Key Points:

- Reconstructed SSS shows realistic small-scale variability near the Gulf Stream and an overestimation in the Sargasso Sea inherited from SMAP
- Enhanced small-scale salinity variability is concentrated along the continental shelfbreak and the Gulf Stream mean position
- Seasonality of small-scale salinity variability appears to be modulated by the annual cycle of large-scale SSS

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Lagrangian Reconstruction to Extract Small-Scale Salinity Variability From SMAP Observations

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Abstract As the resolution of observations and models improves, emerging evidence indicates that ocean variability on 1–200-km scales is of fundamental importance to ocean circulation, air-sea interaction, and biogeochemistry. In many regions, salinity variability dominates over thermal effects in forming density fronts. Unfortunately, current satellite observations of sea surface salinity (SSS) only resolve scales ≥ 40 km (or larger, depending on the product). In this study, we investigate small-scale variability ($\lesssim 25$ km) by reconstructing gridded SSS observations made by the Soil Moisture Active Passive (SMAP) satellite in the northwest Atlantic Ocean. Using altimetric geostrophic currents, we numerically advect SMAP SSS fields to produce a Lagrangian reconstruction that represents small scales. Reconstructed fields are compared to in-situ salinity observations made by a ship-board thermosalinograph, revealing a marked improvement in small-scale salinity variability when compared to the original SMAP fields, particularly from the continental shelf to the Gulf Stream. In the Sargasso Sea, however, both SMAP and the reconstructed fields contain higher variability than is observed in situ. Enhanced small-scale salinity variability is concentrated in two bands: a northern band aligned with the continental shelfbreak and a southern band aligned with the Gulf Stream mean position. Seasonal differences in the small-scale variability appear to covary with the seasonal cycle of the large-scale SSS gradients resulting from the freshening of the coastal waters during periods of elevated river outflow.

Plain Language Summary Emerging evidence indicates that oceanic structures at scales smaller than ~ 100 km have an important contribution to ocean circulation, air-sea interactions, and biogeochemical cycling. In many regions, the contribution of salinity dominates that of temperature in generating density fronts. Satellites that measure sea surface salinity (SSS) from space have a resolution lower than 40 km and do not allow the observation of small-scale structures (< 25 km). The present work is motivated by the need to develop techniques to exploit satellite salinity measurements to extract signals with the highest possible spatial resolution. We investigate small-scale variability captured in reconstructions of SSS observations made by the Soil Moisture Active Passive (SMAP) satellite in the northwest Atlantic Ocean. Reconstructed fields are compared to in-situ observations, revealing a marked improvement in the reproduction of observed salinity fronts when compared to SMAP fields. Enhanced small-scale salinity variability is found to be concentrated in two bands: a northern band aligned with the continental shelfbreak, and a southern band aligned with the Gulf Stream mean position. Seasonal differences in the small-scale salinity variability are mainly driven by the seasonal cycle of the large-scale SSS induced by the freshening of the coastal waters due to river outflow.

1. Introduction

Changes in sea water salinity have important implications for the water cycle, ocean circulation, climate variability, and marine biogeochemistry (Durack et al., 2016; Vinogradova et al., 2019). Sea surface salinity (SSS) is controlled by the net impacts of evaporation and precipitation, inflow of fresh water from rivers, and formation and melting of ice. Ocean currents and mixing spread the surface salinity anomalies throughout the three-dimensional ocean and determine the salinity characteristics of each ocean basin. Despite its importance, measurements of ocean salinity are limited to (i) relatively sparse in-situ observations from different platforms and (ii) global remote sensing surface observations with low resolution from satellites. Here, we aim to obtain information at high resolution from satellite salinity observations using a Lagrangian reconstruction technique in order to study the small-scale salinity variability around the Gulf Stream (northwest Atlantic Ocean).

Satellite observations of sea surface temperature (SST), SSS, and sea surface height (SSH) have greatly increased our understanding of the global ocean circulation (e.g., Chelton et al., 2011). Observations from satellites have the advantage of covering the global ocean in short periods of time; however, satellite observations are restricted to the ocean surface. Salinity remote sensing observations have improved the study of large-scale ocean processes and the capability to analyze large mesoscale salinity variability, giving a near-global, synoptic view of SSS (see Vinogradova et al., 2019, for a review). However, the effective resolution of satellite salinity observations is ≥ 50 km, which is insufficient to capture the entire range of mesoscale dynamics, and far too coarse to capture submesoscale variability.

Salinity, together with temperature, drives ocean circulation through changes in density. Density fronts can be generated as a result of temperature gradients, salinity gradients, or the combined contribution of both (Drushka et al., 2019). The resulting density fronts can develop high vertical velocities that can result in the vertical exchange of salt, heat, gases, carbon, and nutrients between the upper and deeper layers (e.g., Lévy et al., 2001; Mahadevan, 2016; Thomas et al., 2008). Alternatively, gradients in temperature and salinity can be compensated, meaning that their impacts on density cancel out and density is constant (Rudnick & Ferrari, 1999; Rudnick & Martin, 2002). To study the density variability at the ocean surface, it is necessary to have observations of both SST and SSS to evaluate their combined contribution to the generation of density fronts. Microwave SST observations have global coverage and a resolution of 25 km, while infrared SST observations have high resolution (1–10 km) in clear-sky conditions. Satellite SSS observations have low resolution (~ 40 –100 km) and global coverage. The objective of this study is to explore a Lagrangian reconstruction technique to extract high-resolution information from satellite SSS observations so that they approach the resolution of SST.

