

Dear Andrew,  
Dear reviewers,

please find our detailed answers to the referees' letters below.

### **General remarks:**

1. In this text, we used boldface for our answers and italics for the reviewers' original comments.
2. Line numbers refer to the included revised document.
3. As suggested by the second reviewer, we have used professional language editing support for this revision. Thus, the provided latex-diff document includes also many changes resulting from this process.
4. Figure/Table numbering: We experienced problems with figure and table numbering: After adding an appendix, we received the latex compilation error

! LaTeX Error: Too many unprocessed floats.

Using the `\clearpage` command, the figure numbering is wrong (starting from Fig. 21 etc.). Alternative would be not to use the „`\appendix`“ command. This has to be sorted out with the copernicus publishers.



### **Referee #1:**

*This is a review of the second version of the manuscript : “Metos3D: A Marine Ecosystem Toolkit for Optimization and Simulation in 3-D – Simulation Package v0.3.2” by Piwonski and Slawig.*

*The manuscript has certainly improved from the previous version, the objectives are now outlined and it clearly transpires the effort made by the authors to improve its structure and readability. However, in its present form this manuscript is not ready yet for publication in GMD until further moderate changes are made to the text to eliminate most of the residual confusion. As a general comment, I think the lack of coherence in the terminology used throughout the paper is the reason of the “fugacity” of the main message that I have perceived. In other words, I think that if the authors try to call things the same way throughout the text, after having clearly defined them (if possible) things would improve significantly.*

*Finally, I would like to call the attention of the authors to something that would have made this reviewer's task much easier at little cost. The font chosen for the document where the answers to the reviewer's comments are reported is an incredibly poor one. This, together with the plain editing of the text made reading such document nothing short of painful. Latex is great but sometimes a more popular text editor can do wonders when it comes to*

highlighting text, using bold font etc etc; all things usually appreciated for these types of documents. Below are some comments and suggestions:

Main points:

-Section 1, page 1, lines 64-66. Here three strategies used to accelerate the computation of steady-state are mentioned as they are put together in Metos3D. I was expecting later in the text to find somehow a tighter correspondence to this outline in the organization of the sections/subsections but the correspondence wasn't always obvious to me. Again, I think it could all be explained in a much more linear way when the terminology is well-defined in the introduction and it is used in a coherent way throughout the text.

**We think that the ordering of the Sections 3. Off-line simulation, 4. Steady annual cycles (containing Newton method) and 5. Software description (containing spatial parallelization) corresponds now better to the outline in the introduction.**

For example: it wasn't obvious what you were comparing Metos3D with in Section 7.4. Here you use the expression : "parallel performance of the TMM" but you never explain what you exactly mean by it.

**Here scalability is meant, which is now mentioned explicitly, see line 748.**

I am familiar with the TMM and it took a while to me to understand that you were comparing Metos3D with the implementation provided by Khatiwala together with the transport matrices you use here. In the Introduction you briefly describe this comparison at lines 133-136 where you use the expression : "the one used in Khatiwala (2013)". Here is where you should assign to "the one used in Khatiwala (2013)" a name and stick to it in the rest of the manuscript.

**The name „TMM framework“ has been introduced for this purpose now, see line 82.**

-Section 6.1. It is an improvement from the previous version. The use of the schematic in Figure 1 (note that numbering of the figures start from 11) ...

**Figure numbering: see above.**

... helps to follow the description of the implementation however, the terminology used in this section does not correspond with that used in the figure. For example, at lines 470 and 472, the words "debug" and "utilization" are used in italics and are actually called "layers" however there's no trace of them in the Figure. In general, as a suggestion , I would simplify the description, try to outline the main message of this section and leave the details for the appendix.

