte	2 bytes	4 bytes	8 bytes	16 bytes	32 bytes
Latency ( $\mu$ s)	183	182	183	184	184	186

Bandwidth (MB/s)	1.99	3.91	7.66	14.66	27.3	39.7
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The latency difference between the physical server and the virtualised server is from 10 to 14  $\mu$ s when the message size is less than 32 bytes in our test environment.

- 5 We also tested the HPL of the physical server and the virtualised server. The measured value of the HPL is presented below.

Table R4. HPL performance data of the physical server and the virtualised server

	Physical server (24 core)	Virtualised server (24 core)
Gflops	715	640

- 10 However, the performance difference between these physical and virtualised resources has recently been gradually decreasing. This study aims to evaluate the performance of ROMS in a virtualised server of the latest cloud computing environment.

*Change in the revised manuscript:*

- 15 We cited the references on the performance change in the virtualisation resources (Younge et al., 2011, Gupta et al., 2013) in the revised manuscript and included Tables R1–4 representing the latency difference in the Supplementary section.

- 20 2. Some (not an exhaustive list) information that is lacking:

- The spec sheet memory bandwidth of the nodes - The achievable memory bandwidth (e.g. using the STREAM benchmark) – The spec sheet floating point performance of the nodes. HPL usually achieves close to floating point peak on desktop CPUs.e.g., the first system on the top500 list that just uses Broadwell CPUs (<https://www.top500.org/system/178925>) has a peak flops of 8128TFlops and achieves 7040TFlops for HPL (around 86% efficiency).

- 25 Typical low-order finite difference codes and more likely to be limited by the memory bandwidth, so measurement of that would also be of interest.

Answer:

- 30 Thank you. The bandwidth performance of the memory is important in evaluating the performance of the HPC. It should be measured in addition to the Flops, which measure the CPU performance. Following your suggestion, we compared the memory performance of C4.xlarge of AWS with the local HPC server using the STREAM benchmark (STREAM, 2016). The physical server memory bandwidth is approximately 5–15% bigger than the virtualised server bandwidth (Table R5).

- 35 *Change in the revised manuscript:*

Table R5 was included in the Supplementary section.

Table R5. Memory bandwidth of the physical server and the virtualised server using the STREAM benchmark

Function	Local HPC (MB/s)	C4.8xlarge (MB/s)
Copy	79091	68431
Scale	74515	68259
Add	80834	77424
Triad	83858	77657

3. In section 5.1, discussing the HPL results:

This section does not provide enough information for a reader to attempt to reproduce the data. For example, what size of matrix was inverted? There is some discussion of HPL in section 3.1, but this does not detail the exact setup: Page6, line 5: "The value of N governing complexity of tasks varies from 56000 to 125312". What is N? Why are these numbers so specific? Moreover, the statement that HPL is suitable for assessing the effect of network performance is not borne out either by the cited paper (Rajan et al. 2012), or a cursory analysis of the computational complexity of dense inverse computations. For an NxN matrix, HPL globally moves  $O(N^2)$  data and does  $O(N^3)$  flops. For asymptotically  $O(N)$  flops/byte moved. Even with a very slow interconnect, one does not expect to see any real network effects once N is "large enough".

Answer:

Thank you. More information for reproduction will be included in the revised manuscript. We could achieve a better performance of the HPL test with various options and tuning. However, this study mainly focuses on comparing the performance of the ocean modelling system in cloud cluster and local HPC. We employed the HPL to test the cluster configuration and performance before the intensive usage of the ocean modelling system. Rajan et al. (2012) found a slow performance of the inter-process communication in the 1G interconnect switch using the HPL. The HPL was relatively less insensitive in the network configuration but was a useful tool in evaluating the HPC performance by various configurations.

*Change in the revised manuscript:*

We revised page 5 in line 35 as follows:

'The general performance of cloud and local clusters was tested by the HPL before the intensive usage of the numerical ocean modelling system'.

Tables 6 and 7 have been included in the Supplementary section such that readers may reproduce the data.

