sp-2024-19-author_response-version2.pdf

Final response for reviews for A new conceptual framework for assessing the state of the Baltic Sea

Reviewers' comments: formatted in red italics. Authors' final responses: formatted in black.

Reviewer 1:

Summary: The manuscript presents an analysis of a data set from the Baltic Sea reanalysis, focusing on temperature, salinity, ocean heat content and freshwater content. This data set covers the period 1993-2023. The manuscript investigates long-term trends and the connection between these variables. The conclusions of the analysis are not totally surprising. They identify a warming trend and a strong connection between water temperature and ocean heat content and between salinity and freshwater content.

Recommendation: I have concerns about the manuscript's framing, title, and objectives. I do not see problems with the data analysis. My recommendation is that the manuscript requires substantial revisions.

Main points:

1) The title is misleading. I could not identify any 'new conceptual framework framework' nor find a definition for 'state of the Baltic Sea'. The manuscript is perhaps a valuable presentation of the ocean reanalysis, but it does not present any 'framework#' and leaves many concepts in the title and in the introduction undefined. I think this manuscript is indeed a presentation of this data set, which is fine, but it tries to present it as a more substantial advance than it really is.

If the authors believe the manuscript presents a new conceptual framework, they should explain it clearly in the introduction. I failed to see it.

We have changed the title by adding the term "physical", which means that we are dealing with the physical state, not the biogeochemical or ecological state. We have revised the Introduction providing a more detailed explanation of what we mean about the framework and added how this framework is different from the other existing frameworks.

"We propose a new conceptual framework for assessing the physical state of the Baltic Sea by integrating multiple physical and statistical approaches. The framework is based on two main physical indicators: Ocean Heat Content (OHC) and Freshwater Content (FWC). These indicators are used to describe the energy and mass balance of the Baltic Sea. The study identifies the major variables affecting these indicators, including subsurface temperature, salinity, atmospheric forcing factors, and salt transport. The framework follows a three-stage process: time-series analysis, depth-based variability analysis and causal relationships using machine learning. The initial phase consists of calculating the time series of OHC and FWC for the entire Baltic Sea. This provides insights into long-term trends and interannual variability. In basins covered partially by sea ice, the annual mean ice extent (MIE) is considered an

important integral characteristic. The next step examines the horizontally averaged vertical distribution of temperature (for OHC) and salinity (for FWC) to determine which depth ranges contribute the most to their variations. While this does not directly attribute causal links, the vertical profiles of temperature and salinity provide strong indications of which forcing factors might be responsible for changes in OHC and FWC. The final stage integrates forcing functions and ocean state characteristics to identify causal relationships. A Random Forest (RF) model is employed to highlight statistical dependencies between oceanic state variables and external forcing mechanisms. This machine-learning approach enables the identification of general patterns in the temporal evolution of the Baltic Sea's physical state. Our proposed framework integrates the analysis of ocean heat content (OHC) and freshwater content (FWC) by considering both their bulk integral values and their vertical distributions, allowing for the identification of key depth ranges contributing to their variability – which goes beyond other similar frameworks. Unlike the GOOS Essential Ocean Variables (EOV) framework (https://goosocean.org/), which focuses on structured global ocean monitoring without machine learning-based causal analysis, our approach explicitly incorporates machine learning to identify potential drivers of variability. Compared to the IPCC Climate and Ocean Monitoring Framework (IPCC AR6 (2021) Ocean Observations Chapter https://www.ipcc.ch/report/ar6/wg1/), which relies on dynamical climate models for global-scale processes, our framework is designed for regional-scale Baltic Sea analysis, offering a more localized and detailed assessment. Finally, while the NASA Salinity and Heat Budget Analysis (NASA Salinity Budget Project https://podaac.jpl.nasa.gov) is largely empirical and focused on global salinity and heat transport, our approach provides a structured three-stage methodology, incorporating not only empirical analysis but also a cause-and-effect exploration using machine learning. This makes our framework uniquely suited for regional climate monitoring and actionable insights into the physical state of the Baltic Sea. This conceptual framework is designed as an indicator-based approach relevant to policymakers. It enables the monitoring of climate change impacts on the Baltic Sea while maintaining a balance between scientific rigor and practical accessibility. The framework is not meant to serve as a comprehensive dynamical model but rather as a scientifically robust tool for assessing the state of the Baltic Sea and guiding regional management decisions."