Several studies have demonstrated the fundamental role that horizontal advection plays in the temporal evolution of salinity on different time and space scales (e.g., Foltz et al., 2004; Grodsky et al., 2017). Physical processes that can drive small-scale SSS variability include stirring by mesoscale eddies and stirring induced by mesoscale turbulence near large-scale salinity gradients (e.g., Legal et al., 2007; Pietri et al., 2013). The latter was studied by Desprès et al. (2011) through a Lagrangian model that uses currents derived from altimetry with a resolution of $1/3^\circ$ to passively advect the large-scale salinity from a monthly climatology. With this model, they were able to reproduce the spatial variability of salinity fronts at ~ 10 -km scale in the Irminger Sea, revealing that these fronts are often associated with a nonlocal process. A comparison with in-situ data showed that the number and amplitude of fronts in the advected salinity fields were realistic (Desprès et al., 2011). Hence, the Lagrangian advection by altimetric geostrophic currents of a climatological salinity field was able to reconstruct the location and amplitude of fronts in the Irminger Sea. By showing that the fronts in the advected SSS field looked like the observations, they demonstrated that horizontal stirring of the large-scale SSS climatological field by geostrophic currents controls the salinity structure at small scales in that region. Today, this technique can be extended to other regions using satellite SSS observations having higher spatial and temporal resolution than the climatological field, and using altimetric currents with a resolution of $1/4^\circ$.

Dencausse et al. (2014) used a similar method to advect weekly observation-based SSS fields with $1/4^\circ$ horizontal resolution using currents derived from altimetry in the Southern Ocean south of Tasmania, a region characterized by strong mesoscale and submesoscale structures. Their results show that after 2 weeks of simulation, the advected salinity fields have good agreement with in-situ data. They also demonstrated that the Lagrangian model used to reconstruct small scales, named here “Lagrangian reconstruction technique,” works better in regions with moderate to high eddy kinetic energy, where lateral advection dominates. Rogé et al. (2015) extended this analysis to the western equatorial Pacific and to the subtropical southwest Pacific. They suggested that the Lagrangian reconstruction technique is effective in regions with moderate to high mesoscale energy and a correlation between the mesoscale surface tracer and surface height fields. The previous studies were initialized with an in-situ observation-based salinity product whose accuracy depends on the spatial and temporal coverage of the in-situ observations. This limitation can be overcome using satellite SSS observations, which have global coverage of the ocean surface.

A Lagrangian approach using along-track SSS observations from the Aquarius satellite as input was applied by Mahadevan et al. (2016) to study the salinity evolution in the Bay of Bengal, a region where small-scale SSS variations are critical for ocean mixing and air-sea interaction. The advection of along-track SSS

observations with altimetric currents provided a Lagrangian interpolation of monthly SSS fields that allowed the analysis of the freshwater distribution evolution. This dynamic interpolation method was used to map the distribution of freshwater and revealed a dynamically evolving salinity variability that was not captured by Aquarius gridded monthly products with a 1° of resolution.

In this study, we use for the first time Soil Moisture Active Passive (SMAP) SSS observations, gridded with a resolution of $1/4^\circ$ and an effective resolution of 70 km, to capture small-scale salinity variability through a Lagrangian reconstruction technique using currents from altimetry with a resolution of $1/4^\circ$. The region analyzed is the northwest Atlantic Ocean (Figure 1), which is characterized by large-scale salinity gradients and is strongly influenced by the Gulf Stream.

In Sections 2 and 3 we describe the data and methodology used for the reconstruction, respectively. In Section 4.1 we compare the reconstructed SSS fields with observations from a ship-based thermosalinograph; in Section 4.2 we apply the reconstruction technique to weekly fields of SMAP SSS observations to evaluate the seasonal and regional patterns of small-scale variability in the northwest Atlantic Ocean; and in Section 4.3 we compare the reconstructed SSS fields with a data assimilating model. The discussion of the results and the conclusions are presented in Section 5.

2. Data

2.1. SMAP Sea Surface Salinity

Satellite SSS observations are obtained from the SMAP mission. We use version 4.0 of the Level 3 SMAP SSS 8-days running mean gridded product, produced operationally by Remote Sensing Systems (Meissner et al., 2019). Daily maps are based on SSS averages spanning an 8-days moving time window. The product has a grid spacing of $1/4^\circ \times 1/4^\circ$ with a spatial feature resolution of ~ 70 km. SMAP data begin on April 1, 2015 and are freely available through the NASA Physical Oceanography Distributed Active Archive Center (https://podaac.jpl.nasa.gov/dataset/SMAP_RSS_L3_SSS_SMI_8DAY-RUNNINGMEAN_V4). Due to a SMAP observational safehold event, SMAP SSS data were not produced over the period June 19 to July 22, 2019.

2.2. Geostrophic Currents Derived From Altimetry

Geostrophic currents are derived from multimission altimeter satellite gridded absolute dynamic topography and distributed by Copernicus Marine Environment Monitoring Service (CMEMS). The global ocean gridded L4 altimetry products have daily time resolution and $1/4^\circ \times 1/4^\circ$ grid resolution. The Eulerian maps of altimetric currents represent the mesoscale (and larger scales) in the Gulf Stream, with a first Rossby radius of deformation between 40 and 60 km (Chelton et al., 1998), but their integration over time (i.e., their Lagrangian evolution) can give information about finer scales (e.g., Lehahn et al., 2018). These scales are generated because the cascade of tracer variance from the mesoscale to smaller scales is reproduced by advecting tracers with the mesoscale velocity field. Delayed-time altimetry products are available for the SMAP period until May 13, 2019; after this date, near-real-time data are used until January 15, 2020. The data are freely available at the CMEMS website: <http://marine.copernicus.eu>.

2.3. Thermosalinograph Data From the Oleander Project

To compare the reconstructed SSS fields with in-situ observations, we use ship-based thermosalinograph (TSG) data from the long-term M/V Oleander Project (<http://po.msrb.sunysb.edu/Oleander/>). The Oleander vessel makes weekly round trips from the United States east coast (New Jersey) to Bermuda (Figure 1). A newly calibrated TSG was installed on November 21, 2014; however, shortly thereafter, the operation of the TSG was stopped until September 2016. For the comparison with reconstructed SSS fields, we use Oleander along-transect salinity measurements (taken at ~ 3 -m depth) from September 24, 2016 to February 27, 2019. A comparison of the Oleander TSG salinity with SMAP SSS is described by Grodsky et al. (2018a). In total, there are 145 transects with salinity observations (Figure 2) after applying quality control to remove spurious values and discard two short transects.

