Geosci. Model Dev. Discuss.,
https://doi.org/10.5194/gmd-2017-48-RC1, 2017

Geoscientific Model Development Discussions
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Interactive comment on "Parameter Calibration in Global Land Carbon Models Using Surrogate-based Optimization" *by* Haoyu Xu et al.

Anonymous Referee #1

Received and published: 11 July 2017

This manuscript describes the performance of a surrogate-based approach to calibrating three different soil carbon models relative to three global optimization algorithms and a MCMC algorithm. The results indicate that the surrogate-based optimization employing radial basis functions outperforms the other approaches in nearly all circumstances. Model calibration improves the fit of the models to a global dataset of soil carbon values, with the models incorporating soil microbial dynamics explicitly fitting the data more effectively than a model based on CLM-CASA.

Unfortunately, the quality of the English throughout the manuscript is extremely poor with numerous grammatical errors throughout all the text. Without a great deal of additional editing for language alone this will not be publishable in GMD.

All these English language errors, which are far to numerous to call out individually,

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Discussion paper

make it very difficult to undertake a review of scientific merit, but there are a number of areas that clearly require further elaboration and clarification.

Whilst it is certainly challenging, the authors assertion that it is not possible to optimize parameters directly in land surface models such as CLM is not true – see for example Post et al., 2017 JGR-B and reference there in.

The assertion that the “structures of land carbon cycle” with ESMs “are almost the same” maybe true but requires evidence and references.

It is unclear what are the differences between CLM, CLM-CASA and CLM-CASA C-only. My interpretation is that CLM-CASA C-only is the steady-state approximation detailed in Xia et al, 2012, and the SBO was developed for this. Some additional detail is required here – for example, what are the meteorological drivers, what are the inputs? “NPP” is mentioned, but never explained. This is important, as the relevance, or otherwise, of this work to informing ESM development can only be understood if the implications of using a surrogate model to parameterize a matrix-based approximation of the steady-state of the simplistic soil component of an old land model are fully articulated.

The description of how the specific SBO algorithm and parameter point generation strategies is unclear – what is about the nature of the algorithms chosen that makes them appropriate for this particularly use case?

Given the code available in the supplementary material, it is apparent that the various optimization algorithms were implemented in Matlab and relies heavily on material from the File Exchange. Details of this implementation need to be in the main text.

As the authors highlight, “sample size, the nonlinearity and complexity of the real model” all impact surrogate performance. This is partially addressed through the use of three models with different numbers of pools/parameters but not well explained, nor is there reference back to the role of surrogates with ESMs of full complexity.

The analysis of the results (Section 5) fails to discuss the implications of the optimizations for CLM-CASA C-only. What does it mean for the model if even when optimized it can only explain 40% of observed variation? Why are so many parameter values right at the edge of their prior range? Are the numbers “biological feasible”? To what extent is the improvement in fit with microbial model due to the inclusion of microbes, or rather due to spatially varying base rates?

Overall, the work described in this manuscript has the potential to inform future land surface model developments, and highlights the possibilities of using surrogate-based optimization at a fraction of the computational cost of MCMC-type approaches. With much improved editing, clarification of the points outlined here, and a more involved discussion of the outcome of optimization exercise – which is the point of the whole exercise after all – hopefully it can be considered more favorably for inclusion in GMD in the future.

Interactive comment on Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-48, 2017.

Geosci. Model Dev. Discuss.,
https://doi.org/10.5194/gmd-2017-48-RC2, 2017

Geoscientific Model Development Discussions
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Interactive comment on "Parameter Calibration in Global Land Carbon Models Using Surrogate-based Optimization" *by* Haoyu Xu et al.

M. Braakhekke (Referee)

maarten.braakhekke@gmail.com

Received and published: 21 August 2017

Comments are given in the attached PDF.

Please also note the supplement to this comment:
https://www.geosci-model-dev-discuss.net/gmd-2017-48/gmd-2017-48-RC2-supplement.pdf

Interactive comment on Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2017-48, 2017.

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Discussion paper

Review of a "Parameter Calibration in Global Land Carbon Models Using Surrogate-based Optimization" by Xu et al.

Maarten Braakhekke

General comments

This manuscript presents a novel approach for calibrating global land carbon cycle models that are computationally costly (i.e. need a long time for a single simulation). The approach, dubbed surrogate-based optimization, uses a uses a computationally cheap surrogate model, which mimics the original model, to generate candidate parameter sets at each iteration. Since the original model is only run for "good" new parameter sets, this approach avoids evaluation of the original model for "bad" parameters, thereby substantially reducing the number of model iterations, and thus computation time. The authors apply the algorithm for the CLM-CASA global land surface model in order to optimize parameters related to soil carbon cycling against global gridded soil carbon stocks from the IGBP-DIS dataset. Additionally, the approach is applied for two other soil carbon models, which explicitly represent microbial dynamics. The calibration results are compared to those of four other optimization schemes and a Bayesian MCMC algorithm.

To my mind the approach is very promising and helps to tackle an important issue with calibrating global models: the high computation cost. I'm not very experienced with optimizing global models and thus I cannot say if there are other techniques that achieve the same thing, and how these compare to the approach presented here. Nevertheless, I think the paper is relevant, and a strong contribution to the field of global modelling. Furthermore, I think the authors were quite thorough in testing the new approach by applying it to three models, and comparing the results to five other optimization/sampling schemes.

However, I do have several criticisms that should be addressed. These relate mainly to the text.

1. 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.
2. 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.

3. I find the paper a bit biased towards a positive assessment of the algorithm 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. 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.
4. 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 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.
5. 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".

Specific comments

Abstract

- P1, L11: I suggest to either replace "which can be obviously improved" with "which can obviously be improved", or remove "obviously" altogether

Section 1

- P1, L21: "SOC is the largest pool of global land carbon." please provide a reference for this statement.
- P1, L21: I suggest replacing "a famous" with e.g. "the most important".
- P1, L29: I suggest elucidating "agree with". E.g. "For only half of the 11 models the predicted global total SOC falls within estimated range of the HWSD"
- P1, L29: remove "s" in "coefficients"
- P2, L3: remove "the" before "parameter"
- P2, L4: "replace "expensive" with "high"
- P2, L7: remove "the" before "high"
- P2, L8: put "like CLM" between comma's. Also, CLM has not previously been introduced (it is two lines below)
- P2, L15: remove "also"
- P2, L17: replace "the" at the end of the line with "an"
- P2, L18: add "the" before "surrogate"

- P2, L23-24: “Quite a few…benchmark. This sentence is unclear. Consider revising.
- P2, L25: add a comma after “Here”
- P2, L29-30: “On average…Bayesian MCMC”. This sentence presents results, and should not be in the introduction. However, I admit this may be a matter of style.
- P2, L30: 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.
- P2, L34: Replace “analysis” with “discusses”

Section 2

- P3, L1-2: “…their structures of land carbon cycle are almost the same”. This is statement is a major oversimplification. I would suggest something like “there are many similarities”
- P3, L6: remove the “s” at the end of “carbons”
- P3, L9: “one of the most popular earth system models in the world”. I suggest replacing with “widely used Earth system model”
- P3, L23: add “model” after “CLM-CASA’”
- P3, L24: add “of” after “linear”
- P3, L30: I suggest replacing “The steady solution of equation (1) is solved by Xia et al. (2012):” “the steady state solution of equation is given by (Xia et al. 2012):”
- P4, L1: add a comma after “NPP”
- 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.
- P4, L21: add “be” after “to”
- P5, L12: add “The” to the start of the sentence and remove the “s” in the second “models”
- Figure 2: Why do gridcells near coastlines have no data?
- P5, L22: replace “gird” with “grid”
- Tables 1 and 2: please provide the units of the parameters

Section 3

- Section 3: as discussed above the radial basis functions approach needs to be explained, as well as the approach to generate proposal samples
- P6, L9: I suggest adding “surrogate” before “model”
- P6, L12: I suggest replacing “cancelled” with “avoided”
- P6, L133: I suggest replacing “save much” with e.g. “substantially reduce”
- P6, 24-26: This sentence is rather vague. What is meant with “real variability”?
- P6, L24: please provide a reference for Latin hypercube sampling
- P6, L24: add “which” between “for” and “LHS”
- P7, L3: I suggest replacing “optimum” with “optima”
- P7, L7: I suggest replacing “try to present” with “present” or “try”

Section 4

- 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?
- P7, L21: add a comma after "algorithms"
- P7, L23: add a comma after "(CMA-ES)"
- P7, L24: I suggest removing "the outstanding"
- P7, L26: remove the parenthesis "(" after "SCE-UA"
- P7, L28: the reference "MA H, et al., 2006) is not present in the bibliography
- P7, L31: add "other" before "three"
- P8, L1 & L2: I assume you mean "normal" instead of "norm"
- P8, L2: I suggest replacing "proven" with "shown"
- P8, L3: replace "on" with "in"
- 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 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
- Figure 4. I assume the box plots show means and spread over the 50 calibration runs. Please indicate this in the caption
- Figure 4: I suggest replacing "exceptions" with "outliers"
- P8 L15: I suggest replacing "measure" with e.g. "applied"
- P8, L16: please revise "As the requirement of Bayesian MCMC…"
- P8, L19: I suggest replacing "On" with "for"
- P8, L20: I suggest removing "only"
- P8, L21: remove "of" before "more"
- P8, L21: consider rephrasing "can exploit better results"
- P8, L22: I suggest replacing "from the aspect" with "with respect to"
- P8, L24: replace "get" with "gets"
- P8, L25: consider rephrasing "promising one"
- P8, L26: consider rephrasing "It is because…"
- P8, L28: I suggest "…matrix and thus that…" with "…matrix, hence…"
- P8, L29: consider rephrasing "extremely critical"
- Figure 5: For all three models, the RBF-SBO algorithm starts out with a considerably lower RMSE at the first iteration, compared to the other algorithms. Please explain this difference. I wonder if the setup of the algorithm somehow gives RBF-SBO an advantage. This would make the comparison unfair.
- P9, L1 & L15: replace "till" with "until"
- P9, L2: add "s" after "simulation"

- P9, L7: consider removing “as we know”
- P9, L7: replace “the” with “an” before “approximation”
- P9, L14: remove “that”
- P9, L14: replace “increasing” with “higher”
- P9, L15: consider rephrasing “keeps ahead”
- P9, L24: consider rephrasing “for the samples”
- P9 L24: “on the other hand” indicates that what follows contradicts what was stated previously. This is not the case here.
- P9, L29: replace “are” with “is” (refers to “performance” not “models”)
- P9, L29: consider rephrasing “no one can dominate other two”
- P9, L29: consider rephrasing “all get success”

Section 5

- P10, L1: add “state” after “steady”
- P10, L1: replace “Equateion” with “Equation”
- P10, L2: add “the” before “IGBP-DIS”
- P10, L2: I suggest removing “obviously”
- P10, L13: I suggest replacing “sharp” with “narrow”
- P10, L13: I suggest removing “that those are”
- P10, L15: replace “in” with “for”
- P10, L16-17: “On the other hand”: see comment for P9 L24, above
- P10, L19: replace “approximate” with “close”
- P10, L19: replace “assigend" with “assigned”
- P10, L20: consider rephrasing “not so reasonable”
- P10, L20: replace “reaches” with “approaches” or “is close to”
- Section 5.2: for CUE_slope and CUE_0 there is considerable mismatch between the mode of the parameter distributions derived by MCMC, and the estimate from the SBO algorithm. But this is only mentioned in passing (P11, L19-21). It needs to be mentioned more explicitly and the potential reasons and consequences should be discussed.
- P11, L5: move “both” from its current location in the sentence to before “CLM-CASA’”
- P11, L14: consider replacing “biomass” with “dynamics” or “processes” since CLM-CASA’ also has a microbial biomass pool

Section 6

- 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
- 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
- P11, L27-28: see comment P2, L30
- P11, L30: I suggest replacing “dominates” with “outperforms”
- 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

Dear Editor and Referees,

First of all, the authors would like to thank the reviewer for the valuable comments, suggestions as well as generous recognitions, which would greatly improve the clarity of our presentation in the revised version.

Response to the reviews and the change list in the manuscript

Response to Anonymous Referee #1

Comment 1.1: The quality of the English throughout the manuscript is extremely poor with numerous grammatical errors throughout all the text. Without a great deal of additional editing for language alone this will not be publishable in GMD. All these English language errors, which are far to numerous to call out individually, make it very difficult to undertake a review of scientific merit, but there are a number of areas that clearly require further elaboration and clarification.

