We thank the Referee for his/her time and his/her constructive comments. We have complied with most of the proposed changes. In the following, the comments made by the Referee appear in black, while our replies are in blue.

In this article, the author discuss their successful porting of the Meso-NH model, a mesoscale atmospheric model, from CPU to GPU architecture. The reason is to make use of the faster and more efficient running of certain types of calculations on GPU. The authors indeed report significant improvements in speed and energy efficiency using their new GPU code, and in their article discuss the technical details of the code porting, technical choices that need to be made, bit reproducibility efforts, and at the end a set of demonstrative simulations.

First of all, I would like to congratulate the authors with their new GPU-accelerated code, which no doubt was a big effort. I also like the bit-reproducibility work, which appears crucial in getting reliable results across different hardwares. In reading the article, I came across a few themes that I think need to be clarified, which relate mostly to validation and reproducibility, and a handful of small comments that I list at the end of this review. As my technical knowledge of OpenACC/MPI, compilers, and writing custom libraries is limited I will focus a bit more on the practical side, interpretation, and overal validation.

Major comments

Section 4 shortcomings

After demonstrating technical side of the porting process and the hardware / performance scaling of the model on various architectures using the author's standard validation case, section 4 is set to demonstrate the "physical realism" and even aims to "better understand the mechanisms involved in the formation of small-scale wind gusts" (lines 433-434). However, the discussion of the simulations is limited to qualitative descriptions which ultimately demonstrate little in terms of new understanding or physical realism. At the very least, I would expect comparison to observations here and quantitative measures of skill, for example compared to what is achievable using the same amount of computing power (in time or energy) on CPU-only simulations (which would demonstrate the benefit). Furthermore, to substantiate the claims of "successful cascade of scales" (e.g. line 10), I would expect a power density spectrum of wind and specific humidity at certain levels.

We agree that Section 4 does not demonstrate the "physical realism" of the simulations or "the mechanisms involved in the formation of small-scale wind gusts". However, a quantitative comparison with observations and a detailed study of the physical processes are beyond the scope of the paper. As stated in the same section: "While the detailed processes involved are currently investigated in separate studies, the results illustrate that different types of storms are realistically simulated by Meso-NH and benefit from the combination of large domain and high resolution." Thus, we implemented two changes:

- (1) We rephrased the first paragraph to make it clear that the purpose is to illustrate possible applications of high-resolution simulations on a large grid, without levering expectations about an assessment of their forecasting skill or a detailed examination of the involved physical processes, which are left for future studies.
- (2) We added a new figure to show the benefits of high-resolution simulations (now Fig. 10 in the paper, and the left panel of Fig. 1 below): "Focusing on Atlantic storm Alex prior to landfall over Brittany (Fig. 9, top right panel), Fig. 10 shows the scale cascade as spectrum of kinetic energy in the middle of the boundary layer. The Meso-NH simulation (blue curve) exhibits three distinct ranges: the mesoscale for $\lambda > 10$ km, the inertial subrange approaching the theoretical slope of the Kolmogorov spectrum (grey line) for $\lambda < 1$ km, and an energy accumulation range in between for $10 > \lambda > 1$ km. Specifically, the energy accumulation range includes the fine-scale wind structures at the origin of gusts illustrated in Fig. 9. At smaller scales, the drop in energy for $\lambda < 400$ m in Fig. 10 indicates that the effective resolution of the simulation reaches $4\Delta x$." In addition, we compare the Meso-NH simulation with the highest-resolution operational model data available: "In contrast, the AROME operational analysis that provides the initial and lateral boundary conditions for the simulation (orange curve) diverges from Meso-NH for $\lambda < 10$ km: it captures only the mesoscale and misses the energy accumulation and inertial subrange." We prefer this approach to using the same amount of computing power on CPU-only simulations, as suggested by the Reviewer, which would lead to a large energy consumption for limited added value. Finally, the right panel of Fig. 1 shows the energy spectrum at a lower level: while the

divergence with AROME for λ <10 km is similar, the Meso-NH does not clearly follow the slope of the inertial subrange for λ <1 km. This is due to the smaller scale of eddies closer to the surface, which would require even higher resolution to be represented explicitly. For the sake of brevity, only the left panel showing the spectra in the middle of the boundary layer is included in the paper.