**Section 5.1 has been renamed and rewritten. We replaced the old schematic figure by two new ones showing the software layers (Figure 21) and the call graph (Figure 22). See lines 420 ff.**

-Section 6.3 concerns only the interpolation of the transport matrices so it should be specified

*in the title. Alternatively, you could group all the following parts concerning interpolation under this section. For example Section 6.4 lines 555-569. Also Section 6.5 seems like it could be merged (and shortened with Section 6.3.*

**As suggested, we merged all text passages regarding interpolation into one ,Interpolation' section. See lines 550 ff.**

*-Section 7.3. This part of the analysis is very interesting and very useful for model developers however, I believe it would be useful to present results also in terms of the incremental computing time per tracer vs number of tracers.*

**We agree. However, we would like to perform a more detailed analysis in this regard. Unfortunately, we don't have results by now. If desired we will include them in the final version.**



*Minor comments:*

*-Introduction, page 1, lines 45-50. These two sentences are incomprehensible to me. I don't understand what is "its intended (intended in the text) later usage", perhaps try to be more explicit. What does it mean "and mentioned in the name of" ? It seems like this bit of text got lost in there somehow. Rephrase all this part with a clear structure.*

**Has been reformulated. See lines 47-54.**

*-Introduction, page 2, line 105. "Except for the latter....." what latter?*

**We reformulated this passage and made clear it refers to a load-balancing algorithm. See line 110.**

*-Section 5, line 430. Maybe you mean "current" instead of "actual"?*

**We changed it to ,common', see line 527.**

*-Section 6.3, lines 528-535. How is this different from what is commonly done (I guess in the Khatiwala implementation) ? Maybe try to explain (explicitly) how this procedure is different from the common practice and why is preferred.*

**In general, it is the same what is done in the TMM framework. We just thought it is worth mentioning here as in the TMM references it is not.**



*-Be careful with the order of the Figures as they are mentioned in the text, for example, at line 728 you mention Figure 19 before Figures 14 and 15.*

**The figures are in the right order now.**

*-Section 6.4, lines 570-579. Why are there two different "data alignments" ? I could not figure out what you mean here. Maybe this should have resulted clear from the previous sections but it did not so this paragraph sounds like coming out of nowhere to me. Also in this paragraph you mention the "software utilization layer" of which there is no trace in Figure 1.*

**We added a new Section 5.2 ,Geometry information and data alignment ', which**

**makes this clearer now. See lines 448 ff.**



*-Section 7.1.1, lines 653-668. This part looks like it could go in the Appendix or directly in the instructions.*

**Yes. It is part of the Appendix now, see lines 967 ff.**

*-Section 7.2, lines 738-744. Mind to elaborate a little bit further on the cause of those peaks? We did, see lines 673 ff.*

*-Section 7.4, lines 841-842. You should explain clearly here what you mean by theoretical efficiency.*

**This refers to an idealized hardware, see line 780 ff.**



*-Lines 978-980. This sentence is not clear. Consider rewording.*

**The whole passage has been rephrased, see line 917 ff.**

## **Referee #2:**

*The authors have without doubt clarified and improved the general focus of the paper, I welcome the omission of the somewhat pre-mature optimisation section and in particular the analysis involving a suite of biogeochemical models is a nice addition.*

*However, while I think the contents are generally adequate, the manuscript is still lacking significantly in terms of clarity and precision. I have the feeling that this is partly due to short-comings in English language and grammar, which may be sorted by language editing support, but it is also due to a somewhat careless effort in elaborating and revisiting the text, which at this point of the submission process is a little concerning, so in its current form I cannot recommend the work for publication in Geoscientific Model Development. I can only re-iterate my final comments in this respect in the previous review step.*

*In the following I give some examples of my concerns (all line numbers refer to the manuscript version with track changes in the authors response):*

*I believe the title of the work is inadequate: even if optimisation is the ultimate goal, the work does not currently include it, so the title is misleading.*



**We have designed and implemented a software system that is able to simulate and optimize marine ecosystem models coupled to ocean transport. We assigned the name Metos3D to this system. The name was chosen to reflect its final purpose. As mentioned in lines 47-54, a prerequisite for optimization is simulation. Since the description of the simulation package that is the topic of this work obviously already fills a whole paper, we decided to present the optimization package separately. Here, we followed the recommendations of the reviewers of the first submission. Thus we think that the title of the paper exactly reflects this situation.**



