Many thanks for taking the time to read and review our paper, and for the positive comments on the technical aspects of the work, along with the helpful remarks and suggestions. We have responded to the comments in blue below (with the reviewers original comments in grey). Where we have made changes to the manuscript we've noted these below our comments, with red strikethrough text for deletions, green text for additions and black text indicating regions of no change.

In this paper, the authors present a polynomial regression model that data drivenly predicts the tendency of ocean temperature using the MITgcm ocean model. The study is well conducted, and technically correct. A lot of well-thought-out experiments have been conducted and presented reasonably well with enough details to facilitate reproducibility. The authors have even considered nuances such as correlated training-testing datasets and did a very comprehensive analysis. Having said all that, it must also be pointed out that the statistical model considered here is overly simple (and shows very limited skill of 0.58) and does not contribute to building better (not interpretable) data-driven forecasting models. The authors do acknowledge that throughout the length of the study and have even put an entire section talking about the limitations. In my opinion, although the study is very comprehensive, the model is too simple, and (as pointed out by the authors themselves) do not actually have the capability to iteratively (autoregressively) perform ocean temperature prediction as has been done (although in the context of atmosphere) in several papers that the authors themselves have cited, nor does it show good skill for even one-time-step prediction. Underneath, I list my major concerns with the current version of this paper and while these concerns do not question any technical point in the paper, the method presented does not quite serve as a "model" for geoscientific predictions and thus may not be suitable for publication in this journal.

We acknowledge the limitations you highlight, although we think that the work is still suitable for publication in this journal. We address the particular comment concerning the value of 0.58 as a measure of skill in a later reply below. Here we focus on more general principles. We think that this work is useful to the scientific community. The model, while simple, is still a suitable framework for carrying out sensitivity analysis, which is a critical tool in the Earth system sciences. Added to this, our efforts provide a new use for data-driven methodology in ocean modelling. As far as we are aware, there are no examples of use of data-driven techniques being used in this way for ocean models; existing work focuses on atmospheric models or on using machine learning to improve components of ocean models. While the underlying physics is similar across atmospheric and oceanic systems, the applications and regimes of interest are often very different. Data-driven methods are best tested and analysed in both systems, building trust within both communities. We note the concerns over the predictive skill of the model and address these below, but even taking this into account, we think these results are interesting in themselves, and they provide a new baseline for further work, by both the authors and others, and a framework in which to begin addressing oceanographic applications.

Importantly, we note that while the model presented is not designed to be used in a forecasting sense, the GMD guidelines note that the journal considers manuscript types including 'geoscientific model descriptions, from statistical models to box models to GCMs'¹, indicating that even very simple models such as ours, which increase understanding rather than providing tools usable for real-world predictions, fit well within the scope of the journal. Added to this, GMD

¹ <u>https://www.geoscientific-model-development.net/</u>

scope also includes 'New methods for assessment of models'. Here we present an important aspect of assessment of data-driven models, which is again well suited to publication in this journal. While acknowledging the limitations and simplicity of this model, we think the work presented nonetheless provides a key step towards future capability, providing a 'proof of concept' for an oceanographic application and a baseline for further work. It also increases understanding and confidence in the growing field of statistical geophysical models, and therefore is of value to this journal.

We've made the following changes to the manuscript to help better emphasise the focus and relevance of the paper:

~Line 6:

We develop a simple regression model of ocean temperature evolution, Ocean Temperature Regressor v1.0, and investigate its sensitivity to improve understanding of whether data-driven models are capable of learning the complex underlying dynamics of the systems being modelled, or if they instead learn statistically valid, but not physically based patterns.

~Line 78:

... the skill shown in using data-driven methods for predictions of the atmosphere suggest that these same methods could provide skilful predictions for the evolution of the ocean.

The model developed here is highly simplified, both in terms of the idealised GCM configuration we train the model on, and the data-driven methods used. However, the underlying configuration captures key oceanic dynamics, enabling a suitable test bed to see if data-driven methods can capture the dynamical basis of these systems. Similarly, while we use a simple regression technique, this has sufficient skill to assess the ways in which the model works and improve understanding for the potential of data-driven methods more generally.

