Dear Referee,

we would like to thank you for the careful reading of the manuscript and the constructive comments that substantially helped to improve and clarify the paper. Answers to all your comments are detailed hereafter. Corrections to the English grammar were adopted in the revised version of the manuscript according to the reviewer's recommendations, but are not reported or discussed here. All authors agree with the modifications made to the manuscript. The comments by the referee are reported in bold followed by our response (in blue). The text added to the revised manuscript is reported in italic font. The line numbers reported in the answers referred to the revised manuscript. The revised manuscript that includes track changes is also provided in pdf format.

In the following answers, we use ‘Figure’ to identify the figures in the updated manuscript and we use ‘Plot’ to identify the figures in this document.

General comments:
I believe that some scientific choices need further explanations.
1) I suggest answering the following questions by adding the information in the INTRODUCTION
-Both NNs and numerical models are able to cover 7 days of forecast. While the NNs take less computational time, the numerical models have higher accuracy in the last days of the forecast (SST).
- What are the main advantages of using NN to predict ocean physics? Are the advantages only computational ones? (NN can approximate nonlinear function (Hornik et al., 1989)
- What are the main limitations in applying NN to real-world scenarios? (e.g. NN algorithms do not know when they are violating the laws of physics, e.g. Buizza et al., 2022)
The goal of the work is to “create competitive predictive tools”. You use the RMSE to assess the feasibility of NNs in predicting SST and MHWs and you validate all the NN tests (also) comparing the results with a numerical model.
- In this case I believe that the Figures (time-series) you have chosen are sometimes contradictory and sometimes do not show what you are describing (see detailed comments)
Some interesting information on this work can be found in the discussion. I expected to read them in the introduction (see detailed comments).

Thank you for your thorough review and insightful comments regarding our study's objectives and introduction. We extended the introduction taking into account your comments. We extend the text at line 33:”...*In recent years, increasing interest has been given to machine learning (ML) techniques, even though, in contrast to the dynamical model, ML techniques do not know when they are violating the laws of physics (Buizza et al., 2022). As a "learning from data" approach, machine learning has the advantages of computational efficiency, accuracy, transferability, flexibility and ease-of-use in ocean forecasting studies (Boukabara et al., 2019; Li et al., 2020; Wei and Guan, 2022; Taylor and Feng, 2022), Moreover, it is also less prone to model bias errors (Jacox et al., 2020) and, beyond computational efficiency, ML techniques excel in approximating nonlinear functions (Hornik et al. 1989).* ”

2) I suggest answering the following questions by adding the information directly in the METHODS section:
In the text I have the impression that you are sometimes contradicting your scientific choices. For example when you write: "For instance, the numerical approach is better suited for predictions over a wider area, while the data-driven techniques are more applicable for location-specific studies" (L.39). Based on this:
- Why are you proposing predictions over a wider area with data-driven techniques?
Since the MedFS forecast used for validation covers 10 days:
- Please explain why you chose a time interval of 7 days for the forecast (instead of 10 days).
- Have you considered or tried to extend the duration of the prediction? Following your results, I can infer that by extending the duration of the experiment (10days) for SST:
NN's RMSE >> MedFS RMSE
NN's computational time << MedFS computational time
(please specify the computational time of the model in the text).

Thank you for your suggestions.For the sentence you are referring to, there was a misinterpretation in our statement. We initially perceived "location-specific" studies as pertaining to time-series analyses. Consequently, we've removed this sentence from the introduction to avoid confusion. We extended the methodology taking into account your comments. We extend the text at line 146: *"MedFS predictions, part of the Copernicus Marine Service since 2017, offer SST forecasts for lead times up to 9 days averaged across specified regions. Since the accuracy of the ML forecast decreases almost linearly with time, we decided to limit the comparison with the MedFS forecasted SST averages for lead times of 1, 3, and 5 days. "*

We want to highlight to the reviewer that the MedFS forecasts are operationally provided as averaged SST time-series over the selected regions for lead times of 1,3,5 and 9 days.