*Throughout the main body of the text it appears that all states were treated equally in the analysis, while from some figures and the model descriptions in the appendix it appears that only or mainly inorganic phosphate was considered. This should be clarified.*

**We added information on the regarded tracer variable in each figure caption. Otherwise all states are treated equally, which has been made clear in Section 3, see lines 206 ff..**

*Lines 29 following: State explicitly first that the tool has been tested with 6 biogeochemical models.*

**Done, see line 11.**

*Line 87: I can see that the effort increases, but why would it get more complex?*

**Changed to computational complexity, see line 58.**

*Line 132-135: language*

**We rephrased the paragraph, see lines 100 ff.**



*Line 144: versions of what?*

**Versions of load balancing algorithms. See lines 106 ff.**

*Line 145: it's not clear to me what the latter refers to*

**We reformulated this passage and made clear it refers to a load-balancing algorithm. See lines 110 ff.**

*Line 172: is->are*

**Corrected.**

*Section 2 is a brief mathematical description of the pdes of the coupled system, but not a description of marine ecosystem dynamics. Title of the section needs changing.*

**We changed the section title to „Model equations for marine ecosystems“ see line 156**

*Line 265: While I accept that the overall application of the Neumann condition is good enough in the context of testing this software package, for a realistic implementation of a steady state solution of the annual cycle of marine biogeochemistry, I'm not sure how reasonable a general Neumann condition is. I would have thought that atmospheric deposition of nutrients and riverine discharges have a role here.*

**The corresponding paragraph has been extended to describe how this (and also Dirichlet b.c.) can be handled, see lines 193 ff.**

*Line 274 Kappa is diffusivity, not diffusion, diffusion is the process described by the full term.*

**Corrected. See line 209.**

*Lines 185 following: the 128 appears as a general rule here, while I'd expect it to depend on the number of grid points and the strategy of parallelization, which restricted to horizontal domain decomposition. Also it's anticipating results and shouldn't be placed in the introduction.*

**We omitted the number of processes. See line 139.**

*Eq. 4: what is z?*

**It is an arbitrary vector in  $R^{n_y n_x}$ . This is stated at line 293.**

*Line 404: other*

**Corrected. See line 299.**

*Line 406: "are equivalent with": I suspect what is meant is that all norms fulfill that condition? Equivalent is a different thing.*

**We refer to the mathematical definition of norm equivalence. We changed the sentence. See lines 299 ff.**

*Line 520: which number?*

**The number of inner iterations. We rephrased the sentence. See lines 387 ff.**

*Lines 555-556: Unclear what is meant by this sentence, I'd drop it.*

**Dropped.**

*Line 565: nx I suppose?*

**Yes. Corrected.**

*Line 744-756: I can't find any if the following represented in the figure it refers too up to Lin 754? E.g. what is the bottom layer, what is it's role within the software package?*

**Section 5.1 has been renamed and rewritten. We replaced the old schematic figure by two new ones showing the software layers (Figure 21) and the call graph (Figure 22). See lines 420 ff.**

*Line 784 it's not true that it can't be split, but that would require message passing between processes.*

**Corrected. See lines 601 ff.**

*Line 788-790 not clear what's meant by its mid in relation to the vector length and how that is used for balancing then?*

**We reformulated the text. See lines 612 ff.**

*Line 849 following: sounds like a lot of memory operations to reorganise the data structure in the memory space. Should be possible to avoid this using pointers.*

**To our knowledge, this is not possible. If you define a Fortran routine like**

```

subroutine sub(nz, n, y)
  integer :: nz, n
  real*8  :: y(nz, n)
  ...
end subroutine

