



# Data User Manual

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# Acronyms

*Table 1: Acronyms to be used within DUM.*

| | |
|---|---|
| ATBD | Algorithm theoretical basis documents |
| BEC | Barcelona Expert Center B |
| CMEMS | Copernicus Marine Monitoring and Forecasting Service |
| DUM | Data User Manual |
| ESA | European Space Agency |
| ITT | Invitation to tender |
| JPL | Jet Propulsion Laboratory |
| L2 | Level 2 |
| L3 | Level 3 |
| L4 | Level 4 |
| OA | Objective Analysis |
| OSTIA | Operational Sea Surface Temperature and Sea Ice Analysis |
| QC | Quality Control |
| QUID | Quality Information Document |
| RBD | Requirements baseline document |
| SMAP | Soil Moisture Active and Passive |
| SMOS | Soil Moisture and Ocean Salinity |
| SoW | Statement of work |
| SR | Scientific roadmap |
| SSS | Sea Surface Salinity |
| SST | Sea Surface Temperature |
| TB | Brightness Temperature |
| WP | Work package |

# 1 Introduction

## 1.1 Scope of this document

This document holds the Data User Manual (DUM) prepared by Baltic+ Salinity team, as part of the activities included in the [WP200] of the Proposal (Task 2 from SoW ref. EOP-SDR/SWO/086-17/DFP).

The objective of this document is to provide a detailed description of the dataset and the related metadata.

## 1.2 Structure of the document

The DUM is structured as follows:

Chapter 1 Covers the introduction of this document.

Chapter 2 Describes the datasets to be used within the Baltic+ Salinity project to generate the L3 and L4 SSS products.

Chapter 3 Describes the format of the datasets to be produced in the project.

# 2 Baltic+ Salinity Dataset

## 2.1 Satellite data

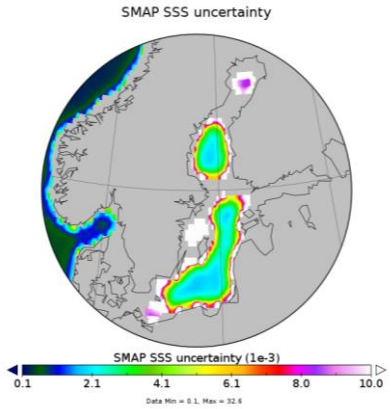
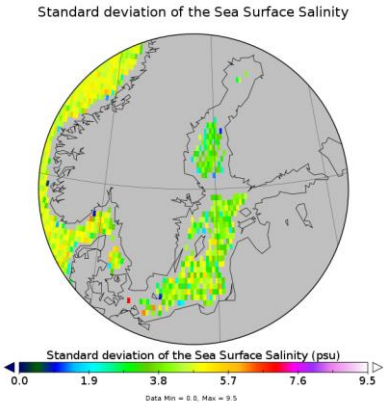
Three satellites have been designed and flown carrying an L-band radiometer, which allows measuring SSS: ESA SMOS (Soil Moisture and Ocean Salinity), NASA Aquarius and SMAP (Soil Moisture Active and Passive). Only SMOS and SMAP provide SSS data in the Baltic region. Several laboratories generate SMOS L3 SSS products and SMAP L3 SSS products, but not all of them provide data in the Baltic Sea due to several technical limitations and difficulties associated to the salinity retrieval in this area. In this project, we will use the products with better performances in terms of spatial coverage in the Baltic Sea [RBD, 2019], namely:

- Global SMAP L3 SSS product version 4.2 generated by the Jet Propulsion Laboratory (JPL) [SMAP JPL, 2019]. This dataset will be used as external reference to compare with the resulting Baltic+ SSS products developed during this project.
- Global SMOS L3 SSS product v1.0 [Olmedo et al. 2017] [BEC, 2017] generated by the Barcelona Expert Center (BEC). This is a global product that needs specific validation in the Baltic Sea. Some limitations in this product are expected in the Baltic Sea due to specific processing issues particularly important over this region, such as residual land-sea and ice-sea contaminations; radio frequency interference effects; and the lower sensitivity of TB to SSS due to cold waters. Methodologies aimed at addressing these issues are refined for the Baltic region in this project. The global SMOS BEC product will be used as a reference to compare with the new products to be generated in Baltic+.

The specifications of these products are described in Table 2.

*Table 2: Specifications of the satellite products to be used in the comparison of the Baltic+ SSS products.*

| Product | SMAP JPL SSS | SMOS BEC global SSS |
|---|---|---|
| Short description | L3 binned product. | Two products are available:<br>L3 containing objectively analysed SMOS salinity fields, L4 with a higher spatio-temporal resolution salinity field computed by merging SMOS L3 salinity and high-resolution Sea Surface Temperature from OSTIA. |
| Accessible at: | ftp://sealion.jpl.nasa.gov/pub/outgoing/smap/v4.2/L3/ | http://bec.icm.csic.es/ocean-experimental-dataset-global/ |
| Format file | netCDF | netCDF |
| Temporal resolution | 8 days, generated daily | 9 days, generated daily (L3);<br>daily (L4) |
| Spatial resolution | 0.25° x 0.25° | 0.25° x 0.25° (L3);<br>0.05° x 0.05° (L4) |

| | | |
|---|---|---|
| Temporal coverage | From 2015-04-04 to present | 2011-2016 |
| Spatial coverage | Global | Global |
| Uncertainty estimation |  <br>In the most part of the basin the uncertainty is ~2 psu but it largely increases close to coasts/ice edges. |  <br>No uncertainty information is provided in this product. However, information about the standard deviation of the set of L2 SSS used for the generation of the OA field is provided. This value is approximately 5 psu in the full region. |
| Variables provided | `smap_sss`: SMAP sea surface salinity | **L3 product:** |
| | `anc_sss`: HYCOM sea surface salinity | `WGS84`: grid mapping name |
| | `anc_sst`: sea surface temperature | `oa_sss`: objectively analysed sea surface salinity |
| | `smap_spd`: SMAP 10m wind speed | `std_sss`: standard deviation of the L2 sea surface salinity of each grid point |
| | `smap_high_spd`: SMAP 10m wind speed (using ancillary SSS) | `totalmeasures`: Total number of L2 measurements of each SMOS grid point |
| | `weight`: Sum of Gaussian weighting factors | `usedmeasures`: Number of measures used for the computation of the objectively analysed salinity value |
| | `land_fraction`: Average of land fraction | `uncorrected_binned`: intermediate SSS data obtained during the non-Bayesian retrieval. |
| | `ice_concentration`: ice concentration | **L4 product:** |

| | | |
|---|---|---|
| | `smap_sss_uncertainty`: SMAP SSS uncertainty | `l4_sss`**:** Sea Surface Salinity analysis using Data fusion of SST. |
| | | `quality_flag`**:** When the flag is equal to 1 the corresponding value of salinity has been extrapolated. |

## 2.2 In situ dataset for validation

All the available in-situ observations, including both historical datasets (i.e. already publicly datasets like Argo) and new datasets to be made available through established scientific networks between the Baltic+ team and other research groups external to the project (see section 4.1 in [RBD, 2019]) are collected and distributed via FTP hosted by BEC. The project website will contain a brief description of the datasets included in this document.

