Author response to reviewers for "Correcting a bias in a climate model with an augmented emulator" by McNeall et al. (2019)

We thank the reviewers for their constructive, fair, and thorough review. In this response, reviewer comments are in black text and author responses are in blue text. Several of the figures used in this response to reviewers have been added to the supplementary material, or to the main text. We identify these with dual labels outlining their position in this response, and in the updated manuscript and supplementary material. Responses to both reviewers are contained in this supplement, and a list of references not used in the main text can be found at the end.

Reviewer 1

In this paper the authors present a technique to determine the set of plausible parameter combinations that lead to a credible version of the climate model FAMOUS, in the presence of a significant model bias. This study follows on from the work described in McNeall et al. (2016), using the same perturbed parameter ensemble of model runs from the FAMOUS climate model. McNeall et al. (2016) identified the land surface input space of FAMOUS that was consistent with observations of the output 'forest fraction' for different forest regions, and found that there was very little overlap between parameter space that was consistent with observations of the Amazon region and parameter space that was consistent with observations of the other forest regions. This led them to conclude that there is either a local climate bias and/or some missing/incorrect process(es) in the land surface model of FAMOUS. Here, the authors extend the approach of McNeall et al. (2016) to develop a method that accounts for a climate bias in the model-observation comparison, by bias-correcting emulator-predicted model output before it is used in the statistical 'history matching' procedure that determines the plausibility of each tested realisation (combination of land surface model parameters) of FAMOUS. The authors bias correct the climate of the Amazon using an 'augmented' Gaussian process emulator, where temperature and precipitation outputs are treated as model inputs alongside the uncertain land surface input parameters. They find that the forest fraction in a region is sensitive to these climate variables, and by bias correcting the climate in the Amazon region the authors are able to correct the forest fraction in the Amazon to tolerable levels for many of the tested realisations of FAMOUS, including the default parameter set, thus increasing the amount of valid input space shared with the other forest regions (from 1.9% of the parameter space in McNeall et al. (2016) to 28.3% here). This approach is a novel adaptation to current methods for climate model-observation comparison, which shows potential for improving and simplifying the model tuning process for coupled climate models, as well as aiding in the identification of model errors. The manuscript is well-written and definitely falls within the scope of GMD and EGU. like the concept of the 'augmented emulator' that includes the localised climate outputs as inputs, however, I do have some concerns about the true validity of the augmented emulator, in particular for the bias corrected climates of central Africa and to an extent the Amazon in the application (see Specific comments below). If these

concerns, along with the other comments listed, can be addressed then I would recommend the publication of the manuscript in GMD.

Specific Comments:

Reviewer 1

Page 7 Line 11 – Page 8 Line 2: I'm confused by the role of the 'beta' parameter in the ensemble set-up. I don't think I understand this. The simulations in the ensemble have each been run with one of 10 different configurations of the atmosphere? Was it randomly assigned as to which 'atmosphere configuration' each simulation had? What are the implications of this? Doesn't this introduce biases into the ensemble (into the ensemble outputs) for identifying the parameter combinations that are plausible, if the ensemble members do not have the same starting point in the atmospheric set-up? Please clarify this in the text.

Author response

The reviewer is correct the simulations in the ensemble have each been run with one of 10 different configurations of the atmosphere and ocean. The beta parameter indexes each of these sets, with the lowest values of beta being the best performing according to Gregoire et al. (2010). The performance of FAMOUS was evaluated in that paper using a wide range of model outputs, and so the "best performing" parameter sets are not necessarily the best performing in temperature and precipitation over the Amazon region, and are drawn from a relatively large region of input parameter space.

The fact that atmospheric and oceanic parameters are also perturbed does indeed have implications for identifying the (land surface and vegetation) parameter sets that are plausible, as the climate of the system - important for land surface behaviour - is affected. Correcting these potential biases in climate is the aim of the augmented emulator, effectively using temperature and precipitation model output to summarise perturbations across the 10 atmospheric and oceanic parameters perturbed in the previous ensemble. We have made changes to the text in section 2.1 "Biases in FAMOUS" to clarify this point, and the explanation of the beta parameter has been expanded. The updated paragraph now reads:

"The ensemble of 100 members perturbed 7 land surface and vegetation inputs (see supplementary material, table S1 along with a further parameter denoted "beta" (β). Each of the ten values of beta provides an index to one of ten of the best-performing atmospheric and oceanic parameter sets used in a previous ensemble with the same model (Gregoire et al 2010) with the lowest values of beta corresponding to the very best performing variants. The beta parameter therefore summarised perturbations in 10 atmospheric and oceanic parameters that impacted the climate of the model, randomly varied with land surface input parameters, and potentially leading to different climatologies in a model variant with the same land surface parameters but different values of beta. Variations in the beta parameter did however not correlate strongly to variations with any of the oceanic, atmospheric or land surface parameters in the ensemble, and so the parameter was excluded from the analysis in M16. In this analysis we recognise that the different model climates caused by variations

in the atmospheric and oceanic parameters will have an impact on the forest fraction, and so we summarise those variations directly using local temperature and precipitation."

Reviewer 1

Page 8 Line 7-8; Section 3.1:'The study only considers regions dominated by tropical broadleaf forest, so as not to confound analysis by including other forests which may have a different set of responses to perturbations in parameters, rainfall and temperature'. Even though the forest regions are of the same 'type' (tropical broadleaf forest), are there other factors in the model that might affect the forest response between regions that are not accounted for? Such as topography that might affect how the forests respond to the parameter perturbations? The analysis is based on an assumption that the forests in the different regions will have the same responses to changes in the land surface parameters, rainfall and temperature. How realistic is this assumption? I'm not saying this assumption should not be made (we have to make assumptions for modelling and statistical analysis!), but I think the authors should state more clearly (in section 2 or 3) that they make this assumption (it is implied in the set-up of the augmented emulator, but not openly said), and discuss any possible implications of it on the results. This could be a further reason why the other forests 'do slightly less well' (e.g. Page 16, Line 11; Page 13 Line 12; Table 2).

Author Response

The reviewer makes a good point. We have added two paragraphs to the main text. At the end of section 2.1 "Biases in FAMOUS", we have added:

"We are assuming here that tropical forests can be represented by a single set of forest function parameters. Whilst such an assumption risks missing important differences across heterogeneous tropical forests, modelling the system with the smallest set of common parameters avoids overfitting to present day data. Avoiding overfitting is important if we are to use these models to project forest functioning in future climates outside observed conditions. One of the questions that the analysis presented in this paper addresses is whether current forest biases in the simulations reflect limitations of this single tropical forest assumption, or whether biases in the simulations of the wider climate variables play a more important role."

We have added a paragraph at the end of section 3.1 "An augmented emulator", explicitly outlining the assumptions of the augmented emulator, and briefly highlighting what might happen if such an assumption was unjustified:

"We note that the augmented emulator depends on the assumption that modelled broadleaf forests in each location respond similarly to perturbations in climate and input parameters. This assumption may not hold for the behaviour of the forests in the model, or indeed the real world. For example, particularly deep rooting of forests in the Amazon would respond differently to rainfall reductions but these processes are not represented in the underlying climate model. Similarly, differing local topology that is captured in the climate model, may influence the forests in a way not captured by our emulator. In both cases, the emulator would show systematic errors of prediction."

Reviewer 1

Section 3.2 –validation of the augmented emulator: The augmented emulator is validated using a 'leave-one-out' approach. However, I am not convinced that this approach fully validates the emulator for its use in the following analysis in Section 4. The emulator looks to be sampled from beyond the range of its training data where it is not validated, which could be affecting the results obtained. The augmented emulator is only trained to predict the forest fraction for climates (P and T variable combinations) that occur in the original simulations of the ensemble for the 3 regions. Figure 3 shows that coverage of the climate variables [P,T] 2-dimensional state-space is not uniform, and has sparse (if any) coverage in many areas of that 2-d space. In particular, there is rather limited coverage around the 'observed' climate (P,T combination) for the Amazon, and for Central Africa there looks to have no training points particularly close by. How the information for P and T augment onto the 7-dimensional space-filling design of the land-surface parameters to produce the final 9-dimensional input design with which the emulator is constructed is not shown (I imagine the actual coverage is some weird and complicated shape with some potentially large gaps) and so I wonder what the training data coverage, and hence emulator skill, is like for the areas of that 9-dimensional parameter space that are used in the bias correction analysis for these observed climates? The leave-one-out validation approach is only testing the emulator in the areas of space that have training runs, and so although the validation plots in Section 3.2 seem reasonable, it looks to me that the emulator is not tested (and so not validated) for the 'bias-corrected' climate of central Africa, and the Amazon, where the emulator is densely sampled for the analysis in Section 4. Outside the trained area of parameter space (e.g. where the observed climate for Central Africa is) prediction from the emulator becomes extrapolation from the emulator, the emulator prediction uncertainty can quickly increase and prediction values from the emulator will return back towards the form of the prior specification of the mean functional form from the GP emulator construction (the emulator mean response surface will bend/shape back towards that form), here a linear function of the inputs [stated in the supplementary information]. Hence, how do we know that the bias corrected predictions used in the analysis for these regions are sensible?

Can the authors provide some further validation for the emulator predictions for the observed climates of central Africa and the Amazon? If not, then the authors should explicitly state this limitation of the emulator in the paper and discuss the possible consequences of this on the figures and results presented in Section 4, and in the discussion and conclusion Sections 5 and 6. Also, could the emulator predicted responses to climates not covered by the training data (including the observed climate for Central Africa and the top left area in Fig 3) be dependent on the emulator's prior (linear) form, and change if this specification was changed? If yes, how confident are the authors in the prior emulator form (linear) being representative of the climate model's actual behaviour in parameter space beyond the training data? If they are not confident in it, then it either shouldn't be used or it needs to be more carefully specified so that it can be used.

In particular:

The results shown in Fig 8 are obtained by sampling with the climate variables set at the observed values (shown in Fig 3). Hence, this means that for central Africa (and the Amazon

to some extent), the sampled predictions come from extrapolating from the emulator beyond the extent of the training data. The responses to the climate variables are reasonably linear and I wonder if this response is at least partially driven by the form of the prior specification of the GP emulator mean function?

Author response

The reviewer raises an important point about emulator extrapolation. We hope that the following further validation of the emulator and exploration of the importance of the prior emulator specification will allay the reviewer's concerns, and that any remaining concerns are sufficiently addressed in the text. We have added section 2 "Further validation" to the supplementary material, with the indicated figures from this response included.

The reviewer is concerned first that the design points do not offer enough coverage near the observed temperature and precipitation for Central Africa and the Amazon, in particular that the emulator is forced to extrapolate, and may be poor at these locations. Further, given that the emulator is extrapolating, the reviewer is concerned that the prior form of the emulator may be dominant, and the prediction overly dependent on that prior form.

In an ideal world, we would generate ensemble members at or near the observations in question, as a way to validate the emulator and ensure our predictions are correct. This is impractical for two reasons 1) we don't have access to the model and setup in order to generate new runs. While it sounds like a weakness of the design, this is a feature of the paper, in that this is a common situation when analysts are working with models from other groups, with older versions of the model, or with very computationally expensive models where more runs cannot be afforded. 2) There is no way to directly control the temperature and precipitation in the model in order to generate a particular design. These inputs to the emulator are in fact outputs of the model, controlled largely by an inaccessible set of parameter perturbations. Given that we cannot validate the emulator at the observations, we suggest that we can at least show that the emulator performs well, even when required to extrapolate into the broader region of temperature and precipitation where the observations in question lie.

Our initial emulator validation relied on a leave-one-out-metric, but we are able to hold out a larger sample of ensemble members, and check the predictions of the resulting emulator. In this case, we hold out 6 ensemble members in the region of and nearest to the observations of temperature and precipitation of the Amazon and Central Africa. We hold out ensemble members with a precipitation below 0.2 and temperature below 0.4 in the normalised ensemble. These ensemble members occur in the bottom-left of the temperature-precipitation phase space, closest to the Central African and Amazon observations (figure R1, figure S1 in the supplementary material). They consist of three members each from the Central African and Amazon forests. These held-out members include one member at the very edge of the temperature space, that is it must be a marginal extrapolation. In our experience, marginal extrapolation is less accurate than extrapolating within the marginal limits of a multidimensional space. We therefore test the emulator with a much more challenging prediction than the leave-one-out validation.

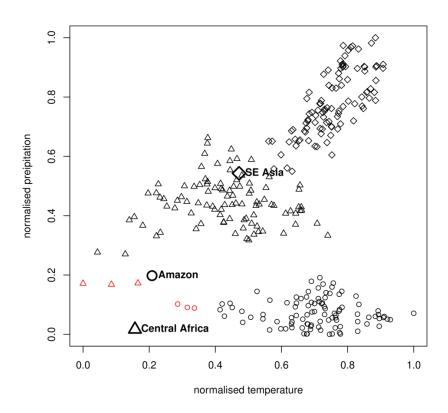


Figure R1/S1. Location of the held-out ensemble members (red points), used to test extrapolation of the emulator.

Figure R2 (also figure S2 in the supplementary material) shows the prediction of the 6 held-out ensemble members (red dots) in the context of the leave-one-out validation (grey dots). In the held-out case, we fit the emulator based on the 294 remaining ensemble members, and predict all 6 held out members at the same time. As the training set is slightly smaller than each leave-one-out training set (299 members), and the emulator is expected to extrapolate further, we might expect a significant degradation in the performance of the emulator in prediction. As we see in figure R2/S2, there is little evidence of such a degradation. Both prediction error and estimated uncertainty are well within the bounds of that found during the leave-one-out validation exercise. Figure R3 (figure S3 in the supplementary material) shows the prediction error for the 6 members, in the context of the histogram of errors from the leave-one-out exercise. None of the errors are near the limits of the distribution, even though they might be expected to be larger, with a smaller training set and deeper extrapolation.

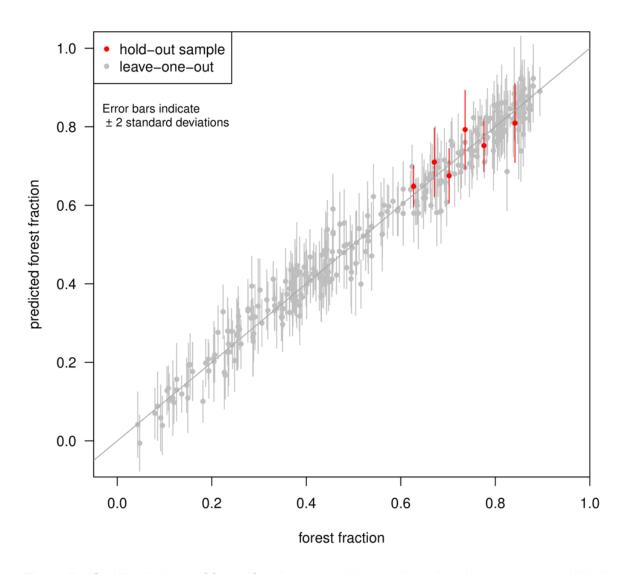


Figure R2/S2. Predictions of forest fraction ensemble members in a leave-one-out validation exercise (grey dots) and for the 6 held-out ensemble members (red dots). Vertical lines represent ± 2 standard deviations.

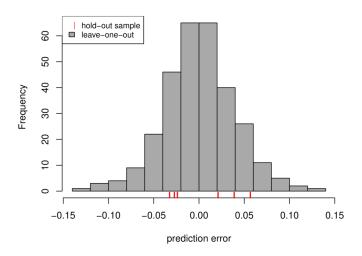


Figure R3/S3. Emulator prediction error (red rug plot) of 6 held-out ensemble members in the context of the leave-one-out validation exercise (grey histogram).

When making a direct comparison of prediction of the 6 held-out members (figure R4 and figure S4 in the supplementary material), we see that there is some small degradation in the performance of the emulator - predictions tend to be slightly further from the held-out ensemble member, and uncertainty bounds wider. However, it should be noted that the error of the held-out samples is 1) only slightly larger than in the leave-one-out case, 2) small when compared to the range of the ensemble, and 3) prediction uncertainty intervals are certainly appropriate and do not increase dramatically. There seems to be no question that even when asked to predict ensemble members that are near the edge of parameter space, and are a significant extrapolation, the emulator performs well. Obviously, this shouldn't be taken as meaning that there is no risk of the emulator performing poorly when extrapolating to the regions of the Amazon and central African temperature and precipitation. However, we hope we have shown that there is little evidence to suggest that the emulator will perform poorly there.

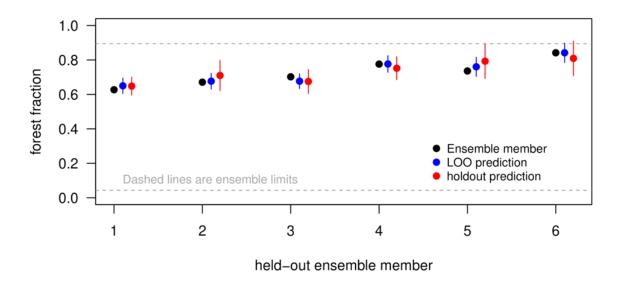


Figure R4/S4. Direct comparison of prediction of the held-out ensemble members in both the leave-one-out (LOO, blue points) and held-out (red points) validation exercises. Vertical lines represent ± 2 standard deviations.