Response*: Thanks. We have tried our best to conduct several rounds of proofreading and substantially improved English presentation in our revised manuscript.*

Changes in manuscript: *We have conducted several rounds of proofreading and substantially improved English presentation (from the beginning to the end of our revised manuscript). We don't mark these changes in the pdf file due to too many modifications.*

Comment 1.2: Whilst it is certainly challenging, the authors assertion that it is not possible to optimize parameters directly in land surface models such as CLM is not true – see for example Post et al., 2017 JGR-B and reference there in.

Response*: We apologize for the confusion. We meant to express the point that optimizing turnover rates and other related parameters with pool-based datasets is computationally too demanding for land surface models. Optimizing flux-related parameters is computationally challenging but possible. The study by Post et al. 2017 was conducted to optimize photosynthesis-related parameters with eddy-flux data. It is a great work. To optimize the parameters, such as those we estimated in this study, has to overcome additional computational challenges. For example, it takes a very long spin-up time to run the whole CLM model. Tuning parameters for the whole model requires the extreme computational and temporal cost.*

Changes in manuscript: *We clarify this point in Section 1 of the revised manuscript by emphasizing the long spin-up time required for carbon cycle simulation (marked as marked as* ***Change 1.2***).

Comment 1.3: The assertion that the "structures of land carbon cycle" with ESMs "are almost the same" maybe true but requires evidence and references.

***Response**: Thanks for your suggestion. Now we cite the paper by Huang et al. 2017, which shows that the matrix equation not only can exactly reproduce the original CLM4.5bgc but also offers the simplicity in coding, diagnostic capacity, and computational efficiency. The latter enables optimizing pool-related parameter estimation.*

Changes in manuscript: *We clarify this point in Section 1 (marked as marked as **Change 1.3***).

Comment 1.4: It is unclear what are the differences between CLM, CLM-CASA and CLM-CASA C-only. My interpretation is that CLM-CASA C-only is the steady-state approximation detailed in Xia et al, 2012, and the SBO was developed for this. This is important, as the relevance, or otherwise, of this work to informing ESM development can only be understood if the implications of using a surrogate model to parameterize a matrix-based approximation of the steady-state of the simplistic soil component of an old land model are fully articulated.
Some additional detail is required here – for example, what are the meteorological drivers, what are the inputs? "NPP" is mentioned, but never explained.

***Response**: Thanks for your questions. We used the term CLM to refer Community Land Model in a general term. CLM-CASA' is a version CLM3.5 of CLM. The CLM-CASA' C-only version is the same model CLM-CASA' only when we consider the C processes of that model. We developed SBO to optimize parameter estimation for the CLM-CASA' C only version using the steady-state approximation. Parameter optimization cannot easily be done at the non-steady state unless time-series data sets are used as did by Zhou et al. 2013 and 2015.*

As the matrix equation results from the re-organization of exact equations as in the original model, the parameter values estimated by SBO can be directly transferred to the original model. Moreover, the matrix representation offers the solution to the land carbon cycle modeling and the National Center for Atmospheric Research (NCAR) land modeling team will adopt the matrix equation as the main frame of CLM in the future version. Thus, any parameter estimation with the matrix equation can be directly used to improve the original model.

We added sentences to clarify this point in our revised manuscript and also to give the detail descriptions of the models.

Changes in manuscript: *We clarify this point in Section 2.1 of our revised manuscript (marked as marked as **Change 1.4***).

Comment 1.5: The description of how the specific SBO algorithm and parameter point generation strategies is unclear – what is about the nature of the algorithms chosen that makes them appropriate for this particularly use case?
Given the code available in the supplementary material, it is apparent that the various optimization algorithms were implemented in Matlab and relies heavily on material from the File Exchange. Details of this implementation need to be in the main text.

***Response**: The initial parameter is generated using LHS (Latin Hyper-Cube Sampling) and we*

agree that the details of the SBO algorithms should be given. An appendix which includes a detail description of SBO has been added in the revised manuscript. The reason why SBO outperformed other global optimization algorithms is that SBO uses a surrogate model to simulate the original model (CLM carbon process) and avoids bad parameter points ('bad' means the high prediction error). By using the surrogate model, the SBO can save many model running times and is appropriate for expensive computation-cost models.

Changes in manuscript: *We totally refactor Section 3 of our revised manuscript (marked as **Change 1.5-1**). We also point out the advantage of our SBO in Section 4.3.1 of the revised version (marked as **Change 1.5-2**). Moreover, an appendix which includes a detail description of our SBO implementation has been added (marked as **Change 1.5-3**).*

Comment 1.6: As the authors highlight, "sample size, the nonlinearity and complexity of the real model" all impact surrogate performance. This is partially addressed through the use of three models with different numbers of pools/parameters but not well explained, nor is there reference back to the role of surrogates with ESMs of full complexity.

***Response**: We agree with the reviewer. To validate this, we carefully choose three different models to evaluate our algorithm. The nonlinearity and complexity of the three models are different. The number of parameters and the equations are different, and the performance of surrogate models are also different. We will add some detailed analysis in the revised version.*

Changes in manuscript: *We clarify this point and point out the value of our SBO for ESMs of full complexity in Section 4.3.1 of the revised version (marked as **Change 1.6**).*

Comment 1.7: The analysis of the results (Section 5) fails to discuss the implications of the optimizations for CLM-CASA C-only. What does it mean for the model if even when optimized it can only explain 40% of observed variation? Why are so many parameter values right at the edge of their prior range? Are the numbers "biological feasible"? To what extent is the improvement in fit with microbial model due to the inclusion of microbes, or rather due to spatially varying base rates?

***Response**: We greatly appreciate the reviewer pointing out this issue. It is still not satisfactory to explain 40% of observed variation with the optimized model. This is similar to another study by Hararuk et al. 2014 and much better than the model with default parameter values, which only explains 33% of the observed variation. The unexplained variation is partly due to uncertainty in observations. Indeed, the world homogenized soil data is grid-based map of soil carbon content, which was developed from pedon data. The equation used for the homogenization only can explain 33% of the variation in the original pedon data. That means that the homogenization itself generates 67% variation. To improve the model-observation fitting, we need to understand uncertainty sources from data, model structure, parameters, and forcing.*

The edge-hitting of estimated parameters is usually related to correlations among parameters. We need information of covariance among parameters to resolve the edge-hitting issues.

It is not very clear to us what the reviewer tried to ask with the question "Are the numbers "Biological feasible? " Is it about the number of parameters that can be constrained by the dataset we used in this study? In general, soil carbon contents rich information to constrain several parameters related to soil carbon pool turnover as showed in this study.

The improvement in fit with microbial model is largely due to the nonlinearity, which is more flexible to fit data. It is not clear to us whether the improved fit has anything to do with spatial variation in base rates. We may design a different study to explore this issue.

Changes in manuscript: *We clarify this point on "only explain 42% of observed variation" in Section 5.1 (marked as **Change 1.7-1**). And we also give more explanations on the edge-hitting issue (marked as **Change 1.7-2**).*

***References**:*

1. *Todd-Brown, K. E. O., J. T. Randerson, W. M. Post, F. M. Hoffman, C. Tarnocai, E. A. G. Schuur, and S. D. Allison (2013), Causes of variation in soil carbon simulations from CMIP5 Earth system models and comparison with observations, Biogeosciences, 10(3), 1717–1736, doi:10.5194/bg-10-1717-2013.*
2. *Weng, E., and Y. Luo (2011), Relative information contributions of model vs. data to short- and long-term forecasts of forest carbon dynamics, Ecol. Appl., 21(5), 1490–1505, doi:10.1890/09-1394.1.*
3. *Luo, Y., L. W. White, J. G. Canadell, E. H. DeLucia, D. S. Ellsworth, A. Finzi, J. Lichter, and W. H. Schlesinger (2003), Sustainability of terrestrial carbon sequestration: A case study in Duke Forest with inversion approach, Global Biogeochem. Cycles, 17(1), 1021, doi:10.1029/2002GB001923.*
4. *Xia, J., Y. Luo, Y. P. Wang, and O. Hararuk (2013), Traceable components of terrestrial carbon storage capacity in biogeochemical models, Global Change Biol., 19, 2104–2116, doi:10.1111/gcb.12172.*
5. *Zhou, T., and Y. Luo (2008), Spatial patterns of ecosystem carbon residence time and NPP-driven carbon uptake in the conterminous United States, Global Biogeochem. Cycles, 22, GB3032, doi:10.1029/2007GB002939.*
6. *Huang YY, XJ Lu, Z Shi, D Lawrence, C Koven, JY Xia, ZG Du, E Kluzek, YQ Luo. (2017). Matrix approach to land carbon cycle modeling: A case study with Community Land Model. Global Change Biology, doi: 10.1111/gcb.13948.*

Response to Referee #2

Comment 2.1: 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 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. The results show that RBF-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.*

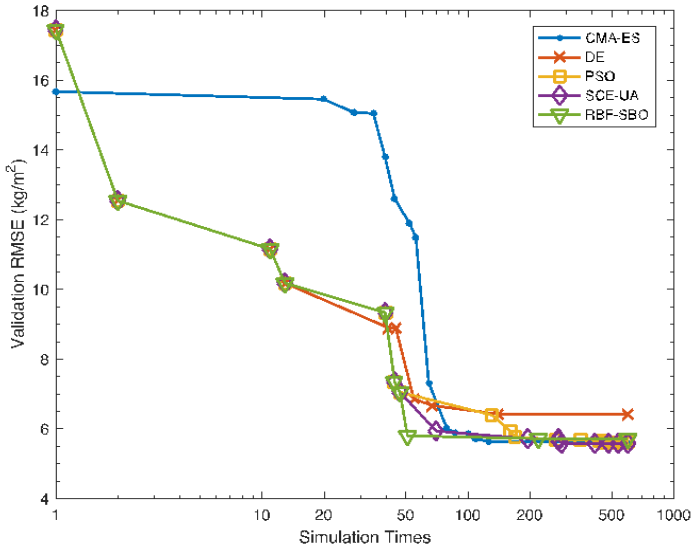

Figure 1: 2-pool microbial model

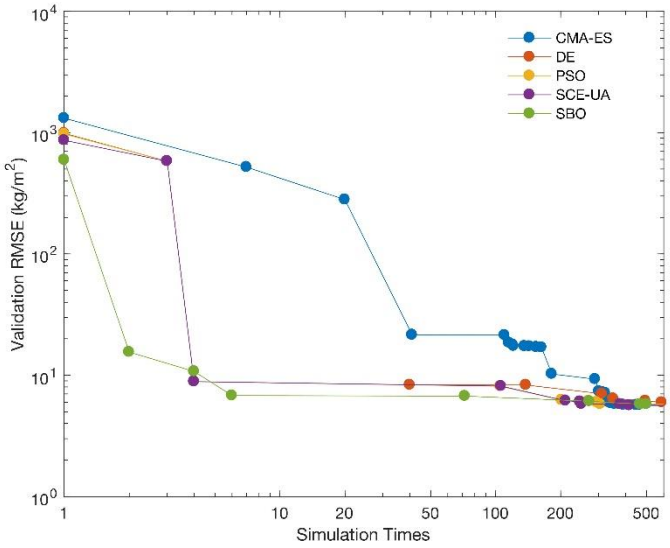

Figure 2: 4-pool microbial model

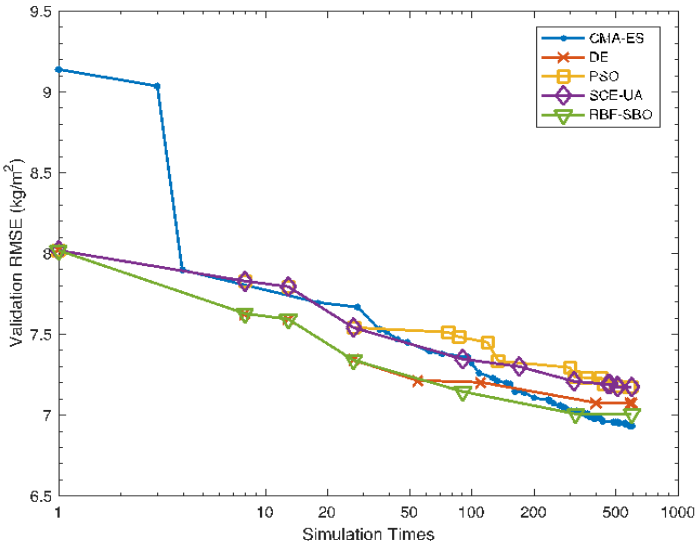

Figure 3: CLM-CASA' Carbon Model

Changes in manuscript: *We clarify the effect of the setup stage in Section 4.3.1 of the revised version (marked as **Change 2.1**).*

Comment 2.2: 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.*

Changes in manuscript: *We totally refactor Section 3 of our revised manuscript (marked as **Change 2.2-1**). Moreover, an appendix which includes a detail description of our SBO implementation has been added (marked as **Change 2.2-2**).*

Comment 2.3: I find the paper a bit biased towards a positive assessment of the algorithm 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 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.*

Changes in manuscript: *We emphasize the reason why our SBO can outperform other global optimization algorithms (marked as* ***Change 2.3-1****) and point out the potential issue of our SBO (marked as* ***Change 2.3-2****) in Section 4.3.1 of the revised version.*

Comment 2.4: 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.
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.*

Changes in manuscript: *We briefly discuss the reason of the mismatch issue for 4-pool microbial model in Section 5.2 (marked as* ***Change 2.4-1****)* and *improve the responding statement in Section 6 of the revised version (marked as* ***Change 2.4-2****)*

Comment 2.5: 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 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.