### 2.2.1 Monitoring data

There are two datasets, partly overlapping, that form the basis for climatological analyses of the conditions in the Baltic Sea: the HELCOM dataset, available at

https://ocean.ices.dk/Helcom/Helcom.aspx?Mode=1

and SeaDataNet v2 Baltic Sea dataset. The SeaDataNet has produced climatologies on the basis of earlier dataset version V1 (these are available at

https://www.seadatanet.org/Products#/search?from=1&to=20).

From most of the monitoring stations there are data from 1-5 times a year, but some stations are monitored more frequently (Figure 1, next page).

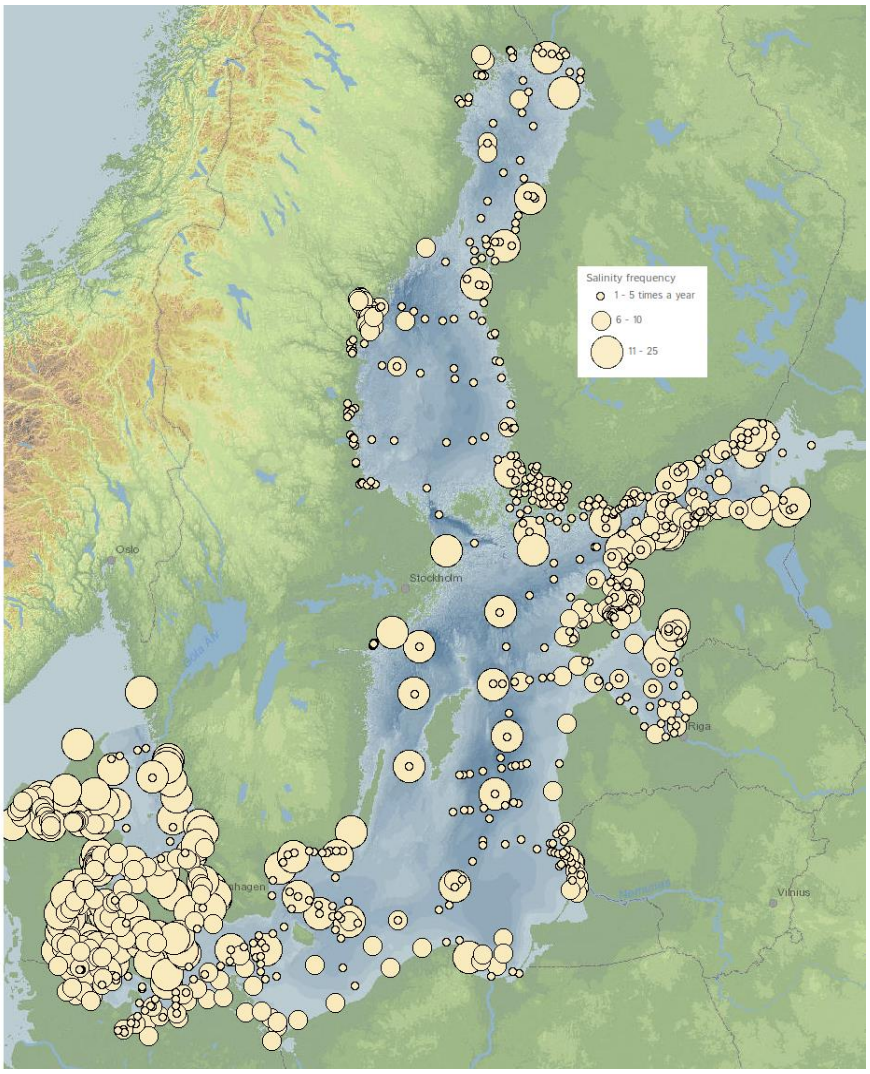



*Figure 1: Frequency of measurements (per year) in the Baltic Sea monitoring stations according to HELCOM. Caption from HELCOM Map and Data Service.*

### 2.2.2 Argo float data

Argo data for the Baltic Sea is available from the Coriolis data portal according to the WMO numbers. There is Argo data available since 2012 and presently there are Argo floats in several Baltic Sea basins: Gotland Deep, Bothnian Sea, Bothnian Bay and Bornholm deep. The Argo data includes TS-profiles and for some floats also Oxygen and biogeochemical parameters are available. Due to the sensor design, the Argo floats measurements are from 4 m downwards . A near-real-time quality control is performed for the Argo data in Coriolis. The NRT QC for the Baltic Sea includes consistency checks for example for time-stamps and locations. In [Siiriä et al. 2018] it has been shown that most of the Baltic Sea Argo data has good quality, but there are some erroneous profiles and the dataset needs to be handled with care, when using it in validation.

The WMO numbers of the Baltic Sea floats and the periods for which the data are available are presented in Table 3, where floats with WMO number beginning with 69 are operated by Finland and those that begin with 39 are operated by Poland, except the 6902036 which is also operated by Poland.