Figure 1. Domain of the Lagrangian reconstruction. (a, b) SMAP SSS observations on February 12, 2017, in (b) the surface currents derived from altimetry on the same day are superimposed, (c) SSS reconstruction on February 12, 2017 after 7 days of Lagrangian advection by altimetric currents, and (d) reconstructed field resampled to the original grid resolution and smoothed with a spatial scale of 70 km. Colored dots running in a line from the United States east coast to Bermuda represent the in-situ salinity observed with a ship-based thermosalinograph on February 12, 2017. SMAP, Soil Moisture Active Passive; SSS, sea surface salinity.

2.4. CMEMS Global Ocean Model

SSS from the CMEMS global ocean physics reanalysis model is also compared to the reconstructed SSS field. The CMEMS global ocean model has a spatial resolution of $1/12^\circ$ and 50 vertical levels, and assimilates observations of along-track altimetry, satellite SST, sea ice concentration, and in-situ vertical profiles of temperature and salinity (Fernandez & Lellouche, 2018). This product covers the period between January 1, 1993 to December 25, 2018; after this date, we use SSS from the CMEMS global ocean physics analysis and forecast model (Law Chune et al., 2020), which has the same resolution and assimilates the same set of observations.

Figure 2. (a) Temporal coverage of the Oleander thermosalinograph data used in this study. Colors represent salinity along each transect. (b) Number of transects per year and (c) per season (January–February–March is winter, April–May–June is spring, July–August–September is summer, and October–November–December is autumn).

3. Methods

3.1. Lagrangian Reconstruction Technique

The Lagrangian reconstruction technique consists of the passive advection of a tracer following the geostrophic currents derived from altimetry. The one-way backward approach used here consists of the backward advection of particles from the final time t_f to the initial time $t_f - n$, where n is the number of days the particles are advected. The SMAP SSS observed at $t_f - n$ is interpolated onto the particle positions that day. With this, each particle has an SSS value that corresponds to the observation at $t_f - n$. Then, we can plot the particles at their final position with their salinity value, and with this create the maps of the reconstructed salinity field. It is important to note that the Lagrangian advection can also be done following a one-way forward approach (Dencausse et al., 2014), which is based on the forward advection of particles from $t_f - n$ to t_f carrying the salinity value from the SMAP SSS observation at $t_f - n$. The advantage of using the backward approach instead of the forward approach is that at t_f we have a regular grid of particles without gaps (Desprès et al., 2011; Rogé et al., 2015). Rogé et al. (2015) also presented a two-way advection technique consisting of the backward advection of tracers, smoothing at the initial position, and relocation to the final position. We found that this technique did not work as well as the one-way technique (for instance, it was highly sensitive to the smoothing scales) and so we do not discuss it further here.

At the final time of the backward simulation, particles are released on a regular grid with 0.04° resolution within the domain limited by 82°W and 63°W in longitude and 25°N and 46°N in latitude (Figure 1). Particles are allowed to leave the domain. After testing different advection times, a value of $n = 7$ days was chosen as it best reproduces the small-scale salinity variability observed in situ. This advection time is shorter than the 14–30 days used in other studies; the Gulf Stream is characterized by high velocities, and features evolve faster than in many other regions. Hence, the lateral stirring during 7 days is enough to create

small-scale salinity fronts and filaments. To obtain the Lagrangian trajectories, we used the Python package OceanParcels, which integrates the altimetry-derived geostrophic velocities with a fourth order Runge-Kutta integrator using a time step of 3 h (Delandmeter & van Sebille, 2019; Lange & van Sebille, 2017). OceanParcels is freely available at <https://oceanparcels.org>.

Figure 1c shows an example of the reconstructed salinity field after applying the Lagrangian reconstruction technique to SMAP observations. The reconstruction method generates SSS variability at smaller scales than the scales observed by SMAP (Figure 1a), allowing the representation of eddies, fronts, and filaments. The correlation coefficient between the observed field (Figure 1a) and the coarse-grained reconstructed field (Figure 1d) on February 12, 2017 is 0.96, indicating that the features in the reconstructed field agree well with those observed by SMAP. Two sets of simulations are considered in this study. The first set is used to compare the advected salinity field with in-situ measurements from the M/V Oleander TSG. For each day having in-situ observations we ran a corresponding simulation. The results of this comparison are shown in Section 4.1. A second set of weekly simulations has been done to analyze the small-scale salinity variability in the northwest Atlantic Ocean. We ran weekly simulations from April 7, 2015 to January 15, 2020, excluding the period between June 19 and July 22, 2019 when SMAP SSS data were not produced. The results of this analysis are presented in Section 4.2. The outputs of both sets of simulations are available at <https://doi.org/10.20350/digitalCSIC/12830> (Barceló-Llull et al., 2020).

3.2. Identification of Fronts

To detect salinity fronts along transects, we apply a gradient-based method that consists of the following four steps:

1. Interpolate data to a regular distance axis with a resolution of 0.2 km, then apply a Loess smoother with a half-power filter cutoff of 10 km, effectively retaining fronts longer than ~ 4 km (Chelton et al., 2011).
2. Isolate large-scale salinity variability by smoothing the interpolated data using a Loess filter with a cutoff of 200 km.
3. Compute residuals of salinity by subtracting the large-scale salinity from step 2 from the interpolated and smoothed field from step 1.
4. Detect fronts in the spatial gradient of the residual from step 3 using a threshold of 0.02 PSU per km, with an additional requirement that at least 25 consecutive data points have to meet the gradient threshold: with this we disregard fronts shorter than 5 km.

