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Interactive comment on "Mechanistic site-based emulation of a global ocean biogeochemical model for parametric analysis and calibration" *by* J. C. P. Hemmings et al.

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1 General comments

In the study of Hemmings, Challenor, and Yool an array of one-dimensional (1D, vertically resolving) ecosystem models is used to emulate the dynamical behaviour of a three-dimensional (3D) global marine biogeochemical model, with same biological equations, at selected ocean locations.

Ideally, variations of parameter values of an ecosystem model would cause alterations in results of the 1D model version that would reflect one-to-one changes in correspond-

ing outcomes of the global 3D model at all local ocean sites. This way the local 1D ecosystem model could act as a perfect site-based emulator of local 3D model behaviour. Thus, if an optimum set of biological parameter values were found so that the 1D model results give a best fit to local data then the 3D model's fit to the same data would be alike (e.g. same maximum of same likelihood).

But these ideal conditions are impossible to accomplish. To run a 1D setup at any particular site requires results of the 3D model that are themselves sensitive to values chosen for parameters of the biological model component: 1) horizontal gradients of tracer concentrations and 2) vertical profiles to initialize tracers for 1D simulations. It means that for 1D simulations (with any particular set of parameter values) a corresponding output from the 3D simulation would also be needed, which would make the 1D model to act as an emulator superfluous.

The authors' idea is instead to refine the error information used in the likelihood. Their refinements consider different sources of uncertainties that are introduced when a 1D ecosystem model is made only dependent on some statistical properties of the 3D simulation output. With a preceding analysis of 3D model results the statistical characteristics of horizontal transport effects and of representative profiles for 1D initialization can be approximated. Based on these approximations, an array of 1D models could be used for parameter optimization without requiring additional 3D runs, which decreases computational time considerably. The better the statistical approximations of the local behaviour of 3D model results the better the capability of a 1D model to act as an emulator. The best set of parameter estimates for the array of 1D models is then expected to be also nearly optimal for global ocean 3D simulation results, provided that the array of local sites covers some of the major and critical ocean regions.

Hemmings, Challenor and Yool approach an important but difficult topic. It is of relevance for deriving large scale biogeochemical mass flux estimates, given a coupled 3D biogeochemical ocean circulation model together with best parameter estimates for its biological equations. Approaches presented here build upon results and findings of

analyses already presented in Hemmings et al. (2012, GMD). I regard their study here as another episode in establishing a meaningful modelling framework for optimizing 3D MEDUSA-NEMO global circulation results. The authors designed their experiments in anticipation of using remotely sensed chlorophyll-*a* data along a North-South transect in the North Atlantic, while setting up a trail of 1D models. They assess the emulator performance and derive the corresponding error information that can eventually be used in a cost function (here a negative log-likelihood multiplied by two) for simultaneous parameter optimisation. Their study does not address the question whether the anticipated use of satellite derived chlorophyll-*a* data along the transect will constrain the values of all model parameters. Also, it remains unclear how the assimilation of chlorophyll-*a* data would affect those parameter values that leave an imprint in mass flux estimates. However, they have done a smart preparatory examination and selected only model parameters whose values affect annual estimates of primary production and export. Thus, variations of these parameters will likely determine mass flux estimates of interest along the North-South transect.

The information and insight provided by the authors are helpful and will likely be appreciated by other readers. To my opinion, their procedure sets the current standard on how to tackle the problem in general. Yet, it does not cover the entire procedure for parameter optimization but it is a fundamental in-between step. The entire topic can become extensive, therefore it is meaningful to investigate and publish individual analysis steps. I can recommend a publication in GMD, since it is novel, inspiring, and helpful.

I would not recommend to everyone to read it in its current form and I feel obliged to suggest to the authors to shorten their text wherever possible. It can be questioned whether all comparisons are really needed, like informed versus uninformed emulator, direct and indirect uncertainties, with or without lateral flux perturbations. The latter, for example, is not required; a better performance is expected when lateral flux perturbations are included. A shortening of the manuscript is recommended also to avoid

possible exhaustion after the first forty pages have been read (which is only about half of all). Although stepwise presented by the authors a reader like I can get lost after page 21 with all the terminology (which is not always intuitively clear) described in the previous paragraphs. The addition of the mathematical variables in brackets in the text would be helpful. In fact, I had to draw my own structural graph to keep track of the different uncertainties and how they are assessed. Figures 1 and 2 do not provide the full picture that is needed to understand the authors' procedures. I appreciate the authors' great care in unravelling all possible uncertainties but I see some possibilities for simplifications. The approaches and individual aspects are not too complicated and are mainly clear but it is their number and combination that sometimes puzzled me.