```

**it is expected that y represents a contiguous piece of memory.**

*Lines 877-879 I don't think there's much value in as adding the code fragment here, there no added information with respect to the equation.*

**We are not sure to what this comment refers to. If it is Listing 1, i.e. the Fortran 95 implementation of the interface, we think it is valuable for the reader.**

*Lines 890 following: The analogy to the treatment of interpolation remains unclear here as that section doesn't mention any of those routines.*

**The interpolation section has been reorganized. See lines 550 ff.**

*Lines 919-921: This sounds more like the section would be a kind of step-through user guide, rather than a description of the software package as the rest of the text. In fact the rest of the section give a lot of details to enable reproduction of the results. This is great and very useful for interested readers, so I think it would be good to mention this in the introduction of the section rather than introducing it as a presentation of results. In fact there is no results in this section until pg 12. Might be worth splitting this into two sections to separate out the part with the actual results from the experiment description.*

**The experimental setup is now part of the Appendix. See lines 962 ff.**

*Line 925 "original implementation" is a bit misleading here as it may sound as it would be an original part of this work, while it was rather introduced in the paper cited shortly afterwards (Dutkiewicz 2005). I'd suggest to drop the "original"*

**„Original“ refers to the implementation that is provided together with the MITgcm and that is used here.**



*Line 976 "filled in", does that mean it has been set to land?  
If so it would be interesting to state the reasoning of this choice.*

**Yes. This originates in the data provided by Khatiwala.**



*Lines 980-983: What is the relevance of these volumes?*

**They are used to compute a weighted norm. We dropped them here and used them to compare the solution of spin-up and Newton (cf. Section 6.1 line 658 and Table 29).**

*Lines 1038-1040: Looking at the figure, I don't understand what the phrase "We observe that the solutions converge to the same difference in between consecutive iterations." means?*

**This was reformulated. See line 656.**

Table 16: What is the difference between the two columns, i.e. that does the V stand for?  
**It stands for volume. This has been added to the figure caption.**

Figures 110,111,... what happened to the figure numbering?  
**See remark at the beginning.**

Figures 19 and similar: the states used in the formula of the norm are not normalised as far as I can see, so what are the states and units we are looking at in the norm? Is this just phosphate? Is it all states? If it is all, shouldn't there be different weights between different states?

**It is phosphate only and the units are mmol P/m<sup>3</sup>. We added this information in each caption.**

Line 790: Figures 117-115?  
**The figures are in the right order now.**

Lines 1132-1134: It is unclear to me how the Sievertsen work has impacted the profiling capacity in this work.

**This seems to be a misunderstanding. The passage has been rephrased. See lines 738 ff.**



Lines 1143-1147: Does the TMM use the same boundary and initial conditions and time steps? I suppose so, but it might be worth mentioning it.

**Yes, the configuration is the same. We added this information. See lines 748 ff.**

Lines 1165-1166: "Here, we use the given output, which is the timing for the whole run. Overall, for the calculation of the speed-up and efficiency results we use the minimum timings for a specific number of cores." Not clear to me.

**Rephrased. See lines 758 ff.**

Line 1185 How is the theoretical speed-up computed?

**We reformulated the text. See lines 779 ff.**

Lines 13002-1312 I don't understand the "On one hand ..., on the other hand..." here, isn't the point simply that the implementation of different biogeochemical models underlines the flexibility and generality of the interface?

**Rephrased. See lines 859 ff.**

Lines 1444-1447: meaning of "whose" is unclear.

**The sentence has been omitted and the paragraph has been rephrased. See lines 911 ff.**

Lines 1485: Not sure what is meant by the investment in the simulation itself.



## **Dropped.**

*A1.1 and A1.2: The formulation that phytoplankton is treated "implicitly" in these models is misleading, when it is actual a free model input parameter and should be treated as such (particularly with view on optimisation!).*

**We added a remark here and also to the description of the NP-DOP model.**

**However, we sticked to the used formulation to be consistent with Kriest et al (2010). See lines 1061 ff.**