4. Results

4.1. Comparing the Reconstructed Fields With In-Situ Data

To evaluate our method, we compare the reconstructed SSS field with ship-based salinity observations at high-spatial resolution from the Oleander project. Figure 3 shows five transects of in-situ observations on different dates, and the reconstructed and SMAP SSS fields interpolated onto the transect position. On September 24, 2016, the reconstructed salinity captures the sharp front at the Gulf Stream position at $\sim 71^\circ\text{W}$, while the original SMAP field has a gradual increase from the fresher coastal waters to the saltier offshore waters without capturing this front (Figure 3a). In the eastern part of the transect, the in-situ observations have a nearly constant value of 36.31 ± 0.07 PSU east of 70.7°W , while the reconstruction has higher variability, with a mean value and standard deviation of 36.46 ± 0.15 PSU. On February 12, 2017, the SMAP observations show a smooth SSS field, while the in-situ data show an increase of salinity between 72.3°W and 71.7°W that corresponds to the eddy reconstructed using the Lagrangian method (Figure 1) and represented along this transect as two well-defined fronts (Figure 3b). East of 70.7°W the reconstruction has a mean value of 36.56 ± 0.16 PSU, while the in-situ data have lower salinity and variability (35.95 ± 0.02 PSU). The higher values in the reconstructed salinity are similar to the observed salinity from SMAP that has a mean value of 36.53 ± 0.21 PSU. The transect sampled on January 14, 2018 (Figure 3c) has a set of fronts west of 69°W that are not seen in the SMAP observations but that the reconstruction is able to reproduce remarkably well, albeit with a small displacement along the longitude axis. As in the previous example, the in-situ salinity has an almost constant value at the eastern side (36.32 ± 0.03 PSU), while the reconstruction has higher salinity mean value and variability (36.71 ± 0.16 PSU). In this case, the higher salinity in the

Figure 3. Salinity measured by the Oleander thermosalinograph (solid black line), reconstructed (dashed violet line) and SMAP (dotted dashed orange line) salinity fields interpolated onto the transect position for different dates. Data along transects are interpolated to a regular distance axis with 0.2-km resolution, and smoothed by applying a Loess filter with a half-power filter cutoff of 10 km. Dates are given in the upper left of each panel. SMAP, Soil Moisture Active Passive.

reconstruction is different from the SMAP salinity mean value (36.39 ± 0.21 PSU). Note that the reconstruction method advects the SMAP SSS observed 7 days before the end of the simulation, at which time the SMAP SSS observation had higher values. The in-situ data on June 2, 2018 reveal a high-intensity salinity front at $\sim 70.8^\circ\text{W}$ that is well reconstructed by the Lagrangian method but not at all captured by SMAP (Figure 3d). The salinity transect sampled on January 6, 2019 shows a set of fronts west of 71.2°W that are not observed by SMAP but that are represented by the reconstructed salinity field (Figure 3e).

These five examples demonstrate that the reconstructed salinity field represents realistic salinity fronts in the western side of the domain, corresponding to within and west of the Gulf Stream. In the eastern side, i.e., the Sargasso Sea, the in-situ data show almost constant salinity values while the reconstructed salinity field represents higher variability. To go deeper into this comparison, we detect fronts along each Oleander transect for each salinity field (TSG, reconstruction, and SMAP) following the method explained in Section 3.2. Figure 4 shows the relative number of fronts detected from each field within $0.25^\circ \times 0.25^\circ$ bins with respect the number of transects crossing each bin, and the mean intensity of these fronts. Fronts detected

Figure 4. Occurrence of salinity fronts detected in (a) thermosalinograph data, (b) reconstructed field, and (c) SMAP observations. The probability in each $0.25^\circ \times 0.25^\circ$ bin is computed as the number of detected fronts divided by the number of transects crossing each bin. Only bins crossed by at least 15% of the maximum number of transects crossing bins (120) are shown. Mean intensity of salinity fronts detected in (d) thermosalinograph data, (e) reconstructed field, and (f) SMAP observations inside each bin. In (d), (e), and (f), bins having a frontal probability <0.15 are masked. Cyan solid line shows the 200-m isobath representative of the shelfbreak position (Richaud et al., 2016). Cyan dashed line represents the mean position of the Gulf Stream approximated as the 0.5-m isoline of the mean dynamic topography MDT-CNES-CLS18 (freely available from Aviso at <https://www.aviso.altimetry.fr/en/data/products/auxiliary-products/mdt.html>). SMAP, Soil Moisture Active Passive.

from the in-situ data show a clear difference between the regions west and east of 70°W (Figure 4a). On the western side, the probability of finding a salinity front is maximum (>0.7), while on the eastern side the probability is minimum (<0.1). The SMAP salinity has a small number of fronts (probability of up to 0.2) near the coast and near 70.3°W , but in the other bins the number of salinity fronts is zero (Figure 4c). The reconstructed salinity represents significantly more fronts than the SMAP field (Figure 4b). As in the in-situ data, the number of fronts detected from the reconstructed salinity is maximum on the western side of the transect, although fewer fronts are detected near the coast than from the TSG data. As expected from the individual transects shown in Figure 3, in the Sargasso Sea east of 70°W , the reconstruction represents fronts that are not detected from in-situ observations; these fronts are unrealistic and are generated due to the higher variability of SMAP observations in comparison with in-situ data in the Sargasso Sea. This comparison reveals regions with high probability of fronts in each data set. Figure 5 shows the fronts detected from each product, and the fronts detected in both TSG data and the reconstructed field, and in TSG data and SMAP observations. As observed in Figure 4, the SMAP field has a small number of fronts. The reconstruction represents more fronts than SMAP observations, many of them at the same position and time as

Figure 5. Fronts detected in (a) thermosalinograph data, (b) the reconstructed field, and (c) SMAP observations. Blue points represent fronts detected in each data point, while orange points highlight the fronts detected in both the thermosalinograph data and the reconstructed field (b) and the SMAP observations (c). SMAP, Soil Moisture Active Passive.

in the TSG data. More fronts are detected from the in-situ data and reconstructed fields west of 70°W , while unrealistic fronts are detected on the reconstruction east of this longitude. The intensity of salinity fronts is defined as the difference between the maximum and minimum salinity values for each front, and its bin average is shown in Figures 4d–4f. In-situ and reconstructed salinity have two regions with high-intensity fronts (>0.7 PSU/km), one at the shelfbreak represented by the 200-m isobath (Richaud et al., 2016) and the other at $\sim 38^{\circ}\text{N}$ west of the Gulf Stream mean position. In the latter region, the in-situ observations have fronts with higher intensity (~ 1.2 PSU/km) than the fronts detected in the reconstruction (~ 0.7 PSU/km), suggesting that the intensity of fronts is underestimated in the reconstruction. The number of reconstructed fronts near the coast is underestimated, while the location of fronts is realistic.

