Review of manuscript gmd-2024-30

June, 22, 2024

Title: NeuralMie (v1.0): An Aerosol Optics Emulator.
Reference: gmd-2024-30

General review

Topic: The manuscript describes the development of NeuralMie tool, an aerosol optics emulator based on machine learning methods, specifically neural networks that uses TensorFlow as its main external library. The manuscript also discusses the future implementation as part of E3SM, but the applications of the presented tool are not limited to the original one. The reviewers have had access to the code and data used to create this tool.

Overview: The manuscript content fits well within the scope of the journal Geoscientific Model Developments, and the tool described may be beneficial for other projects in the context of climate and atmospheric modelling.

Evaluation: The manuscript is well written: the scientific questions are properly explained and the model/method is reasonable. The main core of the article, which I understand is the NeuralMie tool, is interesting, and potentially useful (beyond the initial motivation of the authors are part of E3SM), for the community of scientists that implements optical properties of aerosols in climate models and for this reason I recommend **to accept the paper with minor comments** that I will explain in the review.

1 Main review

Here it is included a short evaluation of general points of the research presented:

Key results In my opinion, the key result is the NeuralMie tool and its development, while the TAMie is more a step of the development than a novelty in this research field.

Validity The full process of developing and implementing the tool is provided in sufficient detail to meet strict reproducibility requirements. The code/datasets are provided to reviewers and along the manuscript new developed tools compared well with established/checked tools. Therefore, it is expected that results are valid. Note however that the code is not provided with any help to reviewers to be executed (README or make files).

Originality The originality of the research is acceptable. There are earlier *emulators*, but the authors adequately justify the advantages of NeuralMie over current alternatives. However, I am a bit skeptical of the TAMie tool as a novelty; nevertheless, presented as part of the NeuralMie development process, it is reasonable to include it either in the main manuscript or in the typical supporting paper.

Review data & methodology The data set used (created) and the methodology are well described in sufficient detail, and the process followed by the authors is easy to follow. The evaluation on the performance of TAMie still depends in part on how (and with what) the comparison is made, but I consider these evaluations reasonable, and in any case not critical to this research. I do not evaluate the code provided here.

Figures/Tables The selection and quality of the figures and tables is also good, although probably the results of Table 2 need more information (name and optimization flags of the compiler used).

Discussion From my point of view, the discussion is reasonable and well organized. I appreciate that the authors describe the limitations of their new tool and the challenges of its application (these are the first steps for future improvements). However, the terminology is sometimes a bit confusing. For example, NeuralMie claims to be as accurate as a pure Mie calculation, but in other sentences it is described as "a significant improvement in accuracy". Although it is possible to understand what the authors mean from the context, perhaps they could consider alternative terminology for the first (or second) context just to add more clarity for readers not expert in aerosol modeling. Alternatively, a few words to specify the two contexts of "accuracy" may be helpful.

Code/Datasets The quality of presentation is good if we omit an evaluation of the source code in the review. As I commented, the source code (and datasets) doesn't have any typical README file, a simple make-file or script to help reviewers analyze/use the tool, nor any file describing the future licensing of the software.

Specific comments

- **Abstract** The authors comment: "This work introduces two new contributions to enable a more accurate representation of aerosol optics in atmospheric models. Enable a more accurate representation of aerosol optics in atmospheric models." However, it appears that TAMie has only been introduced to provide a faster Python-based standard Mie code, so it does not allow for a more accurate representation. In fact, TAMie is later described as being comparable in accuracy to the established Mie codes. Therefore, it seems a bit inconsistent.
- **Abstract** The authors mention: "incurring a negligible error". Usually the adjective of an error (negligible, large, small...) depends on the application. If for example the code is used to calculate by "brute force" to guess the refractive index from a given set of bulk optical parameters, the error may be more relevant. I agree that 0.08% is a fairly small error, but I usually give the user the responsibility to judge any error rating according to their application requirements. It is up to the authors to keep "negligible" or not in the summary, but my view is that "negligible" is for the user of the tool to decide.
- **Introduction** The introduction is reasonable for the scope of their manuscript, still here I include few comments. It is the final decision of the authors to take them or not in account (no requirement on my side).
- **[Line 22-23]** *"Recently, machine learning (ML), and neural networks in particular, have emerged as powerful tools for developing new, more accurate, faster, and more capable, physics parameterizations for atmosphere modeling."* This is an strong statement and probably a large number of modelers would say that ML methods could provide a more accurate or more capable parametrization but not always. Also the statement says everything at the same time: accurate, faster and capable. Is this really so general?
- **[Line 24-26]** *"Conventional parameterizations typically take the form of simplified hand-derived physical models, basic statistical models like lookup tables and linear regressions, and sometimes simply rely on expert heuristics to make decisions about the behaviour of a system."* Again I don't think that this is general, and for sure there is not a full agreement in the research community about this statement. A key set of physical parametrization are derived from fundamental physics and chemistry theories. Just two examples (but there are more): many relations of (cloud) microphysics are derived from Molecular Physics and Thermodynamics, also radiative transfer parametrization are not basic statistical models, lookup tables, linear regressions, expert heuristics or simplified hand-derived physical models (despite specific assumptions/datasets used in current radiative transfer schemes could be improved using ML methods)
- **[Line 29-31]** Do the authors think that everything is positive about the use of ML emulators here, or there are some trade-off to consider that could be worth to mention?
- **[Line 41-43]** Just note that several climate models have aerosols that are not coated aerosols but an internal mixture of an aerosols with inclusions of other species. They usually redefine the refractive index using Maxwell Garnett mixing rule [2]
- **[Line 70-75]** Here, I would be cautious, although the authors' evaluations are reasonable. First, the comparison has been done with two specific Fortran Mie codes. Numba probably is correctly setting the best performance for the LVVM tool chain for the TAMie.py code, but this comparison would need to be sure that the optimization flags of the compiler are optimal for the comparison. The performance improvement of TAMie.py with respect to PyMieScatt code is remarkable even without the use of Numba. The general value of PyMieScatt more than speed is the flexibility of their API and very good documentation, two aspects that are not present in TAMie code.
- **Sections 2. to 3.2** In this sections the authors implement Mie scattering methods in a Python tool called TAMie.py, since the definitions and equations are standard and well known, and the

