Baltic Sea Surface Temperature Analysis 2022: A Study of Marine Heatwaves and Overall High Seasonal Temperatures

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9 Abstract. In 2022, large parts of the Baltic Sea surface experienced the third-warmest to the warmest temperatures over the 10 summer and autumn months since 1997. Warm temperature anomalies can lead to marine heatwaves (MHWs), which are 11 discrete periods of anomalous high temperatures relative to the usual local conditions. Here, we describe the overall sea surface 12 temperature (SST) conditions observed in the Baltic Sea in 2022 and provide a spatio-temporal description of surface MHW 13 events based on remote sensing, model reanalyses and in-situ station data. The most MHWs, locally up to seven MHW events, 14 were detected in the western Baltic Sea and the Inner Danish Straits, where maximum MHW intensities reached values of up 15 to 4.6 °C above the climatological mean. The northern Baltic Proper and the Gulf of Bothnia were impacted mainly by two MHWs at maximum intensities of 7.3 °C and 9.6 °C, respectively. Our results also reveal that MHWs in the upper layer occur 16 17 at a different period than at the bottom layers and are likely driven by different mechanisms. Model data from two exemplary 18 stations, 'Lighthouse Kiel (LT Kiel)' and 'Northern Baltic', show a significant increase in MHW occurrences, of +0.73 MHW 19 events per decade at LT Kiel and of +0.64 MHW events per decade at Northern Baltic, between 1993 and 2022. Moreover, we 20 discuss the expected future increased occurrence of MHWs based on a statistical analysis at both locations.

21 **1 Introduction**

Global warming has led to an increase of ocean heat content (OHC) by about 350 ZJ in the upper 2000 meters from 1958 to 2019, with the year 2022 being the warmest on record as of this writing (Cheng et al., 2022; WMO, 2023). Simultaneously, marine heatwaves (MHWs), extreme events of high water temperature (Hobday et al., 2016), have increased in frequency, duration, spatial extent and intensity during the past four decades (Sun et al., 2023). In 2022, MHWs were recorded on 58 % of the ocean surface (WMO, 2023).

27 The Baltic Sea is one of the marine ecosystems with the fastest recorded warming of surface temperatures of 1.35 °C between

28 1982 and 2006, i.e., 0.54 °C per decade (Belkin, 2009). SST data operationally produced by the German Federal Maritime and

29 Hydrographic Agency (in the following BSH, product ref. no. 1 in Table 1) show a warming trend of 0.58 °C per decade for

the period 1990–2022. High SSTs can affect phytoplankton production, while unprecedented high temperatures in the subsurface layers of the sea could have even more devastating effects on the marine ecosystem (Kauppi et al., 2023). Conditions that facilitate the fast warming of the Baltic Sea are the limited exchange between surface and deeper layers due to a permanent halocline at a depth of 60–80 m (Väli et al., 2013) and the limited water exchange between the Baltic Sea and the open ocean through the narrow Skagerrak. That is why local air-sea heat exchange is the main physical factor for the surface layer water temperature and heat content in the Baltic Sea (Raudsepp et al., 2022).

36 Global mean air temperature in 2022 was among the six warmest in the 173-year instrumental record (WMO, 2023). For 37 Europe especially, the Copernicus Climate Change Service/ECMWF (2022a) states that the air temperatures in August 2022 38 were higher than the 1991–2020 average across most of the continent, especially in a band in Eastern Europe stretching from 39 the Barents and Kara seas to the Caucasus. In November 2022, air temperatures were higher than the 1991–2020 average, 40 especially over the west, south-east and far north of Europe, and were unusually mild over the northern European seas 41 (Copernicus Climate Change Service/ECMWF, 2022b). These large-scale weather patterns likely lead to high sea surface 42 temperatures (SST) in marginal seas like the Baltic Sea and are a likely driver of MHWs. This hypothesis is further supported 43 by a study by Holbrook et al. (2019), which found that MHWs at middle and high latitude regions were driven by large-scale 44 atmospheric pressure anomalies which cause anomalous ocean warming. Stalled atmospheric high-pressure systems coincide 45 with clear skies, warm air, and reduced wind speeds. These conditions then lead to quick warming of the upper ocean and 46 increased thermal stratification due to reduced vertical mixing.

47 So far, there generally have been only a few studies on MHWs in the Baltic Sea (Goebeler at al., 2022; She et al., 2020). In 48 this study, we show that remote sensing data revealed several SST anomalies over the entire Baltic Sea in 2022. We thus use 49 model reanalysis and in-situ station data to provide a spatio-temporal description of the corresponding MHWs. Both datasets 50 contain data collected over a long enough period to also provide its own respective climatology, thereby enabling a consistent 51 representation of MHWs. While the in-situ data provides accurate point-wise measurements of the temperature at selected 52 locations, the model reanalysis data allows for a widespread analysis of MHWs over the entire Baltic Sea, including their 53 extension into subsurface layers. Furthermore, we extend our study by providing a climatology of MHWs at two specific 54 mooring locations, namely at the Lighthouse Kiel (LT Kiel) and Northern Baltic stations. The overall aim of this study is to 55 highlight the areas of the Baltic Sea that were (most) affected by MHWs and determine whether surface MHWs can propagate 56 into deeper layers and thus potentially threaten the subsurface ecosystem. Furthermore, analyzing the climatology of MHWs 57 can provide insight into whether the global increase in MHWs can also be expected to occur on a local scale for the Baltic Sea.