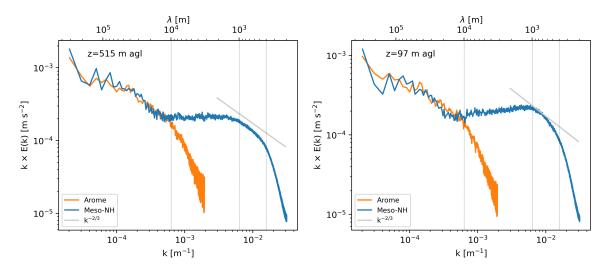


Figure 1: Energy spectrum for Atlantic storm Alex at 515 m agl (left panel) and 97 m agl (right panel) in the Meso-NH simulation (blue curve) and the AROME operational analysis (orange curve). The grey line shows the theoretical slope of the inertial range, while the vertical lines indicate the approximate wavelengths of the lower limit of the mesoscale ($\lambda \approx 10$ km) and the upper limit of the inertial subrange ($\lambda \approx 1$ km), as well as the effective resolution of the simulation ($\lambda \approx 400$ m).

Reproducibility

In light of the previous comment, I thought I'd try and run the code myself on one of the NVIDIA GPU workstations we have available. I use these to run similar GPU-accelerated LES code. After close to an hour, I was not able to compile the library with the documentation supplied in https://zenodo.org/doi/ 10.5281/zenodo.13759713. Some error code was in French (when you run ./configure twice after changing a setting). The top-level README did not guide me through the installation process for a Linux PC, it seemed to be optimized for supercomputer, which is the main purpose, of course. I came across a url for instructions for Linux PCs in the README in the MESONH-v55-OpenACC folder, but that url does not work. The compilation seemed almost done, but there were no clear errors at the end - though I suspect an unlinked NetCDF library was the culprit. I don't doubt the compilation process will ultimately be straightforward, but for a user who has never worked with this model before, the instruction for a model as complex as this were too limited given the time I can spend on a review. I don't have access to the supercomputers used by the authors. We are sorry to hear that you are having trouble compiling Meso-NH. The problem with the NetCDF library sometimes arises because the compilation of the NetCDF library included in the Meso-NH package may conflict with other NetCDF libraries already compiled on the Linux PC, or because other utility libraries (compression, ...) are missing. It is not possible to take account of each user's specific system environment during the installation process. In the case of compilation issue, the user usually mails his/her problem to Meso-NH support, who will help solving it.

Scaling with radiation

Given that this model runs mesoscale domains at LES resolution, I would expected that details in physics parameterizations will start to matter. One example is radiative transfer calculations, see:

Maier, R., Jakub, F., Emde, C., Manev, M., Voigt, A., and Mayer, B.: A dynamic approach to three-dimensional radiative transfer in subkilometer-scale numerical weather prediction models: the dynamic TenStream solver v1.0, Geosci. Model Dev., 17, 3357–3383, https://doi.org/10.5194/gmd-17-3357-2024, 2024.

Veerman, M. A., van Stratum, B. J. H., & van Heerwaarden, C. C. (2022). A case study of cumulus convection over land in cloud-resolving simulations with a coupled ray tracer. Geophysical Research Letters, 49,

e2022GL100808. https://doi.org/10.1029/2022GL100808

Ukkonen, P., & Hogan, R. J. (2024). Twelve times faster yet accurate: A new state-of-the-art in radiation schemes via performance and spectral optimization. Journal of Advances in Modeling Earth Systems, 16, e2023MS003932. https://doi.org/10.1029/2023MS003932

Please clarify:

- What scheme do you use and is it GPU-accelerated? Line 98 should be more specific here. I suspect ecRAD.
- How does the radiation scheme affect the scaling performance of CPU vs GPU code? Line 287 says you call it only every 900s.

We use the radiative code described by Gregory et al. (2000), Revision of convection, radiation and cloud schemes in the ECMWF model, Quart. J. Roy. Meteor. Soc., 126, 1685-1710, https://doi.org/10. 1002/qj.49712656607. This reference is now added Line 98. It describes the radiation scheme used at ECMWF before the ecRad scheme was included in the IFS code. As noted in the text, no attempt has been made to port the radiation scheme to the GPU, so it is included in the performance scaling results, along with other components (Line 286, Figure 3 and "Others" in Figure 4).