Changes in manuscript: ***We have fixed all the grammatical and formatting issues you pointed out.*** *We have also conducted several rounds of proofreading and substantially improved English presentation (**from the beginning to the end of our revised manuscript**). We don't mark these changes in the pdf file due to too many modifications.*

Comment 2.6: 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.*

Changes in manuscript: *The title has been changed to "Parameter Calibration in Global Soil Carbon Models Using Surrogate-based Optimization" in the revised version (marked as **Change 2.6**).*

Comment 2.7: 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.*

Changes in manuscript: *We clarify this point in Section 4.2 of the revised version (marked as **Change 2.7**)*

Comment 2.8: 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.*

Changes in manuscript: *We clarify this point and cite the references Hararuk, 2014 and 2015 in Section 2.2 of the revised version (marked as **Change 2.8**)*

Comment 2.9: 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.*

Changes in manuscript: *We give more description of radial basis function approach in the appendix (marked as **Change 2.9-1**) and also give more descriptions of the sampling methods in Section 3 of the revised version (marked as **Change 2.9-2**).*

Comment 2.10: Section 4.1: The authors state that the calibration process is repeated 50 times. How do you assure that 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.*

Changes in manuscript: *We clarify this point in Section 4.1 of the revised version (marked as **Change 2.10**).*

Comment 2.11: 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 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.*

Changes in manuscript: *We clarify this point in Section 4.2 of the revised version (marked as **Change 2.11**).*

Comment 2.12: 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. Global change biology, 2015, 21(6): 2439-2453.
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, 2014, 119(3):403-417.

Changes in manuscript: *We change the statement in Section 6 of the revised version (marked as **Change 2.12**).*

Comment 2.13: 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, to achieve the same optimization accuracy, the sample size the SBO requires is less than the Bayesian MCMC method and global optimization algorithms for parameter calibration task.*

Changes in manuscript: *We change the statement in Section 6 of the revised version (marked as **Change 2.13**).*

Parameter Calibration in Global Soil Carbon Models Using Surrogate-based Optimization

Haoyu Xu[1], Tao Zhang[1, 2], Yiqi Luo[2, 3], Xin Huang[1, 2], Wei Xue[1, 2]

[1]Department of Computer Science and Technology, Tsinghua University, Beijing 100084

[2]Department of Earth System Science, Ministry of Education Key Laboratory for Earth System Modelling, Tsinghua University, Beijing 100084

[3]Center for Ecosystem Science and Society, Northern Arizona University, USA

Correspondence to: Wei Xue (xuewei@tsinghua.edu.cn)

Abstract. Soil organic carbon (SOC) has a significant effect on the carbon emission and climate change. However, current SOC prediction accuracy of most models is very low. Most evaluation studies indicate that the prediction error mainly comes from parameter uncertainties, which can be improved by parameter calibration. Data assimilation technique has been successfully employed for parameter calibration of SOC models. However, data assimilation algorithms such as sampling-based Bayesian Markov Chain Monte Carlo (MCMC) generally require a large amount of computation cost and are not appropriate for complex global land models. This study proposes a new parameter calibration method based on surrogate optimization techniques for improving the prediction accuracy of SOC. Experiments on three types of soil carbon cycle models, including Community Land Model with Carnegie-Ames-Stanford Approach biogeochemistry sub-model (CLM-CASA') and two microbial models show that surrogate-based optimization method is more effective and efficient than MCMC on both accuracy and cost. Compared to the predictions using the tuned parameter values through Bayesian MCMC, the root mean squared errors (RMSEs) between the predictions using the calibrated parameter values with surrogate-base optimization and the observations could be reduced up to 12% for different SOC models. Meanwhile, the corresponding computation cost required is only one thousandth of that with Bayesian MCMC.

1 Introduction

Soil organic carbon (SOC) is the largest pool of global land carbon (Todd Brown et al., 2013; Luo et al., 2015). The emission of CO2, the most important greenhouse gas, from the land ecosystems greatly depends on the amount of carbon stored in soils. Simultaneously, more emitted CO2 increases the climate warming (Houghton et al., 2001) and the climate warming intensifies soil carbon release, resulting in a positive feedback cycle between the carbon cycle and climate warming (Melillo et al., 2003;

Friedingstein et al., 2006; Luo, 2007). In the fifth Coupled Model Intercomparison Project (CMIP5), the outputs of 11 Earth system models (ESMs) show great uncertainty in the SOC predictions and simulations. Despite the similarity in model structures (Huang et al., 2017), simulated soil carbon content varies six-fold among the models with the simulation results ranging from 510 to 3040 PgC (Todd-Brown et al., 2013). There are only half of 11 models whose the predicted global total SOC falls within the estimated range of the Harmonized World Soil Database (HWSD) and the highest correlation coefficient between the model output and the observation is even lower than 0.4 (Todd Brown et al., 2013; Luo et al., 2015).

Considering the high similarity in the carbon cycle component structures of the 11 ESMs, the difference of SOC simulations mainly comes from the parameterizations (Todd Brown et al., 2013); thus parameter calibration can improve the simulation of carbon cycle obviously (Luo et al., 2016). However, the parameter calibration with global observations has not been widely applied owing to the high computational cost. Take an example, the Bayesian Markov chain Monte Carlo (MCMC) algorithm has ever been used for parameter calibration of SOC simulation and microbial process successfully (Harauk et al., 2014 and 2015). Bayesian MCMC is a sampling-based approach and usually requires a large number of simulations for building an acceptable parameter chain. For instance, over 500,000 simulations are required during parameter calibration of soil carbon models (Harauk et al. 2014 and 2015). Even using high performance computer to provide the computation power, some carbon-enabled complex models, like the latest version of Community Land Model (CLM), require a very long spin-up time for carbon cycle simulation, leading to several hours or days for one simulation. Therefore, Bayesian MCMC cannot be extended to expensive global land models. More effective and efficient parameter calibration algorithms are intensively demanding.

Parameter calibration of SOC models can be formulated as an optimization problem that aims to minimize the output of a metric function. This metric function evaluates the difference between the outputs of model simulation and the corresponding observations and returns a single value (e.g. RMSE) to represent the model error. Global optimization algorithms are introduced to find the minimum value of the non-linear, non-convex and black-box problems (Hapuarachchi et al., 2001; Ma H, et al., 2006; Rocha H, 2008). Unfortunately, the number of required simulations of most global optimization is still very large.

To reduce the number of simulations and decrease the computational cost, we for the first time present the surrogate-based optimization method for calibrating the soil carbon models. Surrogate models serve as computationally cheap approximations of expensive simulation models (Booker et al., 1999), such as complex geoscientific models. During the optimization process, the surrogate model can be used to determine the new promising point in the parameter space at which originally the expensive simulation model has to be evaluated. With the help of surrogate model, many unnecessary simulations with bad parameter values, which lead to high prediction errors, are avoided. Surrogate-based optimization has been proved to be able to find the near-optimal parameter values within only few hundred simulations for different problems (Aleman et al., 2009; Giunta et al., 1997; Regis, 2011; Simpson et al., 2001).

Most studies on both global and surrogate optimizations focus on the mathematical function benchmarks like Comparing Continuous Optimisers, abbreviated as COCO (Hansen et al., 2010; Wang and Duan, 2014). However, the optimization of the mathematical functions may extremely different from the parameter calibration of complex real-world models. In this paper, for the first time, we try to exploit state-of-the-art surrogate optimization method for the parameter calibration of three types of soil organic carbon (SOC) models and compare the performance of surrogate-based optimization to advanced global optimization algorithms and the data assimilation method. The evaluation and analysis based on these representative SOC models prove that surrogate-based optimization has potential to be extended to other complex SOC models or even Community Land Model (CLM).

This paper is organized as follows. Section 2 presents the structure and parameters of three representative SOC models. In Section 3, we introduce the algorithm design of surrogate-based optimization. The parameter calibration results and the analysis of different parameter calibration algorithms are presented in Section 4. Section 5 discusses the calibrated results by using the surrogate-based optimization. Finally, we draw conclusions in Section 6.

2 Global Land Carbon Models and Metrics

Earth system models (ESMs) are the fundamental tools for simulating climate impacts on carbon cycle at the global scale and there are many similarities among structures of different ESMs. They define different carbon pools such as soil and litter pools. Carbon transfer among these pools by respirations (Todd Brown et al., 2013; Weng and Luo, 2011). In this study, we selected three types of SOC models. These models are summarized and extracted from global land models. They keep the key equations and structures of carbon transferring and can be regarded as the representative models in this field. The first model is the soil carbon component of the Community Land Model coupled with Carnegie-Ames-Stanford Approach biogeochemistry submodel (CLM-CASA') (Oleson et al., 2004, 2008). The CLM is the land model for the Community Earth System Model (CESM), which is a widely used earth system model in the world. It is also a collaborative project between scientists in the Terrestrial Sciences Section (TSS) and the Climate and Global Dynamics Division (CGD) at the National Center for Atmospheric Research (NCAR) and the CESM Land Model Working Group. The other two SOC models are microbial models. These two models consider microbial biomass dynamics explicitly which most conventional SOC models like CLM-CASA' don't take into account. The calibrated models explain more variability of the observed SOC (Hararuk et al., 2015). Considering the similarity in model structures, these three types of SOC models can represent the structures of the SOC components in most current land models (Luo and Weng, 2011).

2.1 CLM-CASA' C-only Version Model

The CLM-CASA' includes biogeophysics and biogeochemistry sub-models based on the CLM3.5. Carbon transferring among various plants, litter, and soil pools are simulated in the biogeochemistry sub-models (Parton et al., 1993). The influx and efflux of each pool determine the carbon content of that pool. Carbon influx into the whole system is partitioned into three live biomass pools. Carbon efflux is heterotrophic respiration which is determined by the decomposition rate of organic carbon in each pool. Heterotrophic respiration is influenced by environmental conditions (especially, temperature and soil moisture), soil texture, tissue lignin and available tissue nitrogen content.

The CLM-CASA' model simulates soil carbon decomposition as a first-order decay process (Todd-Brown et al., 2013b). Based on theoretical analysis, carbon cycle of most ESMs can be summarized to differential equations with linear coefficients (Luo and Weng, 2011; Xia et al., 2013).

$$\frac{dX(t)}{dt} = A\xi(t)KX(t) + BU(t) \quad (1)$$

Where $X(t)$ is the carbon content of different pools; $\frac{dX(t)}{dt}$ is the change of the carbon content; A is a matrix of partitioning coefficients among different pools; $\xi(t)$ and K are both diagonal matrixes, representing environmental factors and baseline carbon exit rates, respectively; $U(t)$ is the carbon influx into the whole system and B represents the partitioning coefficients of the carbon influx. The steady state solution of equation is given by Eq.2 (Xia et al. 2012):

$$X_{ss} = -(A\underline{\xi}K)^{-1}\underline{B}\,\underline{U} \quad (2)$$

Where $\underline{\xi}$, $\underline{B}$, and $\underline{U}$ are long-term averages of the environmental scalars, C partitioning among the three live pools, and NPP, respectively. The structure details of CLM-CASA' C-only model are presented in Fig. 1a and parameters are described in Table 1. The CLM-CASA' C-only version is the CLM-CASA' when we only consider the C processes of CLM 3.5. The steady state soil C generated by this C-only version agreed largely with that simulated by original CLM-CASA' model (Xia et al., 2012).