*Table 3: Argo floats: location in the basin and temporal coverage.*

| WMO | Basin | Mission time span |
|---|---|---|
| 6901901 | Bothnian Sea | 17.05.2012 - 05.12.2012 |
| 6902013 | Bothnian Sea | 13.06.2013 - 02.10.2013 |
| 6902017 | Bothnian Sea | 30.05.2014 - 24.10.2015 |
| 6902018 | Bothnian Sea | 30.04.2014 - 13.11.2014 |
| 6902021 | Bothnian Sea | 23.09.2015 - 13.05.2016 |
| 6902022 | Bothnian Sea | 13.05.2016 - 11.10.2016 |
| 6902023 | Bothnian Sea | 13.07.2016 - 25.01.2018 |
| 6902025 | Bothnian Sea | 09.05.2017 - 02.10.2018 |
| 6902028 | Bothnian Sea | 07.08.2017 - 04.09.2018 |
| 6902029 | Bothnian Sea | 06.08.2017 - 27.10.2017 |
| 6902030 | Bothnian Sea | 10.07.2018 - present |
| 6902026 | Bothnian Bay | 06.06.2017 - present |
| 6902014 | Gotland Deep | 14.08.2013 - 21.08.2014 |
| 6902019 | Gotland Deep | 21.08.2014 - 05.08.2015 |
| 6902020 | Gotland Deep | 05.08.2015 - 03.08.2016 |
| 6902027 | Gotland Deep | 15.06.2017 - 15.10.2018 |
| 6903697 | Gotland Deep | 15.10.2018 - present |
| 6902036 | Bornholm Deep | 29.11.2016 - 01.02.2017 |
| 3902100 | Bornholm Deep | 15.03.2017 - 07.01.2018 |
| 3901940 | Bornholm Deep | 20.09.2017 - 04.10.2017 |
| 3901941 | Bornholm Deep | 21.09.2017 - 21.02.2019 |
| 3902133 | Bornholm Deep | 06.11.2017 - present |
| 3902101 | Bornholm Deep | 06.02.2018 - present |
| 3902104 | Bornholm Deep | 01.06.2018-10.09.2018 |
| 3902106 | Bornholm Deep | 11.9.2018 - present |

### 2.2.3 Ferrybox data

FerryBox systems measure data from the near-surface layer from designated ship routes. Presently, there are seven FerryBox lines in the Baltic Sea. Data is available for example through the Copernicus Marine Monitoring and Forecasting Service (CMEMS) service (marine.copernicus.eu). Some data is also available from https://www.ferrybox.org/ and part of the data is available upon request from the originator.

The Quality Control (QC) methods used are presented in the CMEMS IN-SITU Quality Information Document:

http://marine.copernicus.eu/documents/QUID/CMEMS-INS-QUID-013-030-036.pdf.

The estimated accuracy numbers for the Ferrybox salinity data given in the QUID are 0.003-0.2 psu, depending on the sensor type. The dataset includes the following quality flags for the data: 0 = unclassified, 1 = good data, 4 = bad data and 9 = missing data. More detailed information about the Baltic Sea Ferrybox-lines, from which data is available in the CMEMS is given in Table 4. Shorter FerryBox lines like those from Estonia to Sweden and from Finland to Sweden have daily transects. The longer routes take more time and are twice a week.

*Table 4: Ferrybox-lines spatial and temporal coverages.*

| Vessel | Route | Observed parameters | Period available in CMEMS |
|---|---|---|---|
| Baltic Queen | Tallinn - Stockholm | T, S, Chl-a, turb, (pCO2); nutrients, Chl-a, phytoplankton (weekly sampling in spring-summer) | 2015 - 2019 |
| Romantica | Tallinn - Stockholm | T, S, O2, Co2 | October 2016 |
| Victoria | Tallinn - Mariehamn - Stockholm | T, S, Trb, Chl-a, CDOM | 2015 -2016 |
| Finmaid | Helsinki - Travemunde - Helsinki - Gdynia | T, S, Chl-a, nutrients, Phycocyan, CDOM, TURB, nutrients, phytoplankton | 1992 - 2019 |
| Tavastland (old TransPaper) | Gothenburg - Kemi - Oulu - Lübeck - Gothenburg | T, S, Trb, Chl-a-fluorescence, Phycocyan-fluorescence, CDOM-fluorescence, DO, PAR, airPress, airTemp, pH, pCO2 and CO2 in air, RC (phytoplankton, salinity, chl a, CDOM). | 2009 - 2018 |

| | | | |
|---|---|---|---|
| Silja Serenade | Helsinki - Stockholm | T, S, Chl-a, Turb, Phycocyan, nutrients, phytoplankton | 2010, 2014-2018 |
| Tallinn - Helsinki | Tallinn - Helsinki | T, S, fluorescence | 2009 - 2019 available upon request |

Data from ships of opportunity is also available from the Global Ocean Surface Underway Data (GOSUD) Project:

http://www.gosud.org/Data-access/Web-access.

GOSUD is an Intergovernmental Oceanographic Commission (IOC) programme that is designed as an end to end system for data collected by ships as they traverse their ocean tracks. FerryBox data from the Baltic Sea are included there, too.

### 2.2.4 Moored stations

Data from moored stations can also be used in validation. Data from Huvudskär Ost and Arkona stations are available through the CMEMS service (marine.copernicus.eu). Most recent salinity data from Utö station is available at http://swell.fmi.fi/Uto and older data is provided by FMI upon request.

## 2.3 Model dataset

CMEMS provides two model products for Baltic Sea: the Baltic Sea physics analysis and forecast and the Baltic Sea physics reanalysis. Both products provide SSS as daily mean values. The analysis and forecast product are updated two times a day, providing 5-day forecast and best-estimated time series for the past two years. The reanalysis product provides data from 1993 to 2016. The reanalysis is updated every year. The specifications of these products are collected in Table 5. These models are going to be used as a reference in the assessment of the seasonal and inter-annual SSS variability in the Baltic Sea.

*Table 5: Specifications of the two models over the Baltic Sea available in CMEMS.*

| Model dataset | CMEMS Baltic Sea physics analysis and forecast (BALTICSEA_ANALYSIS_FORECAST_PHY_003_006) | CMEMS Baltic Sea physics reanalysis (BALTICSEA_REANALYSIS_PHY_003_011) |
|---|---|---|
| **Short description** | The Baltic Sea physical model product provides forecasts for the physical conditions in the Baltic Sea. It is updated twice daily providing a new two days forecast. In addition to forecast, best-estimated theme series are given for the past two years the product is based on the 3D ocean model code HBM developed within the Baltic ocean community. | The Baltic Sea Physical Reanalysis product provides a 24 years physical reanalysis for the Baltic Sea (1993-2016) using the ice-ocean model NEMO-Nordic (based on NEMO-3.6, Nucleus for European Modelling of the Ocean) together with LSEIK data assimilation. |

| | | |
|---|---|---|
| | | |
| **Accessible at:** | marine.copernicus.eu | marine.copernicus.eu |
| **Format file** | netCDF | netCDF |
| **Temporal resolution** | Hourly values and daily mean values | Hourly values for sea surface height, ice concentration and total ice thickness. Daily and monthly mean values for salinity, temperature, horizontal current components, mixed layer depth, bottom salinity and bottom temperature. |
| **Spatial resolution** | 2km x 2km | 4km x 4km |
| **Vertical resolution** | from -400 to 0 (25 levels) | from -700.00 to 0.0 (56 levels) |
| **Temporal coverage** | From 2017-03-01 to present | 1993-2016 |
| **Spatial coverage** | Baltic Sea | Baltic Sea |