2) The introduction often presents the manuscript in a too-bright light. For instance, the text states (line 45) that it presents a 'model'. I cannot see any model. Again, the manuscript analyzes the connections between different ocean and atmospheric variables, but it does not contain any model that would allow predictions or that includes any physical mechanisms, equations, etc.

We agree that we have not introduced any model. Therefore we have changed the term "model" to the term "framework" throughout the manuscript.

3) I have problems understanding the 'state of the Baltic Sea'. First, it appears that the manuscript deals only with physical variables and leaves geochemical or biological variables out of the analysis. The use of 'state of the Baltic Sea' on this account alone seems exaggerated. But more importantly, what does 'state' mean here? Is it a snapshot of the ocean at a particular time? Does it mean a more value-centered assessment of the situation in the Baltic Sea (good, bad, etc.)? Readers curious about the title may be vastly disappointed when reading the manuscript.

We mean physical state and have changed the title accordingly. The physical state of the Baltic Sea refers to the condition of its marine environment in terms of physical oceanographic characteristics. These include water temperature, salinity, ice cover, sea levels, circulation patterns, and the vertical stratification of the water column. The revised Introduction also includes a more detailed explanation of what we mean about the physical state of the Baltic Sea in this study.

4) I do not see the need for a Random Forest method. The manuscript applies this algorithm to conclude that the driver for the heat content is the temperature at all layers and that the diver for freshwater content is salinity at all layers. Do we need an RF algorithm? Any reader would be stunned if the results would have been different. Ocean heat content can be directly calculated from temperature, and freshwater can be directly calculated from salinity. I do not see the need or the advantage of using a machine-learning algorithm to identify those connections. They are obvious.

We completely agree that ocean heat content is determined by spatially averaged temperature profile and freshwater content by its spatially averaged salinity profile. Using the Random Forest models in the current context is to understand at which depth layers temperature contribute the most significantly to the overall heat content and salinity to the freshwater content.

A Random Forest method captures complex, non-linear relationships between variables. In this study we use four different RF models: RF1 for Ocean Heat Content (OHC) with meteorological variables, RF2 for Freshwater Content (FWC) with meteorological variables, RF3 for OHC with temperature profiles T(z), and RF4 for FWC with salinity profiles S(z), which are described in Table 2 and extended Methods section.

5) On the other hand, the research question is unclear. What knowledge gap would the manuscript fill? What is unknown in the variability of the Baltic Sea that this data set may help to clarify? The introduction is silent about this.

We have added a paragraph about the aim of the study:

"The study aims to evaluate a framework for assessing the physical state of the Baltic Sea by integrating annual mean values of OHC, FWC, subsurface temperature and salinity, atmospheric forcing functions, salt transport, and river runoff. The objective is to use a data-driven RF approach as the primary analysis tool to parse out nonlinear relationships and feature importances from a broad dataset. This study introduces an integrative, basin-wide approach, defining the entire Baltic Sea as a single water body for analysis. It computes time series of total OHC and FWC for the whole sea. Rather than focusing solely on local variations, the methodology emphasizes these integrated indices as representations of the sea's overall state. This holistic integration marks a shift from the segmented or localized analyses of the past."

Summarizing these previous points, it seems to me that the manicurist tries to push up a correct and useful analysis of the ocean data by using exaggerated terms (which often do not have a clear meaning)

Particular comments:

6) line 33 exceptional increase in global sea surface temperature Exceptional in which sense? At which time scale? Th Earth's temperatures have been warmer than now in the geological past.