We apply model interpretation techniques to our data-driven model to try to understand what the model is 'learning' and how the predictions are being made...

1. The authors very thoroughly investigate the effect of different input variables in the one time-step prediction of the temperature tendency, however, the bulk of the temperature difference between time step t and $t + \Delta t$ is 0. Even for a simple polynomial model, this is probably a simple problem. While the authors claim that there is some skill in predicting high value of ΔT , the plot also shows several such predictions missed by the model. This is not surprising owing to the simplicity of the model.

While much of the difference is near zero, very few points are actually zero, with the majority instead representing small changes to temperature. These changes, whilst small, are still very important to capture as they accumulate to give the large-scale motion seen in the ocean. Predicting these small changes is a key first step in being able to model the ocean.

A correlation coefficient of 0.58 in validation really shows that the model is just not skillful. Doing any analysis on such a model, in my opinion, may not be the best path forward in this field of machine learning/data-driven forecasting of weather/climate.

Whilst we are certainly not claiming large skill for the particular model being considered, we do emphasise the limitations of the correlation coefficient as a measure of skill and the resulting interpretation of the value of 0.58 as implying that there is no skill.

We note firstly that different statistical measures of skill provide different insights into the performance of the model. While correlation coefficients are useful, they are heavily influenced by extremes. Our main focus is on providing a useful estimate of increments in temperature taken across all model grid points, rather than capturing extreme values of increments that occur infrequently and at a small number of locations (see below for further comments on 'extreme values'). For this we feel that RMS statistics offer a more meaningful measure of skill. RMS errors are also a far more commonly used statistic when validating forecast models, and while the model developed here is not intended as a forecast model, our aim is similar in trying to represent the general behaviour of the ocean, and so here RMS errors are a very important measure of skill. We also note that it is important to interpret statistics in relation to some baseline. In short term prediction, across atmospheric and oceanographic applications, a common first baseline is persistence (Mittermaier 2008²). When comparing across RMS statistics, we see notable skill in the control when compared to a persistence forecast (an RMS of 9.89e-05 compared with 1.15e-04 over the validation set).

Regarding correlation coefficients, a value of 0.58 still implies that there is a substantial amount of useful information in the predictions -- especially when comparing that against the value zero which would correspond to a model with no useful information. Here it would still be best to compare to persistence however it is not trivial to obtain a correlation coefficient for a constant dataset (i.e. the persistence forecast data set, where $\Delta t = 0$ for every sample). We can however see from Fig. 5 that in the experiment where nonlinear terms are withheld predictions are comparable to a persistence forecast. Here the correlation coefficient is 0.11 over the validation set. Based on this, we can confidently infer that a correlation coefficient for a persistence forecast would be at most 0.11 (potentially even lower) over the validation set, and so again when comparing to this baseline the score of 0.58 for the control model shows considerable skill.

Importantly, we note that unlike similar papers in this area, we have trained the model to learn the temperature increment and assessed the model on these predicted increments, rather than the future temperature. While this should have minimal impact on RMS errors, correlation coefficients are hugely impacted by the framing of this question. Calculating correlation coefficients on these increments gives considerably lower scores than if we were to calculate them on the model's predicted field. Looking at both correlation coefficients and anomaly correlation coefficients calculated the predicted future temperature rather than the increment, these are very close to one. We have added the following to the manuscript to highlight this. ~ Line 279:

As expected we can see from Table 2 and Fig. 2 the regressor performs less well over the validation dataset, however it still outperforms the persistence forecast. It should be noted that the regressor developed here is trained to predict the increment in temperature (δ T), rather than the future temperature (T), and importantly is assessed on this increment prediction. If we assess predictions of future temperature, rather than predictions of the temperature increment, we see correlation coefficients and anomaly correlation coefficients very close to one (differing at the 9th and 6th decimal place respectively) over both the training and validation datasets.

Predicting extremes in the field of weather and climate has been done with data-driven models and authors should probably take a look at those literature, e.g., https://arxiv.org/abs/2103.09743, and

² Mittermaier, M. P. (2008). The Potential Impact of Using Persistence as a Reference Forecast on Perceived Forecast Skill, Weather and Forecasting, 23(5), 1022-1031.

https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2019MS001958. The major issue that the authors face in predicting the extremes is essentially addressing the class imbalance problem which is well studied in the ML literature.

