gmd-2024-117 – Reply to referee #2

Dear referee #2,

Thank you for your supportive review. Please find our replies to your comments below. Your original comments are repeated in italics, our replies – for easier reading –in blue, normal font, and text passages which we included in the manuscript are in bold.

Kerkweg et al. describe in their study the new basemodel DWARF, which is implemented in the MESSy infrastructure. DWARF is a simplified basemodel, which comprises the elementary contents of a basemodel. For example, DWARF defines a model grid, implements a time control (including the possibility of reruns), specifies the type of parallelization and data transfer (MPI) and give the possibility to create and initialize base variables. This makes it possible to perform simplified MESSy model simulations using DWARF as a basemodel instead of more comprehensive and time consuming GCMs such as ECHAM5, COSMO or ICON.

This has advantages for tasks, where the use of the comprehensive legacy base models lead to poor performance and at the same time not all the content of the used base model is required. For example the use of DWARF is for example, as the authors describe, useful in the case of porting of a small set of submodels to a new HPC architectures, for example to a GPU system, or in the case that you want only investigate local processes in a box or in a column.

The authors describe in their paper first the general infrastructure of MESSy and its workflow, also going into more detail on the MESSy submodels that are directly involved in this infrastructure. Then they present the technical realization and the design concept of DWARF and at the end the paper is completed with four application examples using DWARF.

In my opinion, the paper is very interesting and I can highly recommend it for publication. I think it's very good that the general infrastructure of MESSy is described first, and I see this as an added value of the paper, as it really helps to understand how the basemodel DWARF can be combined with MESSy and how it has to be set up. The description of the DWARF basemodel itself and how it works is comprehensively explained and understandable and therefore very useful if you want to use DWARF. I also think that the examples of what can you do with DWARF are sufficient and illustrate very nicely how DWARF can be used effectively.

Therefore I think that the paper is of great scientific importance and significance. Moreover it is written clearly and has a reasonable and understandable structure, language and figures. In my opinion the paper is already in an almost finished state. The paper complies with GMD guidelines and is fully suitable for publication in this journal.

Thank you very much for this positive assessment of our work!

Remarks/Suggestions: A general comment from me concerns the abstract. I think it has partly more the form of an introduction. It refers very strongly to MESSy and in my eyes to less to DWARF itself. It should be underlined what advantages there are to use this new DWARF basemodel and to make the reader more curious to read the paper.

Specifically, I would shorten the description of MESSy in the abstract, make the description of DWARF more detailed, indicate which examples are discussed in the paper, and do a bit more advertising for the DWARF tool as a new useful and good application.

As suggested, we shortened the original abstract and added more details about DWARF to it:

Adaptation of Earth system model (ESM) codes to modern computing architectures is challenging, as ESMs consist of a multitude of different components. Historically grown and developed by scientists rather than software engineers, the codes of the individual components are often interwoven, making the optimisation of the ESMs rather challenging, if not impossible. Thus, in the last years the codes became increasingly modularised and with that, different components are disentangled from each other. This helps porting the code section by section to modern computing architectures, e.g. to GPUs.

Since more than 20 years, the modularisation is the fundamental concept of the Modular Earth Submodel System (MESSy). It is an integrated framework providing data structures and methods to build comprehensive ESMs from individual components. Each component, e.g., a cloud

microphysical scheme, dry deposition of trace gases, or diagnostic tools, as output along satellite orbits, is coded as an individual, so-called submodel. Each submodel is connected via the MESSy infrastructure with all other components, together forming a comprehensive model system. MESSy was mainly developed for research in atmospheric chemistry, and so far it is always connected to a dynamical (climate or weather forecast) model, what we call basemodel. The basemodel is a development outside the MESSy framework. Running a full dynamical model for technical tests when porting only one submodel is a tedious task and unnecessarily resource consuming. Therefore, we developed the so-called MESSy DWARF, a simplified basemodel based on the MESSy infrastructure. We implemented the definition of a very simple grid, parallelisation scheme, and a time control to replace a fully-fledged basemodel.

The MESSy DWARF serves as a valuable tool for technical applications, such as porting individual component implementations to GPUs and performance tests, or as easy test environment for process implementations. Due to the MESSy structure, the applied components can be used in a dynamical model without any changes, because the interface is exactly the same. Furthermore, the MESSy DWARF is suited for scientific purposes running simplified models (with only a selection of components), e.g., a chemical box model for the analysis of chamber experiments, or a trajectory box model imitating an air parcel rising slowly into the stratosphere. Column and plume models could also easily be build based on the DWARF.

In this article we introduce the technical setup of the MESSy DWARF and show four example applications: (1) a simple application using a component calculating orbital parameters, (2) a chemical kinetics model including photolysis frequencies calculation, (3) an application of a chemical box model, and (4) some details on a GPU performance test of the chemical kinetics model.

In total the paper is already in very good condition. I personally have found very few mistakes:
Line 8: "Since" → "For"

Done

Line 80: "asf". Personally, I wouldn't use the abbreviation etc. as it's not necessarily familiar, but maybe I'm wrong.