4.2. Small-Scale Salinity Variability in the Northwest Atlantic Ocean

After comparing the reconstructed SSS field with in-situ observations, in this section we analyze the small-scale salinity variability in the northwest Atlantic Ocean through weekly reconstructions of SMAP SSS observations from April 7, 2015 to January 15, 2020.

To analyze salinity variability, we calculate the standard deviation of SSS within spatial bins of different sizes for each reconstructed date. The SSS standard deviation is representative of the spatial variability at scales shorter than the bin size (Drushka et al., 2019). In Figure 6a, we show the temporal average of the standard deviation of the SMAP SSS observations within bins of $0.75^{\circ} \times 0.75^{\circ}$, 3 times the SMAP grid resolution. For the reconstructed SSS field, we compute the standard deviation within the same bin size (Figure 6b) and within bins of $0.24^{\circ} \times 0.24^{\circ}$, 6 times the particle grid spacing, to analyze the small-scale salinity variability, defined here as scales smaller than ~ 25 km (Figure 6c). Comparing standard deviations computed over the same bin size, the reconstructed SSS field has higher variability than the SMAP observations. This variability is higher in the northern part of the domain, while in the Sargasso Sea it remains low in both SMAP and reconstructed SSS (Figures 6a and 6b). The relatively weak salinity variability in the Sargasso Sea can be explained by considering the weak mean salinity gradients in this region (Figure 7). In contrast, the northern part of the domain has strong mean gradients because the Gulf Stream separates fresher and colder water near the coast from saltier and warmer water in the Sargasso Sea. This difference in water masses can generate salinity fronts on a range of scales that are reflected in maps of horizontal salinity variability. SMAP observations represent the large-scale salinity field, while the reconstructed SSS has higher resolution and also represents the small-scale salinity variability. The enhanced variability in the reconstructed SSS field within bins of $0.75^{\circ} \times 0.75^{\circ}$ suggests that the variability at this bin size is caused by small-scale SSS signals.

By computing standard deviation over a smaller bin size, we isolate the small-scale salinity variability captured by the reconstructed salinity fields, enabling us to study its distribution in the northern part of the domain (Figure 6c). Higher values of small-scale salinity variability are concentrated in two bands. The

Figure 6. Standard deviation of the (a) observed SMAP SSS and (b) reconstructed SSS inferred in bins of $0.75^\circ \times 0.75^\circ$ (3 times the SMAP grid resolution) and averaged over all of the simulation dates. (c) Standard deviation of the reconstructed salinity field inferred in bins of $0.24^\circ \times 0.24^\circ$ (6 times the particle grid spacing) and averaged over all of the simulation dates. For the advected fields, bins that have $<80\%$ of particles with valid salinity values than the total number of particles within bins are masked. In (a) the same mask as in (b) is applied to better compare both fields. The cyan solid line shows the 200-m isobath, representative of the shelfbreak position (Richaud et al., 2016). The cyan dashed line represents the mean position of the Gulf Stream, approximated as the 0.5-m isoline of mean dynamic topography. SMAP, Soil Moisture Active Passive; SSS, sea surface salinity.

northern band is aligned with the shelfbreak front (Fratantoni & Pickart, 2007; Richaud et al., 2016) represented in SMAP fields as a region with high horizontal SSS gradients along the 200-m isobath, while the southern band is aligned along the western side of the Gulf Stream mean position (Figure 7). In the northern band, the geostrophic shelfbreak currents observed by altimetry are weak but there is a preexisting strong large-scale salinity gradient along the shelfbreak. This region is also characterized by meanders and

Figure 7. Temporal average of the (a) SMAP SSS and (b) SMAP SSS gradient magnitude, calculated as $\left(\left(dSSS / dx \right)^2 + \left(dSSS / dy \right)^2 \right)^{1/2}$, where dx and dy are the grid spacing along longitude and latitude, respectively, in km, considering observations on the simulated dates. Blue arrows in (a) are mean altimetric currents from the mean dynamic topography MDT-CNES-CLS18 freely available from Aviso (<https://www.aviso.altimetry.fr/en/data/products/auxiliary-products/mdt.html>). For clarity, only one out of five current vectors are plotted. The cyan solid line in (b) shows the 200-m isobath, representative of the shelfbreak position. The cyan dashed line in (b) represents the mean position of the Gulf Stream, approximated as the 0.5-m isoline of mean dynamic topography. SMAP, Soil Moisture Active Passive; SSS, sea surface salinity.