The computational time for MedFS is 10 minutes to simulate 1 day. We added this information in the manuscript at line 163.

3) I suggest answering the following questions by adding the information directly in the DISCUSSION section:
I have the impression that the reader should follow the NN "branch" instead of the numerical models (to predict SST and MHWs). But "NN algorithms do not know when they are violating the laws of physics" . On the basis of this:
- Do you think that this limits the NNs-skills along the prediction interval?
- Have you considered adding physical constraints to your NN models?
- Have you considered the possibility of predicting SST and MHW by modifying the inputs of the NNs? (e.g. by adding ocean variables to atmospheric variables)
- Would you suggest using NNs to predict SST and MHWs in a 3/5-days interval and MedFS for a longer period?

Buizza, Caterina, et al. "Data learning: Integrating data assimilation and machine learning." Journal of Computational Science 58 (2022): 101525.

We extended the discussion taking into account your comments. We added some text at line 347: "*Furthermore, the neural network algorithms applied lack inherent knowledge of physical laws, potentially leading to violations of fundamental physical constraints. This limitation likely restricts the proficiency of NNs in maintaining accuracy throughout the prediction interval (Boukabara et al. 2019, Dueben et al. 2018). It prompts a need for cautious interpretation and validation of results, especially in scenarios where physical constraints significantly influence outcomes. While this study primarily focuses on predictive skill, future iterations could explore methodologies to infuse ML frameworks with physical laws governing ocean dynamics. For instance, Zanetta et al. (2023) propose achieving physical consistency in deep learning-based postprocessing models for temperature and humidity by incorporating meteorological expertise through analytic equations. Incorporating these constraints could potentially enhance the reliability of NN predictions, mitigating the risk of straying from physical realities. One may consider, due to the strengths of NNs in shorter-term predictions (3/5-days interval) and the potential limitations discussed, to use the ML model alongside models like MedFS for longer prediction intervals.. Utilizing MedFS for longer-term forecasts could leverage its established reliability over extended periods, while ML could excel in shorter-term predictions.*"

Detailed comments (minor):
4) Abstract:
To facilitate the reader, you might explicitly write the number of the Experiments.

- **L 4: MHWs acronym already introduced in Line 1**
- **L 9: Following the outline of the manuscript I think it could be clearer to insert in L9 the sentence L 15-16**
- **L 11 and CNN RMSE?**

Thank you for your comments, we rephrased the abstract:
"*Marine heatwaves (MHWs) have significant social and ecological impacts, necessitating the prediction of these extreme events to prevent and mitigate their negative consequences and provide valuable information to decision-makers about MHW-related risks. In this study, machine learning (ML) techniques are applied to predict Sea Surface Temperature (SST) time series and Marine Heatwaves in 16 regions of the Mediterranean Sea. ML algorithms, including Random Forest (RForest), Long short-term memory (LSTM), and Convolutional Neural Network (CNN), are used to create competitive predictive tools for SST. The ML models are designed to forecast SST and MHWs up to 7 days ahead. For each area, we performed 15 different experiments for ML techniques, modifying the training and testing periods. Alongside SST, other relevant atmospheric variables are utilized as potential predictors of MHWs. Datasets from the European Space Agency Climate Change Initiative (ESA CCI SST) v2.1 and the European Centre for Medium-Range Weather Forecasts (ECMWF) ERA5 reanalysis from 1981 to 2021 are used to train and test the ML techniques. For each area the results show that all the ML methods performed with minimum Root Mean Square Errors (RMSE) of about 0.1°C at a 1-day lead time and maximum values of about 0.8°C at a 7-day lead time. In all regions, both the RForest*

and LSTM models consistently outperformed the CNN model across all lead times. LSTM has the highest predictive skill in 11 regions at all lead times. Importantly, the ML techniques show results similar to the dynamical Copernicus Mediterranean Forecasting System (MedFS) for both SST and MHW forecasts, especially in the early forecast days. For MHW forecasting, ML methods compare favorably with MedFS up to 3-day lead time in 14 regions, while MedFS shows superior skill at 5-day lead time in 9 out of 16 regions. All methods predict the occurrence of MHWs with a confidence level greater than 50\% in each region. Additionally, the study highlights the importance of incoming solar radiation as a significant predictor of SST variability along with SST itself."