My specific comments will include only few corrections and questions. Comments will mainly include recommendations on how the manuscript can possibly be simplified and shortened.

2 Specific questions and comments

Abstract
lines1-3: This very first sentence is incorrect, as the parameters do not compensate for missing complexity. Rather, the plankton ecosystem models rely on parameterizations whose parameters have to represent a mixture of diverse plankton species that are pooled together and attributed to single state variables of plankton biomass.

Introduction
page 6329
lines10-13: biota is part of nature! A plankton ecologist would disagree when stating that the biogeochemical models are mechanistic.
line 20: "...un-modelled..." I think is better to write "... unresolved..."

pages 6331, 6332
lines 27-10: The work of Nerger and Gregg (2008, Journal of Marine Systems) is a good reference her.

page 6334
lines 11-16: This paragraph should be revised according to the refined structure of the paper.
line 19: I would rather talk of an "approximated", "simulation" or "emulation error", not "predicted error" in ff.

page 6335
Equation (1): is not needed if Equation (2) is the one of primary interest for the authors

Equation (2): The terms "R" and "P" are later again used but with different meaning. Therefore, a different terminology should be used. Actually "R" is part of Equation (1) and is not really needed here at all.

page 6336
line 6: The full covariance is not used in the study. A reference to the covariance matrix "R" is not needed.
lines 22-23: sentence is somehow clear to me but could be better formulated.
lines 25-28: I know what the authors want to say but the sentence is too difficult to understand. Since this is an important explanation at this point, the authors should consider a better explanation.

pages 6337, 6338
lines 20 (6337) -26 (6338): The concept of distinguishing between primary and secondary tracers is fine, but it in the text it appears more complicated as it actually is. To write about a subset of tracers is confusing. Perhaps: "The perturbation term represents the effect of horizontal flux divergence. It is only applied to those state variables that determine nutrient concentrations and the biomass of the plankton. Other state variables (secondary tracers) like chlorophyll-*a* concentrations follow the flux cor-

rections of the corresponding biomass (primary tracers). This way chlorophyll-*a*-to-nitrogen and biogenic silicon-to-nitrogen ratios are maintained."

page 6339
line 10: I would talk of "additional variability due to lateral advection effects" instead of "rate of change due to lateral advection of the transformed tracer."
Equations (5, 6, and 7): Here a single equation would be enough. If Equation (6) were already included in Equation (5), then it would be more obvious why the factor of two is needed. Equation (7) is not needed because this had been explained before (see comment above).

page 6340
line 1: "... it must increase towards zero..." This is not clear. Do you mean "... must be set zero..."?
line 15: Some operational oceanographers would disagree as it is not really "predictive skill". Better: "mapping" or "emulation" skill

pages 6340-6348
Subsection 2.2 Informed and uninformed simulators
Subsection 2.3 The uninformed emulator
These subsections definitely require revision. First of all, the authors talk of an "uninformed simulator" first and then use the term "uninformed emulator". Many details in these subsections are confusing. Although correct it is difficult to follow as a reader. Here are my suggestions:

- start with the description of the "uninformed emulator" since this is the ultimate emulator; introduce Equation (9) here and explain "uninformed simulator/emulator residual" and "uninformed simulator/emulator error".
- introduce Equation (11) and explain the residual. I am not happy with the term

"parametric environment residual". Better "parameter induced residual"

- then derive Equation (12) from the combination of Equation (9) and (11).
- now explain Equation (13). The equation is formally correct but cannot be assessed exactly. You therefore consider an informed emulator and derive its error information instead. Equation (8) would then become Equation (14). And "εS" would be set equal to "ε1" of the former Equation (8).
- At this point the different concepts of direct (with reference to the relevant Equation shown before) and indirect uncertainty quantifications are introduced and it is explained how they are computed

Figures 1 and 2: These figures are elaborate already are helpful, but they would become even better if the most important mathematical symbols (as used in the corresponding equations) are also added to the boxes.