58 2 Data and Methods

59 2.1 Satellite data

60 The satellite data service at the BSH compiles daily maps of SST data (product ref. no. 1 in Table 1). These have contributed for example to studies by the BACC Author Team (2008) and Gröger et al. (2022). The SST data are recorded as radiances by 61 62 the Advanced Very High Resolution Radiometer (AVHRR/3) in two thermal infrared channels aboard the NOAA-19 and 63 MetOp B satellites, providing a spatial resolution of 1.1 km, swath widths of 1,447 km and orbital periods of 100 minutes 64 (EUMETSAT, 2015; Minnett et al., 2019). The raw data of eight or nine daytime passes over the Baltic and North Sea are 65 received directly from EUMETSAT and processed using automated, standardized correction procedures (atmospheric correction, cloud masking, georeferencing etc.). Additionally, each flyover is corrected manually in order to preserve as much 66 67 data as possible whilst eliminating any faulty or cloudy pixels. All available single images from a calendar day are combined 68 and averaged, on a single pixel basis, into one daily-mean image. These daily images are then used to produce a weekly 69 analysis on an operational basis. While the BSH has been carrying out the processing of the satellite data itself on the 1.1 km 70 grid since 1990, operational SST analysis for the Baltic Sea did not start until the autumn of 1996. The analysis of the BSH 71 SST dataset presented in this chapter is therefore limited to the period from 1997–2022.

72 **2.2 Station data**

In-situ temperature time series from mooring stations located in the Baltic Sea are used for 1) model validation and 2) cross validation of the MHW computation from model data. Except for SST data from Northern Baltic (K. Hedi, FMI, pers. communication), the station data are obtained from product ref. no. 2 in Table 1. Each available dataset has already been quality controlled by the regional production units (In Situ TAC partners, 2022). The temporal resolution varies from hourly at the German stations to half-hourly at the stations in the northern Baltic Proper and Gulf of Finland. Due to failures, maintenance and other circumstances, no mooring station entirely covers the period from 1st Jan 1993 until now.

79 Of all available mooring stations, we selected those which contain data from 2022 and from at least ten additional years from 80 1993 until 2021 at least one depth. Out of the remaining seven mooring stations that contained surface temperature data, two 81 mooring stations were chosen for the cross validation of MHWs: Lighthouse Kiel (LT Kiel) and Northern Baltic (Fig. 1). Of 82 the observation data, LT Kiel has the greatest time coverage (1989 until the present, missing data: 9.1 % of days). This mooring 83 station lies in the far western part of the southern Baltic, and the water depth there is about 12 m. The station Northern Baltic 84 is located in the northern Baltic Proper. The SST observations there cover the period from 1997 until now (missing data: 8.0 % 85 of days). No mooring station provides a time series in deeper layers long or consistent enough to analyze subsurface MHWs, 86 thus reducing the scope of measurement-based analysis of MHWs to the surface layers.

87 2.3 Baltic Sea Physics Reanalysis Data

88 The Baltic Sea physics reanalysis product (product ref. no. 3 in Table 1) is a model dataset based on the ocean model NEMO 89 v4.0 (Gurvan et al., 2019). The model system assimilates satellite observations of SST (EU Copernicus Marine Service 90 Product, 2022b) and in-situ temperature and salinity profile observations from the ICES database (ICES Bottle and low-91 resolution CTD dataset, 2022). The product provides gridded information on SST and subsurface temperature conditions. The 92 spatial coverage is 1 nautical mile, i.e., approximately 1.8 km. The grid covers the entire Baltic Sea, including the transition 93 zone to the North Sea, with a vertical resolution of 56 non-equidistant depth levels. This multi-year product (MYP) covers the 94 reference period from 1993 up to 2022. The model setup is described in the Product User Manual (PUM, Ringgaard et al., 95 2023).

96 **2.4 Heat wave detection**

97 Marine heatwaves refer to a discrete period of unusually high seawater temperatures. While several definitions describe MHWs 98 quantitatively, the most commonly used method defines them as periods when temperatures exceed the 90th percentile of the 99 local climatology for five days or more (Hobday et al. 2016). We use open-source tools to detect MHWs (Oliver, 2016; Zhao 100 and Marin, 2019) in station and model data. The identified MHWs can be classified following Hobday et al. (2018), in which 101 the MHW category is based on the maximum intensity in multiples of threshold exceedances, i.e., the local difference between 102 the 90th percentile threshold and the climatology. If the threshold is exceeded less than 2 times, the MHW is classified as 103 moderate (Category I), at 2 to 3 times it is classified as strong (Category II), at 3 to 4 times it is classified as severe (Category 104 III), and at 4 or more times it is classified as extreme (Category IV).

Here, the occurrence of MHWs in the Baltic Sea in 2022 is analyzed based on the Baltic Sea MYP (product ref. no 3 in Table
1). The following statistical metrics of MHWs are computed at every third surface grid point of the MYP, resulting in a
resolution of approximately 5.4 km: cumulative intensity, mean intensity, duration of the longest heatwave, number of
heatwaves (frequency), maximum intensity and total days of MHW conditions.

Then, in order to evaluate the development of those MHW metrics over time, block averages (using a block length of one year) for each MHW metric are computed for both the observations (product ref. no 2 in Table 1) and the model data (product ref. no 3 in Table 1) at two stations: Lighthouse Kiel and Northern Baltic. The yearly MHW metrics from observations and the model are correlated for evaluation, and linear trends (95 % significance) are calculated for each of those metrics. Finally, the correlation of the annual MHW metrics to the annual mean temperature based on model data was assessed using a linear leastsquares regression and a two-sided t-test for significance.

All MHW assessments in the following sections use the period from 1993 to 2021 for the climatology, except for Sect. 3.2.1,

in which the comparison of the multi-year evolution of MHWs at Northern Baltic uses the overlapping period from 1997 to
2021 due to the lack of observations at this station before 1997.

118 2.5 Model validation

The MYP data has already been extensively validated in the corresponding Quality Information Document (QuID; Panteleit et al., 2023). In this document, the MYP data are validated within the time period from 1st January 1993 to 31st December 2018. The validation shows a negative bias at the surface with a shift towards more positive values at deeper levels. A variation of statistical values with depth is also clearly visible in the estimated accuracy number (EAN), which represents the root-mean square difference (RMSD) of a specific depth layer. The RMSD varies between 0.29 °C at 200–400 m over 0.63 °C at the surface to 1.3 °C at 5–30 m depth.