presentation is straightforward I see no need for any changes in these sections since the authors have been clear on the origin and references for these definitions/equations.

- **Table 2**, as I already commented, would be good to be specific of the Fortran compiler and the optimization flags used to have a more robust performance comparison. On the other side, in drawing conclusions from Table 2, I think it should be remembered that the performance is comparable "to these Fortran codes" and is an improvement over Python's PyMieScatt code. Probably, the conclusions are fairly general, but with the evidence provided the readers cannot be sure if there is other Fortran/C code better optimized than those used in the comparison (in particular the Fortran codes used seems to be for the references at least two or three decades old). For the authors information, and thinking in future developments there a project that collects Mie codes: List of Mie codes.
- **Equation (20) and the discussion in lines [238-240]** There are modal aerosols where include internally and externally mixture of aerosols. If this something considered when the NeuralMie was developed?
- **Figure 2**. These are interesting results to undertand how increase the complexity of the model it not always improving the accuracy. Still in the case of the core-shell it seems to have an asymtopic decay. In this figure if the two branches have an structural difference they can be represented with different colors. If I understand well this figure is specific of k_e because the Table 6 gives for it the higher errors. However, it the authors have results analogous to Figure 2 for the other parameters ω and $\bar{g}$ are they similar?

Final Comment

As the authors correctly explain, "the main limitations are not necessarily specific to the machine learning model and originate from simplifying assumptions about particle shapes and particle size distributions". This means that the practical improvements provided by the NeuralMie emulator still have the limitations due to the assumptions of the Mie solution (spherical and homogeneously coated particles). One implication is that comparison with observations will remain a challenge, as the emulator provides higher resolution in the parameters with the Mie approximation is based on, but is still using an approximation that has varying degrees of accuracy to represent each type of actual observed aerosols. Even in this case, to the extent that the refractive index estimated from observations is based on inverse methods using the Mie scattering approximation, it seems to me that the emulator may have practical utility.

But possibly the most immediate utility is its application to model comparison. If we look at the results on aerosol diversity *mass extinction efficiency* between climate models, specifically with respect to mineral dust, see reference [1], the use of these emulators may provide additional information that explains or helps to better trend these differences, as still most of them are based on Mie calculations.

As far as the code is concerned, I have not carried out an exhaustive review. For this, a README would be necessary/useful, possibly accompanied by make files. I also recommend to always include a file called LICENSE with the chosen licence and the name of the authors/institution. In a practical way, more detailed headers can also increase the usability and recognition of the code in other projects, even for relatively simple code such as TAMie.py core-suite (about 200 lines).

References

[1] R. Checa-Garcia et al. "Evaluation of natural aerosols in CRESCENDO Earth system models (ESMs): mineral dust". In: *Atmospheric Chemistry and Physics* 21.13 (2021), pp. 10295–10335. DOI: 10.5194/acp-21-10295-2021. URL: https://acp.copernicus.org/articles/21/10295/2021/.

[2] M. Sand et al. “Aerosol absorption in global models from AeroCom phase III”. In: *Atmospheric Chemistry and Physics* 21.20 (2021), pp. 15929–15947. DOI: 10.5194/acp-21-15929-2021. URL: https://acp.copernicus.org/articles/21/15929/2021/.