5) Introduction

I appreciated the description of the impact of MHWs on ecosystems, but since the article does not deal with ecological studies I would expect to have: (i) less information on the ecological impacts (1-2 lines) (ii) more information on the techniques chosen and their pros and cons, including a comparison with numerical models (iii) a brief overview of the main characteristics of the Mediterranean Sea with respect to the objective of your work (e.g The reason why you have chosen the Mediterranean Sea as your study area?). Please describe if there is a sector (western-central-eastern) that is more susceptible to these events.

Thank you for your feedback, we considered all your comments. We choose to retain the impacts paragraph as we believe this information is crucial for comprehending the objectives of our work, following reviewer1's observation. We add specifications on ML methods at line 50: " … *It is important to note that within the methods explored in this paper, LSTM stands out as the sole technique explicitly crafted for handling time series data. In contrast, CNN algorithms are commonly tailored for image processing tasks and are not inherently designed for time-series forecasting. To the best of our knowledge, just a few studies employed the RForest model to predict sea surface temperature…*" . We add justification of the choice of Mediterranean Sea at line 70: "*The Mediterranean Sea is a well-studied hot spot for MHW events (Garrabou et al., 2009; Giorgi, 2006; Cramer et al., 2018; Pastor et al., 2020; Pastor and Khodayar, 2022; Garrabou et al., 2022; Ciappa, 2022). As detailed in the study by Bonino et al. (2023), the Adriatic Sea, the Gulf of Lion, and the Alboran Sea encountered the highest occurrence, shortest duration, and most severe MHWs. The Mediterranean Sea serves our study area due to its relevance for marine management activities, For instance, over 95% of the global production of seabream and seabass comes from aquaculture, with Mediterranean countries contributing to 97% of this production. (Carvalho, N., & Guillen, J. 2021).* "

About 25% of your abstract focuses on NN's improvements compared to numerical models (MedFS) which you mention in P9. I suggest adding a sentence on the MedFS model used to compare the results (at line 70).

- **L 18-29: I think this part could be shortened.**
- **L 44-65: If in your opinion it is important, please highlight if there is a method (shallow/deep) that better fits the SST/MHWs prediction goals (from literature).**
- **L 44-65: Too many citations. I suggest reducing the number of citations and adding more detailed information (i.e. the duration of the predictions from the**

cited literature). Moreover, in many works you cited (Corchado ,Liu, Xie etc.) the duration of the prediction is higher than 7 days.

Thanks for your feedback. We've considered all your comments and, indeed, made substantial revisions to the literature review. We rephrased at line 46: "... *Pioneering works on SST prediction using deep learning methods are, instead, more recent. In the last few years, as reported in a recent review paper (Haghbin et al., 2021), the deep learning-based models such as the RNN, the Long Short Term Memory (LSTM, e.g. Xiao et al. 2019, Liu et al. 2018 and Xie et al. 2019), and CNN (e.g. Han et al. 2019) have attracted progressively more attention in the research community, providing accurate estimates among the models considered…*"

6) Methodological Framework:
Data collection and preprocessing

- **L 83: Add the spatial resolution of the datasets e.g. "daily satellite-derived Sea Surface Temperature (SST) data".**
- **L 86: the L4 dataset provides interpolated data (L3 does not). I assume that you have decided to use the L4 dataset to numerically enrich the dataset for training and test evaluation. Is this the case?**
- **L 102-114: In my opinion, table 1 is a result (as you write in the abstract L15-16)**