125 We additionally evaluated the model data in more detail using a clustering approach, which offers insights into the overall 126 accuracy of the model by grouping the errors. This clustering procedure employs the K-means algorithm (Raudsepp and 127 Maljutenko, 2022). In this evaluation, all available data within the model's domain and simulation period are considered. A 128 two-dimensional error space (dS, dT) is established using simultaneously measured temperature and salinity values as the 129 foundation for clustering. Here, $dS = (S_{mod} - S_{obs})$ and $dT = (T_{mod} - T_{obs})$ represent the differences between the model (S_{mod} and T_{mod}) 130 and observed (S_{obs} and T_{obs}) salinity and temperature, respectively. The dataset employed in this validation study was sourced 131 from the EMODNET dataset compiled by SMHI (product ref. no. 4 in Table 1). It consists of a total of 3,094,089 observations 132 aligning with the simulation period of the Baltic Sea physics reanalysis (product ref. no. 3 in Table 1) and covering the years 133 1993 to 2022. A comprehensive explanation of the k-means-method and detailed results describing the model's accuracy can 134 be found in Appendix A1. The results can be summarized as in that approximately 82 % of all validation points exhibit 135 relatively low temperature bias, STD, and RMSD (Table A1). The surface layer validation shows that less than 10 % of 136 comparison points have significant temperature errors (Figure A1c). Due to the low proportion of these validation points we 137 do not expect a significant impact on the determination of the surface MHWs and their statistics. Below the surface layer, i.e., 138 at depths ranging from 0.5-40 m, up to 25 % of the points correspond to clusters with temperature errors greater than +/-139 2.0 °C; in deeper layers, this percentage gets smaller again (Figure A1c). Consequently, we anticipate that the model reanalysis 140 data provide sufficiently accurate information for calculating subsurface MHWs and their statistics for the Baltic Sea as well. 141 The model is also validated in terms of how accurately it reproduces the MHWs of 2022 and how well it represents their 142 characteristics during the overlapping time periods of data availability at the two locations (1993–2022 for LT Kiel, and 1997– 143 2022 for Northern Baltic). For this, the model data was compared to the available station data (product ref. no 2 in Table 1 for 144 LT Kiel and K. Hedi, FMI, pers. communication for Northern Baltic) at these locations. Table 2 shows the Pearson correlation 145 coefficients for the MHW metrics in Fig 4 between observational and model data for the two stations, which show overall 146 good agreement between the model and the observation data with respect to MHW detection.

147 We also compared the annual temperature curves resulting from both the model and the station data at each location (Fig. A2).

148 Overall, the curves show the same progression. The temperature from the MYP is generally slightly lower, and consequently

this results in a slightly lower temperature climatology and threshold (here, the 90th percentile) on which MHW detection is

150 based. In general, though, the MHWs and their respective intensities and lengths are detected equally in both the station and

151 model data.

152 **3 Results**

153 **3.1 Sea surface temperature anomalies in satellite data**

In the summer of 2022, large parts of the Baltic Sea featured strong warm anomalies based on the BSH SST analysis (product ref. no. 1 in Table 1, Fig. 2). The highest values were up to 3 °C above the long-term mean (1997–2021) in the Bothnian Sea in June and in the Bothnian Bay in July. In August however, these areas were neutral or exhibited cold anomalies, while the Baltic Proper as well as the Gulf of Finland and the Gulf of Riga showed the warmest anomalies of +1.5 °C to 2.5 °C. At the beginning of autumn, the Baltic Sea is marked by a substantial east-to-west gradient of SST anomalies due to a series of upwelling events along its eastern shores. In November, the whole Baltic Sea features strong warm anomalies, again with peak values above +2 °C around Southern Sweden.

161 To provide some climatological context for the observed SST anomalies in a straightforward way, we also present maps 162 ranking the SST anomalies for the summer and autumn months of 2022 against the same months in previous years (right two 163 columns of Fig. 2). These anomaly rankings provide information on how extreme an anomaly of a given magnitude is. For 164 every grid point and for each calendar month, the monthly anomalies are ranked by magnitude. The warm anomalies over 165 large parts of the Baltic Sea during the summer and autumn of 2022 are among the warmest eight on record for the respective 166 months. In September, coastal upwelling led to cold anomalies along the eastern shores, but the other five months of the 167 summer and fall of 2022 (June, July and August as well as October and November) show large areas of the Baltic Sea with 168 warm anomalies that are among the four most pronounced on record. In August and November, we see several large areas 169 along the coastlines of the Baltic countries as well as off the Polish coast and around Gotland that according to the BSH SST 170 analysis dataset featured highest-ever surface temperatures.

171 **3.2 Marine heatwaves**

MHWs describe exceptionally warm temperature anomalies. As the monthly overview in Fig. 2 already provides an indication
of possible MHW conditions in 2022, the MHW metrics defined by Hobday et al. (2016) are assessed using the Baltic Sea
MYP (product ref. no. 3 in Table 1). Each region of the Baltic Sea experienced different MHW characteristics during 2022
(Fig. 3, Table 3).

The most MHWs during 2022 occurred in the Inner Danish Straits and the Western Baltic (Fig. 3d); mainly, four to five MHWs were detected, with some assessed locations experiencing up to seven MHWs and a maximum of 94 total days of MHW conditions (Fig. 3f). The mean and maximum intensities of all MHWs in the Western Baltic reached up to 3.8 °C and 4.6 °C,

179 respectively (Fig. 3b and 3e). The highest mean and maximum intensity values were reached in the northern Baltic Proper and

- 180 in the Bothnian Sea and Bothnian Bay (Fig. 3b and 3e), though these regions were affected mainly by only two MHWs. The
- 181 maximum intensity in the Bothnian Bay even reached 9.6 °C, the highest within the entire studied period from 1993 to 2022.
- 182 The longest MHW is found in the Baltic Proper (32 days), followed by the Bothnian Sea (31 days) and the Inner Danish Straits
- 183 (29 days) (Fig. 3c). The highest values of cumulative intensity (of a single MHW), with up to 119.3 days °C, are found in the
- 184 Kvarken, a strait between the Bothnian Sea and the Bothnian Bay (Fig. 3a).