The reviewer suggests that the prior form of the emulator may be important in extrapolation to the regions of the observations. In figure R5 (figure S5 in the supplementary material), we look at the error of prediction for an emulator trained using a constant, or "flat" prior form (our standard emulator is built using a linear model prior). We find that the performance of the emulator is very similar in both situations, suggesting that the prior form is not critical in determining the performance of the emulator in extrapolating at least as far as the observations that we have. We summarise this finding in section 2.1 "The importance of the prior form for emulator predictions" in the supplementary material.

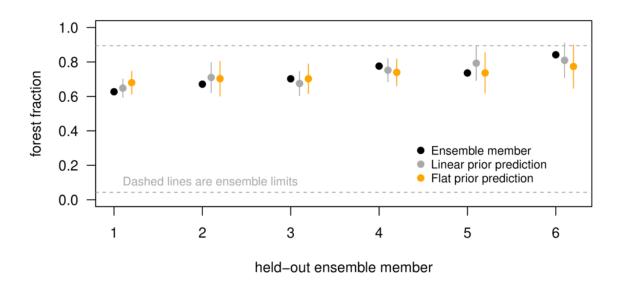
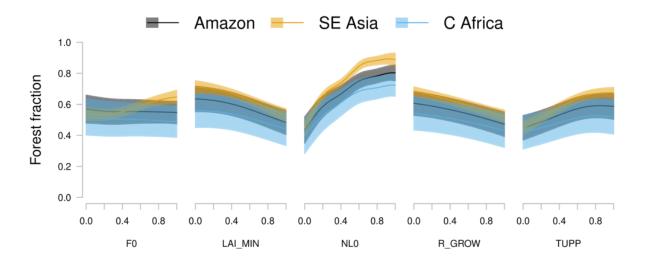


Figure R5/S5. Comparison of emulators for prediction of held-out ensemble members. Black points are the held-out ensemble members, with grey points representing the standard (linear model prior) emulator, and vertical lines ± 2 standard deviations. Orange points represent prediction with a "constant" or "flat" prior, from which the Gaussian process models deviates.

On the reviewer's specific point concerning the results from the one-at-a-time sensitivity analysis (figure 8) being driven by the prior form of the emulator: we find qualitatively similar results if we use a constant prior form for the emulator, suggesting prior form isn't too important. We plot the result in figure R6.



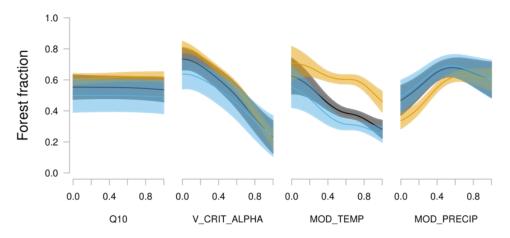


Figure R6. Leave-one-out analysis calculated using a constant or "flat" prior form for the emulator. This is qualitatively similar to that seen in figure 8 of the paper, suggesting that the prior form of the emulator isn't too important. The emulator mea is the solid line, transparent regions represent ± 2 standard deviations.

Reviewer1

Are the results in Fig 9 from the FAST99 algorithm generated by sampling the across the full 2-dimensional climate [P,T] space? How are these results affected by sampling from the emulator where there is no training data, particularly for a cool/wet climate at the top left of Fig 3? Could the sensitivity to the climate variables be over-estimated here? (I cannot easily tell from the plot, but do the individual main effect sensitivities sum to <1?(Main effect + interaction should sum to 1.) I've seen instances where the algorithm produces main effect values that sum to >1 in the presence of noise in the emulator fit.)

Author response

The reviewer is correct: the FAST99 algorithm samples from the full range of 2 dimensional climate space (temperature and precipitation) and there are no ensemble members in the "cool, wet" corner of that space. The emulator estimate of forest fraction is necessarily an extrapolation, and there is therefore a chance that the sensitivity of rainforest to this corner is

overestimated in the FAST99 sensitivity analysis. As far as we are aware, the Sobol indices calculated by the FAST99 algorithm need to be calculated on the unit hypercube, precluding the option of changing the FAST99 algorithm to take into account the shape of the sample in temperature/precipitation space. We have acknowledged this in the text, and offer another form of sensitivity analysis, in order to place the FAST99 results in context.

First, we address the reviewer's question about the FAST99 indices. The FAST99 algorithm calculates first order effects that sum to 0.982, and the total order effects (including interactions) that sum to 1.114 (see table R1).

Input	First Order	Total Order
F0	0.034	0.046
LAI_MIN	0.029	0.041
NL0	0.126	0.148
R_GROW	0.012	0.016
TUPP	0.026	0.043
Q10	0.000	0.003
V_CRIT_ALPHA	0.314	0.347
MOD_TEMP	0.190	0.205
MOD_PRECIP	0.250	0.266
Sum	0.982	1.114

Table R1. Sensitivity indices calculated using the FAST99 algorithm.

The reviewer highlights a larger problem of producing an effective sensitivity analysis when there are dependent inputs - for example, in our case when two inputs are not uniformly sampled. At the moment, this is an active research question, with seemingly no perfect standard solution for the circumstances we find ourselves in in this analysis. There appear to be some solutions for the case of dependent or correlated inputs (see e.g. Mara et al., 2015), but these rely on knowing (or assuming a distributional form for) the conditional densities - a situation we are not in, as the conditional density in the T/P space does not appear drawn from a standard distribution. The problem of sensitivity analysis when there is a non-uniform and non hyper-rectangular input space must surely be a priority for the history matching community, as history matching often provides highly irregular constrained input spaces.

We have identified a type of sensitivity analysis that may give useful information on the relative importance of each parameter in determining whether model output is close to

observations. We believe that this may be a good alternative to the variance-based sensitivity of FAST99, and will give modellers useful feedback about the way the system behaves. It also fits neatly into the History Matching framework. The technique is called Monte Carlo Filtering (MCF), or Regional Sensitivity Analysis. A recent description and references can be found in section 3.4 of <u>Pianosi et al. (2016)</u>. The basic idea of MCF is to split samples from the input space into those where the corresponding model output meets (or not) some criteria of behaviour. Examining the differences between the cumulative distributions of those inputs where the outputs do or do not meet the criteria provides a measure of sensitivity of the output to that input. For example, we might split model behaviour into those outputs above or below a threshold.

We integrate the MCF sensitivity analysis into the history matching framework. We examine the differences in the univariate distributions of each parameter, in those samples where the output is ruled out by history matching, against those that are "Not Ruled Out Yet" (NROY). To measure the differences between the distributions we perform a two-sided Kolmogorov–Smirnov (KS) test and use the KS statistic as in indicator that the output is sensitive to that input. A larger KS statistic indicates that the cumulative distribution function of the respective inputs are further apart, that that input is more important for determining if the output falls within the NROY part of parameter space, and therefore the output is more sensitive to that input in a critical region. We note that MCF is useful for ranking parameters in order of importance, but not for screening, as inputs that are important only in interactions might have the same NROY and ruled out marginal distributions. In this case they would have a sensitivity index of zero.

We include an MCF analysis in the main text in section 4.4 "Sensitivity analysis", with some supporting analyses in the supplementary material.

We apply MCF in two modes: first, on the 300 model runs in our ensemble, and second, using the emulator fitted to all 300 of those ensemble members. When using the original runs, we remove the problem of sampling from the unit hypercube in temperature and precipitation space. The MCF is calculated using the inputs of the runs as they appear in that space. We simply assign an implausibility measure to each run, and then examine the difference in empirical cumulative distribution functions between those that are ruled out or NROY (implausibility < 3) in each input dimension. We assume zero discrepancy and zero discrepancy uncertainty, and there is zero emulation uncertainty as these are the runs. We assume an observational uncertainty of 0.05 (one standard deviation).

Second, we apply MCF using the emulator. This allows us to examine the difference between distributions given a much larger sample from the input space, and to calculate the uncertainty of the MCF sensitivity indices when calculated using different numbers of runs. This comes at the cost of using an imperfect emulator, which may give different results than if we were using a large ensemble of runs. To avoid the problem of sampling precipitation and temperature from regions where there are no ensemble members, we sample uniformly from across input space for all other parameters, and then append a random temperature/precipitation location from the ensemble.

We calculate a sampling uncertainty by calculating the MCF sensitivity metrics 1000 times, each time using a sample size of between 100 and 3000 points from the input space. In this way, we estimate both the mean and the uncertainty (standard deviation) of that mean, when using a different number of ensemble members to calculate the MCF sensitivity indices, including that for 300 members, our ensemble size. We plot these in figure R7 (also included as supplementary material figure S6).

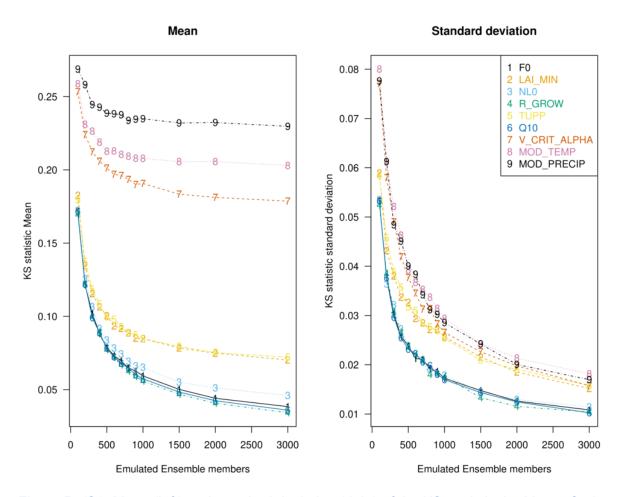


Figure R7/S6. Mean (left) and standard deviation (right) of the KS statistic the Monte Carlo Filtering index of sensitivity, calculated using different sizes of emulated ensembles.

We note that the sensitivity indices are estimated to be higher when a small number of ensemble members are used, as well as with a higher uncertainty. The change in both the estimated statistic and its uncertainty become small by the time 3000 ensemble members are used, suggesting that we should use at least this many emulated ensemble members to obtain an unbiased sensitivity analysis.

We compare the KS statistics for each input, and for a history matching exercise conducted using each tropical forest observation in figure R8. We plot the KS statistic calculated using only the ensemble members as open points, alongside the estimated uncertainty bounds calculated using 300 emulated members. We plot the KS statistic estimated using 5000 emulated members as solid points and error bars. We include a version of this figure plotting only the estimates using 5000 ensemble members in the main text in figure 15.

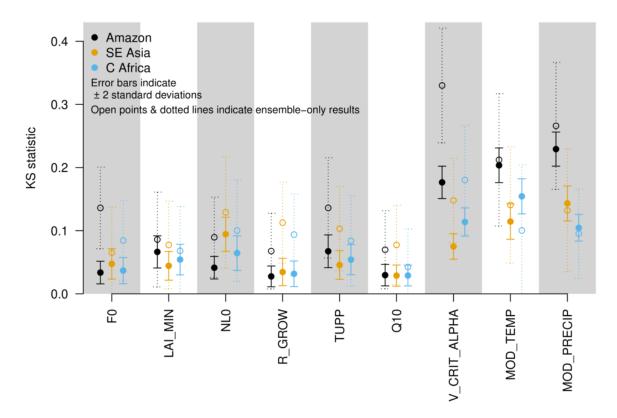


Figure R8. Monte Carlo Filtering estimate of sensitivity of model outputs to model inputs. Solid points are estimated using 5000 emulated ensemble members. Open points are estimated using 300 actual ensemble members, with uncertainty estimated using 300 emulated ensemble members.

We can check the strength of the relationship between the MCF sensitivity measures and the FAST99 sensitivity measures, by plotting them together (figure R9, supplementary material S7). We plot only the FAST99 first-order sensitivity, as we do not expect MCF sensitivity to be able to measure interactions between inputs accurately. We find a fairly strong relationship between the two sensitivity measures, although we would expect some differences, as they are measuring different things, and MCF is not sampling from locations in temperature and precipitation space where there are no ensemble members.

The reviewer asked if the FAST99 algorithm might overestimate the sensitivity of forest fraction to temperature and precipitation, due to sampling a corner of input space with no tropical forest. We find some evidence of this being the case, using the emulated MCF sensitivity index, that avoids this issue by only sampling from locations in temperature and precipitation space that exist in the ensemble. The FAST99 algorithm produces very similar sensitivity indices (perhaps fortuitously, as they measure on a different scale) for temperature and precipitation as the MCF algorithm for the Amazon forest, but the Southeast Asian and Central African forests appear less sensitive to these inputs when estimated using the MCF algorithm.

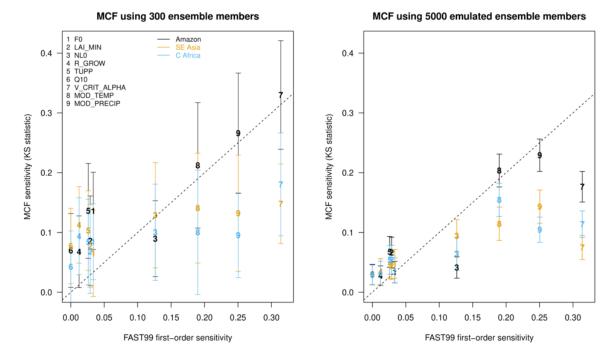
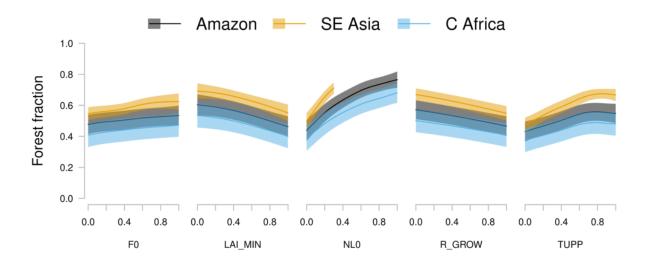


Figure R9/S7. Relationship between the first-order sensitivity of input parameters calculated by the FAST99 algorithm, and that calculated by the Monte Carlo Filtering (MCF) algorithm. The sensitivity indices calculated only using the ensemble members are plotted on the left, with uncertainty estimated by using an emulated 300 member ensemble. On the right, we plot the sensitivity indices when calculated using 5000 emulated ensemble members.

Finally, we can look at the effect of excluding inputs ruled out by history matching has on our leave-one-out sensitivity analysis, with the impact of ruling out some of the higher forest fractions found in the "cool, wet" part of parameter space that is far from any design points. We do this by simply excluding inputs where the calculated implausibility for the outputs is above 3, when assuming observational uncertainty is 0.05 (1 standard deviation), and discrepancy uncertainty is zero. We plot the results in figure R10 (now fig. 14 in the main text, replacing fig. 8 in the original text), and note that very high and very low forest fractions are excluded, somewhat reducing the calculated sensitivity of the forests to various inputs.



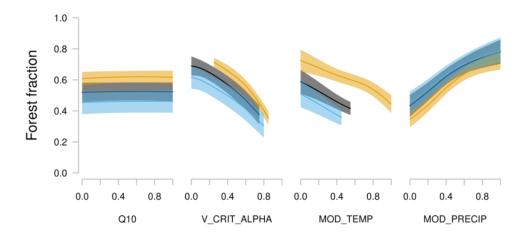


Figure R10/14. One-at-a-time sensitivity analysis, excluding any inputs with a calculated implausibility above 3. Semi-transparent regions represent ± 2 standard deviations

A summary of actions taken:

- We moved sensitivity analysis section (now section 4.4) to after the history matching section (now section 4.3).
- We now report only NROY input space in the one-at-a-time analysis (i.e. the history-matched version). Figure 8 in the original text has been replaced with fig. R10, and is now fig. 14 in the updated manuscript.
- We added Monte Carlo Filtering (MCF) results in the main text sensitivity analysis section, and added the comparison of MCF and FAST99 sensitivity indices in the supplementary material.

Reviewer 1

In Figure 10 the emulator is used to simulate across the entire range of simulated temperature and precipitation with all other inputs fixed at the default setting. How might this result be affected?

Author response

We compare our results in figure 10 with an emulator that uses a different form - a constant (or "flat" prior. The different emulator does indeed change the result of the two-at-a-time sensitivity analysis (see figure R11), but not significantly in the areas near design points (i.e. the ensemble members), or in the regions near the forest fraction observations for the three forests. The largest difference is in the "cool, wet" corner of the temperature/precipitation space, well away from ensemble members or observations. We note that figure 10 of the paper contained an error - the background emulated surface was normalised to its own range, not the range that included the original data. We have updated the figure, and it is now moved to figure 8 in the revised main text.