We mean exceptional warming in recent history. This is the estimation for the period 1979-2024 (McGrath et al., 2024). Rewritten sentence is:

"In 2023, there was an exceptional increase in global sea surface temperature over the period 1973-2024 (McGrath et al., 2024), and OHC reached unprecedented levels (Cheng et al., 2024)."

7) Figure 1 : Conceptual Scheme of the Baltic Sea State parameters.

Again, what is the conceptual scheme shown in this figure? This figure shows the obvious links between those physical variables and only physical variables.

Yes, while these links are obvious, they are rarely, if ever, combined into a single framework for assessing the physical state of a water basin. We have described this framework in more detail in the revised Introduction, with reference to Figure 1.

8) Some methodological aspects are not clearly explained. For instance, I struggled to find the time scales of analysis. I think it is only mentioned in one figure caption or line 171, which alludes to annual means. I kept wondering for a long time if the authors were anal sing daily means, monthly means, seasonal means or annual means

All analyses are prepared in a common timescale using annual mean values covering the period from 1993 to 2023. We wrote on lines L64-65 "This study evaluates a conceptual model for the Baltic Sea using annual mean values of ocean heat content (OHC), freshwater content (FWC), temperature, salinity, and a selection of forcing functions." In revised manuscript we have rewritten the sentence: "The study aims to evaluate a framework for assessing the physical state of the Baltic Sea by integrating annual mean values of OHC, FWC, subsurface temperature and salinity, atmospheric forcing functions, salt transport, and river runoff."

9) Likewise, it is not all clear whether these variables are considered at the grid-cell scale, water column scale or averaged over the Baltic Sea

This is explained in the manuscript. In the conceptual framework we involve spatially averaged values, either it is averaged over the whole Baltic Sea or at each vertical level. We will specify it more clearly in the revised manuscript.

10) Often, physical units are missing, for instance, when stating trends. Trends must have units of variable per unit of time. It is not clear if the trends refer to changes per year, for instance, or over the whole period

These trends are calculated for z-scored values. Therefore they do not have units for physical variables. All trends have been calculated per year. The only trends with physical units are specified in Table 3 caption and we have corrected km³/year units for FWC trend in line 140.

11) "Surface net solar radiation has a weaker but still significant positive trend of 0.058±0.035, and the evaporation time series shows a negative trend of-0.041±0.039"

Units missing

These trends are calculated for z-scored values. Therefore they do not have units for physical variables. All trends have been calculated per year. We have added asterisk to the trends indicating z-score trends (trend*) to distinguish them from physical trends.

Reviewer 2:

Summary: The presented study analyses interannual variations of ocean heat content (OHC) and freshwater content (FWC) of the Baltic Sea based on modern data analysis techniques (random forests) and puts these into perspective to other state variables of the ocean and atmospheric forcing. The underlying data consist of reanalysis products, covering the period 1993-2003. The authors highlight that interannual basin mean FWC variations refer mainly to FWC variations in the halocline, while OHC variations refer mainly to both, variations in the seasonal thermocline and upper halocline.

In a second step, the study elaborates on the potential impact of atmospheric forcing and some oceanographic factors. The authors suggest that similar analysis techniques might be applicable also to other regions.

Major Comments:

The subject of the study is interesting and I appreciate the use of modern data analysis techniques. Also, the manuscript is well written. Still, I have some points which need in my eyes to be addressed:

(1) My major concern is that I find the fitting procedure for the random forest models not well explained. Generally, I would expect distinct data for the fitting procedure and for testing the fit - to evaluate how well the RF-model generalizes to unseen observations. I am not sure if this has been done. Also, I am not sure how the hyperparameters were chosen and would appreciate some more details (e.g., the number of trees, tree depth, minimum samples for splits).