page 6345
line 20: "For each data set..."? This is not clear enough. Why constructing it only for each data set? I thought that it has to be derived for all (primary) tracers. Please clarify.

page 6346
line 2: "... containing the *n* available instances..." Shouldn't it mean " ... containing the *m* available instances...". If not, then it is needed to better explain the elements of the $\mathbf{Y}_{3D}$ matrix.
Equation (16): this is very nice and helpful! But, here $\mathbf{R}_1$ and $\mathbf{R}_2$ are no covariances; it could be confused with Equation (1). This comment is obsolete if the authors have agreed on removing Equation (1).
line 15: Why is *p*=5 and not 4 or 6?

page 6348
Experimental method

line 16: Add how large the ensemble was here.

page 6353
line 7: "... log-transformed 5 day mean..." Do you mean: five day mean of log-transformed or are have five day means been log-transformed? Please explain.
lines 8-10: "The log transformation..." If log-transformed variables are use then the variance does increase with increasing chlorophy-*a* concentration.

page 6354
Results
Figure 3: The figure hardly resolves the seasonal variations. The upper scale should be set to 10 instead of 100; this might already help.
line 17: "Results are shown for ... with and without lateral flux perturbations."
I suggest that the comparison with/without flux perturbation can be removed from the results section. Figure 4 can be omitted and Figure 6 (a very nice figure) can be discussed and shown in the discussion section. Also, I recommend considering only three sites from Figure 5 for the discussion section. It is good to have additional figures in discussion sections.

page 6355
lines 6-9: The results of parameter sets 10 and 6 are surprising. From parameter set 6 I would expect an early increase in biomass due to the high light-sensitivity. Together with the low half-saturation coefficients the net growth rates should be fairly high and I wonder why this is not expressed in the solution of 6. Parameter set 10 has some of the highest loss rates apart from grazing. Thus, the reduced grazing pressure might be the main reason for parameter set 10 to reveal enhanced net growth conditions.

page 6357
lines 1-4: Note that parameter 6 includes the largest sensitivity to light and it will induce high net growth rates earlier than the other parameter combinations. Therefore a greater sensitivity to the initial "winter" concentrations can be expected.

page 6358
lines 3-4: Parameter set 6 "These were excluded on the basis..." Does that mean the parameter range for α_{Pn} has an upper limit that was too high?

page 6360
line 17: Both parameter sets (1 and 4) have a very low light-sensitivity but at the same time are very susceptibility to any small grazing pressure.

Up to this point I have learned that some of the emulator errors are most apparent when special (extreme) parameter combinations are involved. Can't this information be introduced to the Latin Hyper Cube sampling?

pages 6361-6362
lines 18-9: Is this test really expedient? First, will we know the "true" degree of freedom when using real chlorophyll-*a* data, after these data had been processed with the same algorithm. Second, what do we learn about the "true" degree of freedom when the chlorophyll-*a* model results are "automatically" autocorrelated. To me, this part of the analysis can be skipped. It will become more relevant with new insight once real data are used and when a best parameter set is found. Figures 9 through 11 are just fine.

page 6364
Discussion
It would be good to have the discussion on the role of the flux perturbation (as explained before). The flux perturbation, as proposed by the authors, is of great importance and its potential to improve 1D model behaviour in general, can be discussed. The nice Figures (original 6) and a simplified version (with fewer locations) of Figure (original 5) could be placed here. This would put them into a more prominent position.

page 6365
Subsection 5.1 Mechanistic emulator performance rather **Performance of a process based, dynamical emulator**

lines 17-19: "In a practical application..." How critical is this? How large must an inflation factor be?

page 6327
line 16: But then the transport matrix would be the actual target model and not the original 3D model for which the transport matrix model had been constructed.

page 6375
line 1: " A dynamic, process- and site-based emulator..."

lines 18-28: this will still hold even if the results section is revise.

How about an explicit statement or conclusion based on the findings learned from sampling the parameter space and how extreme parameter combinations affected your analyses?

page 6381
Appendix A3
The parameter selection process is interesting and relevant for the experimental design (e.g. eventually exluding extreme parameter sets in some analyses). This section should be shortened and incorporated into section **3.2 Model parameter space**. In lieu thereof the paragraphs on the Student's t-distribution can be omitted.

Interactive comment on Geosci. Model Dev. Discuss., 7, 6327, 2014.