Table R6 HPL compile environment

Architecture	PII_CBLAS	Intel_64
Compiler	gcc 4.4, openmpi2.0.2	parallel_studio_xe_2018_update1_cluster_edition
Math Library	Atlas	Intel® Math Kernel Library (Intel® MKL) 2018

Table R7 Information on the HPL performance test

Cores	16	32	64	84
N (problem size)	56000, 84000	56000, 84000	56000, 84000, 125312	56000, 84000, 125312
NB (block size)	128	128	128	128
P*Q (process grid)	2*8, 4*4, 8*2	2*16, 4*8, 8*4, 16*2	4*16, 8*8, 16*4,	4*21, 7*12, 12*7, 21*4

4. There are good \*performance models\* for HPL. On commodity hardware, it should be straightforward to report the expected performance. Is 100 GFlop/s on 16 cores a good number?

Answer:

Thank you. This is not an optimised result because the basic architecture option (arch=PII\_CBLAS) without optimisation libraries (e.g. Intel Compiler MKL Library) was used to evaluate the performance. Various performances with a Math supporting library have been evaluated to find the optimal performance. Table R8 shows the results. The optimised performance was close to approximately 70% Rpeak flops. The optimised performance of the AWS and the local cluster (Figure R1) indicated a similar change pattern with the unoptimised performance (Figure 5 in the manuscript) according to the number of cores.

Table R8 HPL performance of the clusters

Cores	Local HPC (GFlops)	AWSC4.8xlarge (GFlops)
16 core	601	566
32 core	1161	973
64 core	1870	1935
84 core	2339	2239

*Change in the revised manuscript:*

5 Figure R1 was added and compared with Figure 5 in the revised manuscript.

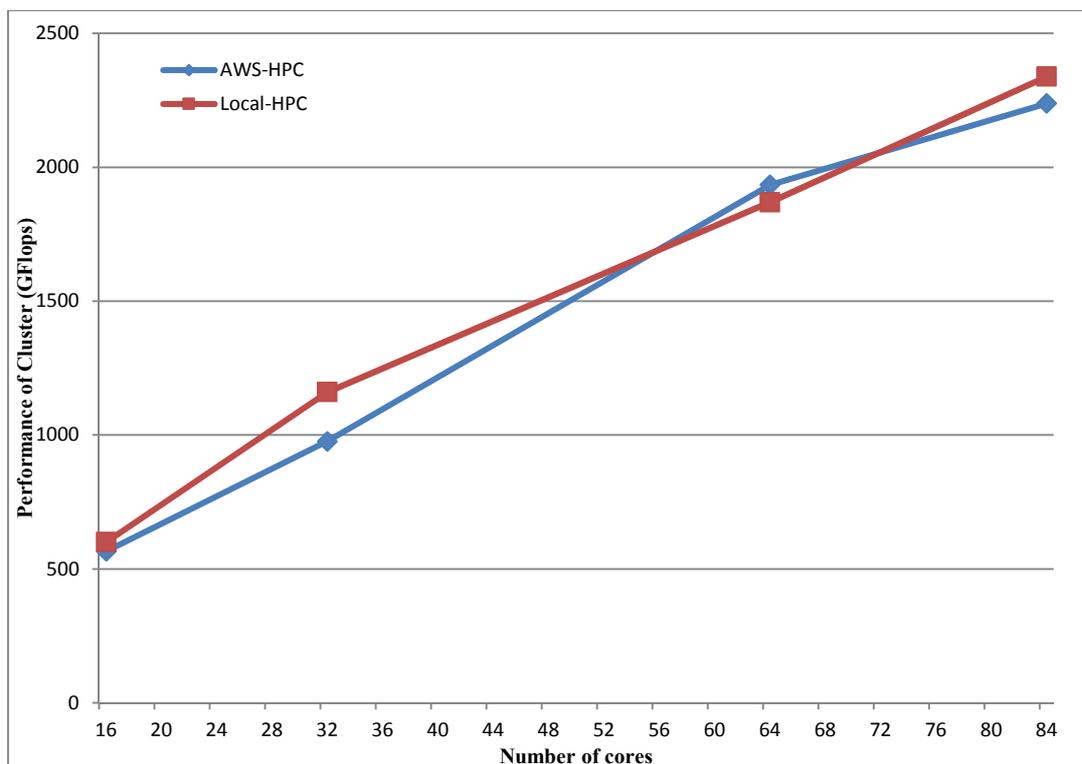


Figure R1. Performance of the cluster using the Intel Compiler and the MKL Math Library

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5. Page 8, Line 6. The statement that "network latency may be smaller than in the AWS cluster" is not really supported by the presented data. As mentioned above, HPL is relatively insensitive to network performance. If you want to make a statement about network latency, then measure it. If you want to characterise the network performance, then the Intel MPI benchmarks are a good place to start (<https://software.intel.com/en-us/articles/intel-mpibenchmarks/>). You can run these on both the AWS instances you have spun up, and the local cluster. These give you direct information about the quality of the interconnect and MPI implementation, rather than attempting to guess from secondary data. For example, see a Supercomputing 2016 poster comparing AWS in-C4 instances with the TSUBAME-KFC supercomputer.