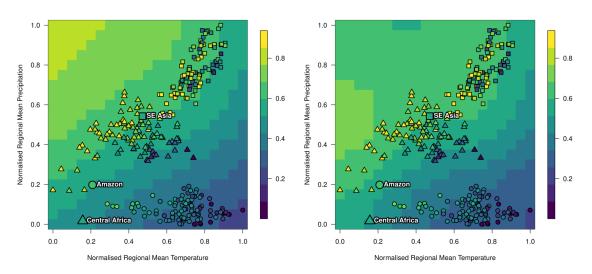


Figure R11. Two-at-a-time sensitivity analysis using the standard emulator with a linear prior form (left), and with a constant or "flat" prior form (right).

Reviewer 1

How might this issue affect the results of the retained parameter space from the history matching (Figures 13-16) for each forest region? In Figure 16, are the regions not covered by the training data more likely to be retained as emulator error is larger, reducing the value of the implausibility metric so that it cannot be ruled out?

Author response

Yes, the issue of extrapolation to unsampled areas of temperature/precipitation parameter space does appear to affect the ruling-out of parameter space. Regions not covered by the training data are more likely to be retained, as the emulator error is larger (but not increasing rapidly - see figure R12). To a large degree, this is the history matching working as it should. There is not enough evidence to rule out inputs where output corresponds to these regions. Recognising that we have other knowledge not accounted for here, this could perhaps be further developed by including an implausibility measure that also includes measures of temperature and precipitation, before bias correction.

We have included the following paragraph at the end of the history matching section (section 4.3):

"It is possible that the estimate of shared NROY input space is larger than it could be, due to the lack of ensemble runs in the ``cool, wet" part of parameter space, where there are no tropical forests. Inputs sampled from this part of parameter space may not be ruled out, as the uncertainty on the emulator may be large. This is history matching working as it should, as we have not included evidence about what the climate model would do if run in this region. Further work could explore the merits of including information from other sources (for example, from our knowledge that tropical forests do not exist in a cool wet climate) into the history matching process."

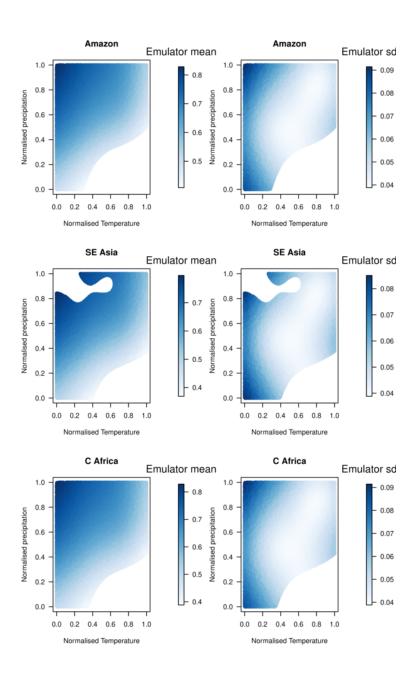


Figure R12 Mean (left) and standard deviation of the standard emulator, with all land surface inputs held at their best values, and only temperature and precipitation varied. White regions are "ruled out", as the emulated forest fraction is deemed statistically too distant from any of the observed forests.

Reviewer 1

Page 15 Line 3-4, Figure 15 (and discussion): guiding further runs, choosing high density regions to run new ensemble members. This is a useful outcome. My question here really relates to how the results trace back to improve model performance... How does the bias correction information feed back for the modeller to know what 'atmospheric configuration' should be used (the 10 atmospheric parameters, or beta?) with the inputs selected as good for any new runs? Can a good representation of forest fraction for all forests simultaneously be obtained in new runs at these parameter combinations without bias correction? Or, would any new runs always need to be bias corrected too, until further work to understand the true cause of the climate bias is completed and the climate model updated? As obviously, just running the model at more combinations in this identified joint space will induce climates as shown in Figure 3, away from the observed climates for each forest. Could the authors comment on this in the discussion?

Author response

It would be difficult in this particular case to directly feed back bias correction information to help the modeller select "good" atmospheric and oceanic parameter sets. This is because 1) the original parameter sets for the atmosphere and ocean are not available, 2) only a small selection of the best performing of parameter sets were chosen from a larger set. That larger set was carefully chosen to sample the parameter space effectively, but there is no guarantee that the best-performing sets have this property. In the case that they do not, it would make it difficult to build an accurate emulator of the relationship between the atmospheric and oceanic parameters, the climate bias, and the modelled forest fraction.

It would be simplest to build an emulator that modelled and perhaps minimised directly the climate biases, given the original perturbations of atmospheric and oceanic parameters. The fact that forest fraction seems so strongly influenced by temperature and precipitation suggests that minimising climate biases would be a good way of minimising forest fraction errors. In this paper we have outlined some of the impacts of the climate biases on forest fraction, which should help to motivate efforts to bias correct the climate of the model directly. However, as implied by the results of Gregoire et al. (2010), this might be at the expense of the performance of other parts of the climate model. Informing the modellers of this fact might motivate more work on fundamental structural errors within the model.

Reviewer 1

Further Comments: Page 3 Line 18: 'Without strong prior information...' What is meant by 'prior information' here? What kind of information? On observations? On model skill? On both? This is a bit vague and needs more clarity.

Author response

Added "Without information about known errors (for example, knowledge of an instrument bias, or a known deficiency of a model) ..."

Reviewer 1

Page 5 Line 9: What reasons? Please give more details here: '...whereas there were a number of reasons one might reject the proposed parameter space, including...'

Author response

We have restructured the paragraph and given more detail about why we might choose the default parameters over a new region of parameter space.

Reviewer 1

Section 1.3 (Page 5 Line 11): It might give more context to the first listed aim on line 11, and for the detail coming in the second paragraph of the section (discussing the results of McNeall et al (2016), which are not 'aims of this paper') to connect that this study is extending the analysis of McNeall et al. (2016) at the start of the section in the first line (first aim?)?

Author response

We have restructured the section as suggested.

Reviewer 1

Page 6 Line 9-11:Sentence starting 'Parameter perturbations...'. Are there any references for examples of such findings?

Author response

We have added references as follows:

Parameter perturbations and CO2 concentrations have been shown to influence the simulation of tropical forests in climate models (Boulton et al., 2017; Huntingford et al., 2008), with increases in CO2 fertilisation and associated increased water use efficiency through stomatal closure offsetting the negative impacts of purely climatic changes (Betts et al., 2007; Good et al., 2011).

Reviewer 1

Page 6 Line 19: ... was sensitive to perturbations in parameters, . This is vague... What kind of parameters? Edit to say '... was sensitive to perturbations in parameters such as...'

Author response

Poulter et al (2010) perturbed 41 parameters they identified as being important in modeling ecosystem processes in LPJmL and affecting the carbon and water cycle, and vegetation dynamics. The criteria they used to estimate the importance of the parameters used a number of model outputs in calculations and so it is difficult to concisely summarise their importance in an overview. We've edited the paragraph to include the fact that the parameters were concerned with ecosystem, carbon, water cycle and vegetation dynamics.

Reviewer 1

Page 6 Line 31 –Page 7 Line 1:I realise that the details of the ensemble are in McNeall et al (2016), but I think it would be useful to give minimal details of the parameters perturbed in this paper also. Their effects are being compared to the climate variables in Section 4.1, with parameter names (acronyms) given in the text, and yet I have to go to a completely different paper to find a description of them /what they correspond to in the model. Please add a small summary table (to the supplementary file, if not to the main paper) that lists the parameters with short descriptions.

Author response

We have added a table of input parameter details to the supplementary material, and added a reference to that in the main body of the text.

Reviewer 1

Page 7 Line 4:What is meant by 'global values'? Global values of what? Please clarify.

Author response

To clarify, we have changed the text to: "The strong relationships between the global mean forest fraction and the mean forest fraction in each region implies that perturbations in input parameters exert a larger control over all forests simultaneously, and individual forests to a smaller extent."

Reviewer 1

Page 8 Line 30: Please provide a reference for GP emulation.

Author response

We have added references to Sacks et al. (1989) and Kennedy & O'Hagan (2001).

Page 9 Line 13:'...the 10 atmospheric parameters perturbed in a previous ensemble, summarised by the β parameter'. I'm struggling to picture how the effects of 10 parameters can be summarised by 1 parameter. A lot of information is being condensed here? This needs more explanation. (Also see first comment above under 'Specific comments'.)

Author response

We have amended the paragraph to clarify the role of beta, and the atmospheric and oceanic parameters as follows:

"These new inputs are outputs of the model when run at the original inputs X, and are influenced by the 10 atmospheric and oceanic parameters perturbed in a previous ensemble in a configuration unavailable to us in this experiment. Performance of the model under those perturbations is summarised in the parameter, beta which has smaller values for the better performing models. The performance metrics included temperature and precipitation, along with a number of other measures so the beta parameter therefore contains information about temperature and precipitation across the ensemble, without being a perfect representation of its behaviour. We cannot control the atmospheric and oceanic parameters directly and thus ensure that they lie in a latin hypercube configuration, although the

ensemble is ordered in a latin hypercube configuration according to the performance of the model at each parameter set."

Reviewer 1

Page 9 Line 14: This sentence: 'We cannot control them directly and thus ensure that they lie in a latin hypercube configuration' is confusing and could be interpreted in different ways. I first read 'and thus ensure' as that you do ensure that they lie in a LH configuration. But on second read I see the meaning you want is that you can't ensure this. Please re-phrase.

Author response

Rephrased (see above).

Reviewer 1

Also, the 'latin' in 'Latin hypercube' should have a capitol L. Please update here and elsewhere.

Author response Corrected.

Reviewer 1

Page 10 Line 12: '3% of the maximum possible value of the ensemble.' What does this really statement tell us? The maximum forest fraction is 1 so the error of 0.03 is 3% of this forest fraction value, but this is the minimum percentage of an output value that it could be. The majority of predictions will be less than 1, and so the error of an 'average prediction' is in general a larger percentage than this. It seems a bit of a misleading statement, and I suggest removing it here and on line 14.

Author response

The inclusion of the 3% figure was an attempt to offer some context and concreteness for a small number (0.03). We take the reviewer's point that this choice might flatter the emulator somewhat, and therefore present the number as a proportion of the mean forest fraction (0.54), meaning the figure is around 6%, for the augmented emulator and 12% for the standard emulator.

Reviewer 1

Page 10 Line 25: I don't understand how the 'rank histogram' indicates that we have 'reliable' uncertainty estimates? It shows the predictions are a mixture of over and under-estimations of the actual model, but it gives no indication of the size of errors, which could be large and therefore not reliable? Maybe I misunderstand this.

Author response

Although the reviewer is correct that the rank histogram does not address the size of the errors, it does ensure that the size of the errors are consistent with the predicted error distributions. Therefore, the size of the errors is not beyond what we thought it should be (this is what we mean by "reliable"). This information, coupled with the fact that the errors themselves are not large should be enough to have confidence both in the accuracy of the

emulator, and its uncertainty estimates. We have added the sentence "Do the error estimates of the augmented emulator match the true error distributions when tested in leave-one-out predictions?" at the beginning of this section to make the intention of the analysis clearer.

Reviewer 1

Section 4.2 and Figure 10: The interpretation of this plot needs clarification. Would the contours be similar at different parts of the land-surface parameter space? (Fixing at a different simulation to the default?) On Page 11, Line 26, it suggests that for central Africa, moving any ensemble member (small triangle point) to the observed (big triangle) would not cross many contours, but the central Africa points with wetter climates (normalised T at approx. 0.4, normalised P at approx. 0.5 to 0.6) would cross between 3 and 4 contours to be in the same one as the observed (big triangle), so I'm not sure this is true? Please clarify this.

Author response

On the first point, the reviewer is correct, there would be some differences if the land surface parameters were fixed at a different point. However, 1) the analysis of this paper supports the conclusion that the default parameters for the land surface are perfectly valid, and 2) given that they are unlikely to be large (sensitivity analysis indicates small interaction terms) we question whether summarising a very large number of possible perturbations will add value to the analysis. On the second point, the reviewer is correct. We have amended the paragraph as below, to make clear that we are talking about a "typical" ensemble member (i.e. one from the centre of each forest sub-ensemble), rather than about any of the ensemble members.

Updated paragraph:

"Moving an indicative ensemble member from the centre of these forest sub-ensembles to observed values of temperature and precipitation would shift them primarily in the same direction as the contours of forest fraction value. South East Asian and Central African ensemble members are therefore simulated with a roughly accurate forest fraction. In contrast, the Amazon is simulated slightly drier, and considerably warmer than the observed Amazon and many ensemble members consequently have a lower forest fraction than observed. Shifting a typical ensemble member for the Amazon to its observed temperature and precipitation would cross a number of contours of forest fraction. This figure provides strong evidence that a significant fraction of the bias in Amazon forest fraction is caused by a bias in simulated climate."

Reviewer 1

Page 12 Line 8-11: Are the values given in this paragraph mean absolute error between model and observations? The first line says 'difference', but this must be an average? Please clarify. Also, could the lack of training data near the observed climate for central Africa be a contributing factor to why central Africa is worse (Line 9) in this metric?

Author response

The numbers given in this paragraph are the difference between observations and 1) predictions of forest fraction at the default land surface parameters using a standard emulator and 2) predictions of the forest fraction at the default land surface parameters and the corrected local climate, using the augmented emulator. We have restructured the paragraph to make it clearer exactly what we have done. The reviewer makes a good point about the lack of training data near the central African forest, and we have included this. The paragraph now reads:

"The bias correction reduces the difference between the prediction for the modelled and observed Amazon forest fraction markedly, from -0.28 using the standard emulator to -0.08 using the augmented emulator. It makes the predicted modelled forest in central Africa worse (-0.11 from -0.03), and slightly improves the SE Asian forest fraction (0.07 from 0.1). Overall, bias correcting the climate takes the mean absolute error at the default parameters from 0.14 to 0.09 for the three forests. It is possible that the predicted forest fraction for central Africa is slightly worse because the observed climate is towards the edge of the parameter space of temperature and precipitation, and there are no runs near."

Reviewer 1

Section 4.4: It might be better for the flow of the results section if the first part of Section 4.4 (up to Page 13 Line 2) describing the history matching methodology was moved into Section 3 on methods?

Author response
Amended as requested.

Reviewer 1

Page 13 Line 12:Could more detail be given as to why the implausibility value at the default settings rises for central Africa and SE Asia on bias correction?

Author response

This is due to the slight rise in predicted error in the case of central Africa, and in the reduction of uncertainty in the case of SE Asia. Both of these would be expected to raise the Implausibility score somewhat. The paragraph has been amended to acknowledge this.

Reviewer 1

Page 17 Line 14-16: Summarising the 10 parameters using 2 outputs is useful, but this is likely to have little traceability back to the original 10 input values? Many different combinations of the 10 inputs could lead to a similar combination in the 2 outputs, so how would one know what combination of the 10 inputs is best when setting up any further runs of the model? Also, the 'O(10xp)' rule is when training points are space-filling across the parameter space being emulated. There is no guarantee (as seen in this example) that this property will hold when outputs are used as dimension reduction, so more points, or even less points, could easily be required. This should be acknowledged.

Author response

The reviewer is correct that there is likely little traceability back to the original 10 input values, and the original ensemble must be examined to get that information. To address the reviewer's points we have added the following paragraph:

"We acknowledge however that in order to trace back information about the performance of the model in forest fraction to the original 10 oceanic and atmospheric parameters, we would need access to the original ensemble. We have used temperature and precipitation to reduce the dimension of the parameter space, but there is no guarantee that the relationship between the original parameters and the local climate is unique. There may be multiple combinations of the 10 parameters that lead to the temperature and precipitation values seen, which would mean that we would require a large ensemble to estimate the relationships well. Alternatively, there may be an even more efficient dimension reduction for forest fraction, meaning we would need even fewer model runs to summarise the relationship."

Technical corrections:

Reviewer 1

Page 1 Line 13-14: 'This might be due to...'. I think this sentence might be easier to read if the number/list format is replaced with 'This might be due to either ..., or...., or a combination of both.'

Response: Amended as requested.

Reviewer 1

Page 1 Line 16-17: '...alongside regular land surface input parameters.'.Is the term 'regular' needed here? Maybe remove this word. [The 'regular' suggests to me that there may be other types of land surface input parameters that are 'not regular' which are not included, which I don't think is the case.]

Response: Amended as requested.

Reviewer 1

Page 1 line 15: Should '...a climate model...' be '...the climate model...'? This is now the specific climate model used by McNeall et al (2016).

Response: Amended to clarify that we are using the augmented emulator on the specific climate model from McNeall (2016).

Reviewer 1

Page 1 Line 17-18: For readability, please change 'is nearly as sensitive to climate variables as changes in its land surface parameter values.' to 'is nearly as sensitive to climate variables as it is to changes in land surface parameter values.'

Response: Amended as requested.

Reviewer 1

Page 2 Line 9: Should '...processes sufficiently to trust...' be '...processes sufficiently and to trust...'?

Response: Added "well", so the sentence now reads "We wish to choose input parameters where the output of the model reproduces observations of the climate, in order to have confidence that the model represents important physical processes sufficiently well to trust projections of the future."

Reviewer 1

Page 2 Line 28:The sentence here is hard to read. Change: '...practices, there appear no standard procedures for climate model tuning however -as the authors...' to '...practices, there appear to be no standard procedures for climate model tuning. However, as the authors...'.