We have included a paragraph in the Methods section explaining the configuration of the Random Forest (RF) models, along with a new Table 2 that details the hyperparameter settings. Additionally, we conducted a sensitivity analysis on the number of trees, which is now presented in Figure A2. Given our goal of training models that capture complex, nonlinear patterns as accurately as possible, we justify the use of the entire dataset for training to maximize the model's learning capacity. We have added following paragraph to Methods

In this study we have trained the four different Random Forest (RF_) models to fit the OHC and FWC timeseries with the hyperparameter configurations shown in Table 2. Two models are trained to predict the OHC and FWC values from the set of the meteorological variables (var suffix) and two from the horizontally averaged temperature and salinity profiles (zax suffix). To optimize the performance of the Random Forest models while ensuring robustness and generalizability, a set of hyperparameters was selected based on sensitivity analysis conducted for number and depth of the trees (Fig A2). The minimum leaf size (MinLS) was set to 1, allowing the trees to fully grow and capture complex data patterns. The number of predictors to sample at each split (Pred2Samp) was dynamically determined as one-third of the total number of predictors, tackling a balance between feature randomness and predictive strength. This approach promotes diversity among trees while preventing excessive correlation. The number of trees (NumTrees) in each RF model was set to 100, providing sufficient ensemble stability while maintaining computational efficiency. Since this study employs RF models to investigate nonlinear relationships between predictors and state variables, we use the entire dataset as the training set to maximize the models' ability to learn patterns. To further enhance predictive reliability, assess uncertainty, and evaluate the

stability of both predictions and feature importances, an ensemble of 150 independently trained RF models was constructed.

(2) I must admit that I find it sometimes difficult to keep overview over all the RF-models. I would find it helpful if the many random forests would be described in an extra sub-section in the Methods and/or a table of all RF-models mentioned in the text might be nice (including some respective measures of the goodness of fit).

We have added a paragraph and Table 2 describing the Random Forest (RF) models in detail. An additional sensitivity analysis illustrating the goodness-of-fit response to the number of trees is presented in Figure A2.

Specific Comments:

Introduction, Ln.38ff: Winsor et al. (2001) and Rodhe and Winsor (2002) might be interesting to mention here for FWC. For OHC Dutheil et al. (2023) might be interesting.

We have added reference to the paper by Winsor et al. (2001) and Rodhe and Winsor (2002). Also we include reference to Dutheil et al. (2023).

Windsor et al. (2001) demonstrated that long-term variations in the freshwater content (FWC) of the Baltic Sea are closely linked to accumulated changes in river runoff. Building on this work, Rodhe and Winsor (2002) concluded that the recycling of Baltic Sea water at the junction between the Baltic Sea and the North Sea is a crucial process in determining the sea's salinity. An increase in freshwater supply to the Baltic Sea will intensify water recycling, resulting in lower salinity, and vice versa.

In the Baltic Sea, the temperature trends for the period 1850-2008 show fast warming at the surface ($\sim 0.06 \, \text{K}$ decade– 1) and bottom ($> 0.04 \, \text{K}$ decade– 1), and slow in the intermediate layers ($< 0.04 \, \text{K}$ decade– 1) (Dutheil et al., 2023). Surface warming has progressively increased over time, primarily due to the sensible heat flux and latent heat flux (Kniebusch et al., 2019).

Ln. 55/56: I would suggest rather to talk about Granger-causality here (https://en.wikipedia.org/wiki/Granger_causality) because statistical relationships cannot identify "real" cause-and-effect relationships.

We note that if one variable consistently improves the prediction of changes in another (in our RF analysis), it suggests a lead–lag relationship consistent with Granger causality, though not proof of mechanistic causation. Our analysis is about identifying statistical dependencies and potential causative links, without overstating them. Still, we would like not to use the term Granger-causality. Granger causality and random forest are different in their approaches to understanding relationships between variables. Traditional Granger causality assumes linear relationships between variables. Random forest can model non-linear dependency. Indeed, Granger causality and RF can be used in combination.

