RESPONSE TO REVIEWER @thomasgillis – RHEA: an open-source Reproducible Hybrid-architecture flow solver Engineered for Academia #4637

The authors would like to thank the reviewer for the valuable comments, suggestions and remarks. We have answered all of them below.

General comments:

1. Is your code 2D or 3D? Please mention it. The distributed computing needed on a 2D code is difficult to support with the architectures nowadays though.

The solver is three-dimensional (3D). Two-dimensional (2D) problems can be considered utilizing one cell in the third direction together with imposing Neumman boundary conditions. We have added this information in the "Computational design" section of the manuscript: "RHEA solves the three-dimensional (3-D) compressible equations of fluid motion …" .

2. I understand timing in parallel with MPI but it seems that there is still an issue there. From the code below I still don't understand the need of MPI_Barrier(). If you remove it you would get an exact timing and the code would work the same way (production or not) as you have the MPI_Allreduce. There is no need for this Barrier if I understood your code correctly.// https://gitlab.com/ProjectRHEA/flowsolverrhea/-/blob/master/src/ParallelTimer.cpp#L34

```
// function stop()
MPI_Barrier(MPI_COMM_WORLD);
time_array[str][1] = getTime_cpu();
time_array[str][2] = time_array[str][1] - time_array[str][0];
// [...]
ltime = time_array[str][2];
MPI_Allreduce(&ltime,&maxtime,1,MPI_DOUBLE,MPI_MAX,MPI_COMM_WORLD);
MPI_Allreduce(&ltime,&mintime,1,MPI_DOUBLE,MPI_MIN,MPI_COMM_WORLD);
MPI_Allreduce(&ltime,&avgtime,1,MPI_DOUBLE,MPI_SUM,MPI_COMM_WORLD);
```

Following this comment, we have removed the MPI_Barrier in the stop function of ParallelTimer.cpp.

3. I would remove the claims "easy", "easily", with "ease". This is extremely subjective and is not supported by quantitative data.

We have removed the words "easy", "easily" and "ease" from the manuscript.

4. Fig1: this figure is still very puzzling to me. I don't fully understand what you did: which test case, how many unknowns per rank, which time-integration, etc.

The test case is described in the “Application example” section. In detail, the computational domain is $4\pi\delta \times 2\delta \times 4\pi\delta/3$ in the streamwise, wall-normal, and spanwise directions, respectively. The streamwise and spanwise boundaries are set periodic, and no-slip conditions are imposed on the horizontal boundaries. The KGP convection scheme [@Coppola2019-A] is utilized for solving the transport equations together with a third-order Runge-Kutta time-integration method. The grid is uniform in the streamwise and spanwise directions, and stretched toward the walls in the vertical direction with the first grid point at y+=0.1. We have added to the manuscript the following information regarding the number of grid cells per node: “The number of grid points utilized for the strong (total quantity) and weak (quantity per node) scalability tests correspond to 256×256×256 (Hybrid) and 384×384×384 (BSC).”.

Additional comments:

5. A traditional way of presenting results is to begin with "time-to-solution" (and for you, energy-to-solution), if you replace your figure by that, then the ratio makes sense. There is no need to have a figure for a ratio, you can simply put it in the text. Also how do you get the energy information? Was it on 1 node?

Following this comment, we have removed the time-to-solution and energy-to-solution plot from the figure. In addition, to avoid confusion, we have clarified the analysis by focusing on the time-to-solution results. Consequently, we have modified the text of the paragraph to: “... Three main observations can be inferred from the results. First, focusing on the time-to-solution when using CPUs+GPUs with respect to only CPUs, the solver is accelerated approximately 2.5x and 5x on the Hybrid and BSC computers …”.

6. On the right: you did a weak scalability so you should mention it before, in the first part of the paragraph (where you mention the strong scalability). Usually the weak scalability metric is referred to as the "efficiency" as the number is between 0 and 1 and not the "speedup".

We have modified the first sentence of the manuscript to “The computational performance of RHEA is analyzed by carrying out performance and scalability tests based on 100 time iterations of the 3-D turbulent channel flow configuration described in the next section.”. In addition, we have changed the labels of the vertical axis of the plots to: (i) Strong Scalability Speedup, and (ii) Weak Scalability Efficiency.

7. I disagree with saying that your CPU and CPU+GPU code scale the same. If you compute the parallel percentage of the software from the scalability study I guess you will find a factor 2 there (or close). Also you mention 90% in the text but we are unable to verify that claim with the graduation of the figure.

The solver on BSC is roughly 5x faster on CPUs+GPUs than on CPUs. In this regard, what we mean is that, for a particular computing configuration (CPUs or CPUs+GPUs), the solver scales similarly keeping in mind the time-to-solution ratio. To clarify this, we have modified the text to "Second, as shown in Figure 1(left), on BSC for a fixed-problem size and noting that on CPUs+GPUs the solver is roughly 5x faster, the solver presents similar speedups in terms of strong scalability when running on CPUs and CPUs+GPUs up to 32 nodes (640 cores and 128 GPUs) until communication overheads become important in relative value.".

8. The CI/CD you have added seems very short to me. It looks like you only check the solution on a problem in 1D? I cannot really check that box, sorry. Maybe add some details.

We have added an additional multidimensional test to CI/CD. In particular, the 2d_taylor_green_vortex, which is a 3D case (16x16x1 grid) that exercises all the main functionalities of the solver, has been added to CI/CD, and the correctness of the result is checked against a "figure of merit" calculated by means of a python script. The test is "passed" if the result is correct, whereas it crashes if it is not correct.

Subjective comments:

9. I understand your strategy to produce reproducible science. However I am not sure that the fact of adding a test folder with some test case justifies that adjective in the title. To me the results (of a paper, presentation, etc) can be reproducible (and should be!), but I am not sure what it means to have "reproducible software". To reproduce results, you need the source code but also the same infrastructure etc. For example one could argue that a CI/CD suite increases reproducibility while the test folder does not. Changing the title would also change the acronym which is maybe not a suitable option at this point.

We understand these arguments. In this regard, our approach to "reproducible results" is also to provide access to the data generated from simulations through: (i) locally storing the data in our clusters to subsequently share files upon making proper arrangements with the requesters; and (ii) sharing selected files through online data repositories, like for example the "Johns Hopkins Turbulence Databases (JHTDB)". In addition, we want to make publicly available the solver, configuration files and post-processing scripts used to generate the data in case that other groups want to regenerate the data and/or extend the range of the simulations

performed. At this point, however, changing the title is not a suitable solution, but, following this comment, we have added an additional multi-dimensional test to CI/CD as described above.

10. "*is named RHEA, which stands for open-source Reproducible Hybrid-architecture flow solver Engineered for Academia, and is inspired by the Titaness great Mother of the ancient Greek Gods, and goddess of female fertility, motherhood and generation. Her name was RHEA and means flow and ease, representing the eternal flow of time and generations with ease.*" I understand that the choice of a name for a software is personal, but I don't think that this level of detail is relevant here. Also the information stated here repeats the title.

Following this comment, we have removed this text from the manuscript.