2.2 The Microbial Models

Microbial process has various kinds of effects on the land carbon cycle, such as the real priming effects and temperature increase caused by soil microbial biomass (Kuzyakov et al., 2000; Luo et al., 2001; Peng et al., 2009). However, most conventional SOC models including CLM-CASA' do not explicitly represent microbial processes. Considering the microbial processes, the SOC decomposition rate is controlled by extracellular enzyme concentrations rather than simple decay constants in the CLM-CASA' and other traditional SOC models (Schimel and Weintraub, 2003). In this study, we focused on two enzyme driven decomposition models, one has two pools (Fig. 1b) introduced by German et al. (2012) and Hararuk et al. (2015), and the other has 4 pools (Fig. 1c) introduced by Allison et al. (2010). We call these two models 2-pool microbial

model and 4-pool microbial model, respectively. The 2-pool microbial model is described as the following equations (Hararuk et al., 2014 and 2015).

$$\frac{dMIC}{dt} = CUE \times V_{max} \times MIC \frac{SOC}{K_m + SOC} - r_d \times MIC \quad (3)$$

$$\frac{dSOC}{dt} = Input_{soil} + r_d \times MIC - V_{max} \times MIC \frac{SOC}{K_m + SOC} \quad (4)$$

Where

$$CUE = CUE_{slope} \times T_s - CUE_0 \quad (5)$$

$$V_{max} = V_{max_0} \times exp\left(-\frac{E_a}{R \times (T_s + 273)}\right) \times exp(-par_{clay} \times clay) \quad (6)$$

$$Km = Km_{slope} \times T_s + Km_0 \times exp(par_{lig} \times lignin) \quad (7)$$

MIC represents the microbial biomass and SOC represents the soil organic carbon pool. $Input_{soil}$ is the carbon influx to soil. The other parameters listed in Table 2 are to be calibrated. Only the first eight ones in Table 2 are the parameters of the 2-pool microbial model.

The 4-pool microbial model from Allison et al. (2010) is described as follws:

$$\frac{dMIC}{dt} = V_{maxup} \times MIC \frac{DOC}{Kmup + DOC} \times CUE - r_d \times MIC - r_{EnzProd} \times MIC \quad (8)$$

$$\frac{dDOC}{dt} = a_{lit\text{-}to\text{-}DOC} \times Input_{soil} + r_d \times MIC \times (1 - a_{MIC\text{-}to\text{-}SOC}) + V_{max} \times ENZ \frac{SOC}{Km + SOC} + r_{EnzLoss} \times ENZ - V_{maxup} \times MIC \frac{DOC}{Kmup + DOC} \quad (9)$$

$$\frac{dSOC}{dt} = a_{lit\text{-}to\text{-}SOC} \times Input_{soil} + r_d \times MIC \times a_{MIC\text{-}to\text{-}SOC} - V_{max} \times ENZ \frac{SOC}{Km + SOC} \quad (10)$$

$$\frac{dENZ}{dt} = r_{EnzProd} \times MIC - r_{EnzLoss} \times ENZ \quad (11)$$

Where

$$CUE = CUE_{slope} \times T_s - CUE_0 \quad (12)$$

$$V_{maxup} = V_{maxup_0} \times exp\left(-\frac{E_{aup}}{R \times (T_s + 273)}\right) \quad (13)$$

$$Kmup = Kmup_{slope} \times T_s + Kmup_0 \quad (14)$$

$$V_{max} = V_{max_0} \times exp(-\frac{E_a}{R\times(T_s+273)}) \times exp(-par_{clay} \times clay) \quad (15)$$

$$Km = Km_{slope} \times T_s + Km_0 \times exp(par_{lig} \times lignin) \quad (16)$$

ENZ and *DOC* are enzyme and dissolved organic carbon pools, respectively. Compared to the 2-pool version, the 4-pool microbial model has additional 7 parameters to be calibrated. Total 15 parameters of the 4-pool microbial model are described in Table 2.

2.3 Data and Metrics

Microbial models and CLM-CASA' C-only models divide the world into 64*128 grid cells and output SOC content at each grid (Fig. 2). The observed SOC data for parameter calibration comes from the International Geosphere Biosphere Programme – Data and Information System (IGBP-DIS) dataset (Global Soil Data Task Group, 2000). The IGBP-DIS dataset includes a 1-km resolution global land carbon data set and the dataset has been widely used in many studies to evaluate and improve models (Zhou et al., 2009; Smith et al., 2013).

The goal of parameter calibration is to improve SOC predictions to better fit the observations. Therefore, we use the root mean squared errors (RMSEs) between the model SOC predictions and the observations at all grid cells as the metric function. This metric function can be described as the following formula:

$$r = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(X_i - O_i)^2} \quad (17)$$

Where N denotes the total number of grid cells, X_i and O_i are the SOC of model prediction and IGBP-DIS observation, respectively. To avoid overfitting and evaluate the calibrated parameters more fairly, we separate all grid cells into training set and validation set. The training set is used to guide the parameter calibration process and the validation set is used to evaluate the calibrated results. Hararuk et al. (2014 and 2015) also used this method when calibrating SOC parameters with the Bayesian MCMC approach. The experiment results in Section 3 and 4 refer to the results for the validation set.

3 Surrogate-Based Optimization Algorithm Design

3.1 Introduction to Surrogate-Based Optimization Algorithm

The parameters of most soil carbon models and land models are tuned manually or based on gradient searching algorithms. Manual tuning method might be effective but highly depends on expert experience. Moreover, complex models may consist

of various components from different disciplines and then require different experts working collaboratively during tuning process.

Considering the difficulty of manually tuning scheme, different parameter calibration algorithms have been developed based on optimization theory. The gradient search algorithms like the quasi-Newton method are introduced to search a set of parameters with better performance in the parameter domain. The gradient search algorithms are usually efficient and fast. However, the gradient search algorithms are designed for finding the local optimum. Essentially it cannot be used to solve the multimodal problems derived from complex earth system models. In addition, the gradient search algorithms are based on the gradient information, which is unavailable for most soil carbon and land models. These models are too complex to get the gradient information, and thus the parameter calibration usually leads to solving a black-box optimization problem. Global optimization algorithms, such as genetic algorithms, particle swarm optimization algorithms, are based on parameter generation and selection strategies and keep gradient independent, which can be easily used for parameter calibration of complex earth system models. Global optimization algorithms are designed to find the global minimum. However, for complex models with large number of parameters, the number of samples (model runs) might be too large to comfortably afford (Jones et al., 1998). Moreover, complex earth system models, for example CLM, require several hours over hundreds of cores for only one sample run and pose a special challenge to the feasibility of automatic parameter calibration.

The surrogate-based optimization is an efficient and effective automatic parameter calibration framework. The surrogate-based optimization fits a surrogate model (or response surface) based on the previous samples and use this surrogate model to emulate the output behaviours of original models with an acceptable accuracy. The main idea of the surrogate-based optimization is to save computational cost during global optimization process by using the surrogate model instead of the original model, and to continuously improve the surrogate model by exploiting new sample runs with the original model. With the surrogate model, the algorithm can make full use of previous samples information and reduce the sample size, time-to-solution as well as the computation cost. The surrogate-based optimization is proved to be successful in solving parameter calibration of computationally expensive black-box problems (Vu et al., 2016).

3.2 Key Components of Surrogate-Based Optimization Algorithm

The flowchart of the surrogate-based optimization (referred as SBO hereafter) is presented in Fig. 3. Firstly, initial sets of parameter values are generated using a sampling method. These sets are then used as inputs to run the real simulation model. Secondly, a surrogate model is constructed by fitting the outputs of these sample runs. The surrogate model serves as a computationally cheap approximation of the expensive simulation model (Booker et al., 1999). Then in each iteration, new sample points simulated by the real model are generated according to specific strategy. This strategy can make use of the information gained from the surrogate model and only exploits the avoidable real model runs to meet the accuracy requirement. The new sample points and their simulation outputs are used to update the surrogate model at the same time. Finally, when

some stop criteria (usually the maximum number of simulations allowed) are met, the algorithm return the optimized parameter values. During the surrogate-based optimization process, quite a few sample runs are generated based on the evaluation of the surrogate model and most meaningless simulations with terrible parameter values are avoided. As a result, the computationally expensive model is simulated at only a few selected promising parameter points and the surrogate model will replace the real model during the calibration process; thus the computation cost is reduced substantially.

There are three key components in the surrogate-based optimization algorithm: the surrogate model, the initial sampling and the parameter point generation for real model run. There are various surrogate models such as multivariate adaptive regression splines (Friedman, 1991), polynomial regression models (Myers and Montgomery, 1995), radial basis functions (RBFs) (Gutmann, 2001; Müller et al., 2013; Powell, 1992; Regis and Shoemaker, 2007, 2009; Wild and Shoemaker, 2013), kriging (Davis and lerapetritou, 2009; Forrester et al., 2008; Jones et al., 1998). Many machine learning regression models are also introduced like support vector regression (Zhang et al., 2009), artificial neural network (Behzadian et al., 2009) and random forest (Breiman, 2001).

As for the initial sampling, the Monte Carlo sampling and Latin Hypercube sampling (LHS for short) are two main sampling methods (McKay et al., 1979; Iman et al., 1981). The Monte Carlo sampling samples values from a probability distribution, which is usually a uniform distribution unless we have additional knowledge about the model and the parameters. During LHS procedure, the range of each parameter is divided into M equally probable intervals. M sample points are selected to cover all intervals of each parameter. Compared to the random sampling, LHS ensures that the ensemble of random numbers is representative of the real variability of the parameters.

The strategies of parameter point generation are iterative algorithms that use data acquired from previous iterations to guide new parameter point generation. Most strategies convert the parameter point generation to optimization problems using an evaluation criterion (Fig. 3). There are many different generation strategies, including Minimizing an Interpolating Surface (MIS) (Jones, 2001) and Maximizing Expected Improvement (MEI) (Schonlau et al., 1997; Picheny et al., 2013). In MIS, the minimum of the surrogate model response surface is found and treated as the new parameter point to evaluate the real simulation model and then update the surrogate model. MEI introduces the “expected improvement” criterion. This criterion estimates the uncertainty of the surrogate model and balances the exploration and exploitation. Another parameter generation strategy is candidate point approach (CAND) (Regis and Shoemake, 2007). In the CAND strategy, the criterion for exploitation is MIS and the criterion for exploration is the distance of the candidate point to the set of sampled parameter points from previous iterations. The previous sampled points represent the explored region and we can estimate the uncertainty with the distance to the explored region. A weighted sum of these two criteria is used to determine the new parameter point during the surrogate-based optimization.

3.3 Design of Surrogate-Based Optimization Algorithm for Soil Carbon Models

Based on the previous introduction of SBO, the detailed procedure of SBO can be found as follows. It is worthy noted that the best parameter set of the real model can be iteratively searched in Step 4 during looking for the new sample points.

Step 1: Generate an initial sampling set S_0.

Step 2: Run the real model and calculate the output error of the parameter points of S_0.

Step 3: Build the surrogate model using the parameters and the outputs generated in Step 2.

Step 4: Predict the output errors of those points which do not belong to S_0 using the surrogate model and determine the points at which to run the real model.

Step 5: Run the real model again for the new parameter points of Step 4 and calculate the output errors of these selected points.

Step 6: Update the surrogate model with the new data of Step 5.

Step 7: Iterate through Steps 4 to 6 until the end condition has been met.

The surrogate-based optimization scheme mentioned in previous sections is a parameter calibration framework, and the key components introduced in Section 3.2 have to be selected during tuning the parameters of soil carbon models. We assume that the soil carbon models (especially together with land model) are computationally expensive and at most several hundred samples can be afforded. The LHS can cover the whole parameter space with limited number of sample points while Monte Carlo sampling usually requires much larger number of samples. Therefore, we choose the LHS as the initial sampling strategy. As mentioned in the previous section, many kinds of surrogate-based models have been introduced and developed. The Machine learning regression models perform not so well as RBF and kriging models according to the evaluation on similar cases (Wang et al., 2014). In this study, we use the RBF surrogate model (RBF-SBO) as our default choice because it has been proved to perform better than other surrogate model types (Müller and Shoemaker, 2014) and has easy-to-use implementation. Moreover, we also implement other surrogate models including Kriging and Mars in our algorithm framework and can also introduce other advanced surrogate models later.

The soil carbon models are usually complex, nonlinear and not smooth and the surrogate model are not accurate when the SBO starts. The MIS can be very efficient but easy to trap into local optima, since the strategy does not consider the uncertainty of the surrogate model and only select the optimum of the surrogate model. The MEI eliminates the disadvantage of MIS but can only be used for the kriging surrogate model because the calculation of the expected improvement requires the standard error at the parameter point and only the kriging (Gaussian Process) surrogate model can provide the standard error (Jones et al., 1995). Finally, we use the CAND strategy as the parameter generation strategy in our algorithm, which has the advantage of balancing the exploitation and exploration of uncertain region.