Figure 8. Standard deviation of the reconstructed salinity field computed over $0.24^\circ \times 0.24^\circ$ bins (6 times the particle grid spacing) and averaged over (a) late winter (February–March–April) and (b) summer (June–July–August). Bins that have $<80\%$ of particles with valid salinity values are masked. Cyan solid line in (a) and (b) shows the 200-m isobath representative of the shelfbreak position. Red and blue dashed lines in (a) and (b) represent the Gulf Stream mean position in late winter and summer, respectively, approximated as the 0.5-m isoline of the seasonally averaged absolute dynamic topography.

eddies with moderate velocities that detach from the Gulf Stream, which are not represented in the mean currents because they evolve over time. The horizontal stirring (or Lagrangian advection) of the preexisting strong large-scale salinity gradient by time-varying mesoscale features detached from the Gulf Stream triggers the generation of small-scale salinity variability (for instance, see the example in Figure 1, in which numerous mesoscale eddies are observable in the surface velocity and reconstructed SSS fields). At the southern band of high small-scale salinity variability around 38°N (Figure 6c), the large-scale salinity gradient observed from SMAP is moderate (Figure 7b). However, the strong Gulf Stream currents at Cape Hatteras (Figure 7a) advect the fresher shelf waters along the Gulf Stream north wall, generating a strong salinity front (for instance, see the example in Figure 1c, in which a salinity front is generated northeast of Cape Hatteras). Additionally, this region is characterized by (i) a contrast in water masses between the fresher water at the continental slope and the saltier water of the Sargasso Sea and (ii) strong mesoscale features generated at the Gulf Stream. The integration over time of the time-varying Gulf Stream currents acting on the preexisting moderate salinity gradient and on the reconstructed salinity front triggers the generation of fine-scale salinity features. An example of this can be seen as the filaments observed around eddies in Figure 1c. Note that due to high current speeds in the Gulf Stream, some particles were outside the domain 7 days before the backward simulation start-date. These particles advect no salinity value and are masked in the final maps (for instance, in Figure 1c see gap with no data at 80°W , 30°N). In temporal averages of the reconstructed SSS standard deviation (Figures 6 and 8), the bins having $<80\%$ of particles with valid salinity values are masked.

The analysis of the seasonal cycle of the small-scale salinity variability inferred from the reconstructed salinity field highlights differences in both seasonal and spatial patterns (Figure 8). In the northeast Gulf of Maine the small-scale salinity variability is higher in late winter compared to summer. In contrast, north of 35°N and west of 70°W (within and east of the Middle Atlantic Bight), the salinity variability is enhanced in summer relative to winter. The seasonal cycle of salinity variability in the Gulf of Maine may be related to the freshening of the coastal waters in spring and summer due to river outflow (Feng et al., 2016; Geyer et al., 2004). The discharge of fresh water would generate salinity fronts in the Gulf of Maine while the fresher water propagates along the Gulf at the beginning of the river outflow season (Figure 9a). Once the fresher water is spread throughout the Gulf (Figure 9b), the number and strength of salinity fronts, and

Figure 9. (a) Late winter (February–March–April) and (b) summer (June–July–August) average of the SMAP SSS observations on the simulated dates. Vectors represent the seasonal averages of the altimetric currents on the simulated dates (one vector out of two is plotted in both dimensions). (c) Late winter and (d) summer average of the SMAP SSS gradient magnitude, only considering observations on the simulated dates. Cyan solid line in (a) and (b) shows the 200-m isobath representative of the shelfbreak position. Red and blue dashed lines in (c) and (d) represent the Gulf Stream mean position in late winter and summer, respectively, approximated as the 0.5-m isoline of the seasonally averaged absolute dynamic topography. SMAP, Soil Moisture Active Passive; SSS, sea surface salinity.

Figure 10. (a) SSS from the global ocean model on February 12, 2017, (b) temporal average of the model SSS, (c) temporal average of the model SSS gradient magnitude, (d) standard deviation of the model SSS in bins of $0.75^\circ \times 0.75^\circ$ and (e) in bins of $0.24^\circ \times 0.24^\circ$. To infer statistics, we only consider the model outputs on the SMAP reconstructed dates. The cyan solid line shows the 200-m isobath, representative of the shelfbreak position. The cyan dashed line represents the mean position of the Gulf Stream, approximated as the 0.5-m isoline of mean dynamic topography.

hence the salinity variability, would decrease there (Figure 8b). Outside the Gulf of Maine, the fresher water continues propagating following the equatorward shelfbreak current into the Middle Atlantic Bight, where the salinity variability increases. At Cape Hatteras, the fresher water is advected northeastward by the Gulf Stream, increasing the salinity variability at the Gulf Stream north wall. Hence, the increase of small-scale salinity variability in summer west of 70°W is related to stronger horizontal gradients of SSS in summer (Figure 9d), while in the Gulf of Maine the large-scale SSS gradients are stronger in late winter (Figure 9c). Overall, regions with moderate to strong SSS gradients are characterized by high small-scale salinity variability. We hypothesize that the seasonal cycle of this variability is mainly driven by the seasonal cycle of the large-scale SSS gradients. Based on altimetry maps, the Gulf Stream location and intensity are nearly the same in summer and late winter (Figures 9a and 9b), so it is likely that seasonal differences in currents are not responsible for the seasonal differences in small-scale SSS variability near the Gulf Stream (the southern band of high variability around 38°N). Hence, the annual cycle of large-scale salinity gradients, as observed from SMAP, are the source of the seasonal cycle of the small-scale salinity variability detected in the reconstructed salinity fields at scales shorter than ~ 25 km.

4.3. Comparing the Reconstructed Fields With a Global Ocean Model

A comparison between the reconstructed SSS field and the SSS field from the CMEMS global ocean model (S_{adv} and S_{model} , respectively) on February 12, 2017 reveals similarities and differences between both fields (Figures 1c and 10a). For instance, north of Cape Hatteras the reconstructed and the modeled SSS fields represent the fresher shelf waters advected to the north wall of the Gulf Stream, a feature that has been

widely documented by other authors (e.g., Ford et al., 1952; Gawarkiewicz & Linder, 2006) but not captured by SMAP observations (Figure 1a). However, S_{model} has less structure than S_{adv} and is also different from the original SMAP SSS field. Note that the CMEMS model assimilates vertical profiles of salinity but does not assimilate satellite SSS observations. The reason for this mismatch between both fields could be the low resolution of the in-situ profiles assimilated by the model. An interesting difference between the model data and the original SMAP field is the low variability that S_{model} has in the Sargasso Sea, consistent with the low SSS variability observed in situ by the thermosalinograph. This comparison suggests that the assimilation of SMAP SSS may improve the global ocean model near the coast, but would introduce unrealistic high variability offshore of the Gulf Stream.