185 **3.2.1 Multi-year evaluation of MHW metrics**

Next, we assess the frequency and other characteristics of the MHWs that occurred in 2022 in a climatological context based
on both observations and model data for the two stations, LT Kiel (based on the overlapping climatology period 1993–2021,
Fig. 4a–h) and Northern Baltic (based on the overlapping climatology period 1997–2021, Fig. 4 i–p). Overall, the results for
the yearly MHW metric calculation are well correlated between the observations and the model data (Table 2).

190 In 2022, a total of five MHWs (four in the MYP) occurred throughout the year at LT Kiel (Fig. A2a). Though none of them 191 was extraordinarily long or intense at LT Kiel, the time series of yearly MHW metrics shows that, based on observational data, 192 the number of MHW occurrences in 2022 was the second highest there since 1989 (Fig. 4a). The time series of MHW 193 frequencies per year suggests that the occurrence of MHW events has increased over the last three decades (Fig. 4a). The trend 194 computed from model data is +0.73 MHWs per decade for the period 1993–2022. The number of MHW events per year is 195 positively correlated (R=0.76) with the increasing annual mean SST at this mooring station (Fig. 4b). The maximum (Fig. 4c) 196 and cumulative intensities (Fig. 4e) of observed MHWs do not show a clear trend and are not correlated to the warming annual 197 mean temperatures (Fig. 4d and Fig. 4f). There is no significant trend in total MHW days (Fig. 4g) at LT Kiel, but a positive 198 correlation (R=0.71) with rising average temperatures (Fig. 4h).

199 For Northern Baltic, neither the station data nor the model data exhibits a statistically significant trend in MHW events for the 200 overlapping period (Fig. 4i). But when all of the available model data from 1993–2022 is taken into account, the trend in MHW 201 occurrences becomes significant at the 95 % level, with +0.64 MHWs per decade. Again, the number of events is positively 202 correlated with annual mean temperature (R=0.58, Fig. 4j). The highest maximum MHW intensities were recorded in recent 203 years (2016, 2018, 2021, 2022), with 2022 showing the highest intensity of any MHW, at 7.3 °C (model data) to 7.4 °C (station 204 data) above the climatologically expected temperature (Fig. 4k,l, see also Fig. A2b). The cumulative MHW intensities show 205 no clear trend or correlation with annual mean temperatures at this station (Fig. 4m,n). In terms of total MHW days, 2018 206 shows the highest numbers (Fig. 40), but otherwise no trend is detectable for this metric, though there is positive correlation 207 with annual mean temperatures (R=0.56, Fig. 4p).

208 **3.2.2 Analysis of vertical MHW distribution at Northern Baltic**

At Northern Baltic, which is about 103 m deep and located in the Western Baltic Proper, the surface temperature has been measured continuously over several decades. Unfortunately, no quality-controlled temperature measurements exist for the

- 211 lower layers at this station. The model validation shows that, at other locations, the model represents temperatures generally 212 well, both at the surface and in the lower layers. In order to obtain further insights into heat wave propagation towards the 213 seafloor, we analyzed the MYP model data (product ref. no. 3 in Table 1) along the entire water column.
- 214 A seasonal SST signal is clearly visible in Fig. 5a. In general, the temperature tends to decrease with depth while the bottom 215 temperature is relatively cold and uniform. In early summer (June), a so-called cold intermediate layer (CIL), defined as a 216 minimum of temperature between the thermocline and the perennial halocline (Chubarenko et al., 2017; Dutheil et al., 2022), 217 develops at a depth of 20–60 m and acts as a barrier between the surface and bottom water bodies. At Northern Baltic, the 218 upper boundary of the CIL coincides with the mixed layer depth (MLD), which is depicted in Fig. 5b-c. Starting from around 219 June, a layer of water with a significantly lower temperature than the climatological mean (up to -7 °C deviation) is found just 220 below the MLD (Fig. 5b), which suggests that the CIL was significantly colder at this time in 2022. This also coincides with 221 the onset of significantly higher temperatures at the surface compared to the climatological mean, though these were initially 222 not high enough to result in a MHW (Fig. 5e). The elevated temperatures start with a significant temperature jump of 5 °C 223 above the climatological mean, followed by abrupt and substantial decreases and increases in temperature over a short period. 224 This eventually leads to a MHW which lasts for 15 days starting from the end of June and which contains a one-day extreme 225 MHW (Category IV) event at a temperature of 7.4 °C above the climatological mean, followed by a severe MHW (Category 226 III) for another three days. Significantly high temperature deviations can also be observed at a depth of 10.8 m, i.e., at the 227 MLD, after July 2nd, just after the Category IV MHW at the surface. However, these temperature deviations did not result in 228 a MHW at this depth. Following the extreme heatwave event at the surface, a comparably weaker MHW can be detected in 229 mid-August at both 0.5 m (Fig. 5e) and 10.8 m (Fig. 5f). Thus, this weaker MHW penetrates past the MLD into slightly deeper 230 levels before reaching the comparably cold layer of water underneath.
- As shown in Fig. 5c and Fig. 5d, the intensity of the MHW tends to decrease as the depth increases. Four MHWs in regions close to the seafloor (i.e., below 60 m) were detected during specific periods from February to April, September to October, and in December. These MHWs are mostly moderate, with temperatures reaching up to 1.59 °C above the climatological mean. Only three days at the end of September can be classified as a Category II MHW in one specific depth-layer close to the seafloor. In the bottom-most depth-layer, the corresponding subsurface MHW is interrupted by five days of temperatures below the 90th percentile. However, as the temperatures are only slightly below the threshold and the MHW criteria are still met in the depth-layers above, one might still count this as one continuous MHW. Furthermore, Fig. 5c also shows isolated Category
- I MHWs at depths between 20 and 50 m.