Response: The section is amended for clarity.

Reviewer 1

Page 2 Line 32: Missing word? Edit: 'It might start with single column version...' to be 'It might start with a single column version...'

Response: Amended as requested.

Reviewer 1

Page 3 Line 2: Change word order? Edit: '...might be then tuned...' to '...might then be tuned...'

Response: Amended as requested.

Reviewer 1

Page 3 Line 8: Change 'Golaz et al. (2013) Show...' to 'Golaz et al. (2013) show...'.

Response: Amended as requested.

Reviewer 1

Page 3 Line 20-21: This sentence needs plural 'candidates' at the start, and the second part should be given as more of a negative to make the point? Revise to: 'This means that good candidates for input parameters might be found in a large volume of input space, but projections of the model made with candidates from across that space might diverge to display a very wide range of outcomes.'

Response: Amended as requested.

Reviewer 1

Page 3 Line 23: 'individual parts' Of the tuning process? Or the model? Please clarify.

Response: Clarified that this meant individual parts of the process.

Reviewer 1

Page 4 line 14: Missing full stop after Vernon et al. (2010).

Response: Corrected.

Reviewer 1

Page 4 Line 20, Line 23: References in bracketed format when should be in in-line format.

Response: Corrected.

Reviewer 1

Page 4 line 33: Remove the second 'used'.

Response: Corrected.

Reviewer 1

Page 5 line 1: Missing words. Change to: '...structural bias in the ocean component of the climate model HadCM3 could'

Response: Corrected.

Reviewer 1

Page 5 Line 33: Should this be '...use the augmented emulator to estimate the sensitivity...'?

Response: Yes it should, corrected.

Reviewer 1

Page 7 Line 2: Move the reference to Fig 1 to the next sentence, which is the sentence that is describing what is shown in Fig 1.

Response: Corrected.

Reviewer 1

Page 7 Line 7-8: '...parameter settings which the emulator suggested should lead to an adequate simulations of...'. The emulator provides the predictions of model output but does not indicate adequacy –this comes from the history matching process (as the authors have described). Change to: '...parameter settings which the history matching process suggested should lead to adequate simulations of...'.

Response: Amended as requested.

Reviewer 1

Page 8 Line 9, 12: References to Jones et al, and Adler et al are in in-line format when should be in bracketed format?

Response: Amended as requested.

Reviewer 1

Page 9 Line 10: Change to: ...each of the forests: the Amazon, central Africa and Southeast Asia...' or put the forest region names in brackets?

Response: Added a colon.

Reviewer 1

Page 9 Line 11-12: For readability, move the sentence 'Regional extent of ... supplementary material.' so that it is the second sentence in this paragraph. (The next sentence follows better from the one before it!)

Response: Moved as requested.

Reviewer 1

Page 9 Line 24: Here the work by M16 is referred to as being by the authors of this work ('we built'), but in all previous references to this point it has been referred to as a separate study (e.g. M16 argue..., or M16 speculated...). Update as needed to be consistent.

Response: Amended as requested.

Reviewer 1

Page 11 Line 3: Should this paragraph start with: 'The augmented emulator...'

Response: Amended as requested.

Reviewer 1

Page 11 Line 5: '...predict changes in forest fraction as each variable is changed from the lowest to highest setting in turn...'. Should 'variable' in this sentence be replaced with 'input'? – as this is done for the land surface input parameters as well as the climate variable inputs?

Response: Changed as requested, and updated to refer to the augmented emulator.

Reviewer 1

Page 12 Line 22: Remove the second 'the'.

Response: Corrected.

Reviewer 1

Page 13 Line 21:The term 'the climate-bias forest' sounds weird? Should this be 'the climate-bias-corrected forest'?

Response: Yes, Corrected.

Reviewer 1

Page 16 Line 34: Remove the second 'could'.

Response: Corrected.

Reviewer 1

Page 17 Line 14: 'O(170)' should be in italics?

Response: Yes, Corrected.

Reviewer 1

Page 18 Line 6: Change: 'If trained an ensemble...' to 'If trained on an ensemble...'. Also, remove the second 'which'.

Response: Corrected.

Reviewer 1

Page 18 Line 10: Remove; '(e.g.)'.

Response: Amended as requested.

Reviewer 1

Page 18 Line 19: Should 'learned' be 'learn'?

Response: Yes, Corrected.

Reviewer 1

Page 18 Line 32: Missing word. Change: '...in leave-one-out...' to '...in a leave-one-out...'.

Response: Corrected.

Reviewer 1

Page 19 Line 13:Change 'finding' to 'findings'.

Response: Corrected.

Reviewer 1

Page 27, Fig 5 caption: The brackets for g1are in the wrong place? For gnand yn, should 'n' be replaced with '3', as is shown in the diagram, and written for 'C' in the next sentence?

Response: Yes, both corrected.

Reviewer 1

Supplementary information Line 17: Reference in bracketed format when should be in in-line format.

Response: Corrected.

Reviewer 1

Supplementary information Line 18: Missing word. Change: '...in section 3 the...' to '...in section 3 of the...'

Response: Corrected.

Reviewer 2

The authors seek to produce an emulator that can account for some of the known biases in a climate model when the aim is to find a 'good' parameter set to represent observations. Overall, I think the idea is a good one and the augmenting of the emulator in this case clearly works to make a better emulator for model constraint. The paper is well written and the method easy to follow. The work should be published in GMD. I have a few points to discuss:

I am pretty confused about the 'beta' parameter and what it means in both the original model and the emulator here – can this be clarified in the text please.

Author Response

Reviewer 1 had a very similar comment, we have comprehensively responded in the first response to reviewer 1, adding expanded explanation of the beta parameter at the end of section 2.1 "Biases in FAMOUS".

Reviewer 2

How much do you need to know about the present bias? It's clear the authors had information on this and a good idea from the modellers where the biases came from but it's less clear what they may have done with less information.

Author response

Knowledge about the present bias in (e.g.) temperature and precipitation is certainly useful when it comes to understanding where the model may be wrong, and in attributing the bias in forest fraction to climate rather than model inadequacy. To gain a good insight into what is possible with similar tools, but less understanding of the sources of bias in the land surface model, we refer the reviewer to the analysis of McNeall *et al.* (2016), which was conducted without this understanding. In particular, the understanding of the shape of the combined parameter space that could not be ruled out, and that the default land surface parameters are within this region are knowledge gained from an understanding of the impacts of the climate bias in this paper.

Reviewer 2

Page 11, Line 26: 'Moving any...' I find this sentence confusing. Can you better link it to the figure and clarify?

Author response

We have edited the paragraph for clarity, and it now reads as follows -

"With other inputs held constant, cooler, wetter climates are predicted to increase forest fraction and drier, warmer climates reduce forest fraction. In general, South East Asian and Central African forests are simulated as warmer and wetter than their true-life counterparts. Moving the temperature and precipitation values of a typical ensemble member from near the centre of these forest sub-ensembles to their observed real-world values would shift them primarily in the same direction as the contours of forest fraction value. This would mean that bias correcting the climate variables would not have a large impact on forest fraction values in South East Asian and Central African forests, and that they are therefore simulated with a roughly accurate forest fraction. In contrast, the Amazon is simulated slightly drier, and considerably warmer than the observed Amazon and many ensemble members consequently have a lower forest fraction than observed. Shifting the temperature and precipitation of a typical ensemble member for the Amazon to its real-world observed values would cross a number of contours of forest fraction. This figure provides strong evidence that a significant fraction of the bias in Amazon forest fraction is caused by a bias in simulated climate."

Reviewer 2

Figure 14: There is a clear relationship with V_CRIT_ALPHA and NLO when the augmented emulator is used. Can you discuss this and what it might mean?

Response: It is clear from the sensitivity analyses section that, all other things remaining the same, (e.g.) increasing the value of NL0 raises strongly forest fraction, while increasing V_CRIT_ALPHA strongly reduces forest fraction. We would expect there to be a region, indeed a plane through parameter space where these two strong effects counteract each other, resulting in a forest fraction close to observations.

This feature does not appear in the history matching before bias correcting (figure 13 in the original text). The low value of the simulated Amazon forest fraction before bias correction of the climate inputs rules out much of the input parameter space later found to be Not Ruled Out Yet (NROY) after the bias corrected history matching exercise (figure 14 in the original text). This point has been added to the discussion.

Reviewer 2

Page 17, line 5: Is it temperature and precipitation that should be targeted or how the model treats them? It's not clear to me exactly what you are recommending.

Author response

Edited for clarity. The sentence now reads "Our work here shows this process as an example. We have identified the importance of precipitation and temperature to the correct simulation of the Amazon forest, and flag their accurate simulation in that region as a priority in for the development of any climate model that hopes to simulate the forest well."

Reviewer 2

Page 17, line 18: If you were to this for every grid box would you expect predictability? I could see this method working for elevation and seasonal biases? How might you go about this?

Author response

We have edited the paragraph to further discuss the practicality and predictability of using the emulator at smaller scales, as follows:

"In theory the augmented emulator could be used to bias correct differently sized regions, down to the size of an individual gridbox for a particular variable. This might be useful for correcting, for example, known biases in elevation or seasonal climate. The principle of repeating the common parameter settings in the design matrix, and including model outputs as inputs would work in exactly the same way, but with a larger number of repeated rows.

In the case of using an augmented emulator on a per-gridbox basis, we might expect the relationship between inputs that we are bias correcting (e.g. temperature, precipitation), and the output of interest (e.g. forest fraction) to be a less clear, as at small scales there are potentially many other inputs that might influence the output. An emulator for an individual gridbox might therefore be less accurate. However, with enough data points, or examples (and there would be many), we might expect to be able to recover any important relationships."

References not in main text

Mara, T.A., Tarantola, S. and Annoni, P., 2015. Non-parametric methods for global sensitivity analysis of model output with dependent inputs. *Environmental modelling & software*, 72, pp.173-183. https://doi.org/10.1016/j.envsoft.2015.07.010

Correcting a bias in a climate model with an augmented emulator

Doug McNeall^{1,3}, Jonny Williams², Richard Betts^{1,3}, Ben Booth¹, Peter Challenor³, Peter Good¹, and Andy Wiltshire^{1,3}

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Correspondence: Doug McNeall (doug.mcneall@metoffice.gov.uk)

Abstract. A key challenge in developing flagship climate model configurations is the process of setting uncertain input parameters at values that lead to credible climate simulations. Setting these parameters traditionally relies heavily on insights from those involved in parameterisation of the underlying climate processes. Given the many degrees of freedom and computational expense involved in evaluating such a selection, this can be imperfect leaving open questions about whether any subsequent simulated biases result from mis-set parameters or wider structural model errors (such as missing or partially parameterised processes). Here we present a complementary approach to identifying plausible climate model parameters, with a method of bias correcting subcomponents of a climate model using a Gaussian process emulator that allows credible values of model input parameters to be found even in the presence of a significant model bias.

A previous study (McNeall et al., 2016) found that a climate model had to be run using land surface input parameter values from very different, almost non-overlapping parts of parameter space to satisfactorily simulate the Amazon and other forests respectively. As the forest fraction of modelled non-Amazon forests was broadly correct at the default parameter settings and the Amazon too low, that study suggested that the problem most likely lay in the model's treatment of non-plant processes in the Amazon region. This might be due to (1) modelling errors such as missing deep-rooting in the Amazon in the land surface component of the climate model, (2) to a warm-dry bias in the Amazon climate of the model, or a combination of both.

In this study we bias correct the climate of the Amazon in a climate model the climate model from (McNeall et al., 2016) using an "augmented" Gaussian process emulator, where temperature and precipitation, variables usually regarded as model outputs, are treated as model inputs alongside regular land surface input parameters. A sensitivity analysis finds that the forest fraction is nearly as sensitive to climate variables as it is to changes in its land surface parameter values. Bias correcting the climate in the Amazon region using the emulator corrects the forest fraction to tolerable levels in the Amazon at many candidates for land surface input parameter values, including the default ones, and increases the valid input space shared with the other forests. We need not invoke a structural model error in the land surface model, beyond having too dry and hot a climate in the Amazon region.

The augmented emulator allows bias correction of an ensemble of climate model runs and reduces the risk of choosing poor parameter values because of an error in a subcomponent of the model. We discuss the potential of the augmented emulator to act as a translational layer between model subcomponents, simplifying the process of model tuning when there are compensating errors, and helping model developers discover and prioritise model errors to target.

¹Met Office Hadley Centre, FitzRoy Road, Exeter, EX1 3PB, UK

²NIWA, 301 Evans Bay Parade, Hataitai, Wellington 6021, New Zealand

³University of Exeter, North Park Road, Exeter, EX4 4OE, UK

1 Introduction

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1.1 Choosing good input parameter settings in the presence of model errors

Choosing values of uncertain input parameters that lead to credible climate simulations is an important and challenging part of developing a new climate model configuration. Climate models contain simplifications of processes too complex to represent explicitly in the model, termed parameterisations. Associated with these parameterisations are coefficients called input parameters, the values of which are uncertain and can be set by the model developer. We wish to choose input parameters where the output of the model reproduces observations of the climate, in order to have confidence that the model represents important physical processes sufficiently well to trust projections of the future. This is difficult because: 1) There is uncertainty in the observations, 2) we cannot run the model at every desired input parameter configuration, and there is uncertainty about model output at those parameter sets not run, and 3) the model does not reproduce the dynamics of the climate system perfectly. The latter is termed model discrepancy, and distinguishing between it and a poorly chosen input parameter configuration is a major challenge in model development.

Input parameters have a material effect on the way the parameterisations operate and therefore induce an uncertainty in the output of the model and corresponding uncertainty in projections of future climate states, but often to an extent that is unknown until the model is run. Modern climate simulations are computationally expensive to run, and there may only be a handful of simulations on which to make a judgement about the validity of a simulation at a particular set of parameters. Further, appropriate values for input parameters may be difficult or even impossible to observe, some having no direct analogue in the real system.

Setting input parameters traditionally relies heavily on insights from those involved in parameterisation of the underlying climate processes. Given the many degrees of freedom and computational expense involved in evaluating such a selection, this can be an imperfect process, leaving open questions about whether any subsequent simulated biases result from mis-set parameters or wider structural model errors (such as missing or partially parameterised processes). The process of setting the values of the input parameters so that the simulator output best matches the real system is called tuning, and where a probability distribution is assigned for the input parameters, it is termed calibration. This process is often viewed as setting constraints on the plausible range of the input parameters, where the climate model sufficiently represents the real system.

Hourdin et al. (2017) offer a summary of In summarising current practice in the somewhat sparsely studied field of climate model tuning. While there are common practices, there appear no standard procedures for climate model tuning however – as the authors point out, Hourdin et al. (2017) point out that it remains an art as well as a science. Individual While there appear no universally accepted procedures, individual modelling centres have begun to document their tuning practices with regard to tuning targets and procedures (Schmidt et al., 2017; Zhao et al., 2018; Walters et al., 2017).

Improving a coupled climate model can require an involved and lengthy process of development, and parameter tuning occurs at different stages in that process. It might start with a single column version of the model developed in isolation as

stand-alone code. It can be relatively easy to find a good subset of input parameters given a small set of inputs and outputs and a well behaved relationship between the two as for a subcomponent of a climate model, particularly where there are good observations of the system being studied. The climate model components to be coupled might be then then be tuned with standard boundary conditions - for example tuning a land/atmosphere component with fixed or historically observed sea surface temperatures. Finally, a system-wide tuning might be used to check that there are minimal problems once everything has been coupled together. There is sometimes a tension however, between choosing input parameters that elicit the best performance for the subcomponent (e.g. for a single-gridbox model), and choosing ones that make the subcomponent behave well in the context of the coupled model. Upon integration, some components of the model may therefore be tuned to compensate for errors in others or there may be unknown errors in the model or observations. Golaz et al. (2013) Show-show the potential impact of compensating errors in tuning. They find that two different but plausible parameter configurations of the cloud formations of the coupled climate model GFDL-CM3 can result in similar present-day radiation balance. The configurations did not differ in their present day climate, but showed significantly different responses to historical forcing and therefore historical climate trajectories. More complex models are computationally expensive and so are infeasible to run in enough configurations to be able to identify these kind of errors. No single expert, or even small team of experts may have the cross-domain knowledge required to identify and fix problems that occur as multiple sub systems interact with each other. Output from a climate model run at a particular set of inputs must be evaluated against observational targets of the real system. Individual observations are subject to uncertainties, sometimes large, and there are often multiple observations of the same property, each with its own strengths and weaknesses.

Without strong prior information then, information about known errors (for example, knowledge of an instrument bias, or a known deficiency of a model), it can be difficult to attribute a difference between simulator output and the real system to underlying model errors, to an incorrect set of input parameters, or to inaccuracies in the observations. This means that a good candidate good candidates for input parameters might be found in a large volume of input space, and but projections of the model made with candidates from across that space might diverge to display a very wide range of outcomes. This problem is sometimes referred to as "identifiability", but otherwise known as "equifinality", or the "degeneracy" of model error and parameter uncertainty.