While the prediction of extremes is an interesting problem, with much relevant literature available, this is not the focus of our work. The intention here is to explore the potential for data-driven methods to eventually be used alongside (or instead of) traditional forecast models. Traditional forecast models are required to predict all behaviour, and predicting the more commonplace dynamics is often the first goal. Whilst our work is highly idealised, it is motivated by this perspective, and as such, here we instead aim to first predict the more common dynamics. Predicting extremes in the sense of the papers referenced here has a very different significance to our problem – not least because our extremes (unusually large values of increments) may have a limited effect on the overall evolution of the system. This would, however, make for interesting further work, and the authors comments highlight the need for data-driven forecast systems to capture these extreme dynamics alongside the more commonplace. We have made the following changes to the manuscript to better clarify these points.

~ Line 258:

The predictions from the regression model closely resemble the true change in daily mean temperature in both the training and validation datasets (Fig. 2) although there is a tendency to under-predict the magnitude of temperature changes. The model captures the central part of the distribution well. Whilst the majority of the temperature change is dominated by small near-zero changes, capturing these is key to producing a good forecast system. Although the complete development of a data-driven forecast system is not the focus of this work, we are motivated by the potential for data-driven methods to replicate traditional forecast systems. As such, the ability of the model developed here to capture the full range of dynamic behaviour, beginning with the most common dynamics, is key.

To a slightly lesser extent it the regressor also captures the tails of the distribution, where temperature changes are larger, although the under-prediction is more significant here. However, it is noteworthy that the model still shows considerable some skill for these points, given that there are a relatively limited number of training samples in the tails — of the over nearly 650 000 training samples, just over 500 of those samples have temperature changes in excess of ± 0.001 °C, and the model used is very simple. Despite the relatively rare nature of these larger temperature changes, we feel that capturing these alongside the smaller changes is critical to building a robust model. The underlying dynamics of the system, which we hope the regression model is able to learn, drives the full range of temperature changes seen. As such if we build a regressor which is unable to capture the extreme levels of change, this would indicate the model is not fully learning the physical dynamics as was intended. Capturing these extremes is also critical to obtaining a model which could (with further development) lead to a feasible alternative forecast system. While these extremes are limited in their occurrence, their impact on the ocean system is notable, particularly if we were interested in longer prediction timescales. A model unable to capture these fails to provide a useful starting point for development of an ocean forecast system. Although we note that the development of a data-driven forecast system is not the focus of this work, the ability of the model developed here to eapture extremes is to some extent relevant from that perspective.

Given the simplicity of the regressor used here, it is promising that it captures the extremes to the limited extent shown. However, the results also identify the need for

more sophisticated methods which can better capture both the dominant dynamics, and the extreme cases.

We've also added the following to the conclusions,

~Line 513:

That we see this behaviour in a simple model suggests that more complex models, capable of capturing the full higher-order non-linearity inherent in GCMs, are well placed to learn the underlying dynamics of these systems.

The model developed here has a number of limitations, and a similar assessment of a more complex model, particularly one which can better capture the extreme behaviour alongside the more dominant dynamics would be of value to confirm this. The work carried out here uses a very idealised and coarse resolution simulator to create the dataset used for training and validation. Further investigation into how the complexity of the training data, and the resolution of the GCM used to create this dataset, impact the sensitivity of data-driven models would also be of further interest. Similarly, we assess model performance and model sensitivity over a single predictive step, but in forecasting applications data-driven models would most likely be used iteratively. Assessment of how model skill varies when iterating data-driven models has been carried out in the context of alternative data driven models. Looking alongside this to how the sensitivity of the model changes when using models iteratively would also provide further insight into this area.

As data-driven models become competitive alternatives to physics driven GCMs, it is imperative to continue to investigate the sensitivity of these models, ensuring we have a good understanding of how these models are working and when it is valid to rely on them.