239 4 Discussion and Conclusions

During August and November 2022, record-warm sea surface temperatures were observed in substantial areas of the Baltic Sea proper. Large parts of the Baltic Sea exhibited the third-warmest to the warmest temperatures in summer and autumn 242 months since 1997. Both periods, in August and November, coincided with atmospheric temperature anomalies. Over the 243 entire year of 2022, the distribution of quantity and intensity of MHWs within the Baltic Sea is twofold: up to seven individual 244 MHW occurrences were recorded as well as simulated in the south-western part of the Baltic Sea, and as a result this region 245 experienced the maximum number of total MHW days of anywhere in the Baltic Sea in 2022. In the northern Baltic Sea, the 246 number of MHWs was lower, with some locations registering only one MHW; remarkably, however, this one MHW led to the 247 highest mean and maximum MHW intensities in the Baltic Sea since the reanalysis started in 1993. In some areas in the 248 Bothnian Bay, the Baltic Sea MYP revealed temperatures that exceeded 9 °C above the 90th percentile of the climatologically 249 expected temperature values (Fig. 3d,e). This can be considered an extraordinarily high MHW intensity, since maximum SST 250 anomalies above 5 °C have only been observed in about 5 % of the global ocean, and MHW intensities normally peak at 2.5 °C 251 to 3.7 °C (Sen Gupta et al., 2020). In our case, the area in the Bothnian Bay experienced a short period with southerly winds 252 and air temperatures up to 28 °C at the end of June 2022 (SMHI, 2023), which led to a short, but very intense MHW in the 253 shallow areas of the Bay.

254 A significant increase in MHW occurrences is detectable over time at our two exemplary stations, of +0.73 MHW events per 255 decade at LT Kiel and +0.64 MHW events per decade at Northern Baltic. Both MHW frequency and the total number of MHW 256 days are statistically related to rising mean temperatures. This confirms that an increasing number of MHWs can be expected 257 in the future in the Baltic Sea, too, due to global warming (Frölicher et al., 2018; Oliver et al., 2019). The adverse impact of 258 MHWs on the ecosystem's various trophic levels has been widely documented (Smale et al., 2019; IPCC, 2022; Smith et al., 259 2023). The Baltic Sea, which has a relatively vulnerable ecosystem, could experience a significant negative impact from 260 MHWs (Kauppi and Villnäs, 2022; Kauppi et al., 2023), and the analysis of subsurface MHWs opens up further potential ways 261 to study their effects. At the Northern Baltic mooring station, MHWs were found at the surface, propagating into deeper layers 262 until reaching the CIL, and some were also detected close to the seafloor. Isolated MHWs were also observed at depths of 263 between 20 and 50 m. However, these are subject to higher uncertainty compared to the ones in the surface and bottom layers 264 due to a higher uncertainty in modeling variability in the pycnocline (QuID; Panteleit et al., 2023). Among the possible reasons 265 for the development of the four MHWs close to the seafloor at Northern Baltic could be vertical heat transport from the surface 266 or a lateral transport of warmer water due to bottom currents, for example. However, a more detailed evaluation would be 267 required to assess their precise cause.

Potential avenues for future studies include examining whether and how surface MHWs are able to propagate into the deeper water masses close to the halocline as well as examining the correlation between the strength (i.e., the classification category) of the MHW and its propagation into deeper water masses. At Northern Baltic, severe and extreme MHWs occurred at the surface when the CIL was particularly cold compared to the climatology. This therefore raises questions of whether a strong CIL might be linked to the development of MHWs at the surface and whether the one might even favor the development of the other. Additional studies could also focus on the positive feedback on the bottom temperature, as was observed in 2022. It might be interesting to determine if this phenomenon can also be found in other years and whether it is triggered by the superposition of either lateral currents or MHWs or of both together. Understanding the effects that potentially lead to the

vertical propagation of MHWs like those observed particularly in the late summer of 2022 will become increasingly crucial in

277 order to evaluate how the already-increasing occurrences of surface MHWs may affect the ecosystem in subsurface layers.

278 Appendix A1

We apply a clustering approach to evaluate the precision of the hydrodynamic model. This technique offers insights into the overall accuracy of the model by grouping the errors. The clustering procedure employs the K-means algorithm, a type of unsupervised machine learning (Jain, 2010). The original explanation of this technique can be found in a study by Raudsepp and Maljutenko (2022). In our evaluation, all available data within the model's domain and simulation period are considered, even if the observation data is unevenly distributed or occasionally sparse. This strategy enables us to assess the model's quality at each specific location and time instance at which measurements have been acquired.

285 Initially, a two-dimensional error space (dS, dT) was established using simultaneously-measured temperature and salinity 286 values as the foundation for clustering. Here, $dS = (S_{mod} - S_{obs})$ and $dT = (T_{mod} - T_{obs})$ represent the differences between the model 287 $(S_{mod} \text{ and } T_{mod})$ and observed $(S_{obs} \text{ and } T_{obs})$ salinity and temperature, respectively. The dataset employed in this validation 288 study was sourced from the EMODNET dataset compiled by SMHI (product ref. no. 4 in Table 1). It consists of a total of 289 3,094,089 observations aligning with the simulation period of the Baltic Sea physics reanalysis (product ref. no. 3 in Table 1) 290 and covering the years 1993 to 2022. For each observation, we extracted the nearest model values from the reanalysis dataset. 291 The next stage involves choosing the number of clusters, and for simplicity we opted in advance for five clusters. Subsequently, 292 the third step entails conducting K-means clustering on the two-dimensional errors. This clustering process is applied to the 293 normalized errors achieved through separate normalization for temperature and salinity errors using the corresponding standard 294 deviations. The K-means algorithm then identifies the centroids' positions within the error space for the predetermined number 295 of clusters. These centroids' locations signify the bias of the error set for each cluster. In the fourth step, statistical metrics for 296 non-normalized clustered errors are computed. Standard deviation (STD), root mean square deviation (RMSD) and the 297 correlation coefficient are examples of common statistics that can be calculated for the parameters associated with each cluster. 298 The fifth step involves examining the spatio-temporal distributions of errors associated with different clusters. During the 299 creation of the error space, we retained the coordinates of each error point (dS, dT)(x, y), allowing us to map the errors of each 300 cluster back onto the locations where the measurements were conducted. To achieve this, the model domain is partitioned into 301 horizontal grid cells (i, j) of 27x27 km² in size. Subsequently, the number of error points attributed to various clusters at each 302 grid cell (i, j) is tallied. The total number of error points linked to the grid cell (i, j) is the sum of points from each cluster. The 303 proportion of error points in each grid cell affiliated with cluster k is determined by the ratio of the number of error points of 304 cluster k to the total number of error points in each grid cell.