Changed to etc.

Line 120: Would you also consider nudging data as boundary data? If not, I would also mention it here.

Yes, in our understanding nudging data is also some kind of boundary data. To clarify this, we added it in this sentence:
The basemodel data itself separates into (i) initial and boundary data (including nudging data) and (ii) basemodel variables.

Line 211: ",as no basemodel is providing any data," → "as no data is provided to DWARF from another base model,"

We do not agree with the suggested re-wording, as DWARF also means the basemodel itself. We chose the following rephrasing to make it clearer:
The first category is not available in the MESSy DWARF, as in the DWARF set-up there is no data-providing basemodel, i.e., the DWARF is completely driven by imported data. The second category is available from the DWARF.

Line 231: "Figure 5" → "Fig. 5"

The GMD guideline (`https://www.geoscientific-model-development.net/submission.html`) states the following: "The abbreviation "Fig." should be used when it appears in running text and should be followed by a number unless it comes at the beginning of a sentence, e.g.: "The results are depicted in Fig. 5. Figure 9 reveals that..."." . Therefore we keep Figure 5 ...

*Table 3: In Orbit1 and Orbit2 you have mgpcol=83 and dlat=2, with a start point of -70°N the last grid box would be at -70+(83*2)=96, that means at 96°N . . . Is that intentional?*

No. Thanks for spotting this. We re-run the simulation with 71 grid boxes for the latitude and changed the paper accordingly.

Fig.7: "0°E, 60°S" →"0°E, 40°S" (red solid line)

Thanks for spotting this. We corrected it.

Line 281: "Figure 7" → "Fig. 7"

Same as for Figure 5 above.

Fig.8: "... 10 minutes after model start." → "10 minutes after model start (1.6.1998)."

Date added.

Line 300: "... to the defined grid." → "... to the defined grid (from 30°N to 51.5°N and 15°W to 16.5°E)."

We added the requested information.

Line 302: "Figure 8" → "Fig. 8"

Kept. Reason see above

Line 305: "profiles" → "fields" ?

Changed.

Line 306: "... these profiles ..." → "... these temperature, pressure and humidity fields ...". For better clarification (only a suggestion) ...

Done. This will also clarify one remark by referee # 3.

Fig. 9: 1) "Profiles at three ..." → "Ozone profiles at three ..."

Done.

2) "... at model start (left) ..." → "... at model start (0 UTC, 1.6.1998, left)"

Changed.

Fig. 9 (panel top left): "O3 initial profile" → "O3 initial profile (0 UTC)"

Changed.

Fig. 9 (panel top right): Is this really the difference between init – 12 UTC, or vice versa? I would rather expect the latter.

You are right. Thanks for spotting this. We changed the annotation accordingly.

Line 317: "of O1D" → "of O1D $(O3 + hv \rightarrow O(1D) + O2)$

Added.

Line 352ff: I would suggest (but it´s only a suggestion): "The higher the photolysis frequencies are, the faster ozone decrease (J(O1D)), OH increase (O(1D) + H2O → 2OH), H2O2 increase (2HO2 → H2O2 + O2), methane decrease (CH4 + O(1D)), and HNO3 increase (NO2 + OH → HNO3)."

Thanks for the suggestion. We changed it to

The higher the photolysis frequencies are, the faster

- **ozone decreases (mainly due to** $O_3 + h\nu \rightarrow O(^1D) + O_2$ **),**
- **OH increases (mainly driven by** $O(^1D) + H_2O \rightarrow 2OH$ **),**
- H_2O_2 **increases (mainly due to** $2HO_2 \rightarrow H_2O_2 + O_2$ **),**
- **methane decreases (mainly driven by** $CH_4 + OH \rightarrow CH_3 + H_2O$ **), and**
- HNO_3 **increases (mainly due to** $NO_2 + OH \rightarrow HNO_3$ **).**

Fig.11./Tab.5: There is something wrong. Corresponding to the panels in Fig.11 in the redline case OH is emitted at 12 UTC, and NO at 14 UTC, and in the blackline case OH at 14 UTC and NO at 12 UTC. But in Tab.5 and in the legend of Fig. 11 the corresponding times are reversed.

Thanks for discovering this mistake. We corrected the table and the legend accordingly.

Line 367: "HNO3 can only be build, ..." → "HNO3 can only be build (NO2 + OH → HNO3),..."

Reaction added as suggested.

Line 381: "even better performance (greater speedup) on GPU" → "even better speedup on GPU". In my opinion MOM shows a better speedup, but not a better performance (because MIM is still faster).

"even better performance (greater speedup) on GPU" Changed to "greater speedup on GPU"

Line 386: "Tab. 66 ". I find this 6 as exponent from 6 confusing. Maybe you can change that somehow.

We moved the footnote to "run times" to avoid this confusion.

Line 401: "https://www.nat-esm.de/" → https://www.nat-esm.de

Slash was removed.

Line 410: "... is already in use ..." →"... is also used ..."

Changed.

Line 422: "https://dlr-amr.github.io/t8code/ " → "https://dlr-amr.github.io/t8code "

Slash was removed.