4 Parameter Calibration Experiments

4.1 Experiment Configuration

In this study, we select the Bayesian MCMC approach and four advanced global optimization algorithms to compare with our proposed surrogate-based optimization method. Three types of SOC models and their metric functions are introduced in Section 2. The target of parameter calibration is to find the optimal values of parameters to achieve the minimum value of the metric function (average RMSE). Moreover, we repeat the parameter calibration process of each algorithm 50 times and use the average results for algorithm evaluation. We compare the performance of algorithms from both the effectiveness and efficiency. The effectiveness refers to the accuracy of the calibrated results and the efficiency can be evaluated by the required simulation times of the original SOC models.

4.2 Various Global Optimization Algorithms and the Bayesian MCMC Approach

The Bayesian MCMC approach and four advanced global optimization algorithms, including Differential Evolution (DE), Particle Swarm Optimization (PSO), Shuffled Complex Evolution (SCE-UA) and Covariance Matrix Adaption Evolution Strategy (CMA-ES), are used to compare with our RBF surrogate-based optimization.

DE (Storn and Price, 1997) and PSO (Kennedy, 1995; Shi and Eberhart, 2009) are the representative algorithms of the evolution strategy and swarm intelligence, respectively. They both have the ability to converge quickly and outperform many genetic algorithms and simulated annealing algorithms (Price and Storn, 2006; Shi and Eberhart, 2009). SCE-UA is designed for the parameter calibration of hydrologic models and has gained success in various hydrology models such as the TOPMODEL, the Xinanjiang watershed model and short-term load forecasting (Hapuarachchi et al., 2001; Ma H, et al., 2006; Li G, et al., 2007). SCE-UA ensures the effectiveness and efficiency by combining the local (the simplex method) and global optimization methods. Despite the difference in detail, DE, PSO and SCE-UA all generate new parameter points according to some simple mathematical formulas. Different from these three algorithms, CMA-ES (Hansen and Ostermeier, 2001; Hansen and Kern, 2004) creates new parameter points based on a multivariate normal distribution. The dependencies between parameters are represented by the covariance matrix of a normal distribution. CMA-ES has been proven to be the best global optimization algorithm in the BBOB-2009 comparison study (Hansen, 2009).

The Bayesian MCMC approach is usually designed to obtain the posterior distributions of model parameters but it can also be used to calibrate parameters to reduce the prediction error. The Bayesian MCMC approach consists of two steps: the proposing step and the moving step. In the proposing step, the parameter covariance matrix is estimated from a series of parameter sets. A new parameter set is generated from the last accepted parameter set through a uniform proposal distribution (Xu et al., 2006). In the moving step, a probability of acceptance determined by prediction error is calculated (Marshall et al., 2004). The final calibrated parameter set is estimated by Maximum likelihood estimator (MLE) with an accepted parameter chain. Hararuk et

al. (2014, 2015) applies the Bayesian MCMC approach using the Metropolis algorithm to parameter calibration of the CLM-CASA' C-only model and microbial models. During the experiments of Hararuk et al. (2014, 2015), the proposing step requires 50,000 simulations and the moving step requires 500,000 simulations for microbial models and 1,000,000 simulations for the CLM-CASA' model. We have got the code from Hararuk and repeated the calibration experiments. The detailed calibration results with the Bayesian MCMC approach are presented in Table 3.

4.3 Results and Analysis

4.3.1 Effectiveness and Efficiency

Fig. 4 presents the calibrated results (RMSE) of different algorithms we applied. For each algorithm, we only perform 100 simulations for comparison. As the Bayesian MCMC approach requires a large number of samples to reach a stable distribution, over 500,000 simulations have been conducted for algorithm evaluation.

Obviously, the average RMSE of the RBF-SBO is the lowest (0.6 kg/m^2 better than the Bayesian MCMC algorithm) for two microbial models among all the algorithms (Fig. 4b, c). For the CLM-CASA' model, our RBF-SBO algorithm is still the best one compared to the global optimization algorithms. And the Bayesian MCMC approach gets a little better result (about 0.02 kg/m^2) since it has to conduct a lot more simulations for better result (Fig. 4a).

With respect to stability, the results of RBF-SBO also shows a lower variation among the 50 repeated experiments compared with the global optimization algorithms on three types of models. For the same reason mentioned before, the Bayesian MCMC approach gets lower variation than our RBF-SBO algorithm on two microbial models. For the most complicated CLM-CASA' model, our RBF-SBO is still promising on stability. Among the global optimization algorithms, the CMA-ES shows a very significant fluctuation (Fig. 4b, c), indicating CMA-ES is unreliable when the number of simulations is as small as 100. This is because the CMA-ES requires quite a few simulations on the exploration of the parameter domain and the construction of the parameter covariance matrix. Therefore, the RBF surrogate-based optimization is the most effective and stable one when the number of simulations is limited.

Fig. 5 shows the results in terms of average validation RMSE. The Bayesian MCMC is not shown here because it requires at least 50000 simulations in the proposing step. The average validation RMSE of RBF-SBO is lower than other four global optimization algorithms before the number of simulations increases to 600 for two microbial models and to 200 for the CLM-CASA' model, respectively. The number of simulations our RBF-SBO requires is fewer than other global optimization algorithms when they reach the same RMSE value and accuracy range. Thus, our RBF surrogate optimization is also the most efficient algorithm which requires the minimum simulation times and computation cost. The reason why our SBO outperforms other global optimization algorithms is that our SBO can enhance the searching efficiency by using a surrogate model to simulate the real model and avoiding bad parameter points ('bad' means the high prediction error). Moreover, the setup scheme

of our SBO also contributes to the superiority of our algorithm, which conducts several sample runs and selects the good parameter sets for use.

Another important observation is that the difference between the results of our RBF-SBO and other global optimization algorithms decreases as the number of simulation increases (Fig. 5). Moreover, the CMA-ES outperforms the RBF-SBO when the number of simulations exceeds 200 for the CLM-CASA' model (Fig. 5a). Our SBO can build the surrogate model with relatively good accuracy quickly, which contributes to finding the near-optimal solution with less computation cost. However, the surrogate model is only an approximation of the real model and the accuracy might be limited due to the strong nonlinearity and the high complexity of the real model. After gaining enough knowledge of the real model by lots of simulations, the excellent global optimization algorithms, such as CMA-ES, may achieve a similar performance or even outperform our SBO, which suggests that our SBO is better to use for parameter calibration problem of cost-expensive models such as CLM.

4.3.2 Impact of the Model Complexity

Compared to the 2-pool and 4-pool microbial models, the CLM-CASA' model has 13 carbon pools and 20 parameters and thus it is significantly more complex than two microbial models. Despite increasing complexity of the CLM-CASA' model, the SBO gets better results before conducting 200 simulations of the real model (Fig. 5a). Moreover, our SBO is always the best parameter calibration method for the 2-pool and 4-pool microbial models before conducting 600 simulations (Fig. 5b, c). In addition, only one global optimization algorithm, CMA-ES, shows better performance compared to our SBO on the CLM-CASA' model after 200 simulations. Considering the high variance of CMA-ES on two microbial models (Fig. 4b, c), our SBO is more effective and more reliable on average.

4.3.3 Impact of Different Types of Surrogate Models

We select the RBF as the surrogate model in the former experiments because the RBF is the promising choice in many surrogate-based optimization algorithms (Müller and Shoemaker, 2014). In this section, we also test two other typical surrogate models, kriging and the multivariate adaptive regression splines (Mars). The Mars model is simple and has almost no requirements to the sample quality. Mars is very quick to train and predict. The kriging, also Gaussian process regression, is a method of interpolation for which the interpolated values are modelled by a Gaussian process governed by prior covariance. Kriging gives the best linear unbiased prediction of the intermediate values under suitable assumptions on the priors.

Figure 6 presents the results of kriging, Mars and RBF in terms of average validation RMSE. The performance of the three surrogate models is similar. The three surrogate models all get reasonable performance in the parameter calibration of the three types of SOC models and perform better than global optimization algorithms, indicating that our surrogate-based optimization is robust.

5 Analysis of Parameter Calibration Results

5.1 Analysis of CLM-CASA' Model

The steady state global SOC simulations (Eq. 2) using CLM-CASA' with the default and calibrated parameter values are presented in Fig. 7a and b, which are also compared to the observed SOC pools provided by the IGBP-DIS dataset. The SOC simulation result using the calibrated parameter values obtained by the surrogate-based optimization matches the observation better than that with the default parameter values (Fig. 7c) with a relatively lower RMSE. By using the calibrated parameter values, the SOC simulations are significantly improved almost all over the world, except some grid cells in the west of Canada and the east of Russia (Fig. 7a, b and c). As a result, the CLM-CASA' simulation result with the default parameter values can only explain 33% of variation in the observed soil C, whereas that with the calibrated parameter values can explain an improved ratio (42%) of variation in the observed soil C. The unexplained variation is partly due to uncertainty in observations. To further improve the model accuracy, we need to gain more understanding of uncertainty sources from data, model structure, parameters, and forcing.

Figure 8 presents the frequency distributions of the 20 calibrated parameters based on MCMC and the calibrated parameter values by using the proposed surrogate-based optimization (the blue lines in Fig. 8). Narrow posterior distributions indicate highly sensitive parameters, agreeing with the conclusions of Hararuk et al. (2014) and Post et al., (2008). The calibrated parameter values of the surrogate-based optimization are close to the responding parameter values at the peaks of posterior distributions for most highly sensitive parameters such as temperature sensitivity of heterotrophic respiration (Q_{10}) and clay effect on C partitioning from slow to passive pools (t_7). The parameter calibration results (RMSE) of the surrogate-based optimization and Bayesian MCMC are similar, agreeing with the parameter calibration results listed in Table 3.

Some calibrated parameter values are very close to the assigned bounds of the parameters in Fig. 8, which is usually related to the correlations among parameters. Further investigation on the covariance among parameters is necessary to explain this issue. In addition, the unreasonable setting of those bounds might be another possible reason. For instance, the calibrated c(12,12) value (1.01×10^{-3}) reaches its lower bound, indicating that passive SOC residence time almost approaches 1000 years.

As listed in Table 1, the calibrated temperature sensitivity (Q_{10}) decreases from 2 to 1.74. The size of soil microbial and passive pools increase due to longer residence time of passive pool and lower temperature sensitivity (Q_{10}). The size of the slow pool, on the contrary, decreases due to the increase in exit rate from slow pool or the decrease of its residence time. Comprehensively, the size of SOC, which is the sum of carbon capacity in passive pools, slow pools and soil microbial pools, increases and more approximates to the observation.

5.2 Analysis of Microbial Models

According to the calibrated RMSE and r^2, the SOC simulation of the 2-pool and 4-pool microbial models are very similar. Without loss of generality, we only analyze the parameter calibration results of the 4-pool microbial model in this section. After parameter calibration using the surrogate-based optimization, the global SOC produced by the 4-pool microbial model are improved, especially in the regions of China, Russia, Europe and North America (as shown in Fig. 9). Overall, the microbial models explain a higher fraction of global variability of the observed SOC data and have lower spatial RMSEs than the CLM-CASA' model (as listed in Table 3).

The microbial models achieve better SOC predictions than that of the calibrated CLM-CASA' model in terms of the prediction of C capacity in the low-temperature regions (Russia, Europe, North America) and in the regions with small soil C inputs (Fig. 7b and 9). The SOC contents are determined by two main factors: the soil carbon inputs and the SOC residence time (Luo et al., 2003). Considering the same soil carbon inputs of the CLM-CASA' and the microbial models, the improvement is mostly induced by the differences of SOC residence time. In all the three models, the SOC residence time is essentially controlled by temperature (Xia et al. 2013). As a result, the temperature sensitivity (Q_{10}) contributes to the difference across three models. The temperature sensitivity keeps constant in the CLM-CASA'. However, both of two microbial models calculate spatially variable Q_{10} with higher values in the low-temperature regions and lower Q_{10} in the high-temperature regions, which reflects the impact of the temperature to the microbial activity. In addition, the SOC residence time can also be affected by the quality of SOC inputs and is related to the microbial decomposition processes. Fresh C input stimulates the microbial dynamics growth, resulting in the increase of old SOC decomposition rate (i.e., priming effect) (Kuzyakov et al, 2000; Fontaine et al., 2004, 2007). Therefore, the microbial models simulate lower SOC residence times than the CLM-CASA' in the regions with high SOC input and high SOC residence time and the regions with low SOC input. This is due to the nonlinearity of substrate limitation in the microbial models (Eq. 8 and 10), as well as the dependency of residence time in microbial dynamics. Comprehensively, the introduction of microbial dynamics helps the microbial models predict SOC better than the CLM-CASA' model.