- 306 Figure A1 displays the results of the K-means clustering for non-normalized errors. Table S1 presents the corresponding 307 metrics. Within cluster k=5, the salinity and temperature values closely align with the observations, with a bias of dS=-308 0.40 g/kg and dT=-0.02 °C, respectively. This cluster encompasses 57 % of all data points. The points are distributed 309 throughout the Baltic Sea and the great majority of them exceed 0.5 (Figure A1b). Clusters k=3 and k=4 exhibit relatively even 310 spatial distributions across the Baltic Sea, accounting for 11 % and 8 % of the points, respectively. These clusters are 311 particularly noteworthy due to their relatively high temperature biases and variability, both of which are crucial for the 312 calculation of marine heatwaves. The clusters k=1 and k=2 represent points with low temperature but a high salinity error 313 (Table A1). Spatially, these points are predominantly located in the southwestern Baltic Sea (Figure A1b), which points to the 314 occasional underestimation or overestimation of the inflow/outflow salinity.
- 315 Collectively, approximately 82 % of all validation points exhibit relatively low temperature bias, STD and RMSD (Table A1).
- The surface-layer validation shows that less than 10 % of comparison points have significant temperature errors (Figure A1c).

317 Due to the low proportion of these validation points, we do not expect a significant impact on the determination of surface

- 318 MHWs and their statistics. Below the surface layer, i.e., at depths ranging from 0.5–40 m, up to 25 % of the points correspond
- to clusters k=3 and k=4 (Figure A1c). Consequently, we anticipate that the model reanalysis data provides sufficiently accurate
- 320 information for calculating subsurface MHWs and their statistics for the Baltic Sea.

321 Data availability

322 This study is based on public databases and the references are listed in Table 1.

323 Author contribution

324 The idea for and concept behind this chapter were formed by Anja Lindenthal, Claudia Hinrichs, Priidik Lagemaa, Helen E. 325 Morrison and Urmas Raudsepp. The data curation was done by Eefke M. van der Lee and Tim Kruschke for the data from 326 product ref. no. 1 in Table 1, by Claudia Hinrichs and Tabea R. Panteleit for the data from product ref. no. 2 in Table 1 and by 327 Simon Jandt-Scheelke and Tabea R. Panteleit for the data from product ref. no. 3 in Table 1. The formal analyses of the datasets 328 and the resulting investigations were performed by Anja Lindenthal, Claudia Hinrichs, Simon Jandt-Scheelke, Tim Kruschke 329 and Tabea R. Panteleit. The k-means model validation was performed by Urmas Raudsepp and Ilja Maljutenko. Claudia 330 Hinrichs, Simon Jandt-Scheelke, Ilja Maljutenko, Tim Kruschke and Tabea R. Panteleit were responsible for the visualization 331 of the data. Anja Lindenthal, Claudia Hinrichs, Simon Jandt-Scheelke, Tim Kruschke, Eefke M. van der Lee, Tabea R. Panteleit 332 and Urmas Raudsepp were involved in the original draft preparation. The final manuscript was reviewed and edited by Claudia 333 Hinrichs, Priidik Lagemaa, Helen E. Morrison and Urmas Raudsepp with contributions from all co-authors.

334 Competing interests

335 The authors declare that they have no conflict of interest.

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456 Tables

Table 1: Product Table

Product ref. no.	Product ID & type	Data access	Documentation
1	BSH Sea Surface Temperature (AVHRR/3); Satellite data	Upon request; overview and contact data via https://www.bsh.de/EN/TO PICS/Monitoring_systems/ Remote_sensing/remote_se nsing_node.html	https://www.bsh.de/DE/THEMEN/Beob achtungssysteme/Fernerkundung/ferner kundung_node.html
2	INSITU_GLO_PHYBGCWA V_DISCRETE_MYNRT_013_ 030; In-Situ Near-Real-Time Observations	EU Copernicus Marine Service Product (2022a)	Quality Information Document (QUID): Wehde et al. (2022) Product User Manual (PUM): In Situ TAC partners (2022)
3	BALTICSEA_MULTIYEAR_ PHY_003_011; Numerical models	EU Copernicus Marine Service Product (2023)	Quality Information Document (QUID): <u>Panteleit et al. (2023</u>) Product User Manual (PUM): <u>Ringgaard et al. (2023</u>)
4	EMODNET_CHEMISTRY_B altic_Sea_aggregated_ eutrophication_and_acidity_dat asets_1902-2017_v2018; Observations	SMHI (2019)	Buga et al. (2018), Giorgetti et al. (2020)

Table 2: Pearson correlation coefficients from linear regression between the MHW metrics computed from the station data and the model data at the stations Lighthouse Kiel and Northern Baltic.

Station	Station common climatology period		MHW max intensity	MHW cumulative intensity	total MHW days	
Lighthouse Kiel	1993-2021	0.82	0.88	0.66	0.93	
Northern Baltic	1997-2021	0.74	0.89	0.82	0.94	

464Table 3: Statistical MHW parameter values in various subregions of the Baltic Sea for 2022 based on the model data from the465Baltic Sea MYP (product ref. no. 3 in Table 1) using daily values of SST between 1st January 1993 and 31st December 2022. The466climatological period covers the years 1993 to 2021.