To extend this comparison, Figures 10b and 10c show the temporal average of S_{model} and the temporal average of the gradient magnitude of S_{model} , considering only the reconstructed dates for consistency with the SMAP statistics shown in Figure 7. The temporal average of S_{model} has fresher water along the coast than the salinity measured by SMAP. As a consequence, S_{model} has stronger horizontal gradients from the coast to the Gulf Stream mean position.

In addition, we have computed the modeled SSS variability in bins of $0.75^\circ \times 0.75^\circ$ and in bins of $0.24^\circ \times 0.24^\circ$ (Figures 10d and 10e), as is done for S_{adv} in Figure 6. The salinity variability calculated in bin sizes of $0.75^\circ \times 0.75^\circ$ (Figure 10d) has a similar distribution as the reconstructed salinity variability (Figure 6b). However, the modeled field has lower variability than S_{adv} along the north wall of the Gulf Stream. This difference is also observed in the small-scale salinity variability: S_{adv} has high values of small-scale variability along the north wall of the Gulf Stream and along the shelfbreak (Figure 6c), while S_{model} only has high small-scale variability along the shelfbreak (Figure 10e). The Lagrangian reconstruction captures more small-scale variability than the model because the space/time scales of the satellite SSS fields are higher than the data that are assimilated into the model.

5. Conclusions and Discussion

In this study, we have investigated for the first time a Lagrangian reconstruction technique to extract signals with high-spatial resolution from SMAP SSS observations in the northwest Atlantic Ocean (Figure 1), a region strongly influenced by the Gulf Stream and characterized by large-scale salinity gradients. The Lagrangian reconstruction method consists of advecting the SMAP SSS field, gridded with a resolution of $1/4^\circ$ and with an effective resolution of 70 km, using currents from satellite altimetry with a resolution of $1/4^\circ$. The horizontal stirring of the large-scale salinity field by the time-varying altimetric currents integrated over time generates a reconstructed salinity field with realistic small-scale salinity variability (defined here as scales smaller than ~ 25 km) from the continental shelf to the Gulf Stream.

To evaluate our method, we compared the reconstructed, high-resolution SSS field to in-situ thermosalinograph data from the Oleander project. This comparison demonstrated that near the Gulf Stream the reconstructed SSS fields have realistic enhanced small-scale variability compared to the original low-resolution SMAP field. We detected fronts on scales between 5 and ~ 50 km along each ship transect and for each field, showing that the reconstructed SSS field represents more fronts and with higher intensity than SMAP observations (Figure 4). Comparing with fronts detected from in-situ data, reconstructed SSS represents realistic salinity fronts from the United States east coast to the Gulf Stream along the thermosalinograph path. However, the probability of detection of salinity fronts from the reconstruction is slightly too low on the continental shelfbreak, and the intensity of fronts near 38°N (the Gulf Stream north wall) is also underestimated (Figure 4). In the Sargasso Sea, the SMAP SSS observations show higher variability than the in-situ observations (Figure 3) and this is reflected in the higher probability of fronts detected from the reconstructed SSS field. The unrealistic salinity fronts generated by the reconstruction are thus a result of unrealistic SMAP variability. Note that in this study we consider gridded SMAP data; however, along-track (Level 2) SMAP data would show fronts that are smoothed over in the gridded product. Due to SMAP technical implementation, daily along-track Level 2 data have high levels of noise and would have introduced spurious signals into the reconstructed fields, so were not used for this study. The product used for the reconstruction is the 8-days running mean gridded product with an effective spatial resolution of 70 km, as it has significantly lower noise (Meissner et al., 2019). In addition, it should be pointed out that previous studies in this

region have applied different detection methods to identify fronts in satellite SST observations. To evaluate those methods, Ullman and Cornillon (2000) and Chang and Cornillon (2015) applied an along-track gradient algorithm to detect fronts in Oleander temperature observations similar to the method used here to detect fronts in salinity. In future work, some of the methods already developed to detect fronts in SST could be adapted to detect fronts in the 2D reconstructed SSS fields. As an application, the fronts detected in the reconstructed SSS could be compared to those detected in satellite SST observations.

The reconstruction technique has been applied to weekly fields of SMAP SSS observations to evaluate the small-scale salinity variability in the northwest Atlantic Ocean. Higher values of the small-scale salinity variability averaged over time are concentrated in two bands (Figure 6): a northern band aligned with the shelfbreak front characterized by strong large-scale gradients of SSS (inferred from SMAP observations), and a southern band aligned along the western side of the Gulf Stream mean position (Figure 7). In the northern band, the horizontal stirring of the preexisting strong large-scale salinity gradient by (i) meanders and eddies detached from the Gulf Stream and (ii) shelfbreak currents, generates small-scale salinity variability. At the southern band around 38°N, the strong small-scale salinity variability is caused by (i) the salinity front generated along the Gulf Stream north wall resulting from fresher shelf water advected by the Gulf Stream currents at Cape Hatteras (Ford et al., 1952; Gawarkiewicz & Linder, 2006), and (ii) the horizontal stirring of the preexisting moderate large-scale salinity gradient and of the reconstructed salinity front by the time-varying Gulf Stream currents. Note that the two regions with high-intensity fronts detected from in-situ and advected salinity fields (Figures 4d and 4e, respectively) correspond to the two bands of strong small-scale salinity variability. A comparison with a global ocean model reveals the limitations of the modeled SSS to represent small-scale variability in the southern band. This may be because the space/time scales of the satellite SSS fields are higher than the salinity observations that are assimilated into the model. The assimilation of SMAP SSS observations into the model would likely improve this representation; however, it might introduce unrealistic variability in the Sargasso Sea.