Thank you for your comments. We added the resolution of the ESA CCI SST dataset at line 86: "*This dataset consists of daily maps of average SST at 20 cm nominal depth with 0.05 × 0.05 of horizontal resolution, covering the period from September 1981 to December 2016.*". We added the motivation for the L4 dataset at line 304: "*In this study, a group of ML algorithms - Random Forest (RForest), Long short-term memory (LSTM) and Convolutional Neural Networks (CNN) - are used to evaluate their ability in building a competitive prediction tool of SST and MHWS occurrence 7 days ahead in the Mediterranean Sea. The methods use the European Space Agency (ESA) Climate Change Initiative (CCI) Sea Surface Temperature, Sea Level Pressure (SLP), Geopotential Height at 500hPa (GEO), Wind Speed (WS), Sensible Heat flux (SENS), Latent Heat flux (LAT) and incoming solar radiation (INC) from ECMWF ERA5 as input data. We compared the ML predictions against the MedFS prediction system, part of the Copernicus Marine Service since 2017, which offers SST forecasts for lead times up to 9 days averaged across specified regions. It is important to underline that the data used in our work are designed primarily for climate studies and providing a gap-free dataset through interpolation, raises concerns about potential biases introduced into our forecasting model. The interpolation process, while ensuring a comprehensive dataset, might inadvertently smooth variations and obscure critical phenomena like coastal upwelling. Alternative approaches utilizing near real-time operational data, could offer more dynamically responsive and less biased datasets for improved forecasting accuracy. Moreover, our methodology involves averaging SST data to obtain a single representative SST for each zone and the same approach is used for atmospheric predictors. We acknowledge that averaging data in this manner might smooth out localized variations, thereby potentially overlooking the non-linearities of* *variables such as wind speed*". We put Table 1 in the results section titled "Mutual information analysis".

7) Experiments/Evaluation metrics :
● L 147: I would have introduced MedFS earlier in the text (e.g. in the Introduction)
We also added a sentence to introduce the MedFS in the introduction at line 67: "*The ML methods are compared against the Copernicus Mediterranean Forecasting System (MedFS, i.e. dynamical ocean model, (Clementi et al., 2021). MedFS is a numerical ocean prediction system, implemented and developed by the Euro-Mediterranean Center on Climate Change (CMCC), that produces analyses and short term forecasts for the entire Mediterranean Sea and adjacent areas in the Atlantic Ocean (Clementi et al., 2021).* "

8) Results:
If you are going to redo some figures, please increase the font size (especially for the legend).
● L 198: "For instance, in all the techniques, region 15 shows the lowest, or almost the lowest (e.g in CNN) RMSE, while region 11 shows the highest errors" I cannot recognise region 15 in the CNN subplot, it is hardly readable. From figure 3 I can only evaluate the daily variability of RMSE across the Med. basins. Perhaps consider that plotting the average RMSE would be more useful to have a general overview on which method 'outperforms' the others.
● L. 198-200: Is there a reason why RMSE in region 11 is higher and 15 lower? A brief overview of the main physical characteristics of the Mediterranean Sea in the introduction might be helpful.
● L. 205: "They also represent different dynamical areas of the Mediterranean basin." Which ones? Add information in the Introduction.

Thank you for your input. We decided to retain Figure 3 but we added Figure 1 as Figure 4 in the manuscript. Following your suggestion, we decided to plot the mean RMSE error for the LSTM REXPs experiment for each region (Figure 1). We can notice that the areas with larger errors are: (i) the Alboran Sea strongly, characterized by a complex dynamics influenced by the incoming cold Atlantic water through the Gibraltar Strait modulating the water transport; (ii) the North-West part of the basin, which is an area of dense water formation and intense dynamics due to the Gulf of Lion gyre (Madec et al., 1991; Pinardi et al., 2006) and by a boundary intense current called the Liguro-Provenal-Catalan Current (Pinardi et al., 2006); (iii) the Adriatic Sea, especially in its northern shelf, characterized by a complex topography, intense air-sea exchanges, large riverine inputs that contribute to enrich the dynamics of the area. Thus the correct SST representation and forecast in these areas represent a challenging modeling problem. We added Figure 1 in the manuscript and reported this description at line 219. We also added the RForest and CNN mean error as Figure S2.