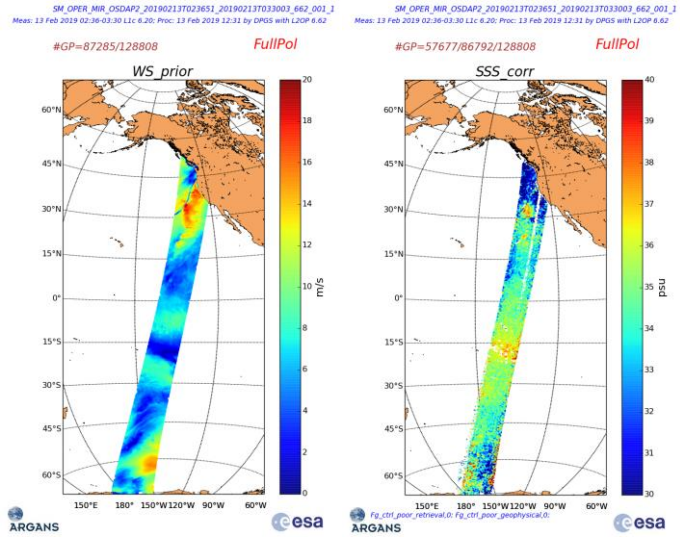
| | | |
|---|---|---|
| **Quality** | Quality of the product is evaluated against measurements. Information available in the Quality Information Document<br>http://marine.copernicus.eu/documents/QUID/CMEMS-BAL-QUID-003-006.pdf | Quality of the product evaluated against measurements. Information available in the Quality Information Document<br>http://marine.copernicus.eu/documents/QUID/CMEMS-BAL-QUID-003-011.pdf |
| **Variables provided** | sea_water_potential_temperature (T) | sea_water_potential_temperature (T) |
| | sea_water_potential_temperature_at_sea_floor (bottomT) | sea_water_potential_temperature_at_sea_floor (bottomT) |
| | sea_water_salinity (S) | sea_water_potential_temperature_at_sea_floor (bottomT) |
| | sea_surface_height_above_sea_level (SSH) | sea_surface_height_above_sea_level (SSH) |
| | eastward_sea_water_velocity (3DUV) | eastward_sea_water_velocity (3DUV) |
| | northward_sea_water_velocity (3DUV) | northward_sea_water_velocity (3DUV) |
| | ocean_mixed_layer_thickness_defined_by_sigma_theta (MLD) | ocean_mixed_layer_thickness_defined_by_sigma_theta (MLD) |
| | sea_ice_area_fraction (SIC) | sea_ice_area_fraction (SIC) |
| | sea_ice_thickness (SIT) | sea_ice_thickness (SIT) |

## 2.4 Auxiliary dataset

### 2.4.1 Dataset used for the SMOS SSS retrieval

The geophysical parameters required for the SSS retrieval in the official Level 2 Ocean Salinity (L2OS) processor are provided by the European Centre for Medium range Weather Forecast (ECMWF) [Sabater and De Rosney, 2010]. For each SMOS half-orbit an auxiliary file co-located in time and space with SMOS data is generated by ECMWF and distributed by the European Space Agency. We will use the same files to retrieve the salinity fields in the Baltic Sea. The specifications of this product are described in Table 6.

*Table 6: Specifications of the two models over the Baltic Sea available in CMEMS.*

| **Product** | ECMWF data |
|---|---|
| **Short description** | ECMWF data on the ISEA 4H9 DGG corresponding to SMOS half-orbit. |
| **Accessible at:** | Provided by ESA |
| **Format file** | The product provides a Header file (HDR) with general information of data and a binary file (DBL) which contains the actual data values. |
| **Temporal resolution** | Interpolated at the SMOS overpasses times |
| **Spatial resolution** | Interpolated to the same grid used for the SMOS L1C product (ISEA 4H9 DGG) |
| **Temporal coverage** | SMOS full mission period (From 2010-01-04 to present) |
| **Spatial coverage** | Each file has the same spatial coverage than the SMOS satellite overpass<br>  <br><br>*Example of the wind speed provided by ECMWF and the retrieved SMOS SSS L2 product corresponding to the same overpass.* |
| **Uncertainty estimation** | The header file contains a flag to assess the quality of the product based on the flags defined in the binary part (overall_quality) |

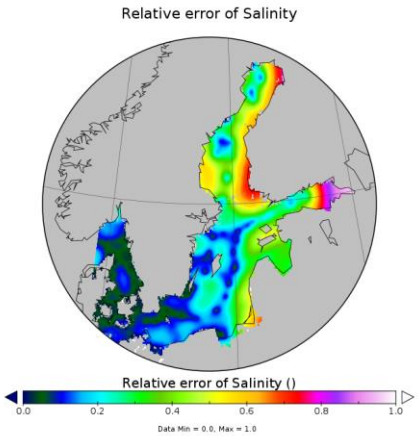
| | |
|---|---|
| **Variables provided in header file** | `Overall_quality`: Flag to assess the quality of the ADF based on the flag defined in the binary part. |
| | `Start_Lat`: Latitude of northernmost DGG grid point used in the generation (positive North) |
| | `Start_Long`: Longitude of westernmost DGG grid point used in the generation (positive East of Greenwich (-180,+180]) |
| | `Stop_Lat`: Latitude of southernmost DGG grid point used in the generation (positive North) |
| | `Stop_Long`: Longitude of easternmost DGG grid point used in the generation (positive East of Greenwich (-180,+180]) |
| | `Mid_Lat`: Latitude of DGG grid point in the middle (rounded down) of the list used in the generation of the product |
| | `Mid_Lon`: Longitude of DGG grid point in the middle (rounded down) of the list used in the generation of the product |
| **Variables provided in the binary file used for the L2 SSS retrieval** | `Grid_Point_ID`: Unique identifier of Earth fixed grid |
| | `Latitude`: Latitude of the DGG node. Range: [-90-90] |
| | `Longitude`: Longitude of the DGG node. Range: [0-360] |
| | `Sea_Ice_Cover`: Sea Ice cover. This parameter is defined both over land and sea. |
| | `Sea_Surface_Temperature`: Temperature of the water surface. This parameter has meaningful value only over sea. |
| | `Rain_Rate`:This parameter is defined both over land and sea. |
| | `Wind_10m_Wave_Model`: Wave model 10 metre wind speed. This parameter has meaningful value only over sea |
| | `Neutral_Equivalent_Wind_Zonal_10m`: 10 meters neutral equivalent wind –zonal component. This parameter is defined both over land and sea. |
| | `Neutral_Equivalent_Wind_Meridional_10m`: 10 metre neutral equivalent wind –meridional component. This parameter is defined both over land and sea. |
| | `Significant_Wave_Height`: Significant height of wind waves. This parameter has meaningful value only over sea |

| | |
|---|---|
| | `Air_Temperature_2m`: 2 meters air temperature. This parameter is defined both over land and sea. |
| | `Surface_Pressure`: Surface Pressure. |
| | `Total_Column_Water_Vapor`: Vertically integrated total water vapour. This parameter is defined both over land and sea. |