Minor comments

Readability of the overal manuscript

As mentioned, I lack the technical know-how of the porting process, and so, feel free to not attribute too much value to this comment. However, if your goal is for the article to be readable to a broader audience, I would advice an approach where the logic and decision making of all steps is written in plain language, with the specific syntax/code not in-line but separate. I understand this may be unavoidable given the topic of the article.

For example, in much of the article, command line options, compiler flags, and run modes are included in parenthesis or in-line in such a way that, for me, the readability of the overal text is challenging and sometimes I lose track of what the purpose of a specific section or paragraph is. In section 4.2, meant to showcase the practical application of the model code, various new technical concepts and run flags are introduced in the first paragraph, and then again at the end of the second paragraph. Lines 106 to 114 may also better be placed in section 2.2? Also the concept of bit-reproducibility can, I think, be explained without the use of inline compiler flags. As you write, we added run flags and other technical elements to show the practical application of porting the Meso-NH code to GPUs. In section 4.2, we have refrained from using these details in the revised version. We prefer to keep lines 106 to 114 in sub-section 2.1, as they are not limited to sub-section 2.2, but include the modifications described in all the following sub-sections. When describing the verification of bit-reproducibility, we prefer to keep the indication of the inline compiler flags, as they are essential to the execution of the MPPDB_CHECK library.

Line 58: No code is bug-free, unfortunately. Do you mean that at least single to multi CPU vs GPU will give the same results, and so there are no bugs related to which architecture it runs on? We agree that no code is bug-free. Here, we state that the implementation for massively parallel executions on CPU or GPU supercomputers is bug free. To clarify, the sentence is now "To our knowledge, Meso-NH is the only atmospheric (or oceanic) model offering bit-level reproducibility. This outstanding capability guarantees that Meso-NH is parallelization bug-free, i.e. there are no bugs in its implementation for parallel executions on CPUs and GPUs."

Line 427: "the use of **single** precision" Changed

We thank the Referee for his time and his constructive comments. We have complied with most of the proposed changes. In the following, the comments made by the Referee appear in black, while our replies are in blue.

This work represents a major GPU porting effort of the Meso-NH model. This model is originally written in Fortran with MPI for distributed-memory parallelization. The work ports significant parts of the model for NVIDIA and AMD architectures using OpenACC. In addition to the directives needed to port GPU kernels, a pre-processor was developed, along with a multi-grid pressure solver as an alternative to the FFT-based one. An extensive performance analysis on different systems is provided.

I found the work insightful and the paper well-organized and written. However, some parts lack the detail needed to fully understand the numerical and computational approach. Without clarifying these details, it becomes quite hard to understand some of the choices that were taken in the effort. I will elaborate below point-by-point.

1. L 78-79: "The current pressure solver consists on [of] a conjugate-residual algorithm accelerated by a flat fast Fourier transform (FFT) precondition." This is insufficient to fully understand the numerical approach to solving the pressure equation. Could you provide more (mathematical) background and mention in which directions FFT(s) are being used and the consequences for the grid spacing and boundary conditions along this and the other directions? Moreover, could you illustrate how this equation is solved in parallel (I could not find a clear answer in the cited references either)?

We now provide the reader with specific references while refraining from adding lengthy mathematical explanations. In section 2.1, we specifically implemented three changes:

- (1) We now refer to Skamarock et al. (1997), Bernardet (1995) and to the 20 pages of Chapter 9, Part I of the Meso-NH scientific documentation devoted to the pressure problem. It reads "The current pressure solver consists of a conjugate-residual algorithm (Skamarock et al. 1997) accelerated by a flat Fast Fourier transform (FFT) preconditioner following Bernardet (1995). The horizontal part of the operator to invert in the elliptic pressure problem is processed with FFT while its vertical part leads to the classical tridiagonal matrix. For a detailed description, the reader is referred to Chapter 9, Part I of the scientific documentation available on the Meso-NH web site (http://mesonh.aero.obs-mip.fr, last access: 16 December 2024)".
- (2) We now mention the initial implementation of the FFT solver for parallel computers done by Giraud et al. (1999). We added "The initial parallel implementation of the FFT pressure solver takes into account two other types of partitioning on each horizontal direction, called x-slice and y-slice. Communication routines have been implemented to move a field between these different decompositions. It is then possible to perform the FFT for each horizontal direction (Giraud et al., 1999)".
- (3) We now mention the adaptation of the FFT pressure solver for massively parallel computers. We added "In the case of FFT, moving data from a vertical beam decomposition to x- and y-slices limits the number of processes to the smallest horizontal dimension. For example, a model on a $512 \times 512 \times 128$ grid can only be run with 512 processes. Instead, a 3-dimensional decomposition of the beam was implemented and optimized. For a run using $p_x \times p_y$ processes, the global domain of size $N_x \times N_y \times N_z$ is divided into z-pencils of size $(N_x/p_x) \times (N_y/p_y) \times N_z$. The FFT is first performed on each x-pencil of size $N_x \times (N_y/p_y) \times (N_z/p_x)$ in the x direction, then on each y-pencil of size $(N_x/p_y) \times N_y \times (N_z/p_x)$ in the y direction. Next, the tridiagonal system is solved in the Fourier space for each y-pencil. Finally, inverse FFTs are calculated on each y-pencil, then on each y-pencil. As a result, the above example can now be run with up to $512 \times 128 = 65536$ processes."
- 2. L. 80. Can you not simply state that it is written in Modern Fortran? If you want to be pedantic, you'd need to state that it has features from older standards (77, 90), too.

Our intention is not to be pedantic. We simply want to point out that Meso-NH uses more recent features than Fortran 95, some of which are useful for porting to GPUs (i.e., do concurrent)

3. L. 122. Just to comment that I found that using 'default(present)' in all OpenACC kernel loops really helps with debugging, as one would get a runtime error whenever something is accessed in a kernel that is not on the device.

The 'default(present)' directive is not really applicable or useful here. As we are porting the code piece by piece to the GPU, not all the data resides on the GPU memory. The code will therefore crash if the data

has been calculated on the CPU and is not yet on the GPU memory. And even if the data is on the GPU memory, an update of the CPU or GPU memory copy is required (! \$acc update host/device ...). Bit reproducibility ensures that no such errors occur.

- 4. I found Figure 1 quite hard to understand. Could you improve the captions so that it is clear what we are looking at? Is the left a serial computation, and the right one an MPI decomposed one with 2D pencils? Following your suggestion, the caption of Fig. 1 is now "Schematic of bit-reproducible verification between primary and replica simulations using the MPPDB_CHECK library. On the left, the primary simulation is a computation performed on the entire domain, i.e. without any domain decomposition on CPU. On the right, the replica simulation is a parallel computation performed on CPU or GPU on the domain broken down into 4×4 pencils."
- 5. L213. Same spirit as comment 1. "the FFT algorithm requires all-to-all communications between MPI processes (...)" Is the FFT algorithm requiring all-to-all communications, or is it the Poisson solver? It is unclear how the pressure equation is being solved numerically (1D or 2D FFTs? + CR along which direction?), and how that is implemented in a distributed-memory paradigm.

To avoid confusion, we changed "The FFT algorithm [...]" into "The FFT pre-conditioner [...]". See our response to comment 1 regarding the details on the FFT pressure solver added in Sect. 2.1.

6. L 218. "The most promising alternative for solving this type of elliptic equation is the use of a geometric multigrid solver for regular structured grid". This claim needs to be substantiated or reconsidered, as it is not obvious, especially for GPUs: As you coarsen in an MG method, the GPU occupancy is being massively reduced, making it perform extremely poorly on GPU-based systems. So, I would say that geometric multigrid solvers do not pair that well with GPUs.

Our claim is now substantiated by adding "In particular, Müller et al. (2015) ported a C/CUDA version of a geometric multigrid algorithm that scaled up to 16384 GPUs."

