

## ***Interactive comment on “Parameter Calibration in Global Land Carbon Models Using Surrogate-based Optimization” by Haoyu Xu et al.***

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First of all, the authors would like to thank the reviewer for the detail and valuable comments, suggestions as well as generous recognitions, which would greatly improve the clarity of our presentation and help our revision.

Comment: The fact that the RBF-SBO starts out with a considerably lower RMSE for all three models (Figure 5) suggests that the calibration setup somehow gives RBF-SBO an unfair advantage over the other algorithms. If this is the case, it would have serious consequences for the paper. Possibly the calibrations would have to be redone in a setup that removes this advantage.

Response: The reason that the setup of RBF-SBO is better than other optimization

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algorithms is that SBO has a sample step and selects the good parameters while other algorithms simply select initial samples randomly. We also repeat the experiments by making the SBO have the same quality setup as other algorithms. The results can be found in the figures below (Figure 1, 2 and 3). The results show that RBS-SBO has the similar performance on 2-pool microbial model and outperforms other algorithms on 4-pool microbial model and CLM-CASA' Carbon Model with the limit of 200 sample runs.

Comment: The description of the methods need to be considerably expanded since much important information is missing, most importantly, on the algorithm itself. Ideally, one should be able to reproduce the approach from the description in the main text, appendix, or supplemental information. However, in this manuscript not nearly enough information is provided for this. For example, I would guess that the algorithm evaluates and rejects several proposal steps using the surrogate model, before a parameter set is deemed good enough to be evaluated by the true model. However, no information is provided as to how these kinds of choices are made. I would suggest including a pseudo-code block to describe the working of the algorithm. Additionally, the surrogate model is constructed based on “radial basis functions” but no additional information is given on how this works. Since the approach for surrogate model is a critical choice (as acknowledged by the authors, P6, L14) this approach needs to be described in much more detail. There are several other places in the text where more information should be provided. These are given in the specific comments below. Parts of these descriptions may be placed in an appendix or online supplement.

Response: Thanks for pointing out the issue. We agree that the details of the algorithms and the “radial basis functions” should be given. The surrogate-based optimization introduction section (Section 3) is refactored in our revised version to make the description more clear and emphasizes the main idea of the SBO. The detailed equations and algorithm procedures are given in the Appendix.

Comment: I find the paper a bit biased towards a positive assessment of the algorithm

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and superiority over other algorithms. The paper would benefit from an additional discussion section on the possible limitations of the approach, which I'm sure exist. For example, the limitations of using a surrogate model for mimicking complex models is briefly mentioned (P9, L5-11), but its consequences are not further discussed.

Response: The experiments are fair to all presented algorithms including global optimization, MCMC and SBO. The sample size is the same and the results on all three models demonstrate that SBO is better than other parameter calibration methods. The reason why SBO outperformed than other global optimization algorithms is that SBO uses a surrogate model to simulate the source model (CLM carbon process) and avoids bad parameter points ( 'bad' means the high prediction error). The limitation of SBO is that it may be overperformed by global optimization algorithms when using more samples. However, the sample size can't be too large for computationally expensive models. Some works such as collaborative tuning are targeted to combine the SBO and global optimization.

Comment: Furthermore, the SBO based estimates strongly disagree with the MCMC estimates for two of the 4-pool microbial model (CUE\_slope, and CUE\_0; Figure 10). This is briefly mentioned (P11, L19) but not further discussed. Comment: P12, L3-4: "it still can find the true parameter values". The mismatch for CUE\_slope and CUE\_0 in Figure 10 shows that this is not always the case.

Response: The Figure 10 shows that some calibrated values of the SBO are different from the Bayesian MCMC, and these different values make the prediction error of SBO results lower than Bayesian MCMC. According to our understanding, the mismatch of these parameters may be due to the different targets of the parameter selection between SBO and Bayesian MCMC.

Comment: The language in the paper is in general quite poor. There are quite a few spelling and grammar errors, and many sentences are semantically incorrect (e.g. missing or incorrect usage of articles), awkward, or use spoken rather than written

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English. I've listed a number of them below, but I strongly advise proof-reading by a proficient an editor proficient in the English language. Please check also the citation references, both in the text and in the bibliography. There appear to be quite a few mistakes.

Response: Many thanks for your valuable suggestions. We have fixed all the grammatical and formatting issues you pointed out, and tried our best to conduct several rounds of proofreading and substantially improved English presentation in our revised manuscript.

Comment: From what I can understand from the paper (P3, L5-15) the authors only ran and calibrated soil carbon models, no full land carbon model. Therefore, I find the title somewhat misleading. The approach can probably be used to optimize a full land carbon model, but this has not been shown. I could imagine that the limitations posed by using a surrogate model would become more relevant for a full land carbon model. Hence, I would suggest replacing "land carbon models" with "soil carbon models", or "the soil carbon component of land carbon models".