### 2.4.2 Dataset used for the generation of the SMOS SSS L3 product

For the generation of the absolute values of salinity from the debiased SSS anomalies we are using a regional climatology as annual reference field of SSS. This regional climatology is distributed by SeaDataNet and it provides temperature and salinity monthly climatologies computed from historical dataset (1900-2012 data by DIVA software v4.6.10) [Baltic Climatology, 2015]. The specifications of this product are described in Table 7.

*Table 7: Description of the regional climatology to be used in the generation of the Baltic+ L3 SSS product.*

| **Product** | DIVA 4D analysis of Salinity from year 1900 to year 2012 |
|---|---|
| **Short description** | Data from SeaDataNet, mainly from CTD and discrete water samplers, region The Baltic Sea. Climatology computed from historical dataset (1900-2012). Weighting have been used with length of 0.5° and 2 days. |
| **Accessible at:** | ftp://ftp2.ifremer.fr/public/seadatanet-baltic_sea-temperaturesalinity_climatologie/SDN_2015-11_TS_Baltic_Sea_Climatology_v1.1.zip |
| **Format file** | netCDF |
| **Temporal resolution** | Monthly climatology |
| **Spatial resolution** | 0.11° longitude x 0.065° latitude |
| **Temporal coverage** | Climatology computed with historical data 1900-2012 |
| **Spatial coverage** | Longitude: [ 9 : 30.89 ]° E  Latitude [ 53 : 65.935 ]° N |
| **Uncertainty estimation** | There are two parameters to describe the salinity error: the error standard deviation of salinity and relative error of salinity. The last one is used to mask poor quality salinity fields in the file. Two different masks are proposed, salinity values with relative error greater than 0.3; and salinity values with relative error greater than 0.5.   |

| | |
|---|---|
| **Variables provided in netcdf file** | `Salinity`: Salinity |
| | `Salinity_err`: Error standard deviation of salinity |
| | `Salinity_relerr`: Relative error of Salinity |

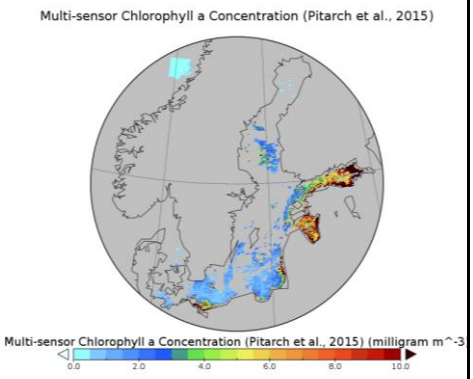
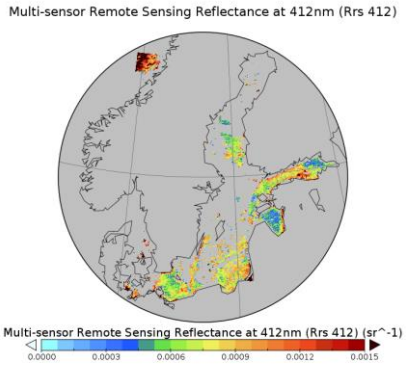
### 2.4.3 Dataset used for the generation of the SSS L4 product

Sea Surface Temperature daily maps from the Operational Sea Surface Temperature and Sea Ice Analysis (OSTIA) is used for the generation of the L4 product. The effective spatial resolution of OSTIA SST fields could be degraded because of the presence of clouds in this region. We will also explore the possibility of using Surface Chlorophyll concentration and multi-sensor remotely sensed reflectance for the generation of the L4 SSS product. More detailed information about SST product can be found in Table 8 and about chlorophyll product in Table 9.

*Table 8: OSTIA SST product to be tested in the development of the Baltic+ L4 SSS product.*

| **Product** | **SST_GLO_SST_L4_NRT_OBSERVATIONS_010_001** |
|---|---|
| **Short description** | For the Global Ocean- The OSTIA global Sea Surface Temperature Reanalysis product provides daily gap-free maps of:<br>Foundation SST (referred to as an L4 product) at 0.05°x 0.05° horizontal resolution, using in-situ and satellite data from infra-red radiometers.<br>SST anomaly from the Pathfinder climatology at 0.25° x 0.25° horizontal resolution. This product provides the foundation SST, which is the temperature free of diurnal variability. |
| **Accessible at:** | http://marine.copernicus.eu/services-portfolio/access-to-products/?option=com_csw&view=details&product_id=SST_GLO_SST_L4_REP_OBSERVATIONS_010_011 |
| **Format file** | netCDF |
| **Temporal resolution** | daily-mean |
| **Spatial resolution** | 0.05° x 0.05° |
| **Temporal coverage** | from 2007-01-01 to present |
| **Spatial coverage** | Global: Longitude [-180 : 180 ]°  E, Latitude [-90 : 90 ]°  N |
| **Uncertainty estimation** | An estimation of the error standard deviation of the SST field is provided |
| **Variables provided** | `analysis_error`: estimated error standard deviation of analysed_sst |
| | `sea_ice_fraction`: sea ice area fraction |
| | `analysed_sst`: analysed sea surface temperature |
| | `mask`: land/open ocean/sea ice/lake mask |