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Although climate model tuning is overall a subjective process, individual parts of the process are amenable to more algorithmic approaches. Statistical and machine learning approaches to choosing parameters to minimise modelling error, or to calculate probability distributions for parameters and model output are known as uncertainty quantification (UQ). The field of Uncertainty Quantification (UQ) has seen a rapid development of methods to quantify uncertainties when using complex computer models to simulate real, physical systems. The problem of accounting for model discrepancy when using data to learn about input parameters is becoming more widely recognised in UQ. It was formalised in a Bayesian setting by Kennedy and O'Hagan (2001). The authors suggested simultaneously estimating a model discrepancy - there called model inadequacy - as a function of the inputs, using a Gaussian process prior. Brynjarsdóttir and O'Hagan (2014) argued that only by accounting for model discrepancy does even a very simple simulator have a chance of making accurate predictions. Further, they found that only where there is strong prior evidence about the nature of that model discrepancy is it possible to solve the inverse

problem and recover the correct inputs. Without this strong prior evidence the estimate of the correct parameters is likely to be overconfident, and wrong, leading to overconfident and wrong predictions of out-of-sample data. Arendt et al. (2012a) offer a number of examples of identifiability problems, ranging from solvable using mild assumptions through to virtually impossible. In a companion paper (Arendt et al., 2012b), they outline a way of improving identifiability using multiple model responses.

1.2 History matching

Some of the dangers of overconfident and wrong estimates of input parameters and model discrepancy can be reduced using a technique called history matching (Craig et al., 1996), sometimes called pre-calibration or iterated refocussing. The aim of history matching is not to find the most likely inputs, but to reject those unlikely to produce simulations statistically close to observations of the real system.

A statistical model called an emulator, trained on an ensemble of runs of the climate model, predicts the output at input configurations not yet run. An implausibility measure (I) is calculated at any input configuration, taking into account the distance between the simulator output and the observation but formally allowing for uncertainty in the observations, the simulator output and the simulator discrepancy. Those inputs that produce a large implausibility score are ruled out from consideration as candidate points. New simulator runs in the remaining input space increase our understanding of the model behaviour and allow more input space to be ruled out in an iterated fashion. An excellent introduction and case studies can be found in Andrianakis et al. (2015), or in Vernon et al. (2010). History matching is perhaps less ambitious but correspondingly more robust than calibration methods, and a full calibration can be carried out once the history matching procedure has been completed.

History matching can be effective in reducing the volume of parameter space that is considered plausible to produce model runs that match the real system. For example, Williamson et al. (2015) report very large reductions (around 99%) in the volume of space considered plausible. History matching does still depend however, on a robust estimate of model discrepancy and associated uncertainty, in order not to produce unjustifiably small regions of not-ruled-out input parameter space. For example, (McNeall et al., 2013) McNeall et al. (2013) studied an ensemble of an ice sheet model and found that using a single type of observation for ruling out input space was not very powerful - particularly if there was not a very strong relationship between an input parameter and the simulator output. The effectiveness of history matching for ruling out input space can be enhanced by using multiple data sets. However (Johnson et al., 2018) Johnson et al. (2018), using history matching to constrain the forcing of a coupled climate and atmospheric chemistry model, find that even with multiple observational targets, a typical example of aerosol effective radiative forcing is only constrained by about 30%.

McNeall et al. (2016) argued that the larger the number of model-data comparisons, the larger the probability that an unidentified model discrepancy rules out a perfectly good input parameter candidate point. Several empirical rules have been used in the literature - for example using the maximum implausibility of a multiple comparison, a candidate input point may be ruled out by a single observation. A more conservative approach is to use the second or third implausibility score, or to use a multivariate implausibility score, both introduced in Vernon et al. (2010). The aim of these scores is to ensure that an unidentified model discrepancy, or a poorly specified statistical model of the relationships between model inputs and outputs does not result in ruling out candidate points that are in fact perfectly good.

While history matching has often been used used to explore and reduce the input parameter space of expensive simulators, its use as a tool to find discrepancies, bias and inadequacies in simulators is less developed. Williamson et al. (2015) argue that what was assumed a structural bias in the ocean component of climate model HadCM3 could be corrected by choosing different parameters. In a different system McNeall et al. (2016) argue that a standard set of parameters for the land surface component of the climate model FAMOUS should be retained, and that a bias seen in the simulation of the Amazon rainforest is a simulator discrepancy not a poor parameter choice. In that case, the model simulated other forests at the standard set of parameters well, and only a tiny volume of parameter space could be found that (barely) adequately simulated all the forests. When cast as a choice between adding a model discrepancy and keeping the default parameters, or rejecting them and accepting the new region of parameter space, they argued that the former was more likely to produce a good model , as presumably scientific judgementand expertise for a number of reasons, whereas were a number of reasons one might reject the proposed parameter space. First, scientific judgement, expertise and experience with previous versions of this and other models will have informed the original choice of parameters, whereas there were a number of reasons one might reject the proposed parameter space. The model simulated other forests at the standard set of parameters well, and only a tiny volume of parameter space could be found that (barely) adequately simulated all the forests. The region of parameter space that apparently simulated all forests well was at the edge of the ensemble, where uncertainty in the emulator is often large, and might dominate the history matching calculation rather than the parameter choices being particularly good. In that case, running more ensemble members in the part of parameter space in question might help rule it out. Three of the forests were well simulated at the default parameters and a highly overlapping region of parameter space, and only the Amazon was poorly simulated at the default parameter setting. Finally, in the region where all forests were adequately simulated, the Amazon forest was under estimated, and the other forests overestimated, suggesting that that choosing that region of parameter space would inevitably force a compromise.

1.3 Aims of the paper

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This paper revisits and extends the analysis of McNeall et al. (2016) (hereafter M16) to attempt to identify the source of model discrepancy in the simulation of the Amazon in FAMOUS. We aim to 1) identify the causes of a low bias in the forest fraction in the Amazon region in an ensemble of the climate model FAMOUS and 2) develop a method that allows us to choose plausible values for input parameters for one component of a coupled model, even when there is a model discrepancy or bias in another subcomponent of the coupled model.

A well simulated and vigorous Amazon forest at the end of the spinup phase of a simulation experiment is a prerequisite for using a model to make robust projections of future changes in the forest. The analysis of McNeall et al. (2016) (hereafter M16)-identified that the land surface input spaces where FAMOUS forest fraction was consistent with observations were very different in the Amazon than they were for other forests. The area of overlap of these spaces - one that would normally be chosen in a history matching exercise - did not simulate any of the forests well, and did not contain the default parameters. M16 suggested that assuming an error in the simulation of the Amazon forest would be a parsimonious choice. Two obvious candidates for the source of this error in the Amazon region were identified: (1) a lack of deep rooting in the Amazon forest,

meaning that trees could not access water at depth as in the real forest and (2) a bias in the climate of the model, affecting the vigour of the trees.

This paper revisits and extends the analysis of M16 to attempt to identify the source of model discrepancy in the simulation of the Amazon in FAMOUS. We simultaneously (1) assess the impact of a bias corrected climate on the Amazon forest and (2) identify regions of input parameter space that should be classified as plausible, given a corrected Amazon climate. To bias correct the climate we develop a new method to augment a Gaussian process emulator, with simulator outputs acting as inputs to the emulator alongside the standard input parameters. We use simulated output of forests at different geographical locations to train the emulator, describing a single relationship between the climate of the simulator, the land surface inputs and the forest fraction. In doing so, we develop a technique that might be used to bias correct subcomponents of coupled models, allowing a more computationally efficient method for final system-tuning of those models.

In section 2, we review the literature on the possible causes of the low Amazon forest fraction in FAMOUS. In section 3.1, we describe how we use the temperature and precipitation to augment the Gaussian process emulator. In section 4.4 we use the emulator to estimate the sensitivity of forest fraction to changes in land surface and climate parameters. In section 4.2 we use the augmented emulator to bias correct the climates of the forest and examine the effect of that bias correction on the input space that is deemed statistically acceptable in a history matching exercise. In section 4.5 we search for regions of parameter space where the bias corrected simulator might perform better than at the default parameters. In section 4.4 we use the augmented emulator to estimate the sensitivity of forest fraction to changes in land surface and climate parameters In section 4.6 we look at regions of climate space where the default parameters would produce statistically acceptable forests. Finally, we offer some discussion of our results in section 5 and conclusions in section 6.

2 Climate and forest fraction

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Previous studies have concluded that the climate state has an influence on the Amazon rainforest. Much of that work has been motivated by the apparent risk of dieback of the Amazon forest posed by a changing climate [e.g. Malhi et al. (2008); Cox et al. (2004)]. We assume that factors that might affect a future simulated Amazon rainforest might also affect the simulated steady-state preindustrial forest in FAMOUS. Parameter perturbations and CO₂ concentrations have been shown to influence the simulation of tropical forests in climate models (Boulton et al., 2017; Huntingford et al., 2008), with increases in CO₂ fertilisation and associated increased water use efficiency through stomatal closure offsetting the negative impacts of purely climatic changes (Betts et al., 2007; Good et al., 2011). A metric linked to rainforest sustainability by Malhi et al. (2009) is Maximum Cumulative Water Deficit, which describes the most negative value of climatological water deficit measured over a year. In a similar vein Good et al. (2011, 2013) find that in Hadley Centre models, sustainable forest is linked to dry-season length, a metric which encompasses both precipitation and temperature, along with sensitivity to increasing CO₂ levels. No forest is found in regions that are too warm or too dry, and there is a fairly distinct boundary between a sustainable and non-sustainable forest. Galbraith et al. (2010) found that temperature, precipitation and humidity had greatly varying influences, and by different mechanisms on changes in vegetation carbon in the Amazon across a number of models, but that rising

CO₂ mitigated losses in biomass. Poulter et al. (2010) found that the response of the Amazon forest to climate change in the land surface model LPJml was sensitive to perturbations in parameters—affecting ecosystem processes, the carbon cycle and vegetation dynamics, but that the dynamics of a dieback in the rainforest was robust across those perturbations. In that case, the main source of uncertainty of dieback was uncertainty in climate scenario. Boulton et al. (2017) found that temperature threshold and leaf area index parameters both have an impact on the forest sustainability under projections of climate change in the Earth system version of HadCM3.

2.1 Biases in FAMOUS

M16 speculated that both local climate biases and missing or incorrect processes in the land surface model - such as missing deep rooting in the Amazon - might be the cause of the simulated low forest fraction in the Amazon region at the end of the pre-industrial period in an ensemble of the climate model FAMOUS. In this study we use the ensemble of FAMOUS previously used in M16, to attempt to find and correct the cause of persistent low forest fraction in the amazon, identified in that paper.

The Fast Met Office UK Universities Simulator, FAMOUS (Jones et al., 2005; Smith et al., 2008), is a reduced-resolution climate simulator based on the climate model HadCM3 (Gordon et al., 2000; Pope et al., 2000). The model has many features of modern climate simulators, but is of sufficiently low resolution to provide fast and simple data sets with which to develop UQ methods. Full details of the ensemble can be found in M16 and Williams et al. (2013).

The ensemble of 100 members perturbed 7 land surface and vegetation inputs, which (see supplementary material, table S1), along with a further parameter denoted "beta" (β). Each of the ten values of beta provides a index to one of ten of the best-performing atmospheric and oceanic parameter sets used in a previous ensemble with the same model Gregoire et al. (2010), with the lowest values of beta corresponding to the very best performing variants. The beta parameter therefore summarised perturbations in 10 atmospheric and oceanic parameters that impacted the climate of the model, randomly varied with land surface input parameters, and potentially leading to different climatologies in a model variant with the same land surface parameters but different values of beta. Variations in the beta parameter did however not correlate strongly to variations with any of the oceanic, atmospheric or land surface parameters in the ensemble, and so the parameter was excluded from the analysis in M16. In this analysis we recognise that the different model climates caused by variations in the atmospheric and oceanic parameters will have an impact on the forest fraction, and so we summarise those variations directly using local temperature and precipitation.

Variation in the parameters across the ensemble had a strong impact on vegetation cover at the end of a spinup period, with atmospheric CO₂ at preindustrial conditions(fig. 1). The broadleaf forest fraction in individual ensemble members varies from almost non-existent to vigourous -(fig. 1). The strong relationships between forest fraction in each forest and global values the global mean forest fraction and the mean forest fraction in each region implies that perturbations in input parameters exert a larger control over all forests simultaneously, and individual forests to a smaller extent.

M16 aggregated the regional mean forest fraction for the Amazon, Southeast Asian, North American and central African forests, along with the global mean. They were only able to find very few land surface parameter settings which the emulator history matching process suggested should lead to an adequate simulations of the Amazon forests and the other forests together.

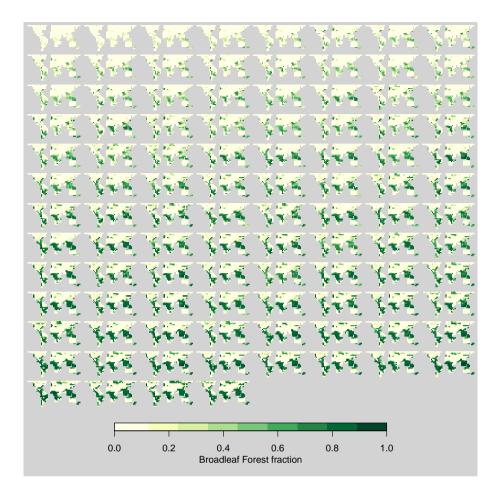


Figure 1. Broadleaf forest fraction in the FAMOUS ensemble, ranked from the smallest to largest global mean value.

Further, these These parameter sets were at the edges of sampled parameter space, where larger uncertainty in the emulator may have been driving the acceptance of the parameter sets.

The ensemble did however have a further perturbation – a parameter denoted "beta" (β), which indexed into one of ten of the best-performing atmospheric parameter sets used in a previous ensemble with the same model. The beta parameter then summarised perturbations in a number of other parameters that impacted the climate of the model. Variations in the parameter did not correlate with any of the land surface parameters in the ensemble, and so was excluded from the analysis in M16.

In this study, we use the same ensemble of forest fraction data used in M16. However, we add temperature and precipitation data, present in the original ensemble but not used to build an emulator in the M16 study, to further our understanding of the causes of the low forest fraction in the Amazon region. The temperature and precipitation data summarise the effects of atmospheric parameters on the atmospheric component of the model, in a way that is directly seen by the land surface component of the model. We consider only regions dominated by tropical broadleaf forest, so as not to confound analysis by including other forests which may have a different set of responses to perturbations in parameters, rainfall and temperature.

For temperature observations we use the CRU global monthly surface temperature climatology Jones et al. (1999) (Jones et al., 1999), covering the years 1960-1990. For precipitation we use the average monthly rate of precipitation, covering the years from 1979-2001 from GPCP Version 2.2 provided by the NOAA/OAR/ESRL PSD, Boulder, Colorado, USA, from their Web site at https://www.esrl.noaa.gov/psd/ Adler et al. (2003) (Adler et al., 2003). Vegetation fraction observations are adapted from Loveland et al. (2000), and are shown in fig. 2. Although the observations all cover slightly different time periods, we expect the differences caused by harmonising the time periods to be very small compared to other uncertainties in our analysis, and to be well covered by our uncertainty estimates.

A plot of regional mean temperature and precipitation in the tropical forest regions in the FAMOUS ensemble (fig. 3) indicates the form of the impact that the regional climate has on forest fraction in the climate model. Central African and Southeast Asian climates in the model simulations run in a sweep across the middle of the plot, from dry and cool to wet and warm.

It appears that a wetter climate - which would be expected to stabilise forests - broadly compensates for the forest reductions induced by a warmer climate. Within the ensemble of Central African forests for example, forest fraction increases towards the "cooler, wetter" (top left) part of the climate phase space. Beyond a certain value however, there are no simulated climates or forests in this climatic region. It is clear from the plot that while central African and Southeast Asian forests are simulated in the large part considerably warmer than recent observations, they are also simulated considerably wetter, which might be expected to compensate forest stability. In contrast, while simulated considerably warmer, the Amazon is also slightly drier than recent observations, which might further reduce forest stability.

We are assuming here that tropical forests can be represented by a single set of forest function parameters. While such an assumption risks missing important differences across heterogenous tropical forests, modelling the system with the smallest set of common parameters avoids overfitting to present day data. Avoiding overfitting is important if we are to use these models to project forest functioning in future climates outside observed conditions. One of the questions that the analysis presented in this paper addresses is whether current forest biases in the simulations reflect limitations of this single tropical forest assumption, or whether biases in the simulations of the wider climate variables play a more important role.

3 Methods

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The climate model FAMOUS is computationally expensive enough that we cannot run it for a large enough number of input parameter combinations to adequately explore parameter space and find model biases. To increase computational efficiency we build a Gaussian process emulator: a statistical function that predicts the output of the model at any input, with a corresponding estimate of uncertainty —(see e.g. Sacks et al. (1989); Kennedy and O'Hagan (2001)). The emulator models climate model output y as a function g() of inputs x so that y = g(x). It is trained on the ensemble of model runs described in section 2.1. The set of land surface input parameters is called the design matrix, denoted X, and the corresponding sample of model output forest fraction is denoted y. The configuration of the design matrix is a latin-Latin hypercube (McKay et al., 1979), as used in

e.g. Gregoire et al. (2010); Williams et al. (2013), with sample input points chosen to fill input parameter space efficiently and therefore sample relationships between input parameters effectively.