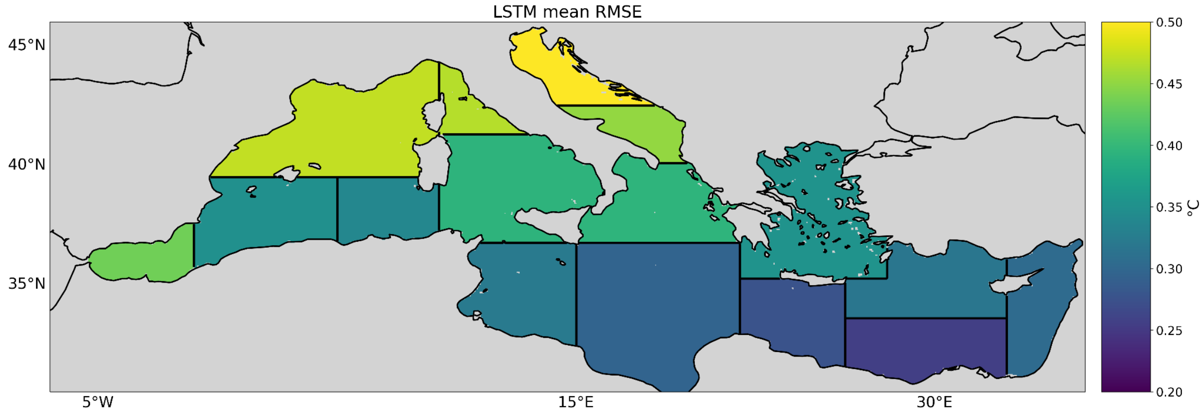

Figure 1. LSTM mean RMSE for REXP for each region

● L. 210: "In contrast to ML methods, the dynamical model's prediction of SST is influenced by atmospheric forecasts throughout the forecast period, which likely prevents the RMSE from increasing with the lead time."
I think this is not a result, I would rather move it into the Discussion section.
● L 215: "ML methods show lower RMSE than the MedFS forecast system for the first 3 days of forecast and they are comparable at lead time of 5 days."
From Figure 4a
- it results that the RMSE of MedFS at day3 is less than the one from NN methods in west and east only.
- why are MedFS bullets plotted only for days 1,3,5?
- UEXPs are called whiskers in the Figure and bar / UEXPs in the text. Better to be consistent with the nomenclature.
● L 221: "It is likely connected to the fact that CNN algorithms are typically designed for image processing rather than time-series forecasting". It would probably be better to have this information right from the introduction.
● L 223: Is there a particular reason to choose the year 2020?
● L 225: The figure shows a very close match between the forecasts and the observations. Hence NNs don't outperform the MedFS.
● L 232: "while Figure 4b shows the variation of the F1 score for all the methods with increasing forecast lead time"
The reader expects at this point an explanation of the figure 4b. It comes at L244. I suggest removing this sentence or adding information previously.

