Comment on gmd-2021-392
Anonymous Referee #2

Referee comment on "Adaptive time step algorithms for the simulation of marine ecosystem models using the transport matrix method implementation Metos3D (v0.5.0)" by Markus Pfeil and Thomas Slawig, Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2021-392-RC2, 2022

First, I have not read the other reviews, so my opinion is given independently.

This manuscript presents novel algorithms for adapting the time step in biogeochemical models driven by the Transport Matrix Method (TMM). The authors present 3 different ways of controlling the time step, and show that while Algorithms 1 and 3 can potentially speed up the spin-up of the biogeochemical models in some (but not all cases), Algorithm 2 generally does not. This work seems worthy of publication after some moderate revisions and further critical evaluation of how well each method works. Some aspects of the data presentation and writing could also be improved.

General Comments

It is striking that the step size control method (Algorithm 1) does not actually do much continuous adjustment of the time step most of the time. While the authors go to great lengths to enable the time step to change responsively, in reality the step size quickly expands out to 32x the original time step, or it stays anchored at 1x the original time step. The adjustment happens very early in the simulations, meaning that for most of the 10,000 years the algorithm simply creates more overhead for the simulation without any additional benefit. This suggests that the whole process of finding the right time step could be restricted to an appropriate initiation period (perhaps 100 years, or whatever minimum envelope is needed), after which the time step is held fixed.
On a related note, I thought the design of the Algorithm 1 could be significantly improved by only running the error checks on a subset of time steps (not every single time step). Presently, the steps 11 and 12 are computed for every time step of the simulation to verify the accuracy of the chosen delta T. This error check could easily be made on a subset of timesteps. Perhaps on every 10th time step, an error check could be run, or if there needs to be a continuous block of time steps, only do this for a limited window at periodic intervals. It seems wasteful to me to run the error check on every time step, when most of the time it will have no influence.

Algorithm 3 appears to have the most utility, since it clearly saves time in the spin-up, and achieves a reasonable approximation to the reference case (correct me if I’ve got that wrong). Algorithm 2 fails because it appears to me that the exclusion of negative tracers is too stringent a condition. The authors mention that negative tracer concentrations sometimes occur in the reference case… so this algorithm should be a non-starter, shouldn’t it?

Overall, I think there could be more critical evaluation in the discussion and conclusions as to which algorithms actually performed well, which are recommended or not, and why.

Line Comments

L36: “parallelization... lowers the computational effort”. Not really, it just speeds up the result. Parallelization results in more computational resources being used not less... the benefit is in human time.
L43-45: There are a lot of different time-saving methods listed here, but there is no evaluation of which methods are pertinent to the current study. I think there needs to be a discussion of why one needs an explicit time-stepping method for the present study. The Newton-Krylov method is briefly mentioned, but the authors don’t explain why they are not using that method (does it prevent the biogeochemistry models from working properly?)

L56: “ignoring and avoiding negative tracer concentrations”. I did not understand this sentence until I had read the whole manuscript. I think this should be rephrased for clarity, to state more simply that a step-size control method was implemented with and without a condition to exclude negative tracer concentrations.

L68: “Due to the fully coupling”. Grammatically this should be “full coupling”

L80-81: In these equations, the terms A, D, qi and dn are shown without any explanation (until later in the manuscript). These new terms should be briefly labelled here for clarify.

L84: You could write here: “advection (A) and diffusion (D)” to partially address the point above.

L84: “in marine water” sounds strange. Why not say “in the ocean”?

L98-99: “is called marine ecosystem model”. Here an article (“a” or “the”) is needed in front of “marine”

L109: “above equations”: please specify which equations you mean

L116: “refer to Kriest…”: I think you mean “refer the reader to Kriest…”

L151: “for the biogeochemistry tutorial”: this is confusing. What is “the biogeochemistry tutorial”? Do you mean this model was created for teaching purposes?

L152: “As the N-DOP model” -> “As in the…”
L171: Why have the equation numbers suddenly disappeared here?
L175-176: Equation numbers?

L188 and L190: Equation numbers?

There are many more examples where equation numbers are not included... this seems confusing to me.

L251: “Despite of such” -> “Despite such”

L245-257: This paragraph could use further discussion on why excluding negative concentrations is justified in the algorithm, given that negative values can occur in the reference case regardless of the accelerated time steps. On balance, it seems to me that this is a poor choice of criterion (the results are not good for Algorithm 2).

L284: I don’t understand the backslash here.

Figure 2: These 6 panels really need titles. It is cumbersome to have to refer backwards and forwards to the caption for the meaning of them.

Figure 3: As in Figure 2, the subplots need titles.

Table 3: I think an extra table, analogous to Table 3, should be added which shows the computational cost saving factor for each model, and the time step multiplication factor m at the end of the simulation.

L458: “Only in half of the simulation runs decreased the algorithm”: Grammar is wrong.

L460: “… applied the entire spin-up large time steps”: grammar is wrong.

L461-463: The sentence starting with “Although the algorithm...” is confusing to read. Please rephrase and clarify.
L466: “an reasonable”: typo

L492: “local error always needed two evaluations of the same time interval”: This highlights my general comment that the algorithm should not be checking the error every single time step.

L493-494: “Due to negative concentrations in the approximations, the algorithm then used nearly always the smallest time step.” This suggests to me that this algorithm should not be recommended in the future.

L515-524: Finishing the paper with a list of dot points is not a good way to conclude. Please rewrite this as a normal paragraph, or if you want to list these points like this, don’t make it the final statement of the paper.

P.S. Sorry for the delay in submitting my review.