*Table 9: Chlorophyll and reflectance products to be used in the development of the Baltic+ L4 SSS product.*

| **Product** | **OCEANCOLOUR_BAL_CHL_L3_REP_OBSERVATIONS_009_080** | **OCEANCOLOUR_BAL_OPTICS_L3_REP_OBSERVATIONS_009_097** |
|---|---|---|
| **Short description** | The Global Ocean Satellite monitoring and marine ecosystem study group (GOS) of the Italian National Research Council (CNR), in Rome distributes surface chlorophyll concentration (mg m-3, 1 km resolution) estimated via the BalAlg algorithm (Pitarch et al., 2016) applied over the Rrs spectra provided by the Plymouth Marine Laboratory using an ad-hoc configuration of the ESA-CCI processor for CMEMS.<br>  | The Global Ocean Satellite monitoring and marine ecosystem study group (GOS) of the Italian National Research Council (CNR), in Rome operationally distributes the Remote Sensing Reflectance (Rrs) and the diffuse attenuation coefficient of light at 490 nm (kd490) data, computed with the ESA-CCI technique for Copernicus at 1 Km resolution.<br>  |
| **Accessible at:** | http://marine.copernicus.eu/services-portfolio/access-to-products/?option=com_csw&view=details&product_id=OCEANCOLOUR_BAL_CHL_L3_REP_OBSERVATIONS_009_080 | http://marine.copernicus.eu/services-portfolio/access-to-products/?option=com_csw&view=details&product_id=OCEANCOLOUR_BAL_OPTICS_L3_REP_OBSERVATIONS_009_097 |
| **Format file** | netCDF | netCDF |
| **Temporal resolution** | daily-mean | daily-mean |
| **Spatial resolution** | 1km x 1km | 1km x 1km |
| **Temporal coverage** | from 1997-09-04 to 2017-12-19 | 1997-09-04 to 2017-12-19 |
| **Spatial coverage** | Baltic Sea: Longitude: [9.25:30.25] E Latitude [53.25:65.85]° N | Baltic Sea: Longitude: [9.25:30.25]° E Latitude [53.25:65.85]° N |

| | | |
|---|---|---|
| **Uncertainty estimation** | Not provided | Not provided |
| **Variables provided** | `CHL`: Multi-sensor Chlorophyll a-Concentration | `RRS412`: Multi-sensor Remote Sensing Reflectance at 412 nm (Rrs_412) |

# 3 Format of the Dataset produced by the project

All the associated data, SSS products and in-situ measurements will be distributed in netCDF-4 format following the Climate and Forecast (CF) Metadata conventions (at least v1.6). Compression will be applied for variables stored in netCDF files and time dimension will be defined as a record dimension.

The format of the generated Baltic+ SSS products will also be complaint with the ESA CCI SSS [SSS CCI, 2019].

Grid mappings used will be described in the netCDF variables section specifying its name by means of the grid_mapping_name attribute and map parameters and coordinates according to the grid mapping used.

As a general procedure, the global attributes included in the produced netCDF files will be the following:

- title (brief description of the dataset)
- institution (where the data was produced)
- sources (list of the ancillary data files used)
- references (ATBD, algorithm…)
- conventions (CF-version)
- product_version (the version of the product)
- date_created (the date in which the file has been created)
- creator_name / creator_url /creator_email
- project (the project name “Baltic+ Salinity Dynamics” )
- funding (“European Space Agency under contract reference 4000126102/18/I-BG)
- license (conditions about data access and distribution)
- time_coverage_start (format "yyyymmddThhmmssZ")
- time_coverage_end (format "yyyymmddThhmmssZ")
- time_coverage_duration (ISO8601 compliant, for instance “P9D”)
- geospatial_lon_resolution (longitude resolution in degrees for regular lat-lon gridded data)
- geospatial_lat_resolution (latitude resolution in degrees for regular lat-lon gridded data)
- geospatial_lon_units (usually "degrees_east" for lat-lon gridded data)
- geospatial_lat_units (usually “degrees_north" for lat-lon gridded data)
- geospatial_lon_min / geospatial_lon_max (minimum and maximum value for longitude, range -180 to +180)
- geospatial_lat_min / geospatial_lat_max (minimum and maximum value for latitude, range -90 to +90)
- key_variables (comma separated list of primary variables)

Data will be distributed through the BEC secure FTP service ftp.icm.csic.es available through port 27500. This ftp server will be available before June 2019.

## 3.1 Description of the regional SSS dataset

A Lambert azimuthal equal area projection of 25 km with center at [20°E, 59°N] has been used to process L1 (geolocated brightness temperatures) and L2 (SSS) levels. The L3 and L4 Baltic+ SSS products will be distributed in a regular latitude-longitude grid (WGS 84 -- WGS84 - World Geodetic System 1984).

The geographical coverage of the regional Baltic+ SSS products is defined as: longitude range [9°E-30°E] and latitude range [53°N-66°N]. Table 10 shows the main specifications of the Baltic+ L3 SSS product and Table 11 the corresponding details of Baltic+ L4 SSS product.

*Table 10: Baltic+ L3 SSS product specification.*

| Baltic+ L3 SSS product | |
|---|---|
| Processing level | L3 |
| Geographical coverage | 5°E -> 30°E; 53°N -> 66°N |
| Spatial resolution | 0.25° x 0.25° |
| Coordinate reference system | WGS 84 |
| Temporal coverage | v1: From 2011-01-01 to 2013-12-31<br>v2: From 2011-01-01 to present |
| Temporal resolution | 9 days average (generated every day) |

