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Interactive comment on "Reviews and syntheses: Parameter identification in marine planktonic ecosystem modelling" *by* Markus Schartau et al.

Markus Schartau et al.

mschartau@geomar.de

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We greatly appreciate the many meaningful suggestions provided by Referee #4. According to some of the Referee's comments we changed parts of the manuscript's structure, which we think has improved the readability. We thank Referee #4 for taking the time to read our manuscript and particularly for some constructive and very helpful comments.

General comments by Referee #4

***Comment* 1**: To make the manuscript more understandable by novices in the field, the authors may want to begin the review with Section 5 "Typical parameterisations of plankton models and their parameters" rather than starting with error models. Given that the title of this article is parameter identification in plankton modeling, it seems strange that theoretical discussion of error models comes before any discussion of actual ecosystem parameterization attempts.

Author's response:
This good suggestion is much appreciated. We followed Referee #4's suggestion, although it required some additional changes of the original structure of (now Sect. 3, former Sect. 5) and of (now Sect. 5, former Sect. 4). The suggested switching of the Sections works well, as it puts more emphasis on biological aspects earlier in the manuscript.

The revised manuscript structure is:
"The paper starts with some theoretical background information (Sect. 2), introducing mathematical notation and depicting prevalent assumptions that are typically made for parameter identification analyses and model calibration (Sect. 2.1). We then branch off from DA theory and discuss the parameters typically dealt with in plankton ecosystem models. In Sect. (3) we disentangle major differences between approaches to parameterising photoautotrophic growth and briefly discuss simple but common parameterisations of plankton loss rates. In this context we also address the utilisation of data from laboratory and mesocosm experiments. Error models are described in order to elucidate error assumptions made in previous ecosystem modeling studies (Sect. 4). This is followed by a description of different approaches to specify uncertainties in parameter values (Sect. 5). An example of parameter estimation with simulations of a mesocosm experiment connects aspects of Sect. (3) with the theoretical considerations of Sect. (5). Thereafter, model complexity is jointly addressed together with cross-validation in Sect. (6), followed by a review of space-time variations in marine ecosystem model parameters (Sect. 7). Emulator, or surrogate-based, approaches are briefly explained and exemplified (Sect. 8) before

we discuss parameter estimation of large-scale and global biogeochemical ocean circulation models (Sect. 9). Finally, we summarise the insights that we gained on parameter identification in Sect. (10), and we will briefly address prospects of some marine ecosystem model approaches that could improve parameter identification."

***Comment* 2**: The manuscript is quite long and certain sections contain significantly more detail than others. As a result, the manuscript would be improved if the sections could be made more consistent in terms of their degree of detail.

Author's response:
To elaborate a meaningful structure was an extensive task and during the preparation of the manuscript we repeatedly discussed the content of respective sections of the submitted version of our manuscript. To achieve a balance that satisfies section authors as well as all other coauthors is somewhat difficult and will always be partially subjective. We think we have found some good trade-off between accessibility and discussion of a wide range of topics. It is extremely difficult to find a balance that could possibly please all readers.

According to the Referee's comment we re-assessed the content and found few places where we could skip details. We decided to skip the two paragraphs that extended on the discussion about Eigenvalue decomposition of the Hessian (now Sect. 5, former Sect. 4). Since we introduced a section that describes the basic theoretical background of the sequential DA approach (Sect. 2.2.2) we could remove the descriptions and equations in Sect. (7.1.3 Time-varying parameters). We also started to revise text and condense the content in Sect. (9) considerably, which will be finalised if the editors invite us to upload a fully revised version of our manuscript. See also response to comment 9.

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Discussion paper

***Comment* 3**: In certain places, e.g. section 2, the article assumes a familiarity of terms, which may benefit from greater introductory explanation. In particular, I found the description of "kinematic model errors" and "dynamical model errors" on page 6 somewhat lacking.

Author's response:

We have added an additional sentence to the paragraph following the kinematic model error equation. The relevant text now reads (with extra sentence highlighted in red color): "A general relationship between the true state and model state can be expressed as:

$$\vec{x}^t = T\left[\vec{x}, \boldsymbol{\zeta}(\theta_\zeta)\right] \tag{1}$$

where T is a truth operator, and $\boldsymbol{\zeta}$ is a set of random variables described by distributional parameters θ_ζ. We will refer to the ζ as *kinematic* model errors because they are associated with the model state, while the *dynamical* model errors $\boldsymbol{\eta}$ in Eq. (1) act to perturb the model dynamics. The true values of the kinematic model errors therefore define the potential discrepancy between the target true state and a hypothetical "ideal" model output (i.e. with the "true" values of the parameters and, if applicable, the "true" values of the dynamical model errors).

How we interpret and specify Eq. (2) depends on the spatio-temporal averaging scales chosen to define the true state $\vec{x}^t$, which in turn depends on the objectives of the modelling study. One approach is to define these averaging scales as equal to or larger than the shortest space and time scales that are fully resolved by the model. Kinematic model errors ζ may then represent the integrated effects of the various dynamical sources of model error, if these are not already accounted for by dynamical model errors $\boldsymbol{\eta}$ in Eq. (1). Alternatively, the true state can be defined over scales smaller than those resolved by the model, possibly at the scales of the observations. This may lead to a simpler model for observational error (see below), but now the ζ

must account for the unresolved scales, in addition to any error effects in the model dynamics otherwise not accounted for. With stochastic dynamical models ($\boldsymbol{\eta} \neq 0$), the true state is usually defined on the scales of the model and assumed to coincide with the model output for some (θ_e, $\boldsymbol{\eta}$), such that no kinematic error model is needed."