3.1 An augmented emulator

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Our strategy is to augment the design matrix of input parameters X with corresponding atmospheric climate model output that might have an impact on the modelled land surface, building an emulator that models the effects of both input parameters and climate on forest fraction. We then use the augmented emulator to bias correct each forest in turn. We use the emulator to describe the relationship between land surface parameters, atmospheric variables that summarise the action of hidden atmospheric parameters, and the broadleaf forest fraction. The relationships between these variables are summarised in fig. 4.

We have a number of forests for each ensemble member, differing in driving influences by a different local climate. Regional extent of each of the broadleaf forests can be found in the supplementary material. We use regional mean temperature, T, and precipitation, P, for each of the forests: the Amazon, central Africa and Southeast Asia as additional inputs to augment our original design matrix of land surface parameters, X. Regional extent of each of the broadleaf forests can be found in the supplementary material. These new inputs are outputs of the model when run at the original inputs X, and are influenced by the 10 atmospheric and oceanic parameters perturbed in a previous ensemble τ in a configuration unavailable to us in this experiment. Performance of the model under those perturbations is summarised in the β parameter, beta parameter, which has smaller values for the better performing models. The performance metrics included temperature and precipitation, along with a number of other measures so the beta parameter therefore contains information about temperature and precipitation across the ensemble, without being a perfect representation of its behaviour. We cannot control them the atmospheric and oceanic parameters directly and thus ensure that they lie in a latin hypercube configuration. Latin hypercube configuration, although the ensemble is ordered in a Latin hypercube configuration according to the performance of the model at each parameter set.

With n=100 ensemble members, we form each $n\times 1$ vector of temperature and precipitation and form an $n\times 2$ matrix of climate variables for the Amazon $C_{AZ}=[T_{AZ}P_{AZ}]$, Central Africa $C_{AF}=[T_{AF}P_{AF}]$ and Southeast Asia $C_{AS}=[T_{AS}P_{AS}]$. We use these to augment the original $n\times p$ input matrix X, creating a unique input location for each forest. We then stack these augmented input matrices together to form a single input matrix X'.

$$X' = \begin{bmatrix} X & C_{AZ} \\ X & C_{AF} \\ X & C_{AS} \end{bmatrix} \tag{1}$$

From an initial ensemble design matrix with n=100 members and p=7 inputs, we now have a design with n=300 members and p=9 inputs. Each member with a replicated set of initial input parameters (e.g members [1,101,201]), differ only in the T and P values. Figure 5 shows a diagram of the augmented emulator along with the composition of the resulting input matrix and output vector.

Where in M16, we the authors built an independent emulator for each output (i.e. regional forest fraction), we now build a single emulator for all forest fractions simultaneously given input parameters, temperature and precipitation. The output vector

for the tropical forests has gone from being 3 sets of 100 values y_{AZ} , y_{AF} , y_{AS} , to a single vector $y' = [y_{AZ}, y_{AF}, y_{AS}]$ of length 300. We model forest fraction y' as a function of X' using the Gaussian process emulator of package DiceKriging (Roustant et al., 2012) in the R statistical language and environment for statistical computing. Details of the emulator can be found in the supplementary material.

We note that the augmented emulator depends on the assumption that modelled broadleaf forests in each location respond similarly to perturbations in climate and input parameters. This assumption may not hold for the behaviour of the forests in the model, or indeed the real world. For example, particularly deep rooting of forests in the Amazon would respond differently to rainfall reductions but these processes are not represented in the underlying climate model. Similarly, differing local topology that is captured in the climate model, may influence the forests in a way not captured by our emulator. In both cases, the emulator would show systematic errors of prediction.

10 3.2 Verifying the augmented emulator

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To verify that the augmented emulator adequately reproduces the simulator behaviour, we use a leave-one-out metric. For this metric, we sequentially remove one simulator run from the ensemble, train the emulator on the remaining ensemble members and predict the held-out run. We present the predicted members and the calculated uncertainty plotted against the actual ensemble values in fig. 6.

It is important to check that the augmented emulator performs well in prediction, in order to have confidence that using emulated runs in our later analyses is a valid strategy. We see no reason to doubt that the augmented emulator provides a good prediction and accurate uncertainty estimates for prediction at inputs points not yet run. We use the mean of the absolute value of the difference between the emulator prediction and corresponding held-out value to calculate the Mean Absolute Error of cross-validation prediction (MAE). Prediction error and uncertainty estimates remain approximately stationary across all tropical forests and values of forest fraction. The mean absolute error of prediction using this emulator is a little under 0.03, or 3 around 6% of the maximum possible mean value of the ensemble.

When compared against the regular emulator using just the land surface inputs, the augmented emulator performs well. The augmented emulator has a mean absolute error of prediction of 0.03 or 3% of the maximum possible value of the ensemble. The regular emulator built individually for each of the forests (as per M16) has a mean absolute error value of 0.058 - nearly double that of the augmented emulator. This indicates that adding temperature and precipitation to the input matrix adds useful information to a predictive statistical model. A breakdown of the mean absolute error of the emulator on a per-forest basis can be seen in table 1.

There is some concern that the emulator might not perform well close to the observed values of temperature and precipitation, particularly for the Amazon and Central African regions. For this reason, we carry out an enhanced verification of the emulator, holding out more ensemble members and demanding further extraoplation (see supplementary material, section 2). We find no reason to doubt that the augmented emulator performs well.

Do the error estimates of the augmented emulator match the true error distributions when tested in leave-one-out predictions? We test the reliability of uncertainty estimates of the emulator by checking that the estimated probability distributions for held-

Table 1. Mean absolute error (MAE) rounded to the first significant figure for the regular emulator, using just the seven land surface inputs, and the augmented emulator, including temperature and precipitation.

Forest	Regular emulator MAE	Augmented emulator MAE
Amazon	0.05	0.03
Southeast Asia	0.06	0.03
Central Africa	0.06	0.03
All	0.06	0.03

out ensemble members match the true error distributions in the leave-one-out exercise. We create a rank histogram (see e.g. Hamill (2001)) for predictions, sampling 1000 times from each Gaussian prediction distribution, and plotting the rank of the actual prediction in that distribution. The distribution of these ranks overall predictions should be uniform if the uncertainty estimates are reliable. Consistent overestimation of uncertainty will produce a peaked histogram, while systematic underestimation of uncertainty will produce a u-shaped histogram. The rank histogram produced by this set of predictions (fig. 7) is close to a uniform distribution, indicating reliable predictions.

15 4 Analyses

3.1 History Matching

3.2 Sensitivity analysis

The emulator allows us to measure the sensitivity of forest fraction to the land surface input parameters simultaneously with elimate variables temperature and precipitation. We measure the one-at-a-time sensitivity to parameters and climate variables, using the emulator to predict changes in forest fraction as each variable is changed from the lowest to highest setting in turn, with all other parameters at the default settings or observed values. We present the results in fig. ??. Parameters NLO and V_CRIT_ALPHA and climate variables temperature and precipitation exert strong influences of similar magnitudes on forest fraction. Shaded regions represent the uncertainty of the sensitivity to each parameter, due to estimated emulator uncertainty of ± 2 standard deviations. This sensitivity measure does not include the extra uncertainty due to the fact that the relationships will change depending on the position of the other parameters. We do however see a measure of how temperature and precipitation affect the marginal response of the other parameters, as the observed climates of each forest are different. For example, we clearly see that the response of the forest fraction to e.g. NLO depends on climate – the forest fraction response is a noticeably different shape when varied under the mean climate of the South East Asian region. History matching is the process of finding and ruling out regions of parameter space where the model is unlikely to produce output that matches observations well. It measures the statistical distance between an observation of a real-world process, and the emulated output of the climate model

at any input setting. An input where the output is deemed too far from the observation is ruled "implausible", and removed from consideration. Remaining inputs are conditionally accepted as "Not Ruled Out Yet" (NROY), recognising that further information about the model or observations might yet rule them as implausible.

One-at-a-time sensitivity of forest fraction variation of each parameter and climate variable in turn across the entire ensemble range. All other parameters or variables are held at their default values while each parameter is varied. Solid lines represent the emulator mean and shaded areas represent ± 2 standard deviations of emulator uncertainty.

A quantitative measure of sensitivity of the model output to parameters that does take into account interactions with other parameters is found using the FAST99 algorithm of Saltelli et al. (1999), summarised in fig. 13. Precipitation and Temperature are the second and third most important parameters, more important than NL0Observations of the system are denoted z, and only slightly less important than V_CRIT_ALPHA. Interaction terms contribute a small but non-negligible part to the sensitivity we assume that they are made with uncorrelated and independent errors ϵ such that

$$z = y + \epsilon \tag{2}$$

Assuming a "best" set of inputs x^* where the model discrepancy δ , or difference between climate model output y and z is minimised, we relate observations to inputs with

$$15 \quad z = g(x^*) + \delta + \epsilon \tag{3}$$

We calculate measure of implausibility I, and reject any input as implausible where I > 3 after Pukelsheim's three-sigma rule; that is, for any unimodal distribution, 95 % of the probability mass will be contained within 3 standard deviations of the mean (Pukelsheim, 1994). We calculate

$$\underline{I^2} = |z - E[g(x)]|^2 / Var[g(x)] + Var[\delta] + Var[\epsilon]$$

$$\tag{4}$$

which recognises that the distance between the best estimate of the emulator and the observations must be normalised by uncertainty in the emulator g(x), in the observational error ϵ , and in the estimate of model discrepancy δ .

Sensitivity of forest fraction to model parameters and climate parameters, found using the FAST99 algorithm of Saltelli et al. (1999)

4 Analyses

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4.1 The joint impacts of temperature and precipitation on forest fraction

What impact do temperature and precipitation have on forest fraction together? We use the emulator from section 3.1 and predict the simulator output across the entire range of simulated temperature and precipitation, while holding the other inputs

at their default values. The marginal impacts of temperature and precipitation on forest fraction are clear in fig. 8. Ensemble member temperature, precipitation and forest fraction, taken from fig. 3 are overplotted for comparison. Temperature and precipitation values are normalised to the range of the ensemble in this plot.

Cooler, With other inputs held constant, cooler, wetter climates are predicted to increase forest fraction and drier, warmer climates lead to very low forest fractionvalues in some simulations reduce forest fraction. In general, South East Asian and Central African forests are simulated as warmer and wetter than their true-life counterparts. Moving any ensemble member to observed values of temperature and precipitation would not cross many the temperature and precipitation values of a typical ensemble member from near the centre of these forest sub-ensembles to their observed real-world values would shift them primarily in the same direction as the contours of forest fraction value, and so ensemble members are. This would mean that bias correcting the climate variables would not have a large impact on forest fraction values in South East Asian and Central African forests, and that they are therefore simulated with a roughly accurate forest fraction. In contrast, the Amazon is simulated slightly drier, and considerably warmer than the observed Amazon and many ensemble members consequently have a lower forest fraction than observed. Shifting the temperature and precipitation of a typical ensemble member for the Amazon to its real-world observed values would cross a number of countours of forest fraction. This figure provides strong evidence that a significant fraction of the bias in Amazon forest fraction is caused by a bias in simulated climate.

4.2 A climate bias correction approach

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With an emulator that models the relationship between input parameters, local climate and the forest fraction, we can predict what would happen to forest fraction in any model simulation if the local climate was correct. In fig. 9, for example, the predicted value is the forest fraction we compare the value of forest fraction predicted at the default set of land surface parameters, with using the standard emulator, with that predicted using the local temperature and precipitation corrected to the observed values -using the augmented emulator. This means that Central Africa becomes significantly drier, and a little cooler than the centroid of the ensemble. Southeast Asia becomes a little cooler and a little drier. The Amazon forest becomes a little wetter, and significantly cooler. The ensemble has a much larger spread of climates in central Africa than South East Asia or the Amazon. We note that we do not have an ensemble member run at the default land surface parameters, so we compare two predictions using the emulator.

The bias correction reduces the difference between the prediction for the modelled and observed Amazon forest fraction markedly, from -0.28 using the standard emulator to -0.08 using the augmented emulator. It makes the predicted modelled forest in central Africa worse (-0.11 from -0.03), and slightly improves the SE Asian forest fraction (0.07 from 0.1). Overall, bias correcting the climate takes the mean absolute error at the default parameters from 0.14 to 0.09 for the three forests. It is possible that the predicted forest fraction for central Africa is slightly worse because the observed climate is towards the edge of the parameter space of temperature and precipitation, and there are no runs near.

4.3 History matching to learn about model discrepancy

In this section we use history matching (see section 3.1) to learn about parts of input parameter space that are consistent with observations, and to find the causes of discrepancy in the model. History matching measures the statistical distance between an observation of a real-world process, and the emulated output of the climate model at any input setting. An input where the output is deemed too far from the observation is ruled "implausible", and removed from consideration. Remaining inputs are conditionally accepted as "Not Ruled Out Yet" (NROY), recognising that further information about the model or observations might yet rule them as implausible.

Observations of the system are denoted z, and we assume that they are made with uncorrelated and independent errors ϵ such that

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$$z = y + \epsilon$$

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Assuming a "best" set of inputs x^* where the model discrepancy δ , or difference between climate model output y and z is minimised, we relate observations to inputs with-

$$z = g(x^*) + \delta + \epsilon$$

We calculate measure of implausibility *I*, and reject any input as implausible where *I* > 3 after Pukelsheim's three-sigma rule; that is, for any unimodal distribution, 95 % of the probability mass will be contained within 3 standard deviations of the mean (Pukelsheim, 1994). We calculate

$$\underline{I^2 =} |z - E[g(x)]|^2 / Var[g(x)] \underline{+ Var[\delta] + Var[\underline{\epsilon}]}$$

which recognises that the distance between the best estimate of the emulator and the observations must be normalised by uncertainty in the emulator g(x), in the observational error ϵ , and in the estimate of model discrepancy δ .

We study the region of input space that is "Not Ruled Out Yet" (NROY) by comparison of the model output to the observations of forest fraction. In the previous section we see that the overall difference between the simulated and observed forest fraction is reduced if the output is bias corrected. In this section, we study how that bias correction affects the NROY space.

In M16, the default input parameters were ruled out as implausible for the Amazon region forest fraction. For the sake of illustration, we assume very low uncertainties: zero observational uncertainty and a model discrepancy term with a zero mean and an uncertainty (\pm 1 sd) of just 0.01. We note that under these conditions the default parameters would be ruled out in the standard emulator. However, if we bias correct the model output using the observed temperature and precipitation, we find that the implausibility measure I for the forest fraction in the Amazon at the standard input parameters reduces from nearly 7 to 1.3 - comfortably under the often-used threshold of 3 for rejection of an input. The implausibility of the SE Asian and Central

Table 2. Mean absolute error of the simulated forest fraction, and Implausibility of the default set of land surface parameters when non-bias corrected and bias corrected to temperature and precipitation observations.

Forest	Error	Implausibility	Error (bias corrected)	Implausibility (bias corrected)
Amazon	0.316	6.94	-0.079	1.31
Southeast Asia	-0.096	1 .61	0.072	1.76
Central Africa	-0.04	0.768	-0.11	1.5

African forest fraction at the default parameter settings rises with bias correction (see table 2), but neither comparison comes close to ruling out the default parameters. We This rise in implausibility is caused by a smaller uncertainty estimate (in the case of SE Asia), and a larger emulation error (in the case of Central Africa). However, we can confidently say that bias correction using the emulator means that observations no longer rule out the default parameters, even with the assumption of a very small model discrepancy.

Another result of bias correction is that it increases the "harmonisation" of the input spaces - that is, the volume of the input space that is "shared", or Not Ruled Out Yet by any of the comparisons of the simulated forest fractions with data. In M16, we argued that the regions of input parameter space where the model output best matched the observations had a large shared volume for the Central African, Southeast Asian and North American forests. In contrast, the "best" input parameters for the Amazon showed very little overlap with these other forests. This pointed to a systematic difference between the Amazon and the other forests that might be a climate bias, or a fundamental discrepancy in the land surface component of the model. Here, we show that the climate-bias climate-bias corrected forest in the Amazon would share a much larger proportion of its NROY space with the other forests. Indeed, the default parameters are now part of this "shared" space, and there is formally no need to invoke an unexplained model discrepancy in order to accept them for all the tropical forests. We show a cartoon of the situation in fig. 10.

We find that when we bias correct all the spaces, the proportion of "shared" NROY input space relative to the union of NROY spaces for all forests increases from 2.6% to 31% - an order of magnitude increase (see table 3). This is driven chiefly by the harmonisation of the NROY space of the Amazon to the other two forests. We see that before bias correction, the South East Asian and African forests share nearly three quarters (74%) of their combined NROY space. This drops to 33% when bias corrected, but with the advantage that the Amazon and Central Africa now share over 90% (91.5%) of their combined NROY space (table 4).