Figure 10 presents the posterior distributions of the parameters calculated by Bayesian MCMC and the calibrated parameter values by our surrogate-based optimization. According to the posterior distribution, r_d, CUE_{slope}, CUE_0, E_a, par_{lig} and par_{clay} are the most constrained and sensitive parameters. The calibration results of the surrogate-based optimization agree with the posterior distributions of these highly sensitive parameters (Fig. 10) except CUE_{slope} and CUE_0. CUE_{slope} and CUE_0 are highly sensitive owing to their influence on temperature sensitivity. Due to the difference between CUE_{slope} and CUE_0, the RMSE of the surrogate-based optimization is 1.4 kg/m^2 and 0.8 kg/m^2 lower than those with Bayesian MCMC for 4-pool and 2-pool microbial models respectively (as listed in Table 3). The mismatch of CUE_{slope} and CUE_0 may be mainly due to the different targets of the parameter selection between two methods.

6 Conclusions

Parameter calibration becomes more and more challenging for SOC model development, especially for the computationally-expensive global land models owing to large number of simulations. In this study, we introduce a surrogate-based optimization algorithm to the parameter calibration of computationally expensive SOC models. The main findings are:

1) Compared to advanced global optimization algorithms, the surrogate-based optimization is more effective and more efficient on average. Our RBF surrogate-based optimization outperforms other parameter calibration algorithms when the number of simulations is no more than 200.
2) The parameter optimization based on RBF surrogate model gains more accurate calibration results than those of the Bayesian MCMC approach in the three soil carbon models. Moreover, the computation cost of the surrogate-based optimization is only 0.1% of that of the Bayesian MCMC.
3) The surrogate-based optimization scheme is robust. Various types of surrogate models have the similar performance in parameter calibration tasks of SOC models.
4) Although the surrogate-based optimization is only guided by a single metric function, it still can find better parameter values compared to the default ones. We carefully analyze the spatial SOC distributions produced by the SOC models with the calibrated parameters using our surrogate-based optimization, which indicates that the surrogate-based optimization truly improves the model prediction and simulation capability.

Nowadays, more and more complex simulation models present challenges to the surrogate-based optimization algorithm. To improve the accuracy of the surrogate-based optimization, better surrogate models are expected. Current surrogate models including our implementation for soil carbon models most employ only one surrogate model, which may limit the successful use for different kinds of models. We will focus on the application of multiple surrogate models using ensemble learning in the future.

7 Code and data availability

The code and data of three models and the related algorithm implementations can be found in the supplement. If you have any problem when using the code and repeating the experiments, please feel free to contact the first author of this paper: Haoyu Xu (ocean920329@gmail.com).

Appendix: The detailed description of the proposed Surrogate-Based Optimization algorithm

The parameter calibration of the soil carbon models can be formulated to the following optimization problem:

$min_{x \in D} \{f(x)\}$

In which, $f: R^d \rightarrow R$ is a continuous black-box function, representing the prediction error of the real model. And D is a subset of R^d, representing the legal ranges of parameters. A parameter can be represented as a point in R^d. The surrogate-based optimization algorithm conducts several steps as follows.

1. Generate an initial sampling set S_0.
2. Run the real model and calculate the output error of the parameter points of S_0.
3. Build the surrogate model using the parameters and the outputs generated in Step 2.
4. Predict the output errors of those points which do not belong to S_0 using the surrogate model and determine the points at which to run the real model.
5. Run the real model again for the new parameter points of Step 4 and calculate the output errors of these selected points.
6. Update the surrogate model with the new data of Step 5.
7. Iterate through Steps 4 to 6 until the end condition has been met.

Different surrogate-based optimization algorithms may have different choices with respect to the follows:

- ✧ The sampling method to generate the initial set S_0.
- ✧ The surrogate model, which predicts the output y using the given data point x. Before prediction, some (x, y) data pairs should be given to train the model and the data is called training set.
- ✧ How to decide the new points at which to run the real model in each iteration.

As introduced in Section 3, we use Latin hypercube sampling (LHS) to generate the initial set S_0 (Iman et al., 1981). As for the surrogate model, we compare three kinds of surrogate models including Kriging, Mars and RBF.

The Mars model (abbreviation of multivariate adaptive regression splines) is an extension of naïve linear models, which introduced by Friedman J H. (Friedman J H., 1991). The form of Mars is presented as follows:

$$\hat{f}(x) = \sum_{i=1}^{m} c_i B_i(x)$$

Where $\hat{f}(x)$ represents the prediction of y at the point x, and c_i is a constant coefficient to be trained. The $B_i(x)$ is the basis function which can take one of the three forms: a constant, a hinge function like $max\ (0, x - const)$ and a product of more than one hinge function.

The RBF model (abbreviation of radial basis function) is a real-valued function. The prediction at a point x using RBF model only depends on the distance between x and other points in the training set, whose outputs have been already given. The distance $r = \|x, c\|$ is usually Euclidean distance. The radial function is the function satisfies the property $\phi(x, c) = \phi(\|x, c\|) = \phi(r)$. The prediction at point x with RBF model is formulated as:

$$\hat{f}(x) = \sum_{i=1}^{N} w_i \, \phi(\|x, x_i\|)$$

Where the x_i represents the point of the training set which has N points in total. Many different radial functions have been introduced and some commonly-used ones are Gaussian $\phi(r) = e^{-(\varepsilon r)^2}$, Multiquadric $\phi(r) = \sqrt{1 + (\varepsilon r)^2}$, and Polyharmonic spline: $\phi(r) = r^k ln(r)$. In our experiments, we choose the Gaussian radial function.

Both the Kriging model and the Gaussian process regression model predict the output using a Gaussian process governed by prior covariance. Before used to train the kriging model, the x and y should be normalized to satisfy a normalization distribution where the means is 0 and the covariance is 1. The Kriging predictor can be found as follows:

$$\hat{f}(x) = \hat{\mu} + \sum_{i=1}^{n} c_i r_i(x)$$

Where $\hat{\mu}$ is the estimated mean of the gaussian process, c_i is a constant representing the weight and $r_i(x) = Corr(x, x^{(i)})$ is the correlation between the x and the ith point $x^{(i)}$ in the training set. $\hat{\mu}$ and c_i can be trained with the training set.

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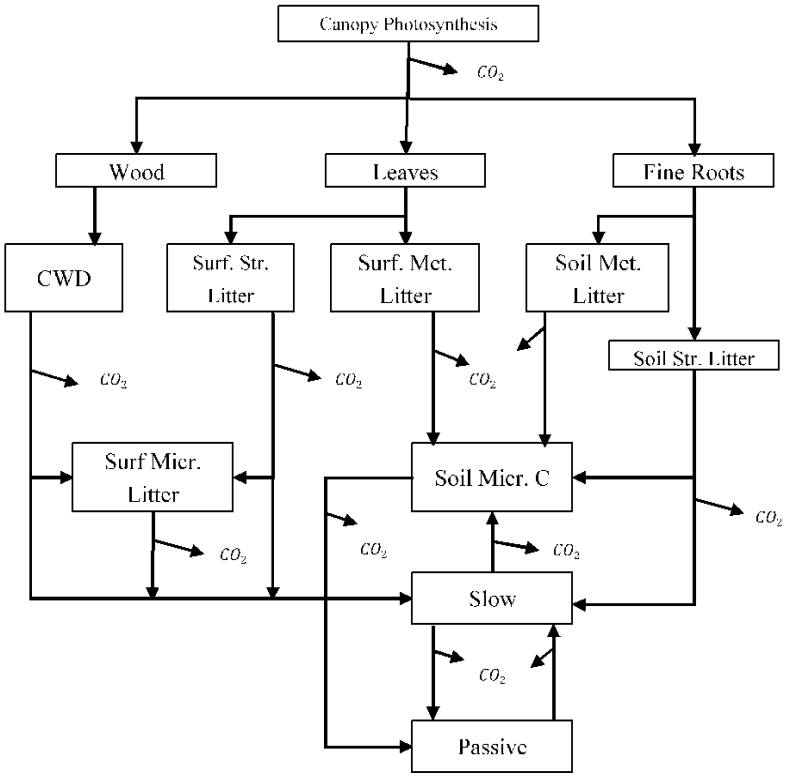
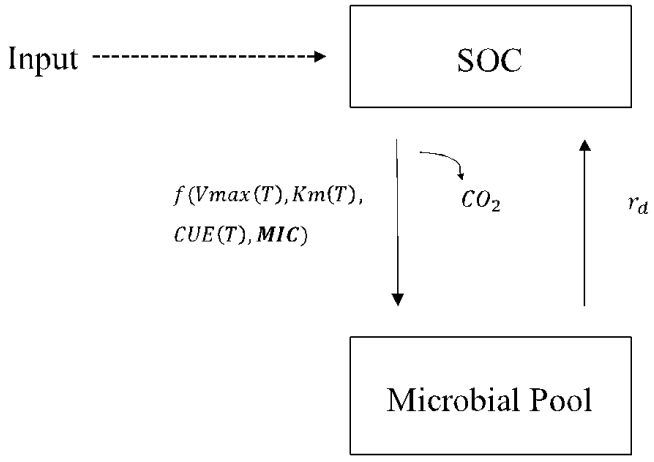
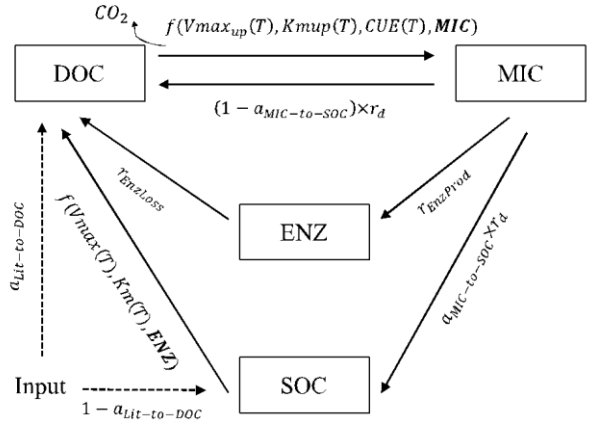


(a) **The CLM-CASA' model**



(b) **2-pool microbial model**



(c) **4-pool microbial model**

Figure 1. Schematic representations of (a) CLM-CASA model, (b) 2-pool microbial model and (c) 4-pool microbial models

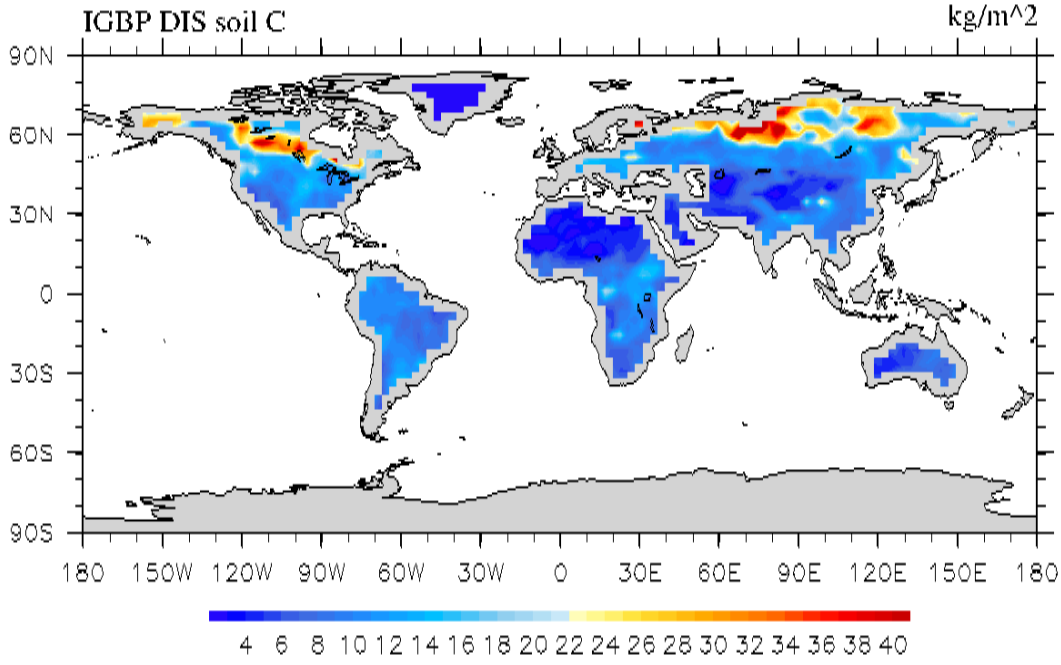


Figure 2. IBGP-DIS soil carbon distribution. Soil carbon varies from 0 kg/m^2 in deserts to 60 kg/m^2 in boreal regions