15

20 Answer:

Thank you. The N/W latency with Linux-qperf and Intel-mpibenchmark (intel-mpi-benchmarks, 2017) was measured according to the message size. The latency showed a performance difference between the AWS cluster and the local cluster on the message size.

Change in the revised manuscript:

We added Figure R2 to the Supplementary section.

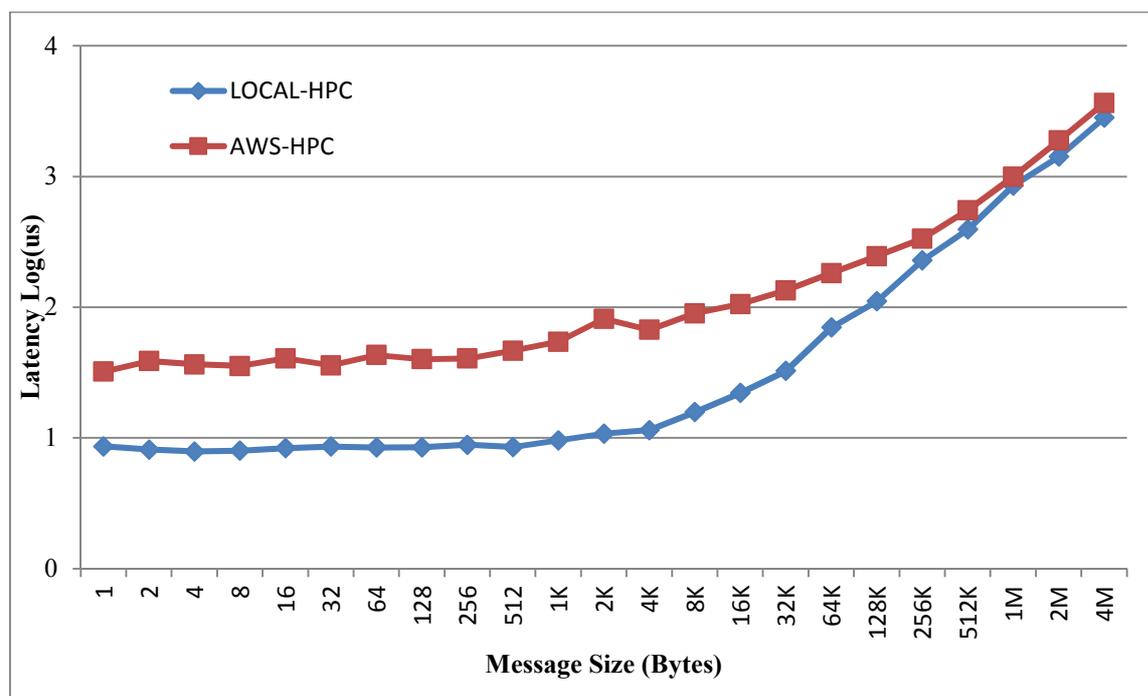


Figure R2. Comparison of the latency between local-HPC and AWS-HPC according to the message size

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6. Although the two experimental testbeds give approximately the same floating point performance, it is not possible to determine if the effect of virtualisation is introducing a penalty (because the peak performance of the hardware is not reported anywhere). Are these two lines similar because the hardware is approximately the same, and being used with similar efficiency? Or, does the AWS instance in fact have twice as much "spec sheet" performance, but you lose 50% for some reason (or vice versa)?

10

Answer:

Thank you. You might have been misled on the performance of the two clusters (Figure 5) because of the insufficient H/W information in the manuscript. More information on H/W has been added to help the readers better understand our study. The CPU configuration of each node in AWS and local HPC (e.g. Threads, Core, Sockets and CPU Clocks) has also been added. Furthermore, we configured both clusters with Intel Compiler and MKL Library to measure the optimised performance. The cluster performance of AWS was similar to that of the local cluster despite the faster CPU, which might be caused by the performance penalty of virtualisation in AWS.