When compared to the initial input parameter space covered by the ensemble, the shared NROY space of the non-bias-corrected forests represents 1.9%, rising to 28% on bias correction.

We visualise two dimensional projections of the NROY input parameter space shared by all three forests before bias correction in fig. 11 and after bias correction in 12. The two dimensional projections of high density regions of NROY points are dramatically shifted and expanded in the bias corrected input space, and the default parameters now lie in a high density

Table 3. Measures of the NROY input space shared by all three forests. The intersection is NROY for all three forests, the Union is NROY for at least one forest. The initial space is that defined by the parameter limits of the initial experiment design.

	Intersection / Union (%)	on / Union (%) Intersection / Initial (%)	
Non bias-corrected	2.6	1.9	
Bias-corrected	31	28.3	

Table 4. Proportion of shared NROY input space for each forest pair compared to the total NROY space covered by the same forest pair. Non bias corrected (top) and bias corrected (bottom).

Non bias-corrected	Amazon	Southeast Asia	Central Africa
Amazon	1		
Southeast Asia	0.034	1	
Central Africa	0.075	0.741	1
Bias-corrected			
Amazon	1		
Southeast Asia	0.329	1	
Central Africa	0.915	0.337	1

region. For example, a high-density region of NROY points is apparent in the bias-corrected input parameter space (fig. 12), in the projection of V_CRIT_ALPHA and NLO. It is clear from sensitivity analyses (sect. 4.4) that, all other things remaining the same, increasing the value of NLO raises strongly forest fraction, while increasing V_CRIT_ALPHA strongly reduces forest fraction. We would expect there to be a region, indeed a plane through parameter space where these two strong effects counteract each other, resulting in a forest fraction close to observations. This feature does not appear in the history matching before bias correcting (fig. 11). The low value of the simulated Amazon forest fraction before bias correction of the climate inputs rules out much of the input parameter space later found to be Not Ruled Out Yet (NROY) after the bias corrected history matching exercise (fig. 12).

It is possible that the estimate of shared NROY input space is larger than it could be, due to the lack of ensemble runs in the "cool, wet" part of parameter space, where there are no tropical forests. Inputs sampled from this part of parameter space may not be ruled out, as the uncertainty on the emulator may be large. This is history matching working as it should, as we have not included evidence about what the climate model would do if run in this region. Further work could explore the merits of including information from other sources (for example, from our knowledge that tropical forests do not exist in a cool wet climate) into the history matching process.

4.4 Sensitivity analysis

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The augmented emulator allows us to measure the sensitivity of forest fraction to the land surface input parameters simultaneously with climate variables temperature and precipitation. A quantitative measure of sensitivity of the model output to parameters that does take into account interactions with other parameters is found using the FAST99 algorithm of Saltelli et al. (1999), summarised in fig. 13. Precipitation and Temperature are the second and third most important parameters, more important than NLO, and only slightly less important than V_CRIT_ALPHA. Interaction terms contribute a small but non-negligible part to the sensitivity. This form of quantitative sensitivity analysis is useful to understand initial model behaviour, but could be vulnerable to error, as it is assumed that all parts of the input space are valid. Our experiment design does not control temperature and precipitation directly, and the "cool, wet" part of this parameter space does not contain tropical broadleaf forest. It is possible therefore that a sensitivity analysis that relies on input samples from this region might mis-specify sensitivity indices. Below, we outline two methods that tackle this problem: One-at-a-time sensitivity analysis with history matching, and Monte Carlo filtering.

We measure the one-at-a-time sensitivity to parameters and climate variables, using the augmented emulator to predict changes in forest fraction as each input is changed from the lowest to highest setting in turn, with all other inputs at the default settings or observed values. We present the results in fig. 14. In this diagram, we exclude emulated forests that are deemed implausible according to the criteria in section 3.1. This is to avoid potentially over-estimating the sensitivity of forest fraction to (for example) temperature and precipitation by including results from regions of parameter space far from existing ensemble members, and in very different climate regimes from existing broadleaf tropical forests.

Parameters NL0 and V_CRIT_ALPHA and climate variables temperature and precipitation exert strong influences of similar magnitudes on forest fraction. Shaded regions represent the uncertainty of the sensitivity to each parameter, due to estimated emulator uncertainty of ± 2 standard deviations. This sensitivity measure does not include the extra uncertainty due to the fact that the relationships will change depending on the position of the other parameters. We do however see a measure of how temperature and precipitation affect the marginal response of the other parameters, as the observed climates of each forest are different. For example, we clearly see that the response of the forest fraction to e.g. NL0 depends on climate - the forest fraction response is a noticeably different shape when varied under the mean climate of the South East Asian region.

A technique called Monte Carlo Filtering (MCF), or Regional Sensitivity Analysis is useful in situations where input parameter distributions are non-uniform, correlated, or not all parts of parameter space are valid. The basic idea of MCF is to split samples from the input space into those where the corresponding model output meets (or not) some criteria of behaviour. Examining the differences between the cumulative distributions of those inputs where the outputs do or do not meet the criteria provides a measure of sensitivity of the output to that input. For example, we might split model behaviour into those outputs above or below a threshold. A recent description of MCF and references can be found in section 3.4 of Pianosi et al. (2016).

We integrate the MCF sensitivity analysis into the history matching framework. We examine the differences in the univariate cumulative distributions of each parameter, in those samples where the output is ruled out by history matching, against those that are "Not Ruled Out Yet" (NROY). To measure the differences between the distributions we perform a two-sided

Kolmogorov–Smirnov (KS) test and use the KS statistic as in indicator that the output is sensitive to that input. A larger KS statistic indicates that the cumulative distribution function of the respective inputs are further apart, that that input is more important for determining if the output falls within the NROY part of parameter space, and therefore the output is more sensitive to that input in a critical region. We note that MCF is useful for ranking parameters, but not for screening, as inputs that are important only in interactions might have the same NROY and ruled out marginal distributions. In this case they would have a sensitivity index of zero.

We apply MCF using the emulator. This allows us to examine the difference between model output distributions given a much larger sample from the input space than when using only the ensemble. This comes at the cost of using an imperfect emulator, which may give different results than if we were using a large ensemble of runs. To avoid the problem of sampling precipitation and temperature from regions where there are no ensemble members, we sample uniformly from across input space for all other parameters, and then append a random temperature/precipitation location from the ensemble. We calculate a sampling uncertainty by calculating the MCF sensitivity metrics 1000 times, each time using a sample size of 5000 emulated ensemble members. In this way, we estimate both the mean and the uncertainty (standard deviation) of the MCF sensitivity measures. We note that the sensitivity indices are calculated higher when a small number of ensemble members are used, as well as with a higher uncertainty. The change in both the estimated statistic and its uncertainty have begun to become small by the time 3000 ensemble members are used, suggesting that we should use at least this many emulated ensemble members to obtain an unbiased sensitivity analysis (see supplementary material). We compare the KS statistics and their associated uncertainty for each input in fig. 15.

We can check the strength of the relationship between the MCF sensitivity measures and the FAST99 sensitivity measures, by plotting them together. We examine this relationship in the supplementary material (fig. S7).

4.5 Doing better than the default parameters

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We can use the emulator to find locations in parameter space where there is a potential that the difference between the modelled and observed forest fractions could be smaller than at the default parameters. Figure 16 shows the density of parameter settings in each 2-dimensional projection of the input space, where the emulator estimates the model performs better than at the default parameters, once bias correction has been applied. That is, the absolute difference between each estimated forest fraction and the observed values is smaller than the absolute difference of the mean estimate at the default parameters. Out of 100000 samples from the uniform hypercube defined by the range of the experiment design, only 2451, or around 2.5% match this criterion and are plotted. This diagram might help guide further runs in the ensemble, choosing high density regions to run new ensemble members. The convergence of NL0 and V_CRIT_ALPHA seems particularly focussed, and suggests that a lower value of V_CRIT_ALPHA might be a way to reduce error in the forest fraction. There is another, although less densely populated region of high NL0 and V_CRIT_ALPHA that might fulfil the criteria of lower estimates of error for each forest. These regions would be good targets for supplementary runs of the climate model, and for particularly careful emulator checking. A poorly performing emulator could guide a model developer into wasting model runs at locations which, in reality, did not produce forest fractions close to the observed values.

4.6 Allowable climate at default parameters

We use history matching to find the set of regional mean climates that are most consistent with the observations for each tropical forest. To illustrate the best case scenario we set model discrepancy, its associated uncertainty, and observational uncertainty artificially low (0, 0.01 and 0 respectively), so that implausibility is almost exclusively a product of the emulator uncertainty. We find the set of NROY temperature and precipitation values when the remaining input parameters are held at their default values. Figure 17 shows the density of NROY points in the climate space for each of the observed forest fractions. We see that the Amazon and Central African forests might be well simulated in the model in a very wide range of cooler and wetter climates, with only the "hot, dry" corner showing zero density of potential inputs that produce similar forest fraction to observations. The Southeast Asian forest fraction is matched by a swathe of inputs running diagonally through the centre of input space. Neither the hot-dry or cool-wet corners of input space produce forests that match the observations, though the warm-wet and cool-dry corners do.

5 Discussion

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5.1 Simulating the Amazon

We have shown that the simulation of the broadleaf tropical forest in FAMOUS is almost as sensitive to temperature and precipitation as to any land surface parameter perturbation in the ensemble. However, the calculated sensitivities are dependent on the chosen limits of the parameter perturbations themselves. The precise order and size of sensitivities might change given updated parameter ranges, but there is little doubt that the climate variables are a strong influence on broadleaf forest fraction. This version of FAMOUS when run with the default land surface input parameter settings would successfully simulate the Amazon rainforest to within tolerable limits if regional climate biases were substantially reduced. As such, there is no need to invoke a missing process in the land surface in order to explain the forest fraction discrepancy in the Amazon. We have strengthened the case made by M16 that the low Amazon forest fraction is not a result of poorly chosen parameters. There is a broad region of climate space where the effects of temperature and precipitation on forest fraction compensate for each other. This gives room for a number of possible sources of model discrepancy, and by extension makes it unlikely that the default input parameters are optimal. There are indications from the emulator that a small region of parameter space exists where there is even smaller overall error in the simulation, offering a target for exploration using further runs of the model.

There is a feedback from the land surface to the atmosphere implicitly included in the emulated relationship. We cannot control this feedback directly with the emulator, and so work out the impact of this feedback on the forest fraction as it is present in the training data. This feedback would have to be taken into account if we were to simulate the correct climate independently of the land surface.

It is possible that were we to include a process seen to be missing from the Amazon (such as deeper rooting of trees allowing them to thrive in drier climates), our map of NROY input space would alter again. Given that there is a measure of uncertainty in observations and the emulator, as well as the possibility of further compensating errors, we cannot rule out a model discrepancy

such as a deep rooting process. The fact that the other forests do slightly less well when their climates are bias corrected points to a potential missing process in the model, compensated for by parameter perturbations. However, the impact of this missing process is likely much smaller than we might have estimated had we not taken the bias correction of the forest into account.

5.2 Uses for an augmented emulator

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By building an emulator that includes temperature and precipitation - traditionally used as climate model outputs - we are able to separate the tuning of one component of the model (here the atmosphere) from another (the land surface). Perturbations to the atmospheric parameters, tested in a previous ensemble but not available to us except through an indicator parameter, are summarised as inputs through the climate of the model.

We have used the augmented emulator as a translational layer between components of the model. The augmented emulator allows us to ask "what would it mean for our choice of input parameters if the mean climate of the model in the Amazon region were correct?" This means that we will have less chance of ruling out parts of parameter space that would lead to good simulations or keeping those parts that lead to implausible simulations. An augmented emulator as a translational layer might be built as part of a model development process, making it computationally cheaper and faster. Traditionally, the components of computationally expensive flagship climate models are built and tuned in isolation before being coupled together. The act of coupling model components can reveal model discrepancies or inadequacies. A model discrepancy in one model component can mean that a connected subcomponent requires retuning from its independently-tuned state. There is a danger that this retuning leads to a model that reproduces historical data fairly well, but that makes errors in fundamental processes and therefore is less able to predict or extrapolate - for example, a climate model when projecting future changes under unprecedented greenhouse gas concentrations. Given the time and resources needed to run such complex models, these errors might persist much longer than necessary, and have profound consequences for climate policy.

A translational layer would allow parameter choices to be made for a model when run in coupled mode, even when there was a significant bias in one of the components that would affect the other components. The translational layer would bias correct the output of a component of the model, allowing an exploration of the effects of input parameter changes on the subcomponent of the model, in the absence of significant errors. Using the augmented emulator could could eliminate some of the steps in the tuning process, help the model developer identify potential sources of bias, and to quickly and cheaply calculate the impacts of fixing them. In doing so it would aid model developers in identifying priorities for and allocating effort in future model development.

Our work here shows this process as an example. We have identified the importance of precipitation and temperature to the correct simulation of the Amazon forest, and flag them as priorities in future climate model development accurate simulation in that region as a priority in for the development of any climate model that hopes to simulate the forest well. We have identified regions of the space of these climate variables where the Amazon forest might thrive, and related that back to regions of land surface parameter space that might be targeted in future runs of the model. We have achieved this in a previously-run ensemble of the model, allowing computational resources to be directed towards new climate model runs that will provide more and better information about the model.

There are also potential computational efficiencies in our approach of decoupling the tuning of two components (here the atmosphere and the land surface) in the model. A good rule of thumb is that a design matrix for building an emulator should have $O(10 \times p)$ training points, where $p \cdot p$ is the number of input parameters, in order to adequately sample parameter space to the extent it is possible to build a good emulator. With approximately 10 atmospheric and 7 land surface parameters, we would need $O(170) \cdot O(170)$ runs. Here, we have summarised those 10 parameters as two outputs that have a material impact on the aspect of the land surface that we are interested in. Adding these two to the 7 inputs, we need $O(10 \times (2+7) = 90)$ runs, well covered by our available ensemble of 100 runs.

We acknowledge however that in order to trace back information about the performance of the model in forest fraction to the original 10 oceanic and atmospheric parameters, we would need access to the original ensemble. We have used temperature and precipitation to reduce the dimension of the parameter space, but there is no guarantee that the relationship between the original parameters and the local climate is unique. There may be multiple combinations of the 10 parameters that lead to the temperature and precipitation values seen, which would mean that we would require a large ensemble to estimate the relationships well. Alternatively, there may be an even more efficient dimension reduction for forest fraction, meaning we would need even fewer model runs to summarise the relationship.

5.3 Limitations

In theory the augmented emulator could be used to bias correct, for example, every gridbox in a field for a particular variable differently sized regions, down to the size of an individual gridbox for a particular variable. This might be useful for correcting, for example, known biases in elevation or seasonal climate. The principle of repeating the common parameter settings in the design matrix, and including model outputs as inputs would work in exactly the same way, but with a larger number of repeated rows. In the case of using an augmented emulator on a per-gridbox basis, we might expect the relationship between inputs that we are bias correcting (e.g. temperature, precipitation), and the output of interest (e.g. forest fraction) to be a less clear, as at small scales there are potentially many other inputs that might influence the output. An emulator for an individual gridbox might therefore be less accurate. However, with enough data points, or examples (and there would be many), we might expect to be able to recover any important relationships.

The computational resources needed to fit a Gaussian process emulator when the number of outputs estimated simultaneously becomes even moderately large limits the use of our technique. The design input parameter matrix used for training the emulator grows to $n \times d$ rows, where n is the number of ensemble members in the original training set, and d is the number of separate output instances to be considered. In our example, d is 3, and so we only have $100 \times 3 = 300$ in the new training set. Given an initial ensemble of a few hundred, this could easily result in a training set with hundreds of thousands or even millions of rows. Gaussian process emulators are currently limited to using training data with perhaps a few hundred rows as current software packages must invert an $n \times n$ matrix, a potentially very computationally expensive process (see e.g. Hensman et al. (2013) for examples). At the time of writing this limitation would preclude using our specific technique for correcting biases on a per-gridbox basis. To make use of the translational layer for large data sets we would need new Gaussian process technology, or specific strategies to deal with large data sets. These strategies might involve kernel based methods, keeping the scope

of training data local to limit the size of any inverted matrices. Alternatively, they might involve building emulators using only a strategically sampled selection of the outputs. Recent advances in using Gaussian processes for larger data sets can be found in Hensman et al. (2013, 2015); Wilson et al. (2015); Wilson and Nickisch (2015). Our current strategy is to reduce the dimension of the output of the climate model, by taking the regional mean of the output of the climate model (temperature and precipitation). More advanced dimension reduction techniques might offer great potential.

Given that we overcome such technical barriers, we see no reason that such a layer not be built that is used to (for example) correct the climate seen by individual land surface grid boxes, rather than (as here) individual aggregated forests. The process of rejecting poor parameter sets might be aided by having a comparison against each gridbox in an entire global observed surface, rather than aggregated forests. Alternatively, we might allow parameters to vary on a gridbox-by-gridbox basis, effectively forming a map of Not-Ruled-Out-Yet parameters.