Line 79ff: It might also be interesting to add that many studies reported a strong warming of the Baltic during the past decades when compared to the global oceans (e.g. Kniebusch et al, 2019).

We have added the reference to (Kniebusch et al., 2019).

"In the Baltic Sea, the temperature trends for the period 1850-2008 show fast warming at the surface ($\sim 0.06 \text{ K decade}-1$) and bottom (> 0.04 K decade-1), and slow in the intermediate layers (< 0.04 K decade-1) (Dutheil et al., 2023). Surface warming has progressively increased over time, primarily due to the sensible heat flux and latent heat flux (Kniebusch et al., 2019)."

Line 99ff: I would find it nice to get a bit more background information on FWC and OHC – why it is considered so important and how it's calculated? (e.g. I guess the reference salinity from Raudsepp et al. 2023 has been updated?).

We have explained the importance of FWC and OHC in the revised manuscript.

"OHC offers a comprehensive view of oceanic heat storage, crucial for evaluating climate change impacts, energy budgets, and long-term trends (Forster et al., 2024). OHC directly reflects Earth's energy imbalance, making it a key metric for tracking global warming, unlike basin-averaged temperature, which lacks a direct connection to energy budgets (von Schuckmann et al., 2016, 2023). Consequently, OHC is prioritized in climate models and international assessments (IPCC, 2019) due to its direct relationship with anthropogenic forcing and its predictive value for future climate scenarios."

"Ocean FWC is deemed more significant than mean salinity for understanding climate dynamics and ocean processes. FWC provides a holistic measure of freshwater storage and its effects on ocean circulation, climate, and sea-level rise (Solomon et al., 2021; Fukumori et al., 2021). It directly measures freshwater inputs (e.g., ice melt, river runoff, rainfall) or losses (e.g., evaporation), whereas mean salinity only indicates the average salt concentration, ignoring volume (Hoffman et al., 2023). A minor salinity change over a large water volume could signify a substantial freshwater flux, which mean salinity alone would not reveal (Schauer and Losch, 2019)."

We have provided the equations for the calculation of OHC and FWC with updated Tref and Sref calculation compared to Raudsepp et al. (2023).

Methods, Random Forest: Line 109ff: As outlined in the major comments, I find the fitting procedure for the random forest models not well explained. Generally, I would expect distinct data for the fitting procedure and for testing the fit - to evaluate how well the RF-model generalizes to unseen observations. I am not sure if this has been done and how the hyper parameters were chosen.

We have added a paragraph in Methods describing the choice of the hyperparameters. We deviate from the "general" use of RF as our aim is not to predict OHC and FWC for unseen predictors, but we are trying to explain the past "seen" relationships between meteorological variables and OHC, FWC

parameters (see reply to first major comment).

Methods, Line 136: I think it would help the readers if another subsection was introduced, explaining which data were used to generate the random forests, including the thoughts behind the design-choices (e.g. for using annual means and the selected predictors). Given the very limited amount of data I would try to keep the number of predictors as low as possible. Currently, many design information of the RF-models appear in the Result-Section and I found it sometimes hard to keep overview.

We will have added a paragraph in Methods describing the design of the models. The limited amount of data prevented us from conducting a forecasting study to predict future OHC and FWC values. However, by fitting the RF models to the full dataset and allowing the use of all available predictors, we were able to analyze the relative importance of each predictor.

Line 172ff: As said, I would find it easier to follow if the RF-design information would be moved to a respective sub-section in the Methods.

We have added Table 2 and sentences, where the hyperparameters for RF models have been clearly described.

Line 199: Could you provide some measure on the quality of this reconstruction? – for the readers to rate it against the fit when using all predictors. Also, I am not sure if this intermediate step is needed (couldn't deep salinity (or Mohrholz, 2018?) be included directly for FWC based on Fig.3?).

We first conducted the Random Forest (RF) model analysis without detrending the data (Lines 198–216), which was not included in the original manuscript. We have now added the corresponding figure and the goodness-of-fit metrics to Appendix 1 for the models trained on the OHC and FWC time series that include the trends.