Appreciate your feedback. We've considered your comments while revising the results and discussion section. The inclusion of the 2020 year doesn't stem from a specific motivation but rather its availability from MedFS and the forecasted time-series. In Figure 4a, we've plotted bullets solely for days 1, 3, and 5 as these correspond to the available lead times in MedFS, as previously explained in the methodology section at line 147: "*MedFS predictions, part of the Copernicus Marine Service since 2017, offer SST forecasts for lead times up to 9 days averaged across specified regions. Since the accuracy of the ML forecast decreases almost linearly with time, we decided to limit the comparison with the MedFS forecasted SST averages for lead times of 1, 3, and 5 days.*"

As said before, we also added a sentence to introduce the MedFS in the introduction at line 66: "*The ML methods are compared against the Copernicus Mediterranean Forecasting System (MedFS, i.e. dynamical ocean model, (Clementi et al., 2021).*

MedFS is a numerical ocean prediction system, implemented and developed by the Euro-Mediterranean Center on Climate Change (CMCC), that produces analyses and short term forecasts for the entire Mediterranean Sea and adjacent areas in the Atlantic Ocean (Clementi et al., 2021). "

● **Figure 6: impossible to see the lines. Since you only explain INC SST and LAT why plotting the others atmo forcing? (you can merge all the other ones in 1 single line)**

Thank you, we simplified the Figure. The Figure 2 below is now the Figure 7 in the manuscript. We explained it at line 287:
"*The labels of Figure 6 indicate, for each experiment, the driver that has been shuffled in REXPs. For an easier interpretation of the results we are showing only the SST, the INC and the LAT drivers, as they are the most relevant.* ". We comment on this Figure at line 290: "*Nevertheless, it is worth noting that the extent to which the RMSE increases after shuffling SST shows a tendency to decrease as the forecast lead time increases. This result suggests that the SST itself has the strongest predictive power in forecasting SST, slightly losing predictive skill increasing the lead times. The incoming solar radiation, to a lower extent, shows the opposite behaviour: after shuffling, the RMSE tends to increase more than the other drivers with the forecast lead times. The RMSE at L7 reached values of about 1°C, 1.7°C, 1°C for WM, CM and EM, respectively. Surprisingly, in contrast with the mutual information analysis, we can notice that for WM and EM the latent heat plays a role. In particular, for WM the RMSE at L7 reached values of about 0.5 for all the ML techniques, double of the RMSE of REXPs. Overall, the aforementioned analysis suggests that the incoming solar radiation, as shown also by the mutual information analysis, has some predictive power in driving SST variability. It is important to highlight that incoming solar radiation shows a tendency to gain predictive power as forecast leads increase, whereas SST, to a much lesser extent, tends to lose it. This suggests that atmospheric variables could be useful in forecasting SST at longer time scales. Nevertheless, it is worth mentioning that the ML methods look for statistical relations (e.g. linear or non-linear relations) between variables that do not necessarily have a physical meaning (e.g. a cause-effect relation).*"