15

Table R9. CPU specification of the local and AWS clusters

	Local cluster node	AWS cluster instance (c4x8large)
Architecture	x86_64	x86_64
CPU(s)	28	36
On-line CPU(s) list	0-27	0-35
Thread(s) per core	1	2
Core(s) per socket	14	9
Socket(s)	2	2

20

Vendor ID	Genuine_Intel	Genuine_Intel
CPU family	6	6
Model name	Intel® Xeon® CPU E5-2697 v3 at 2.6 GHz	Intel® Xeon® CPU E5-2666 v3 at 2.9 GHz
CPU MHz	2599.843	3100.012
Hypervisor vendor:	-	Xen
L1d cache	32 K	32 K
L1i cache	32 K	32 K
L2 cache	256 K	256 K
L3 cache	35840 K	25600 K

*Change in the revised manuscript:*

Table R9 has been included in the revised manuscript.

5

7. Section 5.2. This again has little analysis of the data, other than to note that when using higher resolution simulations, the scaling efficiency is better. But this is not surprising. When we increase the amount of local work (higher resolution), any effects due to serial fractions (Amdahl's law) from bad parallelisation or similar become smaller. An interesting question is how many degrees of freedom (dofs) are used per core. The C-grid staggering for ROMS means that, if I have done my sums correctly, there are about  $1.7e6$  dofs for each of velocity and pressure on the smallest grid. On 64 cores, this corresponds to around  $3e4$  dofs/core. For explicit schemes that have not been highly optimised, this is generally seen to be close to a break-even point for parallel scaling. So the results at this scale are not surprising that the AWS cluster stops scaling sooner is almost certainly due to network performance. This should be possible to model if one knew what the actual network latency and bandwidth were (you could measure this!). For an example of how to make these predictions I can recommend Fischer, Heisey, and Min (2015).

10

15

Answer:

Thank you. We appreciate your valuable comment. We could measure various networks and band widths according to your suggestion; however, it would be another long story because it needs much time and resource to model based on sufficient data. This is beyond the scope of the present study, which suggests cloud computing as a useful tool for ocean scientists that do not have enough computing resources. We leave further analyses with various configurations, that might be an interesting topic, for the next study.

20

25

8. Section 5.3. Validation of the model notes that there is a small difference in the results between local and AWS run simulations. Probably this is fine, but one wonders. Was the comparison on the same number of cores in both cases? Does ROMS offer bitwise reproducible results when run on the same number of cores (or only statistically the same)? For example, if the authors were to run multiple times on a single system, would they expect a small spread in the results, or would they expect the same numbers every time? If the latter, it is not obvious why this should not transfer to different systems (if using the same number of cores).

30

Answer:

Thank you. We compared the simulation results with the same number of cores between AWS and local HPC. For additional information, the root mean square error (RMSE) of the temperature and the velocities between AWS and local HPC were calculated to validate the model results according to the number of cores. The RMSE between AWS and local HP was tiny, regardless of the ROMS version and the number of cores.

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Table R10. RMSE of the temperature and the velocities between AWS and HPC according to the number of cores using ROMS v 3.6 (revision 783)

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Cores	Temp	U m/s	V m/s
16 core	0.0057	4.7613e-004	5.0426e-004
32 core	0.0097	4.9277e-004	4.8897e-004
64 core	0.0108	5.5478e-004	5.3697e-004

Table R11. RMSE of the temperature and the velocities between AWS and HPC according to the number of cores using ROMS v.3.7 (revision 898)

Cores	Temp	U m/s	V m/s
16 core	0.0112	5.2358e-004	5.7382e-004
32 core	0.0086	5.0863e-004	5.7747e-004
64 core	0.0098	5.7419e-004	5.9089e-004

5 *Change in the revised manuscript:*

Tables R11 and R12 have been included in the Supplementary section.