If trained on an ensemble of model runs which which included all major uncertainties important for future forests, an augmented emulator could be used directly to estimate the impacts and related uncertainty of climate change on forest fraction in the model, even in the presence of a significant bias in a model subcomponent. After estimating the relationship between the uncertain parameters, climate, and the forest fraction, we could calculate the forest fraction at any climate, including those that might be found in the future. This ensemble of climate model runs would project the future forests under a number of (e.g.) atmospheric CO₂ concentrations and parameter combinations. It would be necessary that the training data included any climates that might be seen under the climate change scenario to be studied, as the emulator has much larger uncertainties if asked to extrapolate beyond the limits of the training data. The trajectory of vegetation states through time would also be an important element of the ensemble, as the vegetation state is path dependent. However there would be great potential to save a large number of runs, as not every parameter perturbation would have to be run with every projection scenario. Such a set of runs would serve as a framework upon which a great many post hoc analyses could be done with the emulator. Once the set of runs was complete, they would effectively serve as the definitive version of the model - any new information that needed to be extracted from the model could in theory be found using the emulator. Not only might we be able to identify and correct important climate biases and their impact on the forest, but also update our estimates of forest change as we learned learn more about the uncertainty ranges of the uncertain parameters and forcing trajectory.

25 6 Conclusions

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A previous study (McNeall et al., 2016) concluded that it was difficult to simulate the Amazon rainforest and other tropical rainforests at a set of input parameters in the climate model FAMOUS, pointing to a climate bias or model discrepancy as a source of error. Here we demonstrate that we can correct the simulation of the Amazon rainforest in the climate model FAMOUS by correcting the regional bias in the climate of the model with a Gaussian process emulator. We therefore find it unnecessary to invoke a model discrepancy or inadequacy, such as a lack of deep rooting in the Amazon in the model, to explain the anomalously low forest fraction in an ensemble of forests simulations.

We use average regional temperature and precipitation as inputs, alongside a number of land surface parameters, to predict average forest fraction in the tropical forests of the Amazon, Southeast Asia and central Africa. We assume that the differences in these parameters account for the regional differences between the forests, and use data from all three tropical forest regions to build a single emulator. We find that the augmented emulator improves accuracy in a leave-one-out test of prediction, reducing the mean absolute error of prediction by almost half, from nearly 6% of forest fraction to just under 3%. This allays any fears that the emulator is inadequate to perform a useful analysis, or produces a measurable bias in predictions, once augmented with temperature and precipitation as inputs. In two types of sensitivity analyses, temperature and precipitation are important inputs, ranking 2 and 3 after V CRIT ALPHA (rank 1) and ahead of NL0 (rank 4).

We use the augmented emulator to bias correct the climate of the climate model to modern observations. Once bias corrected, the simulated forest fraction in the Amazon is much closer to the observed value in the real world. The other forests also change slightly, with central Africa moving further from the observations, and Southeast Asia moving slightly closer. We find that the differences in the accuracy of simulation of the Amazon forest fraction and the other forests can be explained by the error in climate in the Amazon. There is no requirement to invoke a land surface model discrepancy in order to explain the difference between the Amazon and the other forests. After bias correction, the default parameters are classified as "Not Ruled Out Yet" in a history matching exercise, that is they are conditionally accepted as being able to produce simulations of all three forests that are statistically sufficiently close to the values observed in the real world. Bias correction "harmonises" the proportion of joint NROY space that is shared by the three forests. This proportion rises from 2.6% to 31% on bias correction. Taken together these finding findings strengthen the conclusion of McNeall et al. (2016) that the default parameters should not be ruled out as implausible by the failure of FAMOUS to simulate the Amazon. We find a small proportion (around 2.5%) of input parameter space where we estimate that the climate model might simulate the forests better than at the default parameters. This space would be a good target for further runs of the simulator.

We offer a technique of using an emulator augmented with input variables that are traditionally used as outputs, to aide the tuning of a coupled model perturbed parameter ensemble by separating the tuning of the individual components. This has the potential to (1) reduce the computational expense by reducing the number of model runs needed during the model tuning and development process and (2) help model developers prioritise areas of the model that would most benefit from development. The technique could also be applied to efficiently estimate the impacts of climate change on the land surface, even where there are substantial biases in the current climate of the model.

Code and data availability. Code and data are available at https://doi.org/10.5281/zenodo.3246103

Author contributions. DM designed the analysis and wrote the paper with the assistance of all other authors. JW ran the climate model and provided the climate model data.

Competing interests. The authors declare no competing interests.

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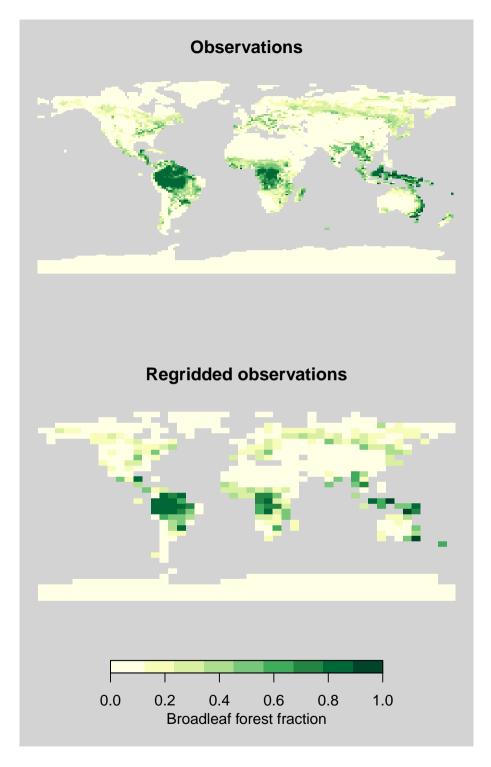


Figure 2. Observations of broadleaf forest fraction on their native grid (top), and regridded to the FAMOUS grid (bottom).

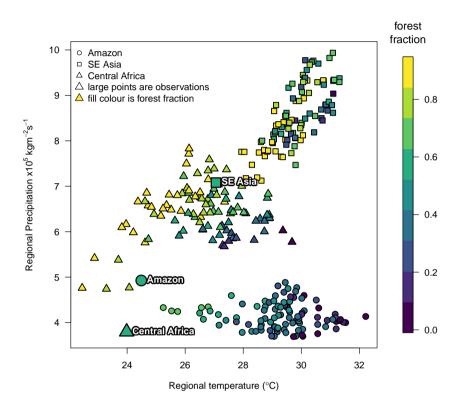


Figure 3. Regional temperature, precipitation and broadleaf forest fraction in the ensemble of FAMOUS compared with observations. Smaller symbols represent broadleaf forest fraction in the FAMOUS ensemble against regional mean temperature and precipitation. Ensemble member forest fraction in the Amazon is represented by the colour of the circles, Central Africa by triangles and SE Asia by squares. Larger symbols represent observed climate and forest fraction.

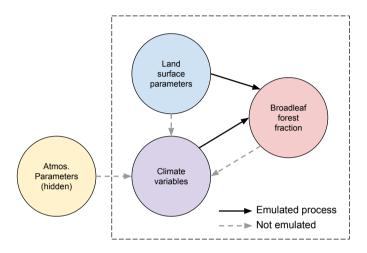


Figure 4. A graph showing the assumed relationship between input parameters, climate variables and forest fraction. An arrow indicates influence in the direction of the arrow. Processes that are directly emulated are shown with a solid arrow, while the processes shown by a dotted arrow are not directly emulated.

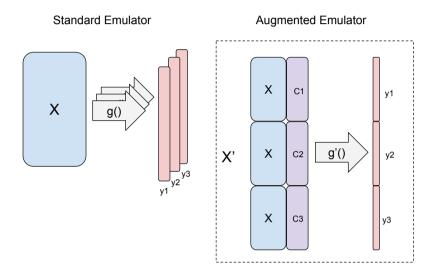


Figure 5. In a standard emulator setup (left), training data consists of an input matrix X and corresponding simulator output y. A new emulator $g_1, \ldots, (g_n), g_1, \ldots, g_3$ is trained for each output $g_1, \ldots, g_n, g_1, \ldots, g_n$ of interest. In the augmented emulator, output from the simulator G_1, \ldots, G_n augments the design matrix, with the initial inputs X repeated.

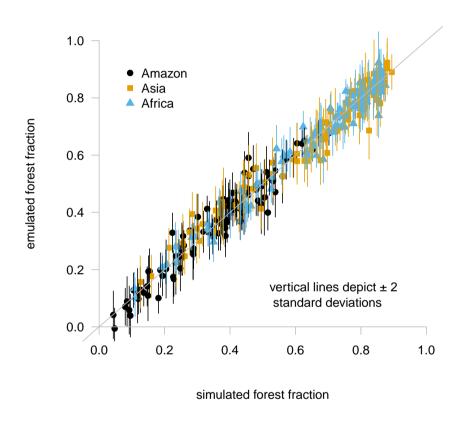


Figure 6. Leave-one-out cross validation plot, with the true value of the simulator output on the x-axis, and predicted output on the y-axis. Vertical lines indicate ± 2 standard deviations.

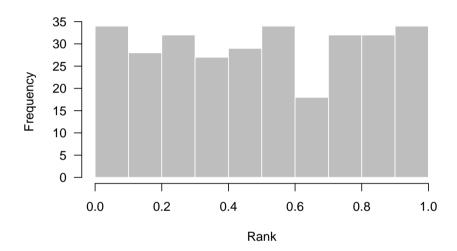


Figure 7. Rank histogram of leave-one-out predictions. For each prediction of a held-out ensemble member, we sample 1000 points from the Gaussian prediction distribution, and then record where the true held-out ensemble member ranks in that distribution. We plot a histogram of the ranks for all 300 ensemble members. A uniform distribution of ranks indicates that uncertainty estimates of the emulator are well calibrated.

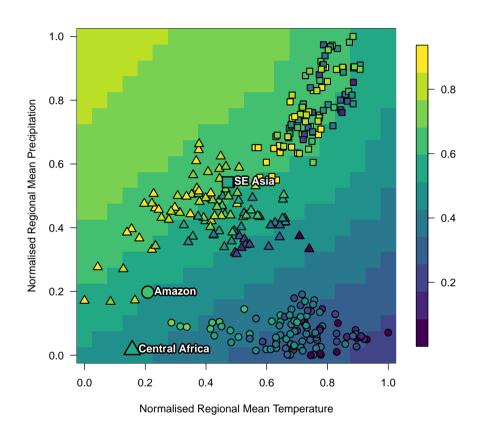


Figure 8. The impact of climate on forest fraction. Background plot colour indicates the mean emulated forest fraction when all land surface inputs are held at their default values. Temperature and precipitation in the ensemble are marked with symbols, with the fill colour representing forest fraction. Larger symbols represent the values observed in the real world.

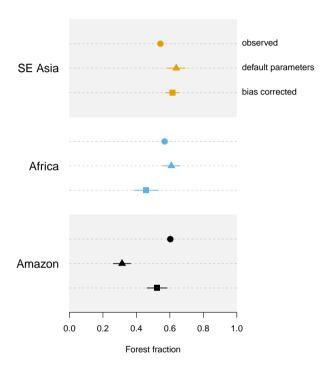


Figure 9. Observed and emulated Forest fraction in each tropical forest. For the emulated forest fraction at default and bias corrected parameters, emulator uncertainty of \pm 2sd is represented by horizontal bars.

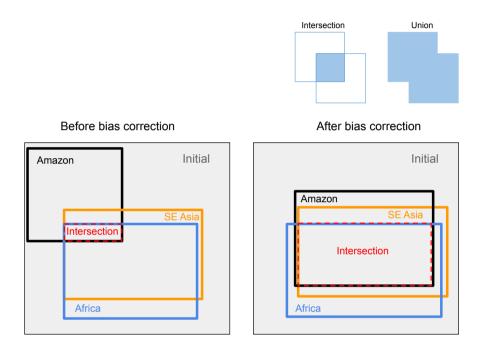


Figure 10. A cartoon depicting the input space that is "not ruled out yet (NROY)" when the climate simulator output is compared to observations of the forest fraction in the Amazon, Africa, and South East Asia before (left) and after (right) bias correction. We measure the "shared" space (the intersection of NROY spaces for each forest) as a fraction of the union (the total space covered by all three forests) of the NROY spaces. The "initial" space represents the total parameter space covered by the ensemble.

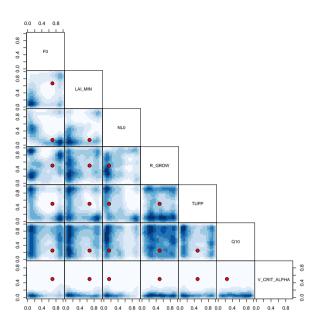


Figure 11. NROY land surface input space shared by all three forests before bias correction. Blue shading denotes the density of NROY input candidates, projected into the two dimensional space indicated by the labels. The default parameter settings are marked as red points.

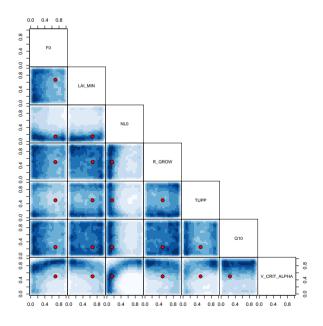


Figure 12. NROY land surface input space shared by all three forests when bias corrected using the augmented emulator. Blue shading denotes the density of NROY input candidates, projected into the two dimensional space indicated by the labels. The default parameter settings are marked as red points.

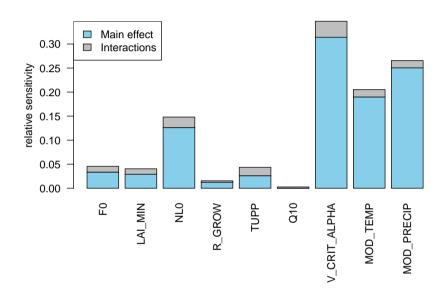


Figure 13. Sensitivity of forest fraction to model parameters and climate parameters, found using the FAST99 algorithm of Saltelli et al. (1999).

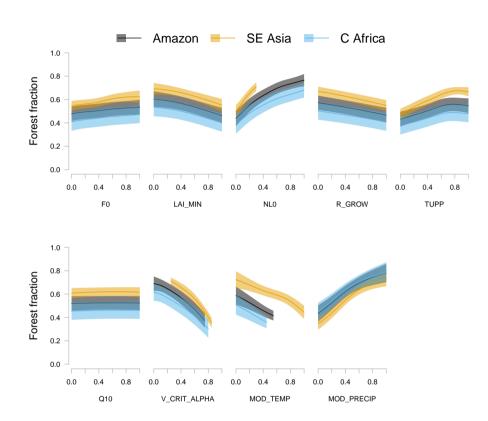


Figure 14. One-at-a-time sensitivity of forest fraction variation of each parameter and climate variable in turn across the "Not Ruled Out Yet" parameter range. All other parameters or variables are held at their default values while each parameter is varied, and values of model broadleaf forest fraction which are statistically far from observations are excluded. Solid lines represent the emulator mean and shaded areas represent ± 2 standard deviations of emulator uncertainty.

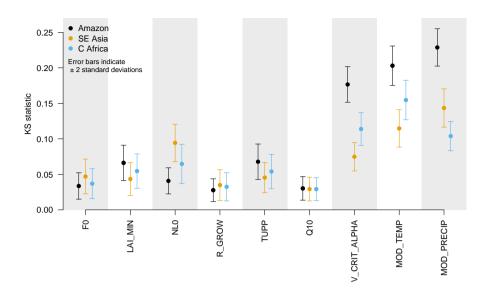


Figure 15. Monte Carlo filtering estimate of the sensitivity of model output to inputs, using 5000 emulated members. Error bars represent \pm 2 standard deviations of uncertainty in the statistic, calculated by repeating the calculation 1000 times.

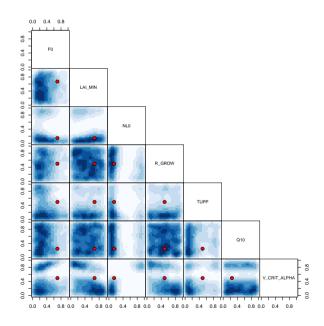


Figure 16. Two dimensional projections of the density of inputs where the corresponding bias corrected emulated forests have a smaller error than the bias corrected default parameters. These regions might be good targets for additional runs of the climate model. Default parameters are shown as a red point.

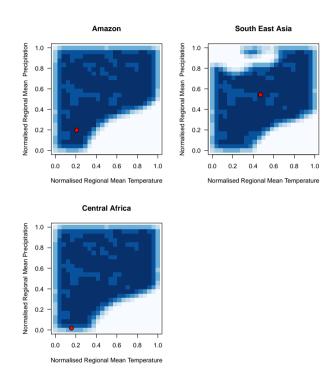


Figure 17. Density of not-ruled-out yet emulated temperature and precipitation pairs for each observed tropical forest fraction, when input parameters are held at their default values. Observed climates for each forest are marked in red.