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Interactive comment on “Metos3D: a marine ecosystem toolkit for optimization and simulation in 3-D – Simulation Package v0.2” by J. Piwonski and T. Slawig

Anonymous Referee #2

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This manuscript presents a steady state offline solver for marine biogeochemical models using two alternative approaches: a iterative procedure towards the fixed point solution or a Newtonian equation solver of the residual norm. While the subject of the work is generally relevant to the journal presenting a novel tool with a high potential for application in the scientific community, it falls short on a couple of important points that need addressing if it was to be considered for a full GMD publication. My main concern is the lack of clarity on what the purpose of the tool in its current state is and what it actually delivers. The abstract promotes it as a tool for parameter identification and a lot of the intrudctory and final discussion mention optimisation. However, it is not stated what is intended by parameter identification and how the tool would

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achieve it. I assume from the discussion that the intention of the authors is the identification of an optimal parameter set for a given biogeochemical model, while what the tool actually delivers is a periodic steady state solver for biogeochemical models using offline ocean physics. This can without doubt be a valuable element for a parameter optimisation toolkit, but is nevertheless only one element of it and moreover it doesn't address the core of the actual optimisation problem, e.g. what should a model be optimised against. In addition, it doesn't give a benchmark that would allow comparison against other optimisation tools. (The work does give some performance indications for the steady state solver, but no generalised performance indications for the optimisation process.) Moreover, the authors demonstrate themselves in their example that the application within the optimisation process is still premature. On this background, I would suggest to change the pitch of the manuscript towards what the tool actually does for (at least to my understanding), and what it actually delivers successfully and reliably, i.e. the periodic steady state solution of the biogeochemical model. I see no reason to limit the tool to a specific application in optimisation that is then treated only superficially and insufficiently if this is given as the main purpose of the tool. On the contrary I can see a series of other valuable applications to any form of large ensemble experiment and examples may be given in the discussions to highlight the utility of such a tool beyond optimisation. As a second point the manuscript lacks generally in clarity (some examples below) and requires a considerable review in grammar and style. For future submissions, I would strongly suggest the authors to review their manuscripts before initial submission on these terms (maybe with the help of a native speaker) as I believe a lot of the points given below could have been addressed in this process leading to a much more beneficial review. Reviewing the work in its current form required a considerable amount of assumptions of what was actually intended.

Some comments in detail:

pg 4402 line 2: what is intended with parameter identification? pg 4403 line 8: when talking about biogeochemical models and their validation in generic term, the obvious

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question concerning the estimation of an optimal model parametrisation beforehand, is what the model should be optimised against? I believe this will be highly application dependent. pg 4403 line 23: "acceptable loss of accuracy" involved in the splitting of ocean physics and biogeochemical processes: any references? pg 4404 line 4-10: I'd suggest to move this to the later section where residual and norm are introduced, it becomes much clearer then, particularly to modellers with a less numerical background. pg 4406, line 15: the dimensionless time "1" here refers to one intra-annual time step, while in the above section (lines 4,6) it refers to one periodic step, i.e. one year. These should be distinct by or using different variables for time within the annual cycle and in the iteration procedure, or by explicitly using time units. pg 4406, line 24 onwards: I'd suggest to introduce necessity for the split explicit and implicit treatment of physical processes first and then specify it's application to the offline solver in order to facilitate understanding for readers that are unfamiliar with the problem. pg 4407 eq 2, lines 16,17: difference between A and A' should be clarified. pg 4407 line 22 - pg4408, line 1: I'd expect the sufficient resolution of the tracer transport process on monthly time steps to be highly configuration and application dependent, rather than hold generically. pg 4408, lines 11-15: "Generally, we assume that a tracer model is implemented for a single water column, synonymously called profile in the following. This assumption does not constrain the interface for the future and, it actually simplifies the current software implementation." The interface to the biogeochemical models is the main point of the tool and being clear here is essential to encourage potential users. I'd suggest spending a couple of words here stating assumptions and limitations clearer, i.e. - any "client" model must be able to take-up its states from the interface in water column format. - no geometrical information on horizontal vicinity of the vertical profiles is preserved in the interface. - any model that requires horizontal structure in it's internal computation requires modification in the internals of the tool. I realise that the vast majority of biogeochemical models currently used will fulfill these requirements, but they should be explicit. pg 4409 eq 3, where have the indices y,k gone? pg 4409, last paragraph, what's the purpose of the initialisation and finalisation

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routines. pg 4410 lines 3,4: confusion in the use of 1 in the time dimension, see above
pg 4412 line 16: Why is the unweighted norm used? pg 4414 line 13 "repository of
the simulation package" pg 4414 line 23 "The next both layers" -> next two layers pg
4416 lines 12-15 "Thus, the matrices and vectors are linearly interpolated to the cur-
rent time step during the iteration. The files of a specific data set are interpreted as
averages of the time intervals they represent. Consequently, we interpolate in between
the associated centers of these intervals." If linear interpolation is used the result will
be non-conservative, which should be noted. pg 4416 line 25: how are the weights
alpha and beta determined, i.e. is this a linear interpolation? pg. 4419 lines 19-23:
so the effective state variables are two, all others are diagnostics? Should be made
clearer. pg. 4419, line25,26: what is the "introduced convention for directory struc-
ture"? pg. 4420 line 20: You may want to consider hosting the binary data outside
the git repository. pg. 4421 line 27: again, wouldn't this number be application and
configuration dependent? pg. 4423 line 27 ratio of what? pg. 4426 line 12 state the
origin of the reference solution and its purpose pg. 4427 lines 15-21 are unclear to
me. Maybe the figure would help, but unfortunately the labels are unreadable at this
scale. pg 4428 line 2 "intended purpose", what is the intended purpose? pg 4428 line
22 "was somehow "natural"" what's meant by this? pg 4428 line 28 "computationally
still too complex", I suppose the authors intend too expensive? pg 4429 line 3-6 I fail to
see why a suitable choice of the time step would have complicated the verification. pg
4429 lines 9-13 Here the authors clearly state that the solver tool in its current form fails
to deliver the intended purpose, i.e. parameter identification, see general comments
above. pg 4429 lines 20-21 what's the expected flexibility? pg 4429 lines 24-25 not a
sentence

Figures 3,4,6,7,8,9,10 are unreadable and require larger labels.

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