9. Section 6.1. The discussion of hyperthreading effects is somewhat confusing. It seems like you are just saying "If you want performance equivalent to X physical CPUs, you should provision X physical CPUs (rather than the X/2 physical CPUs you would get with virtualised hyperthreaded CPUs)". It is unclear from the discussion if allocating two instances each with 16 vCPUs is twice as expensive as one instance with 32 vCPUs. Furthermore, you do not present any evidence of the performance difference between 16 vCPUs and 32 vCPUs (the referenced Figure 10 compares performance between two different compilers).

15 Answer:

Thank you. As shown in Table R9, the actual number of physical CPUs is half of the vCPU provided by instances. If we turn on the hyperthread feature, we can see the number of vCPUs, which is twice the number of real CPUs. Utilizing the hyperthread function to run several operations is advantageous if the amount of CPU usage is small. The effect is negligible if the physical CPU usage is close to 100% like the actual HPC. We included the result for the 16 core and 32 core ROMS run times using the same compiler on the same node to show this fact (Figure R3).

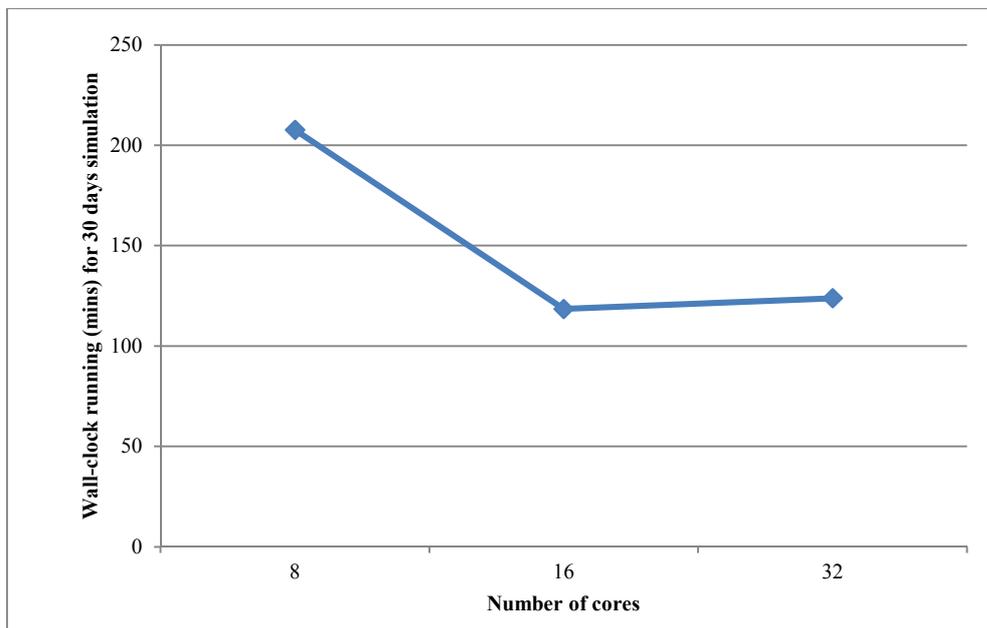


Figure R3. Comparison of the wall-clock running time of vCores with the same compiler

10. Section 6.2. This again does not provide enough information to interpret the data. For example, what compiler versions did you use in both cases, what were the compiler flags? Presumably AWS is not special, and you would expect to see the same difference on the local system as well?

5

Answer:

Thank you. We compiled our model using makefile with the same compiler and the same compile option. The compiler configuration for ROMS was included in the manuscript. We used the default makefile without optimisation options in both cases. More details on the configuration of the environment in AWS have been included in the revised manuscript.

10

*Change in the revised manuscript:*

We replaced Table 2 with Table R12 in the revised manuscript

15

Table R12

Type	CPU	Memory	Node	OS	Compiler
AWS HPC	32 core (vCPU) Intel Xeon E5-2666- v3 (2.9 GHz)	60G	8	Amazon Linux	PGI Compiler 16.10 NetCDF4 gcc 4.4 Intel Compiler 2018 update 1
Laboratory HPC	28 core Intel Xeon E5-2697-v3 (2.6 GHz)	128G	3	CentOS 6.9	PGI Compiler 16.10 NetCDF4 gcc 4.4 Intel Compiler 2018 update 1

. 11. Section 6.3. This compares the time to solution between two different instance types. The difference appears to only be in the frequency of the utilised CPUs. The 2.9GHz CPU is 5% faster than the 2.3GHz CPU. An interesting question is, "how much cheaper is the slower CPU". A 5% slowdown seems like it might be worth paying if the cost is much less. Considering table 1, however, it is much higher (presumably because more memory is expensive).