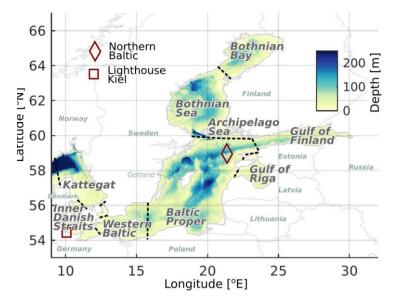
	Kattegat	Inner Danish Straits	Western Baltic	Baltic Proper	Gulf of Riga	Gulf of Finland	Archipe- lago Sea	Bothnian Sea	Bothnian Bay
Cumulative intensity of longest MHW / °C days	81.5	63.8	64	79.4	63	66.5	61.1	119.3	85.1
Mean intensity / °C	3.6	3.5	3.8	5.3	4.9	5.8	4.5	6.4	6.5
Duration of longest MHW / days	24	29	26	32	17	17	21	31	20
Number of MHWs (modal) per year	1-6 (3)	2-7 (4)	2-7 (5)	1-7 (3)	1-4 (3)	1-4 (2)	2-4 (3)	1-6 (2)	1-5 (2)
Maximum intensity / °C	4.5	4.2	4.6	7.3	5.9	6.8	5.1	8.6	9.6
Total days of MHW conditions / days	56	86	94	79	50	48	55	63	47

467

468Table A1: The share (%), bias, root-mean-square error (RMSE), standard deviation (SD), and correlation coefficient (Corr) for469each of the five clusters.

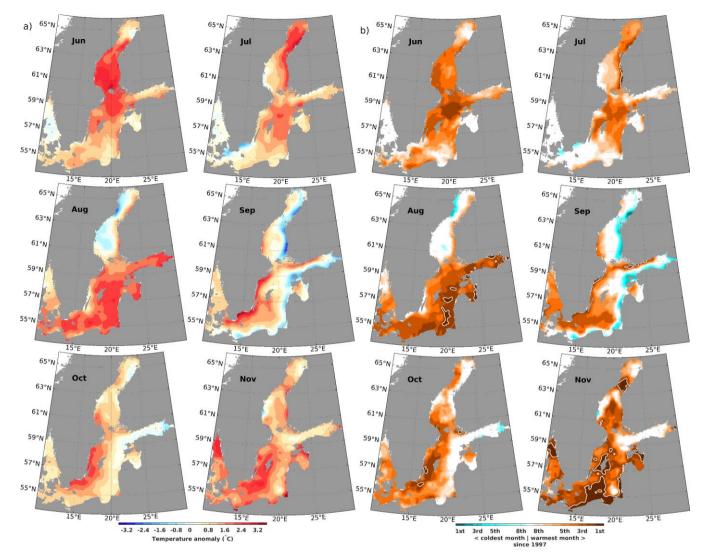
	Shares	Bias		SD		RMSE		Corr		
k	%	dS	dT	dS	dT	S	Т	S	Т	dSdT
		(g/kg)	(°C)	(g/kg)	(°C)	(g/kg)	(°C)			
1	18.6	-4.14	-0.26	1.80	0.85	4.51	0.89	0.90	0.78	-0.09
2	7.4	3.53	0.39	2.16	1.06	4.14	1.13	0.93	0.75	-0.11
3	10.5	-0.62	2.58	2.12	1.28	2.21	2.88	0.97	0.58	-0.06
4	6.3	0.27	-2.29	1.97	1.21	1.99	2.59	0.95	0.71	-0.14
5	57.2	-0.40	-0.02	0.83	0.54	0.92	0.54	0.99	0.89	0.07

471 Figures



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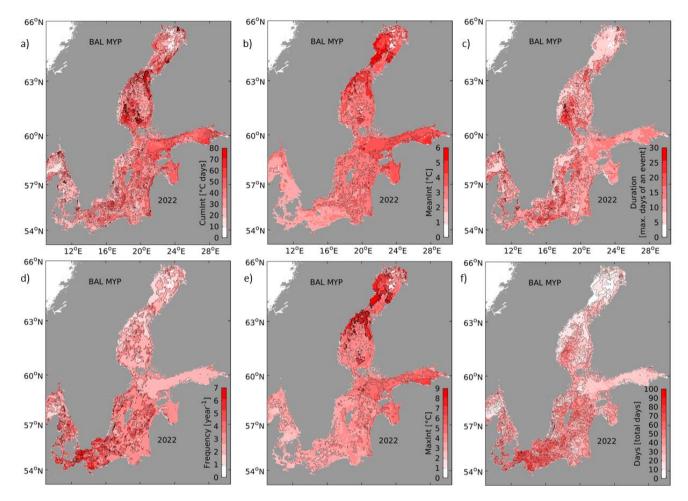
Figure 1: Map of the Baltic Sea with relevant locations mentioned in the study. Boundaries between subregions are marked with
 dashed lines.



476

 Figure 2: Anomalies (difference to climatology of 1997-2021) of SST for the Baltic Sea according to the BSH SST analysis (product ref. no 1 in Table 1) during the summer and autumn months in 2022 (a) and ranks of these SST anomalies (b) when compared to the full dataset starting in 1997. In (b), brownish (cyan) colors denote anomalies belonging to the warmest (coldest) eight anomalies

480 found since 1997. Record warm anomalies (rank 1) are highlighted by white contours.

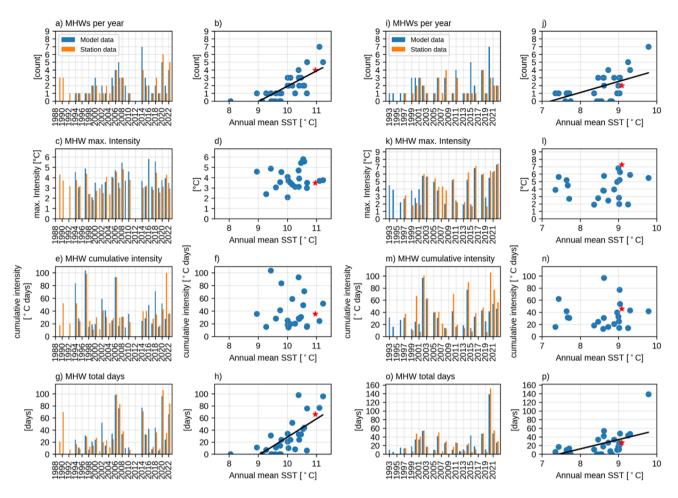


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Figure 3: Statistical metrics of MHWs in 2022 in the Baltic Sea based on SST data of the Baltic Sea MYP (product ref. no. 3 in Table 1) with the climatological period covering the years 1993 to 2021 - (a) cumulative intensity of the longest heatwave, (b) mean intensity, (c) duration of the longest heatwave, (d) number of heatwaves during 2022, (e) maximum intensity during the longest heatwave, (f) summed up days of all heatwave during 2022. The definition of these metrics follows <u>Hobday et al. (2016)</u>.