The format of the netCDF files containing Baltic+ L3 SSS product is described below:

```
dimensions:
        time = UNLIMITED ; // (1 currently)
        lat = 52 ;
        lon = 100 ;
variables:
        int time(time) ;
                time:standard_name = "time" ;
                time:long_name = "time" ;
                time:units = "seconds since 1970-1-1 00:00:00" ;
                time:time = "t" ;
                time:coordinate_defines = "center" ;
                time:_CoordinateAxisType = "Time" ;
                time:calendar = "gregorian" ;
        float latitude(lat) ;
                latitude:standard_name = "latitude" ;
                latitude:long_name = "Latitude" ;
                latitude:units = "degrees_north" ;
                latitude:axis = "Y" ;
                latitude:valid_min = 53.f ;
                latitude:valid_max = 66.f ;
        float longitude(lon) ;
                longitude:standard_name = "longitude" ;
                longitude:long_name = "Longitude" ;
                longitude:units = "degrees_east" ;
                longitude:axis = "X" ;
```

```
        longitude:valid_min = 5.f ;
        longitude:valid_max= 30.f ;
int crs ;
        crs:grid_mapping_name = "latitude_longitude" ;
        crs:longitude_of_prime_meridian = 0.f ;
        crs:semi_major_axis = 6378137.f ;
        crs:inverse_flattening = 298.2572f ;
        crs:datum = "WGS84" ;
        crs:proj4tex = "+proj=latlong +ellps=WGS84"
float sss(time, lat, lon) ;
        sss:missing_value = -999.f ;
        sss:_FillValue = -999.f ;
        sss:standard_name = "sea_surface_salinity" ;
        sss:long_name = "Sea Surface Salinity" ;
        sss:valid_min = 0.f ;
        sss:valid_max = 50.f ;
        sss:grid_mapping = "crs" ;
        sss:coordinates = "time latitude longitude" ;
        sss:units = "1" ;
        sss:description = "Sea Surface Salinity [psu]" ;
float sss_error(time, lat, lon) ;
        sss_error:missing_value = -999.f ;
        sss_error:_FillValue = -999.f ;
        sss_error:standard_name = "sea_surface_salinity_uncertainty" ;
        sss_error:long_name = "Sea Surface Salinity uncertainty" ;
        sss_error:valid_min = 0.f ;
        sss_error:valid_max = 10.f ;
        sss_error:grid_mapping = "crs" ;
        sss_error:coordinates = "time latitude longitude" ;
        sss_error:units = "1" ;
        sss_error:description = "Sea Surface Salinity uncertainty [psu]" ;
float sss_anomaly(time, lat, lon) ;
        sss_anomaly:missing_value = -999.f ;
        sss_anomaly:_FillValue = -999.f ;
        sss_anomaly:standard_name = "sea_surface_salinity_anomaly" ;
        sss_anomaly:long_name = "Sea Surface Salinity anomaly" ;
        sss_anomaly:valid_min = -50.f ;
        sss_anomaly:valid_max = 50.f ;
        sss_anomaly:grid_mapping = "crs" ;
        sss_anomaly:coordinates = "time latitude longitude" ;
        sss_anomaly:units = "1" ;
        sss_anomaly:description = "Sea Surface Salinity anomaly [psu]" ;
```

*Table 11: Baltic+ L4 SSS product specification.*

| Baltic+ L4 SSS product | |
|---|---|
| Processing level | L4 (SMOS L3 SSS fused with OSTIA SST) |
| Geographical coverage | 5°E -> 30°E; 53°N -> 66°N |
| Spatial resolution | 0.05° x 0.05° |
| Coordinate reference system | WGS 84 |
| Temporal coverage | v1: from 2011-01-01 to 2013-12-31<br>v2: from 2011-01-01 to present |
| Temporal resolution | daily |

The format of the netCDF files containing Baltic+ L4 SSS product (SMOS L3 SSS fused with SST from OSTIA) is described below:

```
dimensions:
    time = UNLIMITED ; // (1 currently)
    lat = 260 ;
    lon = 500 ;
variables:
    int time(time) ;
        time:calendar = "Gregorian" ;
        time:long_name = "time" ;
        time:standard_name = "time" ;
        time:units = "seconds since 1970-1-1 00:00:00" ;
        time:time = "t" ;
        time:coordinate_defines = "center" ;
        time:_CoordinateAxisType = "Time" ;
    float lat(lat) ;
        latitude:standard_name = "latitude" ;
        latitude:long_name = "Latitude" ;
        latitude:units = "degrees_north" ;
        latitude:axis = "Y" ;
        latitude:valid_min = 53.f ;
        latitude:valid_max = 66.f ;
   float lon(lon) ;
        longitude:standard_name = "longitude" ;
        longitude:long_name = "Longitude" ;
        longitude:units = "degrees_east" ;
        longitude:axis = "X" ;
```

```
        longitude:valid_min = 5.f ;
        longitude:valid_max = 30.f ;
    int crs ;
        crs:grid_mapping_name = "latitude_longitude" ;
        crs:longitude_of_prime_meridian = 0.f ;
        crs:semi_major_axis = 6378137.f ;
        crs:inverse_flattening = 298.2572f ;
        crs:datum = "WGS84" ;
        crs:proj4tex = "+proj=latlong +ellps=WGS84"
     float l4_sss(time, lat, lon) ;
        l4_sss:missing_value = -999.f ;
        l4_sss:_FillValue = -999.f ;
        l4_sss:standard_name = "l4_sea_surface_salinity" ;
        l4_sss:long_name = "L4 Sea Surface Salinity" ;
        l4_sss:valid_min = 0.f ;
        l4_sss:valid_max = 50.f ;
        l4_sss:grid_mapping = "crs" ;
        l4_sss:coordinates = "time latitude longitude"
        l4_sss:units = "1" ;
        l4_sss:description = "SMOS Sea Surface Salinity fused with OSTIA SST [psu]" ;
    float l4_sss_error(time, lat, lon) ;
        l4_sss_error:missing_value = -999.f ;
        l4_sss_error:_FillValue = -999.f ;
        l4_sss_error:standard_name = "l4_sea_surface_salinity_uncertainty" ;
        l4_sss_error:long_name = "L4 Sea Surface Salinity uncertainty" ;
        l4_sss_error:valid_min = 0.f ;
        l4_sss_error:valid_max = 10.f ;
        l4_sss_error:grid_mapping = "crs" ;
        l4_sss_error:coordinates = "time latitude longitude" ;
        l4_sss_error:units = "1" ;
        l4_sss_error:description = "Uncertainty of L4 Sea Surface Salinity product (SMOS SSS
fused with OSTIA SST)[psu]" ;
    float l4_sss_anomaly(time, lat, lon) ;
        l4_sss_anomaly:missing_value = -999.f ;
        l4_sss_anomaly:_FillValue = -999.f ;
        l4_sss_anomaly:standard_name = "sea_surface_salinity_anomaly" ;
        l4_sss_anomaly:long_name = "Sea Surface Salinity anomaly" ;
        l4_sss_anomaly:valid_min = -50.f ;
        l4_sss_anomaly:valid_max = 50.f ;
        l4_sss_anomaly:grid_mapping = "crs" ;
        l4_sss_anomaly:coordinates = "time latitude longitude" ;
        l4_sss_anomaly:units = "1" ;
        l4_sss_anomaly:description = "Anomaly of L4 Sea Surface Salinity product (SMOS SSS fused
with OSTIA SST) [psu]" ;
```

The file naming will follow the following fixed convention (based on [SSS CCI, 2019]) in order to simplify the access to the users:

`<processing_center>-<processing_level>-<variable>-<area>-<spatial_resolution>-<start_date>_<end_date>-<version>.nc`

for instance:

`BEC-L3-SSS-BALTIC-0.25d-20120201_20120210-v1.0.nc` (for L3 products)

`BEC-L4-SSS-BALTIC-0.05d-20120201_20120210-v1.0.nc` (for L4 products)

## 3.2 Description of the Collection in-situ data

In-situ data which has been identified in the RBD [RBD, 2019] are collected in the WP200. In-situ data collocated with the SMOS measurements will be distributed to facilitate the validation of the Baltic+ SSS products.