Response: Thanks. The title has been changed to "soil carbon models" in the revised version

Comment: It is rather unfair to compare computational cost of the SBO approach presented here to that of Bayesian MCMC, since the latter is a sampling algorithm, whereas the former is a optimization algorithm. Sampling schemes are intended to obtain a detailed approximation of the posterior/likelihood function whereas optimization schemes only yield an estimate of the maximum likelihood point. Comparing the computational cost to that of the other optimization approaches would make more sense.

Response: We agree with the reviewer. The Bayesian MCMC is designed to obtain a posterior likelihood function but it can also be used to calibrate parameters to reduce the prediction error. Moreover, we also compare the SBO with known global optimization algorithms in our manuscript.

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Comment: Section 2.2: The microbial soil carbon models and the corresponding equations (3)-(16) need to be better explained (e.g. what processes do the different terms in the ODEs represent). For someone not experienced with such models it is currently difficult to understand what's going on.

Response: The detail introduction of the microbial soil carbon models can be found in the paper "Hararuk, Oleksandra, M. J. Smith, and Y. Luo. Microbial models with data-driven parameters predict stronger soil carbon responses to climate change." *Global Change Biology* 21.6 (2015)". We have added some sentences for clarification in the revised version.

Comment: Section 3: as discussed above the radial basis functions approach needs to be explained, as well as the approach to generate proposal samples

Response: The introduction and discussion have been included in the Appendix of the revised version.

Comment: Section 4.1: The authors state that the calibration process is repeated 50 times. How do you assure that the you don't get the same result every time? Is the algorithm started with different initial values, or are there stochastic parts in the algorithm?

Response: Thanks for the question. In fact, even if we start these algorithms (MCMC, global optimization, SBO) with the same initial values, the final calibrated results are different in different running time. It is due to the stochastic nature of these algorithms. We ran each algorithm 50 times and used the average results for algorithm evaluation to eliminate the influence of this kind of uncertainty.

Comment: P8, L4-12 concerning the Bayesian MCMC approach: -It appears that the authors used the Metropolis algorithm. If so, please state this. -Have these calibration runs been performed specifically for this study or did the authors use the results from Hararuk et al. (2014, 2015)? -How is the acceptance probability calculated? -How was

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convergence of the MCMC algorithm diagnosed. What criterion was used? -Please provide more information on how the MLE point is determined -It is stated that Table 3 provides the detail of the Bayesian MCMC approach. However, other than the number of iterations no information is given

Response: The Bayesian MCMC (Hararuk et al, 2015, mentioned before) used the Metropolis algorithm. We have got the code from Hararuk and repeated the calibration experiments. This MCMC approach would run 50, 000 samples before ends.

Comment: P11, L23: I don't agree with the statement that "Bayesian MCMC approach has been used to typical SOC models". To my mind most of these models have been tuned either manually or with gradient search algorithms

Response: As far as we know, the Bayesian MCMC approach has been used to the two microbial soil carbon models and the carbon cycle component of CLM.

1. Hararuk, Oleksandra, M. J. Smith, and Y. Luo. Microbial models with data-driven parameters predict stronger soil carbon responses to climate change.

2. Hararuk, Oleksandra, J. Xia, and Y. Luo. Evaluation and improvement of a global land model against soil carbon data using a Bayesian Markov chain Monte Carlo method. *Journal of Geophysical Research Biogeosciences* 119.3(2014):403-417.

Comment: P11, L24-25: "owing to approximate one million simulations". The number of required iterations is completely dependent on the specific calibration problem so one cannot state a specific number for calibrating SOC models in general

Response: We agree with the reviewer. It's difficult to estimate the number for different parameter calibration tasks. We have clarified this in our revision version. According to the experiments we conducted in this work, the sample size the SBO requires is less than the Bayesian MCMC method and global optimization algorithms for parameter calibration task.

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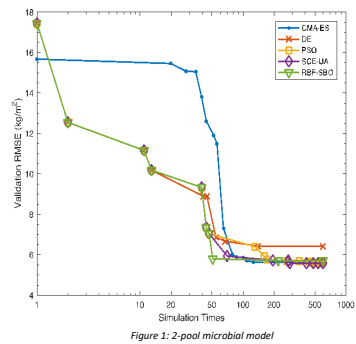


Figure 1: 2-pool microbial model

Fig. 1.

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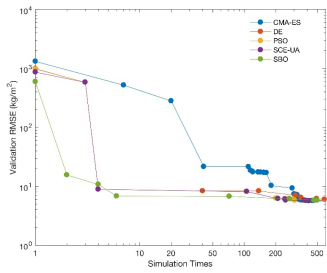


Figure 2: 4-pool microbial model

Fig. 2.

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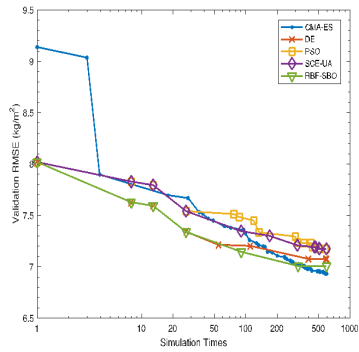


Figure 3: CLM-CASA Carbon Model

Fig. 3.

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