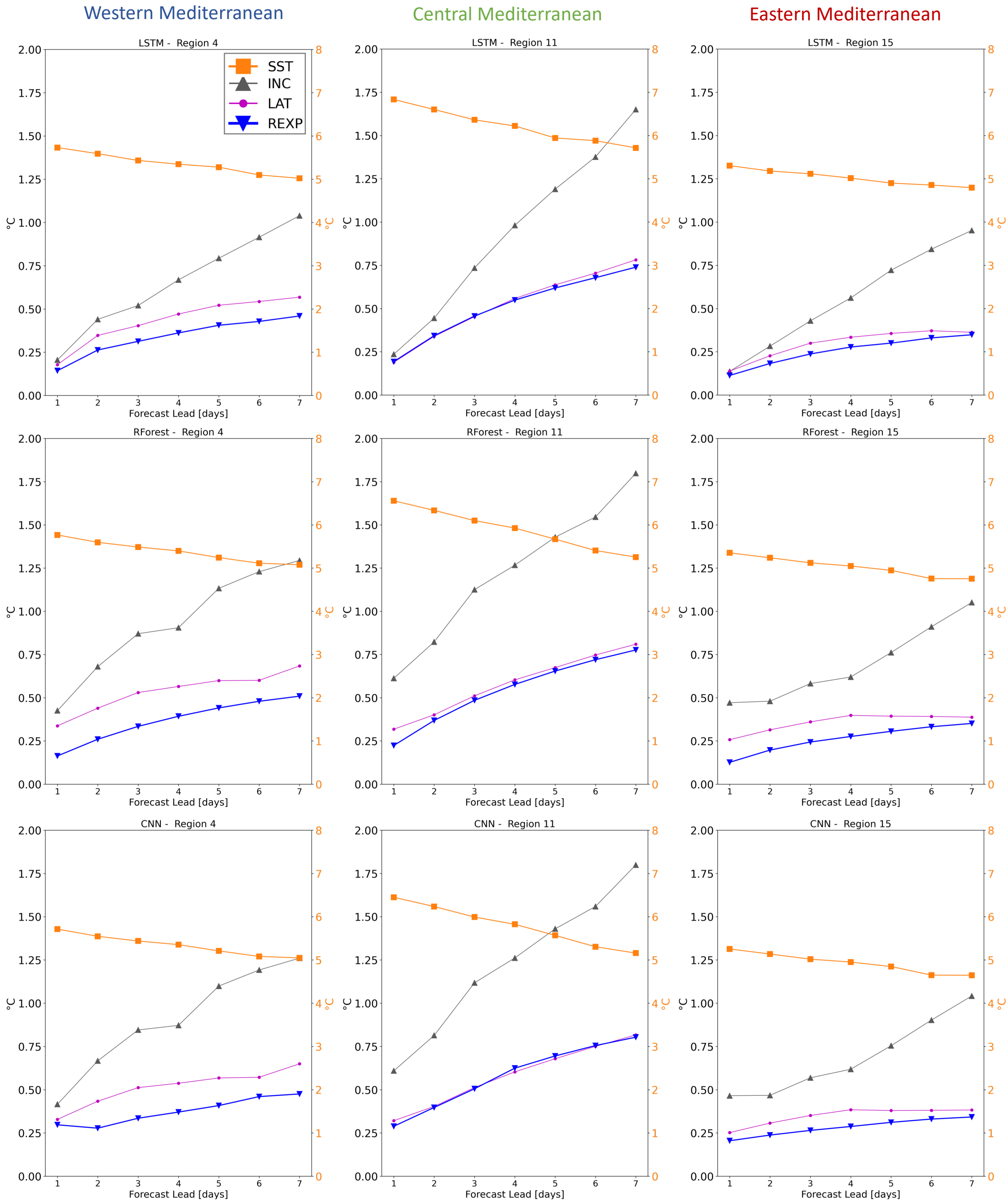

Figure 2. SST Root Mean Square Error (RMSE) of the sensitivity experiments SEXPs for each forecast lead time for: (left column) Western Mediterranean, (middle column) Central Mediterranean, (right column) Eastern Mediterranean. The labels indicate, for each experiment, the driver that has been shuffled. Right y axis (orange ticks) refers to SST driver experiment (orange solid line with square marker), left y axis indicates the other drivers error.

9) Discussion and conclusions:

Can you introduce possible future developments?

- **L278-282: All the abbreviations are already introduced**
- **L299-301: These features are typical of all the NNs methods. I would prefer to have this general info in the Introduction section.**
- **L330-336: Too much information on the impact, I suggest reducing this paragraph.**

Thank you for your comments, but we opt to reintroduce the abbreviation in the Discussion section for readability purposes, particularly in this crucial part of the manuscript. Additionally, we choose to retain the impacts paragraph as we believe this information is pivotal for comprehending the objectives of our work, following reviewer1's observation. However, we plan to relocate the general information about NN methods to the introduction at line 35: "*As a "learning from data" approach, machine learning has the advantages of computational efficiency, accuracy, transferability, flexibility and ease-of-use in ocean forecasting studies (Boukabara et al., 2019; Li et al., 2020; Wei and Guan, 2022; Taylor and Feng, 2022).*"

10) Supplementary:
Correct the description of Figure S4
Figure S4: As Figure S4 but for forecast lead time 3.

Thank you, we corrected it.

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