***Comment* 4**: : Likewise, at the beginning of section 4.1, a few introductory remarks describing the authors' specific intended meanings of "confidence" and "credible" would be helpful when transitioning into this section.

Author's response:
We suggest to use the following revised text:
"Uncertainty regions in parameter space can be determined basically in two different ways, either based on a Bayesian- or frequentist interpretations. Depending on the estimator, uncertainties in the combination of parameter values may either disclose a credible region of a random distribution of parameter values (Bayesian interpretation) or they mark a confidence region that should include the true value with a certain nominal probability of e.g. 95% (frequentist interpretation). The latter means that different data sets (of same type) may yield different confidence regions and e.g. 95% of those regions are expected to include the true "fixed" value, which does not imply that the true value falls into a confidence region with 95% probability. According to the Bayesian interpretation a credible region is specified by the probability of including the true value. For maximisations of the likelihood $p(\vec{y} \mid \Theta)$ it is often stated that credible and confidence regions are practically identical. Such interpretation is imprecise since the methods to confine either regions can be very different with respect to the underlying assumptions, e.g. MCMC versus bootstrap approaches."

***Comment* 5**: Section 2.2 would likely benefit from being split into a few subsections.

Author's response:
A good suggestion, thanks. We have split Section 2.2 into four subsections: "Basic probabilistic approaches", "Sequential methods", "Variational methods", and "Recent approaches".

***Comment* 6**: Should section 4.2 be in section 4? Should section 4.3 come before 4.2?

Author's response: We follow the Referee's suggestion and the section about profile likelihoods has now been placed before point-wise approximations.

***Comment* 7**: Can you mention one or two advantages of mesocosm data to complement your mention of drawbacks in the next sentence?

Author's response:
Yes, the text appears more negative than positive with respect to mesocosm experiments. We considered this and have added text, see rearranged Sect. 5 (now Sect. 3). We wrote: "One advantage is that mesocosms are, apart from the surface, closed systems and measurements of inorganic nutrients, dissolved and particulate organic matter should, in principle, add up to approximately constant concentrations of total nitrogen and total phosphorus. Total carbon concentrations may only vary due to air-sea gas exchange. By design these experiments often integrate valuable series of joint and parallel measurements, yielding detailed data from various scientist with different expertise (e.g., Williams and Egge, 1998; Riebesell et al., 2008; Guieu et al., 2014)."

***Comment* 8**: Can this section include a mention of where the authors think the use of combined emulators is headed? What are the hurdles to overcome?

Author's response:

To Sect. (8.3 Combining dynamical and statistical approaches) we want to add more information in this respect. We suggest the addition of the following paragraph: "The ultimate aim of the two stage procedure would be to use estimates of model output that the dynamic emulator can provide rapidly for 100s of parameter vectors to construct a statistical emulator for a cost function or similar metric that is then used in parameter identification. The dynamical emulator would effectively bridge the gap between a small reference ensemble that is practical to generate with the full 3D model and the statistical emulator that requires a relatively large training set. The metric must incorporate an error model that takes into account all sources of uncertainty in the statistical emulation of the full model. Thus, the uncertainty estimates obtained when training the statistical emulator must be inflated by combining them with the dynamical emulator's own uncertainty estimates. Stage 1 emulation results suggest that it may be important to first extend the latter to include temporal covariance estimates for the parameter-dependent variation. Another important consideration is that longer spin-up times for creating the 3D model reference ensemble would be required in a practical application to truly represent the effects of varying parameters in a global circulation model. The application of dynamical emulation techniques for accelerated spin-up, such as the TM method (Khatiwala, 2007) mentioned in Sect. (8.1), could help to provide a better representation."

***Comment* 9**: After stating that an appropriate treatment of uncertainties for Earth system models is critical, it seems as if this section is going to go into depth on that subject, but it is a cursory overview. I would suggest mentioning here that a full treatment of uncertainties in Earth system models is beyond the scope of this article.

Author's response:

Section (9) is currently revised and will be condensed. So far, we have decided to leave the Sect. (9.4 Impact of parameter uncertainties on climate model projections into the future) as it is but added to the first paragraph the suggested statement: "An appropriate treatment of the uncertainties contained in the applied scenarios and employed models is crucial for correctly interpreting model projections, informing the societal debate about climate policies and thus strengthening the base for developing relevant measures. A full treatment of uncertainties in the projections of EMS is beyond the scope of our review and we can only address this topic here briefly."

***Comment* 10**: It seems that this paragraph is not focused on what the section title states. Half of the paragraph is about a novel thermodynamically inspired ecosystem model. Can the title be reworded, or the text reworded as to relate more to "keeping number of free parameters low". Also, in the title, what does "grasping" mean in reference to complexity?

Author's response:
We suggest to change the clumsy title of Sect. (10.1) simply to "Modelling prospects", which catches the actual content.

We thank Referee #4 for the closer inspection. All technical errors identified and listed by the Referee were corrected.

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