Line 199ff: How do these results and design decisions fit to the foregoing findings that the overall interannual FWC variations are mainly due to changes of FWC in the halocline? (as impacting factors I would thus expect mainly P-E, runoff and inflows form the North Sea?). Ultimately, Fig 3d is a nice result and I think it might help the readability to have it a bit more included in the subsequent argumentation.

We have connected our findings about the halocline (Fig. 3) with our analysis of drivers (Fig. 4) to be consistent in the Discussion (L382-389, in track-changes document). We have added following paragraph to the revised manuscript

The signals of the MBIs are evident in the bottom salinity of the Bornholm Basin. Figure 4 illustrates that interannual variations in FWC are linked to the bottom salinity in the Bornholm Basin, which serves as a proxy for MBIs, as well as zonal wind stress and net precipitation. Therefore, Figure 4 highlights the drivers of FWC, while Figure 3 emphasizes the significance of halocline salinity's response to FWC. Consequently, we can infer that inflows from the North Sea and net precipitation are responsible for

changes in halocline salinity, with zonal wind facilitating these inflows. However, we were unable to directly associate moderate and small inflows from the North Sea with changes in halocline salinity. This aspect requires further investigation and precise simulation of salt transport between the North Sea and the Baltic Sea, which is beyond the scope of the current study.

Line 212 Which criteria were used to identify MLD and UML? Also, I am not sure how to conclude line 216 from this. Maybe this is because I am not sure what is meant by "of the sea". Can you help me out?

We have included an explanation of how mixed layer depth is calculated according to Panteleit et al., (2023) and have added a paragraph to the Methods section. We have deleted the sentence where we used the term "of the sea".

Line 224: So, these were not assimilated?

The model system assimilates satellite observations of SST (EU Copernicus Marine Service Product, 2023) and in situ temperature and salinity profile observations from the ICES database (ICES Bottle and low-resolution CTD dataset, 2022). Even so, the salinity values at the entrance region have notable errors (Lindenthal et al., 2024). Due to data assimilation, the salinity downstream from the Danish straits is acceptable (Lindenthal et al., 2024), but salt fluxes through the cross-section at the entrance to the Baltic Sea are not accurate enough.

We have added reference to Lindenthal et al. (2024).

Line 232: I would call this inflow instead of influx – but both formulations might be right.

We have changed the term influx to inflow to indicate general salt inflow to the Baltic Sea.

Line 235. You lost me a bit here – maybe it helps to mark the strong inflow events in the time series plot and shorten the explanation so it's easier to follow?

We have marked the salt inflow events from the MBI statistics dataset of (Morholz, 2018; https://www.io-warnemuende.de/major-baltic-inflow-statistics-7274.html) to Figure 4 and Figure A1.

Discussion & Conclusion, Line 250: I miss some more arguments why OHC and FWC are considered so important that they define the Baltic Sea state (as opposed to common measures such as temperature and salinity).

We have expanded the Data and Methods section to include the rationale and references for using OHC and FWC. Additionally, we have elaborated on the importance of OHC and FWC in the first paragraph of the Discussion section.

Line 251: I find "the forcing functions" a bit vague here.

We have changed it with "atmospheric and hydrologic variables",

Line 270: replace "correlation" by "relation"? (could be non-linear)

We have changed "correlation" to "relation".

Figures:

Fig.2: I appreciate that the authors aim for as many information as possible in this plot but I am struggling to understand the colored dots in relation to the solid lines.

We have extended Fig 2. caption to explain that the solid lines are probability density functions of the normalised timeseries, which are shown as colored dots.

Fig.4: Could you also describe the symbols in Fig.4 c and d in the caption? Line 244 FWC

The "+" markers meaning - 1 standard deviation spread of the feature importance - has been added to Fig. 4 and Fig. 3 captions.

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