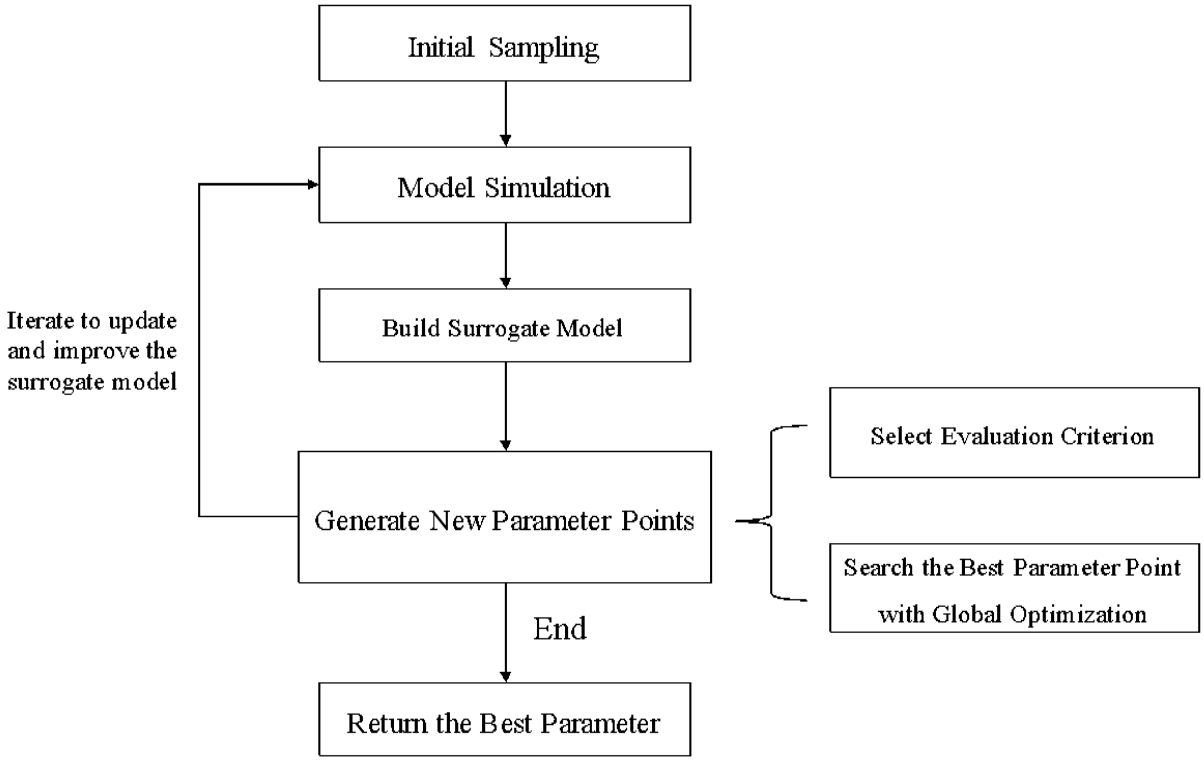
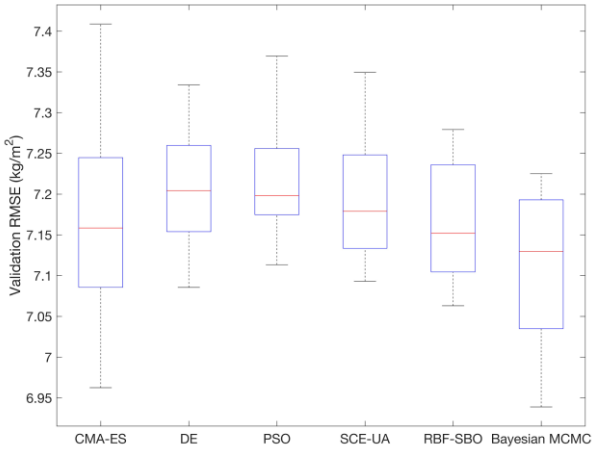
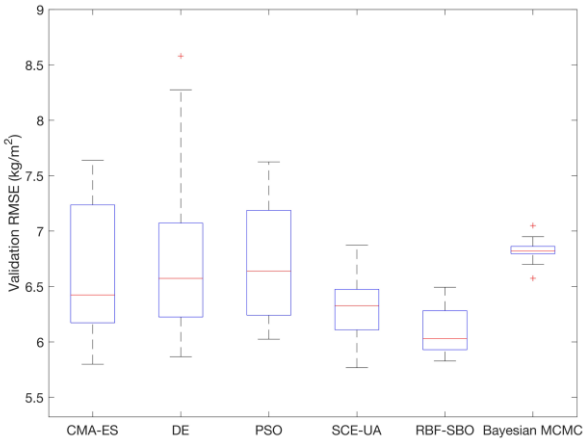


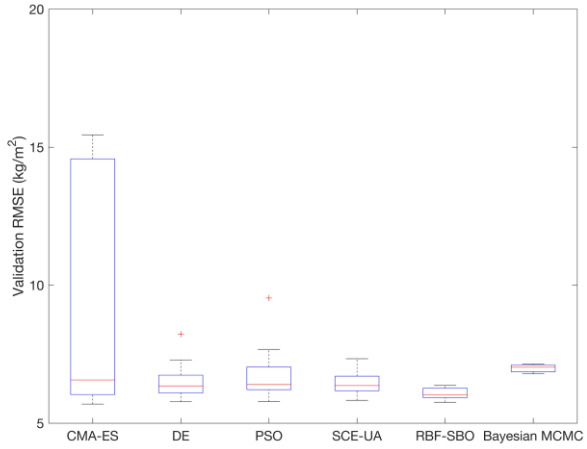
Figure 3. The flowchart of the surrogate-based optimization



(a) CLM-CASA' model

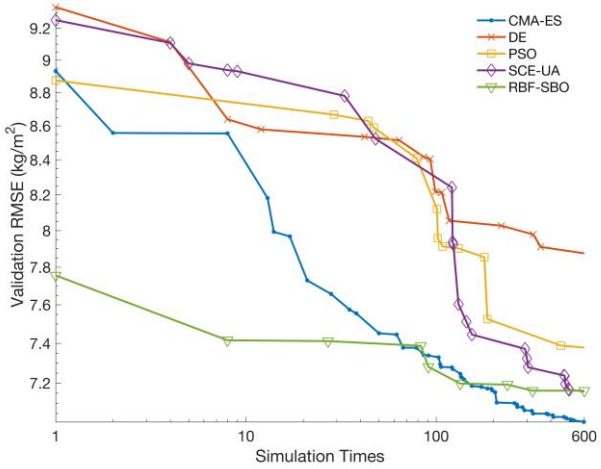


(b) 2-pool microbial model

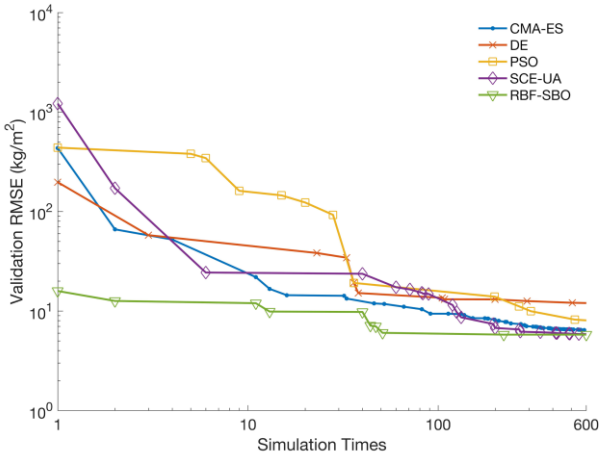


(c) 4-pool microbial model

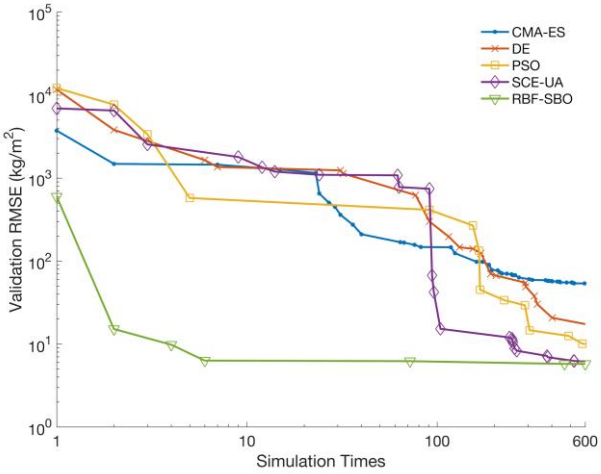
Figure 4. The RMSEs of different optimization algorithms: (a) CLM-CASA' model; (b) 2-pool microbial model and (c) 4-pool microbial model. The box plots show the means and the quartiles spreading over total 50 calibration runs. The central line indicates the median; the bottom and top of the box are the first and third quartiles; the black bottom and top lines out of the rectangles are the maximum and minimum; the red crosses represent the outliers. The simulation times of former 5 algorithms are 100 and the simulation times of Bayesian MCMC are presented in Table 3.



(a) The RMSEs for CLM-CASA' model

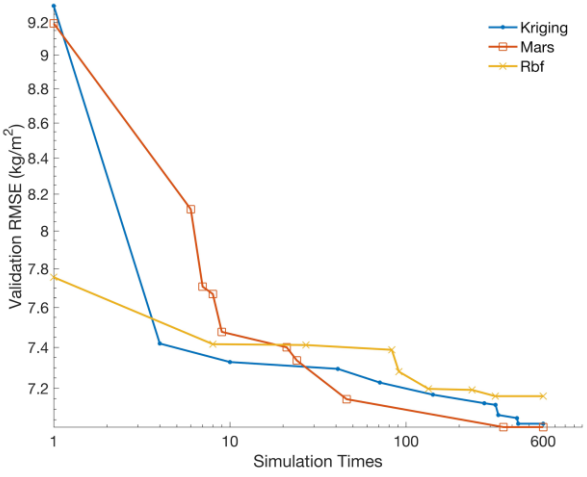


(b) The RMSEs for 2-pool microbial model

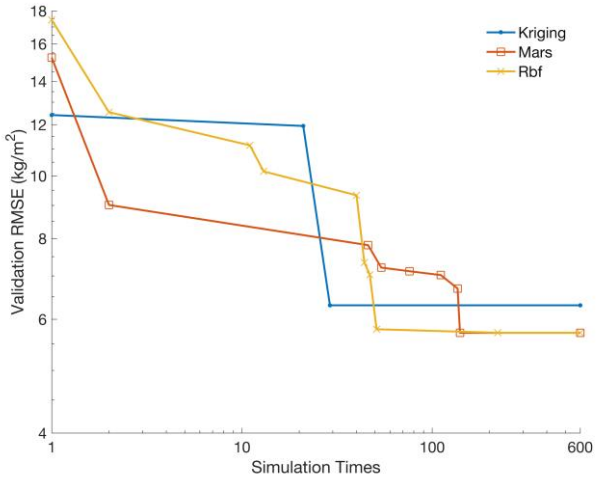


(c) The RMSEs for 4-pool microbial model

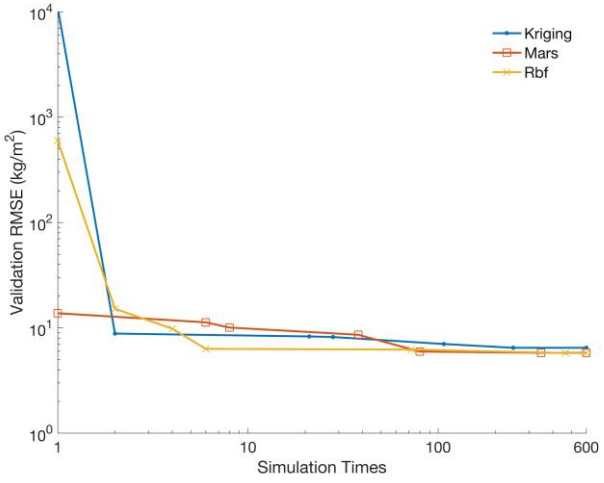
Figure 5. The average RMSEs with the increase of simulation times and different optimization algorithms: (a) the CLM-CASA' model; (b) 2-pool microbial model and (c) 4-pool microbial model.