LT Kiel

Northern Baltic



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Figure 4: Comparison and time series of annual MHW metrics (a,i: MHW events; c,k: maximum intensity [°C]; e,m: cumulative intensity [°C days]; g,o: MHW days) for station data (orange bars) and model data (blue bars) at the stations LT Kiel (left) and Northern Baltic (right). The MHW metrics from the model are plotted against the annual mean SST at that station with the year

490 2022 marked in red. Statistically significant (95 %) correlations are indicated with a black line.

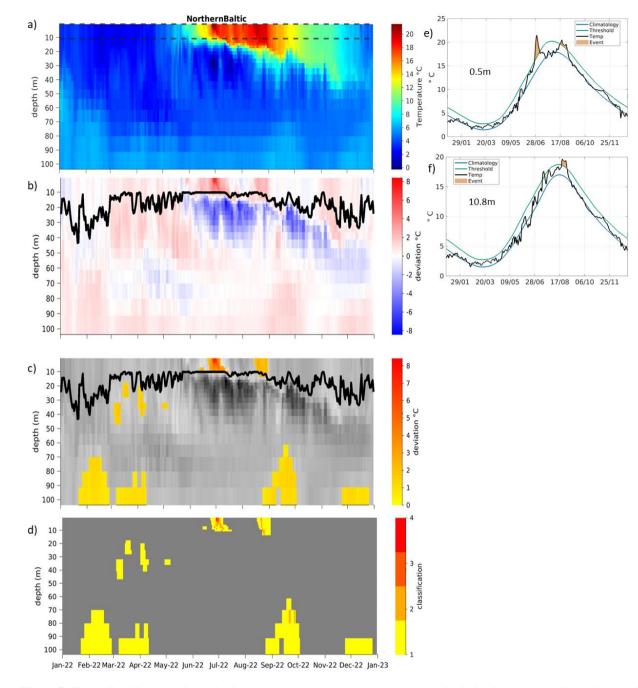
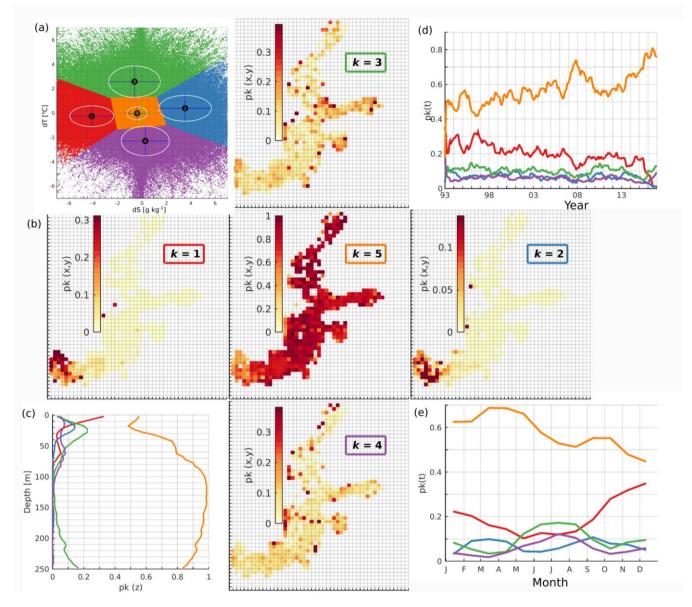
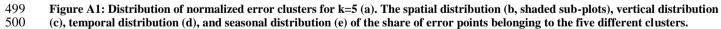


Figure 5: Hovmöller diagrams show absolute water temperature (a), temperature deviation between the climatology and the MYP data for 2022 (b) and MHWs (c) and their classifications (d, 1-moderate, 2-strong, 3-severe, 4-extreme) including the mixed layer depth as the thick black line (b and c) at Northern Baltic based on the Baltic Sea MYP (product ref. no. 3 in Table 1). The time series on the right (e-f) are located at the vertical positions marked as dashed lines in (a) and show temperature (black), climatology (blue), 90th percentile threshold for MHW analysis (green) and MHWs (red shading) based on model data at depths of 0.5 m (e) and 10.8 m (f). The period used for the climatology is 1993-2021.





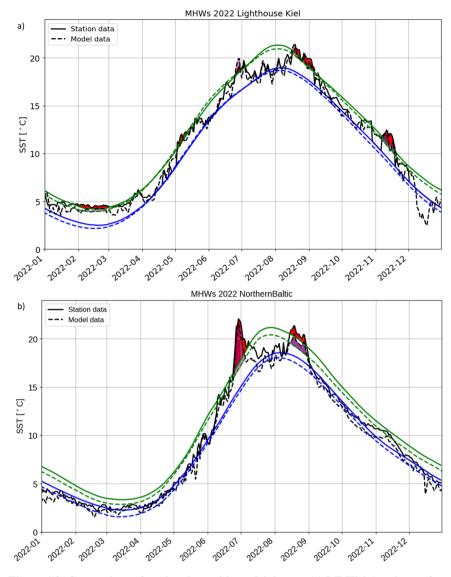


Figure A2: Comparison of station data with model data at (a) LT Kiel (product ref. no. 2 and 3 in Table 1), (b) Northern Baltic (K. Hedi, FMI, pers. communication and product ref. no. 3 in Table 1). The dashed lines correspond to the model, while the continuous lines correspond to the station data. In blue, the climatological mean is shown. The green lines show the 90th percentile threshold for MHW detection and the black lines are the respective 2022 temperature data. The purple (model data) and red (station data) marked areas show the detected MHWs in 2022. The reference period is 1993-2021 for LT Kiel (a) and 1997-2021 for Northern Baltic (b).