We also added a paragraph regarding the cost of FFT-based solvers on supercomputers: "Such a negative impact of all-to-all communications in the FFT pre-conditioner has been seen with Meso-NH running on MIRA, a Blue Gene/Q system at Argonne National Laboratory by showing sub-optimal scalability when using 2 billion threads (Lac et al. 2018; see their Fig. 1). Verma et al. (2023) performed a scaling analysis of their GPU-FFT library for grid sizes of 1024^3 , 2048^3 , and 4096^3 , utilizing up to 512 A100 GPUs. They reported a ratio of communication time to total time of 50% when using 8 GPUs and over 90% when using more than 128 GPUs. Ibeid et al. (2020) showed in exascale projections for grid size of 65536^3 that the FFT total time is due solely to the FFT communication time, which is dominated by the network access cost."

7. L 235. I see that along one direction the (direct) Thomas algorithm is used, while in other two an iterative (MG) method is used. The linear algebra behind this approach is quite unclear to me, so please provide more mathematical details so a reader can easily follow the method without navigating into the code or other references.

For reasons of readability of the manuscript as a whole (a criticism made by the Reviewer #1), we prefer to refrain from adding lengthy mathematical explanations and we refer the reader to the 20-page documentation of the MG method (Müller 2014).

8. L. 250. A comparison between FFT-based and multigrid is performed, but I am missing a lot of details needed for reproducibility and better understanding. What kind of tolerance is being used in the FFT-based flavor (CR method), and in the MG one? What kind of smoother is being used in the geometric multi-grid method? These details need to be clear for better interpreting the results.

To clarify, we added "It should be noted that the comparison between FFT and MG pressure solvers is presented only in terms of computational performance. No reproducibility of pressure between solvers is expected. Similar accuracy, i.e. the same threshold in the residual divergence of the pressure value, is however demanded by both solvers."

9. L 288. "The test case uses advection, turbulence, cloud microphysics, pressure solver and other components". Consider being more exhaustive here.

To clarify, the sentence is now "The test case uses advection, turbulence, cloud microphysics, pressure solver

(see section 2.1 for more details) and other components. These other components include elements not covered by the above-mentioned processes, such as gravity and Coriolis terms (executed on GPUs), radiation (called every 900 s only, executed on CPUs), time advancement of all variables and I/O operations (which are largely disabled in our simulations)."

10. L 322. I read that there can be several MPI tasks per GPU. It is unclear how this is implemented in practice. A sketch with the domain decomposition colored by MPI tasks, along with the GPUs that handle each group of tasks, would be very insightful.

The binding configuration was explained Line 298 ("Binding on CPU cores and GPUs is carefully chosen [...]. If several binding configurations have been tested, only the one giving the fastest results is kept."). Then we added "For example, the best run on an Adastra node with 16 MPI processes uses a 4×4 subdomain grid. To optimize MPI communications, processes with neighboring subdomains are mapped to nearby GPUs, prioritizing proximity and direct network links. To optimize memory bandwidth, each process is pinned to a separate CPU core, evenly distributed across the 8 L3 caches (2 processes per cache) and 4 NUMA nodes. Finally, MPI processes are paired with their closest GPU for optimal host-device memory transfers."

11. Please re-consider the performance analysis in light of the fact that with MG the GPU occupancy decreases at coarse levels, and if this can explain some of the observations.

It is possible that the low occupancy rate at coarse levels explains the behavior of the MG solver. However, we can note that the occupancy per GPU is fixed when the number of GPUs remains unchanged, but that the solver performance decreases if the number of CPUs is increased. Other phenomena (MPI performance, compiler optimizations, software stack...) could probably explain what is going on and are not easy to differentiate. As a result, we believe it is difficult to determine with any certainty the reasons for what is observed.

12. Finally, in other fluid dynamics domains, direct FFT-based solvers (i.e., FFT factorization along two directions, and Gauss elimination along the last one) show 3x to 100x speed-up compared to multi-grid approaches. While their communication patterns are more complex, their fast performance and good GPU utilization make them quite attractive for GPU-based systems. This goes a bit in contrast with the present observations, though the baseline FFT-based solver is not direct here. I would recommend putting this work in perspective w.r.t. other efforts in the literature that have made similar comparisons.

See our response to comment 6 where several papers are cited on the scalability of FFT-based and MG solvers on exascale systems.

Feel free to contact me directly if something is unclear at P.SimoesCosta@tudelft.nl. Your comments are very clear. Thanks again for your time.

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