20

Again, assessing the raw data from this experiment is made needlessly difficult. Given the lower cost and higher performance of the c4 instances, it is unclear why the r4 instance was chosen as a comparison.

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Answer:

Thank you very much for your comment. The r4 instance was selected to compare the effect of the N/W performance. The c4 instance provided 10 Gbps of bandwidth using the Intel 82599 virtual function (VF) interface, whereas the r4 instance provided 20 Gbps of bandwidth using the elastic network adapter (ENA) (AWS, 2016). ROMS is relatively less insensitive to N/W because it showed little difference in the performance of c4 and r4.

30

*Change in the revised manuscript:*

We explained the reason why we chose the r4 instance for comparison in the revised manuscript.

35

Some minor comments:

12. Page 3, line 17. Chen (2017) draw, I think, bad conclusions about the parallel scaling of CESM on AWS. I suspect their local supercomputing resource would have shown the same tail-off (if they had run that far).

Answer:

5 Thank you. We agree with you on this point.

13. Page 5, line 25. It is unclear why setting up the environment for models is time consuming on local HPC services (but not on AWS). Why does copying VMs reduce the time for large scale experiments?

10

Answer:

Thank you for your comment. An easy configuration of the environment is a useful benefit of cloud computing. A large-scale model generally needs a large number of nodes. It takes time to prepare an additional physical environment, such as electric capacity and space. Moreover, the installation of OS and the compiler and the network configuration need additional effort. However, we can easily create a node by cloning a pre-configured image in a cloud system, which is much easier than configuring the environment on a per-node basis in local.

15

14. Page 7, lines 30–32 are copied verbatim from the AWS documentation. Although a citation is provided, it is (to me) not sufficiently clear that these are quotes, rather than description with referenced work. I have not exhaustively checked the rest of the paper for such examples.

20

Answer:

Thank you. The AWS documentations we cited were technical function manuals. We thought that copied verbatim was more desirable to prevent misleading, but we revised this part according to your suggestion.

25

*Change in the revised manuscript:*

The text for the revised manuscript is as follows:

'AWS enhanced networking provides higher bandwidth, higher packets per second (PPS) performance, and lower latencies among instances. AWS recommends placement groups for applications that need low network latency and high network bandwidth (AWS, 2016d).'

30

15. Page 12. The code availability section does not reference HPL at all.

35

Answer:

Thank you. We added the code availability of HPL and STREAM in the revised manuscript.

*Change in the revised manuscript:*

40 The text on code availability for the revised manuscript is as follows:

#### **Code availability**

ROMS is publicly available and licensed under the MIT/X License. (Please see the ROMS website at <http://myroms.org> for details.) Its source code is available for download from the ROMS website via the SVN server. The particular version used for computing the ocean simulations executed in this study is available in trunk, revision 783. How to create and reconstruct the cloud computing infrastructure in AWS and makefile options are explained in Appendix A. The Amazon Machine Image (AMI) is sharable in AWS.

45

The HPL is publicly available and licensed under the HPL Copyright Notice and Licensing Terms. (Please see the HPL website at <http://www.netlib.org/benchmark/hpl/index.html> for details.) Its source code is available for

download from the HPL website.

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25   NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

STREAM is publicly available and licensed under the STREAM Copyright Notice and Licensing Terms. (Please see the STREAM benchmark website at <https://www.cs.virginia.edu/stream> for details.) Its source code is  
30   available for download from the STREAM website.

16. Most of the instance types listed in this table are not referred to elsewhere in the paper, why are they therefore included?

Answer:

35   Thank you. We used the c4 and r4 instances in our study. However, public cloud services and AWS provided various instance types with CPU, memory, and N/W configurations for various purposes and sizes. We introduced various instance types to help users select for their research purposes.

40   17. The listed memory capacity of Table 1 does not tally with Table 2. If I understand the paper correctly, most simulations were carried out with c4.8xlarge instances (which Table 1 claims supply 60GB RAM). But Table 2 claims that 128GB RAM were available. Which is correct? Again, I have not exhaustively checked details.

Answer:

45   Thank you for pointing this out, and we apologise for this typo. 60 GB RAM was corrected appropriately.

## References

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