The analysis of the seasonal cycle of the small-scale salinity variability reveals differences in both seasonal and spatial patterns (Figure 8). In the Gulf of Maine, the small-scale salinity variability is higher in late winter, while it is enhanced in summer north of 35°N and west of 70°W in the Middle Atlantic Bight and at the Gulf Stream north wall. The seasonal cycle of the small-scale salinity variability is mainly driven by the seasonal cycle of the large-scale SSS gradients observed with SMAP (Figure 9). The Gulf Stream location and intensity, based on altimetry maps, are nearly the same in summer and late winter, suggesting that seasonal differences in currents are not responsible for the seasonal differences in small-scale salinity variability near the Gulf Stream. The seasonal differences observed in large-scale SSS gradients are related to the freshening of the coastal waters in the Gulf of Maine resulting from elevated river outflow in spring and summer (Feng et al., 2016; Geyer et al., 2004). In the Gulf of Maine, the gradients are higher in late winter because the fresher water from river outflow is starting to spread along the Gulf (Figures 9a and 9c). After the fresher water is spread throughout the Gulf in summer, the large-scale salinity gradients are weaker there, but enhanced along the shelfbreak where the water is advected (Figures 9b and 9d). Near the coast, the shelfbreak current transports the fresher water equatorward to Cape Hatteras, where the Gulf Stream advects the fresher water northeastward, generating strong salinity gradients west of 70°W and north of 35°N. In summary, the region with highest small-scale salinity variability in the northwest Atlantic Ocean has a seasonal cycle related to gradients in large-scale SSS induced by the freshening of the coastal waters due to river outflow in spring and summer in the Gulf of Maine, the southwestward spreading of this fresher water along the coast, and the northeastward advection along the Gulf Stream north wall. In general, regions with moderate to strong SSS gradients are characterized by strong small-scale salinity variability, and the seasonal cycle of this variability is mainly driven by the seasonal cycle of the large-scale SSS gradients. This suggests that maps of large-scale horizontal SSS gradients such as those that can be estimated from SMAP enable us to determine which regions may have higher small-scale salinity variability generated by horizontal advection of mesoscale currents. In addition, specific intrusion events can also contribute to increase the small-scale salinity variability. For instance, Grodsky et al. (2018b) describe an increase of surface salinity in the Gulf of Maine in winter 2017–2018 related to a salty feature coming from the Grand Banks and entering the Gulf of Maine after interacting with mesoscale structures detached from the Gulf Stream. This intrusion of salty water would induce small-scale salinity variability; the repetition of this type of event in winter would significantly increase the small-scale salinity variability in this season in the Gulf of Maine.

The Lagrangian reconstruction method applies realistic lateral stirring to the initial salinity SMAP observations. The reconstruction at small scales depends on the accuracy of the SMAP observations. For instance, in the Sargasso Sea SMAP detects higher SSS variability than shown by in-situ observations, generating unrealistic high small-scale salinity variability in the reconstruction. In addition, the reconstruction method can be applied to SSS fields with coarse resolution but still retaining enough information to reconstruct small scales. The 70-km SMAP SSS gridded product has been proven to preserve enough initial SSS variability to perform the reconstruction. Quantifying the extent to which the initial SSS fields can be smoothed while still retaining enough variability for the reconstruction could be explored through observing system simulation experiments. The reconstruction also depends on the horizontal currents used to advect the large-scale SSS field. By using altimetric currents, we analyze the role of mesoscale geostrophic stirring on the generation of small-scale salinity variability. Hence, the impact of other physical processes, such as mixing and Ekman transport, is excluded. As a consequence, the representation of fine-scale tracer variability is reliable in regions dominated by large-scale balanced motions and hence well resolved by altimetry (Dencausse et al., 2014; Lehahn et al., 2018; Rogé et al., 2015). However, even in that case, the uncertainty in altimetry-derived currents is inherited by the reconstructed fields and it translates in an offset of the position of reconstructed small-scale features with respect to those detected from in-situ observations. Because of the limitations of the reconstruction method, to extend this analysis to other regions the reconstructed fields should be compared with in-situ observations and the specific limitations of this method in that region should be evaluated. In addition, other current products include additional components of the flow to the altimetric currents (e.g., GlobCurrent, OSCAR). OSCAR (Ocean Surface Current Analysis Real-time) is a global product that combines satellite and in-situ observations of sea surface height, surface vector wind and sea surface temperature to estimate horizontal currents (<https://www.esr.org/research/oscar/oscar-surface-currents/>). We tested the reconstruction of salinity using OSCAR currents and found that the reconstructed fields were similar but smoother than the ones obtained from altimetric currents due to the lower resolution of the OSCAR velocity field ($1/3^\circ$). The next generation of satellite missions (e.g., SWOT, WaCM; Chelton et al., 2019) will provide surface horizontal velocities with high-spatial resolution that may increase the accuracy of the small-scale salinity variability reconstructed from SMAP.

Data Availability Statement

SMAP salinity data are produced by Remote Sensing Systems and sponsored by the NASA Ocean Salinity Science Team. SMAP SSS fields can be download at https://podaac.jpl.nasa.gov/dataset/SMAP_RSS_L3_SSS_SMI_8DAY-RUNNINGMEAN_V4, and the altimetric currents at the CMEMS website (<http://marine.copernicus.eu>). The mean dynamic topography can be downloaded from Aviso at <https://www.aviso.altimetry.fr/en/data/products/auxiliary-products/mdt.html>. OceanParcels is freely available at <https://oceanparcels.org>. Model outputs from the CMEMS global ocean physics reanalysis product can be downloaded at https://resources.marine.copernicus.eu/?option=com_csw&view=details&product_id=GLOBAL_REANALYSIS_PHY_001_030 and from the global ocean physics analysis and forecast product at https://resources.marine.copernicus.eu/?option=com_csw&view=details&product_id=GLOBAL_ANALYSIS_FORECAST_PHY_001_024. The reconstructed SSS fields are available at <https://doi.org/10.20350/digitalCSIC/12830> (Barceló-Llull et al., 2020).

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