(a) The RMSEs for CLM-CASA' model

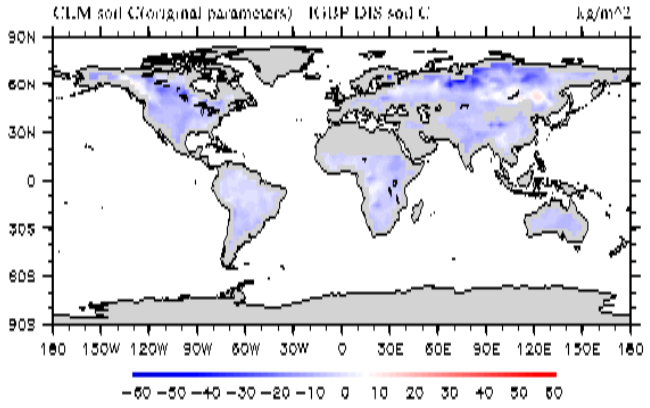


(b) The RMSEs for 2-pool microbial model

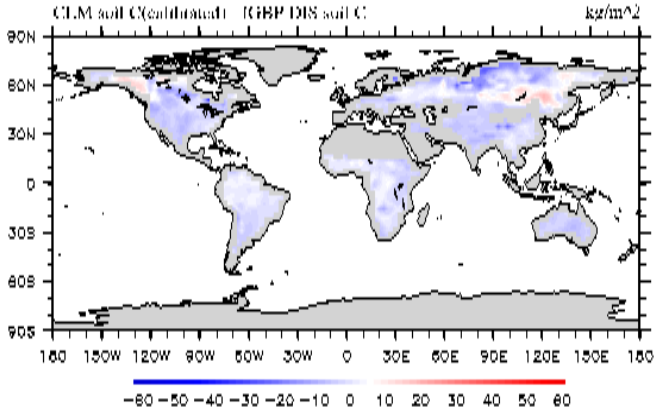


(c) The RMSEs for 4-pool microbial model

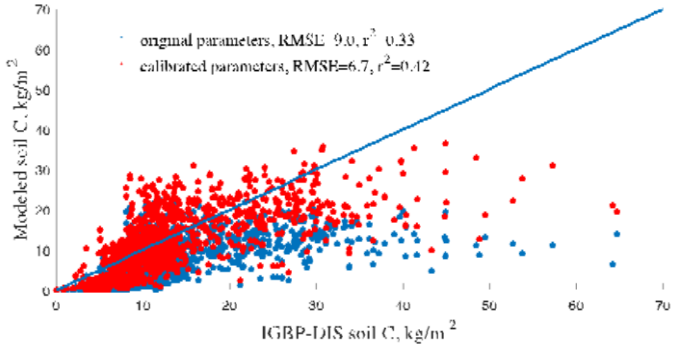
Figure 6. The average RMSEs with the increase of simulation times and different surrogate models.



(a) CLM soil C – IGBP-DIS soil C



(b) CLM soil C (calibrated) – IGBP-DIS soil C



(c) Spatial correspondence between modelled soil and IGBP-DIS soil

Figure 7. Spatial correspondence of SOC produced by CLM-CASA' to SOC reported by IGBP-DIS. The subgraph (a) shows the results using the default parameter values and the subgraph (b) shows the results after parameter calibration using the surrogate-based optimization. The points in Fig. 7c represent the grid cell values (blue ones for the results with default parameter values and

red ones for the results after parameter calibration). CLM-CASA' with the default parameter values explains 33% of variation in the observed soil C, while CLM-CASA' with the calibrated parameter values explains 42% of variability in the observed soil C.

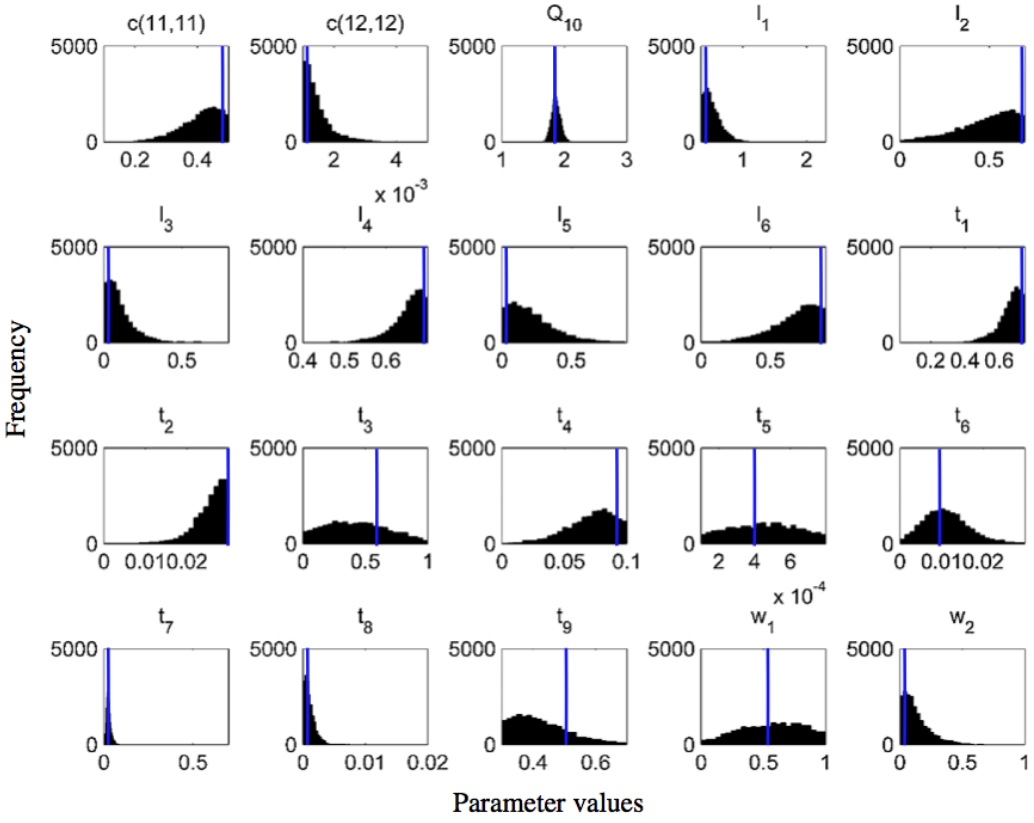


Figure 8. Frequency distributions of 20 calibrated parameters of CLM-CASA' model by Bayesian MCMC approach (Harauk, 2014) and surrogate-based optimization (blue line in each subgraph).

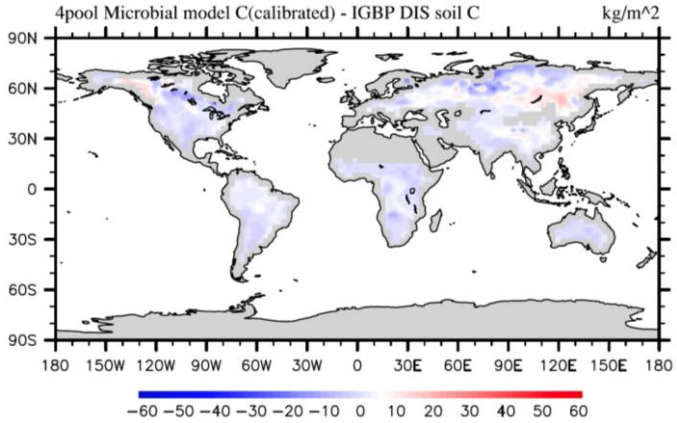


Figure 9. Spatial correspondence of 4-pool microbial model produced SOC to the IGBP-DIS reported SOC.

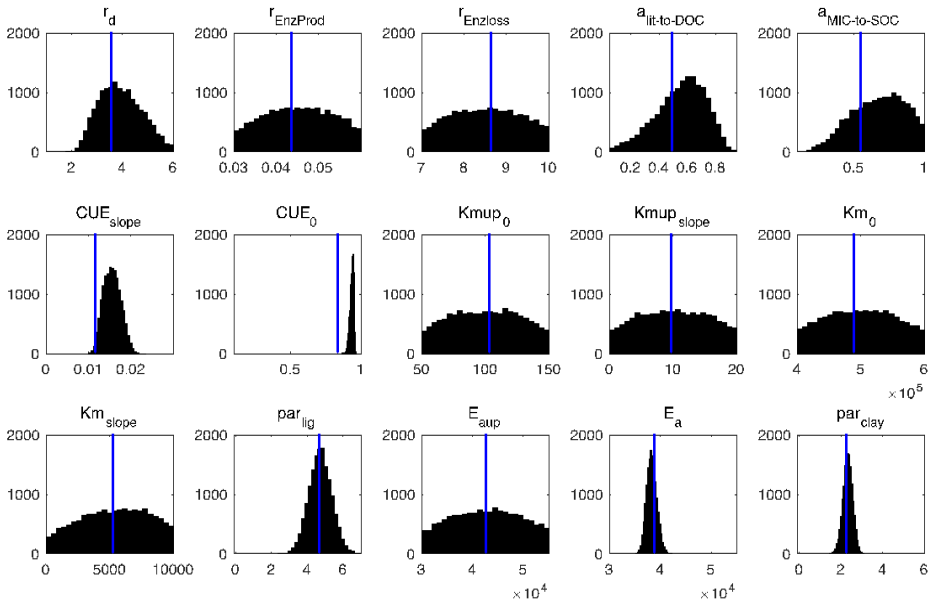


Figure 10. Posterior probability density functions of the 4-pool microbial model parameters (generated by Bayesian MCMC). The blue vertical lines are the final calibrated parameter values by our surrogate-based optimization.

Table 1. Parameter description of CLM-CASA' C-only model

Parameter Description	Symbol	Default Value (x0.001)	Calibrated Value by SBO (x0.001)
Exit rate from slow pool	c(11,11)	200	495.6
Exit rate from passive pool	c(12,12)	4.5	1.01
Temperature sensitivity of C decomposition	Q_{10}	2000	1737
Labile C fraction effect on C partitioning from leaves to surface metabolic litter	w_1	1000	589.04
Labile C fraction effect on C partitioning from roots to soil metabolic litter	w_2	200	4.52
Partitioning from surface structural to surface microbial pool if no lignin in surface structural litter	l_1	400	384.5
Lignin effect of partitioning from surface structural litter to surface microbial litter	l_2	400	689
Lignin effect on partitioning from surface structural litter to soil slow pool	l_3	700	7.499
Partitioning from soil structural to soil microbial pool if no lignin in soil structural litter	l_4	450	697.7
Lignin effect on partitioning from soil structural litter to soil microbial pool	l_5	450	54.46
Lignin effect on partitioning from soil structural litter to soil slow pool	l_6	700	871.5
C partitioning from soil microbial pool to slow pool if no sand or clay	t_1	169	747.7
Clay effect on C partitioning from soil microbial pool	t_2	5.44	29.6
Sand effect on C partitioning from soil microbial to slow pool	t_3	678	636.8
Combined effect of sand and clay on C partitioning from soil microbial pool	t_4	22	99.5
C partitioning from soil microbial to passive pool if no sand or clay	t_5	0.51	0.152
Sand effect on C partitioning from soil microbial to passive pool	t_6	2.04	12.99
Clay effect on C partitioning from slow pool to passive pool	t_7	4.05	24.2
C partitioning from slow to passive pool if no clay	t_8	14	0.012
C partitioning from slow to soil microbial pool if no clay	t_9	449	368.8

Table 2. Parameter and description of the 4-pool microbial models

Parameter Name	Parameter Description	Default Value	Calibrated Value by SBO
r_d	Microbial death rate	4.38	4.89
CUE_0	Baseline microbial carbon use efficiency	0.63	0.965
CUE_{slope}	CUE_0 dependency on temperature	0.016	0.00853
Km_0	Baseline half saturation constant	500000	498467
Km_{slope}	Km_0 dependency on temperature	5000	9751
E_a	Activation energy of SOC decomposition	47000	36669
par_{clay}	Clay limitation	0	2.41
par_{lig}	Lignin-dependent correction factor	0	6.23
$r_{EnzProd}$	Rate of enzyme production	0.0438	0.0361
$r_{EnzLoss}$	Rate of enzyme loss	8.76	8.08
$a_{lit-to-DOC}$	Fraction of $Input_{soid}$ that is transferred to soil	0.3	0.832
$a_{MIC-to-SOC}$	Fraction of dead microbes transferred to soil	0.5	0.716
$Kmup_0$	Baseline half-saturation constants for substrate limitation of DOC uptake	100	134
$Kmup_{slope}$	$Kmup_0$ dependency on temperature	10	4.62
E_{aup}	Activation energy of DOC uptake	47000	34811

Table 3 Calibration results of Bayesian MCMC and our surrogate-based optimization

SOC model	Detail	Method	Lowest RMSE ($kg \cdot m^{-2}$)	Variance Explained	Number of Simulations
2-pool microbial	8 parameters	Bayesian MCMC	6.609	51.6%	50,000+500,000
	2 carbon pools	RBF-SBO	5.785	51.6%	221
4-pool microbial	15 parameters	Bayesian MCMC	7.142	51.3%	50,000+500,000
	4 carbon pools	RBF-SBO	5.756	51.4%	199
CLM-CASA'	20 parameters	Bayesian MCMC	7.000	41.0%	50,000+1,000,000
	13 carbon pools	RBF-SBO	7.162	42.8%	321