2. The authors quite correctly point out that their model cannot do autoregressive/ iterative prediction thus rendering their model not-useful to some extent. Still, interpretability of these models is a big step forward in this field. However, doing so from looking at predictions at a single time step may not be the right approach. There have been several studies that have shown that error propagation in this model is non-trivial and nonlinear. Thus, data-driven models that iteratively forecast the state of the atmosphere/ocean may show variable skill based on how far it directly forecasts and the error analysis may lead to starkly different results e.g., Figure 2 of this paper

(https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2020MS002203) shows the effect of changing the time step of prediction in the data-driven model and so does this paper (https://gmd.copernicus.org/preprints/gmd-2021-71/) . While it is definitely true that a physical variable that actually affects ocean temperature would probably lead to better skill if used as an input, this observation has been reported in the context of atmospheric dynamics in a more complex deep learning model

(https://agupubs.onlinelibrary.wiley.com/doi/10.1029/2019MS00705) and is quite intuitive to be honest. It is still worth mentioning that the authors do a remarkable job at presenting these analyses which are quite comprehensive in the context of this problem.

As noted by the reviewer, the focus of our paper is in the sensitivity analysis of the model, rather than the long term predictive skill. When looking at the sensitivity of a model, the implications of looking over a single predictive step versus looking over an iterative forecast are notably different. When looking at the sensitivity of an iterated forecast (i.e. when applying the model many times to give a forecast multiple time-steps ahead), we see impacts from the way in which errors propagate over iterations. This is interesting, and very important, particularly when considering this is in the context of meaningful predictive models; again however, this is not our focus here. We are especially interested in whether data-driven models can to some extent 'learn' the dynamics of the systems they are modelling rather than finding statistically valid, but not necessarily physically valid patterns. We think that this question is best addressed by firstly looking solely at single-step predictions, in order to avoid the propagation of errors over multiple step predictions confusing the results.

Again though, we note that there are many interesting questions around how errors propagate when iteratively forecasting with data-driven models and the sensitivity of models to this propagation. In particular considering the distinction between changes to forecast skill with forecast period and changes to forecast sensitivity with forecast period. It would make interesting further work to assess this question in the context of a model which can be iterated, as in the paper referenced here by the reviewer. We've added the following to the conclusions to highlight this for future work.

~Line 513:

That we see this behaviour in a simple model suggests that more complex models, capable of capturing the full higher-order non-linearity inherent in GCMs, are well placed to learn the underlying dynamics of these systems.

The model developed here has a number of limitations, and a similar assessment of a more complex model, particularly one which can better capture the extreme behaviour alongside the more dominant dynamics would be of value to confirm this. The work carried out here uses a very idealised and coarse resolution simulator to create the dataset used for training and validation. Further investigation into how the complexity of the training data, and the resolution of the GCM used to create this dataset, impact the sensitivity of data-driven models would also be of further interest. Similarly, we assess model performance and model sensitivity over a single predictive step, but in forecasting applications data-driven models would most likely be used iteratively. Assessment of how model skill varies when iterating data-driven models has been carried out in the context of alternative data driven models. Looking alongside this to how the sensitivity of the model changes when using models iteratively would also provide further insight into this area.

As data-driven models become competitive alternatives to physics driven GCMs, it is imperative to continue to investigate the sensitivity of these models, ensuring we have a good understanding of how these models are working and when it is valid to rely on them.

I would like to emphasize that the analyses conducted in the study are very comprehensive and would had been much more impactful had it been done for a model that was useful for data driven prediction. Of course, with an increase in complexity of the model, these analyses would become non-trivial as well. However, at this current stage, the best validation accuracy of the data-driven model is 0.58 which questions the performance of the model especially for a single time step prediction. One of the reasons could be because of under-predicting the extremes which can be dealt in other ways as well.

Again we refer to our response to point 1 regarding the model skill. There are differing measures of model performance, and we think the RMS error is the most suitable here (and that the correlation coefficient value of 0.58 cannot straightforwardly be interpreted as 'low skill', especially in consideration of the high scores obtained when calculated both correlation coefficients and anomaly correlation coefficients for the predicted temperatures, rather than the

predicted increments.). We also emphasise again that our focus is not on forecasting extremes, but on first capturing the more common dynamics seen in the model. Many thanks again for the comments and suggestions, and for the recognition of the comprehensive nature of this work.