The match-up files provided in netCDF format will contain the collocated SSS for a given satellite/in-situ product pair, auxiliary geophysical parameters such as temperature, and other relevant variables such as distance to the coast, temporal lag between in-situ time and satellite SSS product central time, etc. The in-situ measurements are the drivers of the file, which means that there are as much pairs as in situ measurements, even though several in situ measurements fall in the same satellite cell grid. Match-up files will have the same temporal coverage as their corresponding satellite product. In the case of in-situ measurements provided by moorings, profilers or CTD only the uppermost measurement is included (considering only measurements in the mixed layer depth). The format of the data files delivered under this project follows the format defined in the ESA PI-MEP project:

https://pimep-test.oceandatalab.com/ [Pi-MEP, 2018].

The in-situ based observations have been grouped as punctual measurements (group 1) and continuous measurements (group 2).

Group 1:

- ARGO profilers (CORIOLIS)
- Moored stations
- CTD measurements

Group 2:

- Thermo-Salinograph (TSG) data installed on Voluntary Observing Ships & Research Vessels (LEGOS, GOSUD)
- Dedicated campaign data (see data from PassMe project in [RBD, 2019]).

The format of the files will be slightly different for the different group sensors (see the format of the match up files). File Name convention given to the Match up files is the following:

`ESA_ITT+Baltic-<processing_level>-<area>-<insitu_sensor_type>-<date_ini>-<date_end>-v<product_version>.nc`

`<insitu_sensor_type>` can be ARGO, MOOR, CTD_, TSG_

for instance:

`ESA_ITT+Baltic-L3-BALTIC-ARGO-20120201_20120210-v1.0.nc` (for L3 products)

ESA_ITT+Baltic-L4-BALTIC-ARGO-20120201_20120210-v1.0.nc (for L4 products)

The format of the in-situ match ups is the following:

```
dimensions:
        nmeas = 200 ; // number of the in-situ measurements
variables:
        float latitude_insitu(nmeas) ;
                latitude_insitu:standard_name = "latitude" ;
                latitude_insitu:long_name = "Latitude of the in-situ measurement" ;
                latitude_insitu:units = "degrees_north" ;
                latitude_insitu:axis = "Y" ;
        float longitude_insitu(nmeas) ;
                longitude_insitu:standard_name = "longitude" ;
                longitude_insitu:long_name = "Longitude of the in-situ measurement" ;
                longitude_insitu:units = "degrees_east" ;
                longitude_ insitu:axis = "X" ;
        int date_insitu(nmeas) ;
                date_insitu:standard_name = "time" ;
                date_insitu:long_name = "Time" ;
                date_insitu:units = "seconds since 1970-1-1 00:00:00" ;
                date_insitu:time = "T" ;
                date_insitu:calendar = "gregorian" ;
        float sss_insitu(nmeas) ;
                sss_insitu:missing_value = -999.f ;
                sss_insitu:_FillValue = -999.f ;
                sss_insitu:standard_name = "sea_surface_salinity" ;
                sss_insitu:long_name = "In-situ Sea Surface Salinity" ;
                sss_insitu:valid_min = 0.f ;
                sss_insitu:valid_max = 50.f ;
                sss_insitu:units = "1" ;
                sss_insitu:description = "Sea Surface Salinity [psu]" ;
        float latitude_satellite(nmeas) ;
                latitude_insitu:standard_name = "latitude" ;
                latitude_insitu:long_name = "Satellite product latitude at the in-situ location" ;
                latitude_insitu:units = "degrees_north" ;
                latitude_insitu:axis = "Y" ;
        float longitude_satellite(nmeas) ;
                longitude_insitu:standard_name = "longitude" ;
                longitude_insitu:long_name = "Satellite product longitude at in-situ location" ;
                longitude_insitu:units = "degrees_east" ;
                longitude_insitu:axis = "X" ;
        float sss_satellite(nmeas) ;
                sss_satellite:missing_value = -999.f ;
```

```
                sss_satellite:_FillValue = -999.f ;
                sss_satellite:standard_name = "sea_surface_salinity" ;
                sss_satellite:long_name = "Satellite SSS at in-situ location"
                sss_insitu:valid_min = 0.f ;
                sss_insitu:valid_max = 50.f ;
                sss_satellite:units = "1" ;
                sss_satellite:
        float sst_insitu(nmeas) ;
                sst_insitu:long_name = "In-situ Sea Surface Temperature" ;
                sst_insitu:units = "degree Celsius" ;
                sst_insitu:standard_name = "sea_water_temperature" ;
                sst_insitu:_FillValue = -999.f ;
        float coast_distance(nmeas) ;
                coast_distance:long_name = "Distance to coasts at in-situ location" ;
                coast_distance:units = "km" ;
                coast_distance:_FillValue = -999.f ;
        float depth_insitu(nmeas) ;
                depth_insitu:long_name = "Depth" ;
                depth_insitu:units = "m" ;
                depth_insitu:standard_name = "sea_water_depth" ;
                depth_insitu:_FillValue = -999.f ;
        float time_lags(nmeas) ;
                time_lags:long_name = "Temporal lag between in-situ time and satellite SSS product
central time" ;
                time_lags:units = "days" ;
                time_lags:_FillValue = -999.f ;
        float spatial_lags(nmeas) ;
                spatial_lags:long_name = "Spatial lag between in-situ location and satellite SSS
product pixel center" ;
                spatial_lags:units = "km" ;
                spatial_lags:_FillValue = -999.f ;
        float sss_gradient_insitu(nmeas) ; //this field is for in situ of group 1
                sss_gradient_insitu:long_name = "Sea Surface Salinity gradient" ;
                sss_gradient_insitu:standard_name = "sea_water_salinity_gradient" ;
                sss_gradient_insitu:_FillValue = -999.f ;
                sss_gradient_insitu:units = "m-1" ;
        float sst_gradient_insitu(nmeas) ; //this field is for in situ of group 1
                sst_gradient_insitu:long_name = "Sea Surface Temperature gradient" ;
                sst_gradient_insitu:standard_name = "sea_water_temperature_gradient" ;
                sst_gradient_insitu:_FillValue = -999.f ;
                sst_gradient_insitu:units = "Kkm-1" ;
```

# 4 References

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***End of document***