Matchup Characteristics of Sea Surface Salinity using a High-resolution Ocean Model

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Abstract: Sea surface salinity (SSS) satellite measurements are validated using in situ observations 8 usually made by surfacing Argo floats. Validation statistics are computed using matched values of 9 SSS from satellites and floats. This study explores how the matchup process is done using a high-10 resolution numerical ocean model, the MITgcm. One year of model output is sampled as if the 11 Aquarius and Soil Moisture Active Passive (SMAP) satellites flew over it and Argo floats popped 12 up into it. Statistical measures of mismatch between satellite and float are computed, RMS difference 13 (RMSD) and bias. The bias is small, less than 0.002 in absolute value, but negative with float values 14 being greater than satellites. RMSD is computed using an "all salinity difference" method that av-15 erages level 2 satellite observations within a given time and space window for comparison with 16 Argo floats. RMSD values range from 0.08 to 0.18 depending on the space-time window and the 17 satellite. This range gives an estimate of the representation error inherent in comparing single point 18 Argo floats to area-average satellite values. The study has implications for future SSS satellite mis-19 sions and the need to specify how errors are computed to gauge the total accuracy of retrieved SSS 20 values. 21

Keywords: Surface salinity, ocean modelling, representation error, satellite validation, matchups

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1. Introduction

Since 2009, three satellite missions have been launched to measure sea surface salin-25 ity (SSS), Soil Moisture and Ocean Salinity (SMOS) from the European Space Agency, 26 Aquarius from NASA/SAC-D and Soil Moisture Active Passive (SMAP) also from NASA. 27 These missions utilize sun-synchronous polar orbits with high inclinations, but differing 28 spatial and temporal resolutions, and have provided continuous SSS measurement cov-29 erage of the global ocean [1]. They all measure ocean brightness temperature at 1.4 GHz 30 (L-band) which can be converted to SSS, a process known as retrieval [2,3]. The specifica-31 tions for each of the missions is nicely summarized by [4] (their Figure 2). In terms of 32 spatial (temporal) resolution, it is about 60 km (3 days) for SMOS, 100 km (7 days) for 33 Aquarius and 40 km (2-3 days) for SMAP. 34

In order to gauge the accuracy of the satellite measurements of SSS, they are often 35 compared to measurements taken in situ by instrumentation, a process known as validation. These may take the form of comparisons with gridded Argo products such as that of 37 [5] or [6] ([2,3,7-12]). There may also be comparisons with individual observations such 38 as floats, saildrones, thermosalinographs or moorings [8-10,13-20]. Comparisons may be 39 done using satellite data at level 2 (L2) (e.g. [8,9,13]) or level 3 (L3) (e.g. [15]). 40

In general, in situ measurements of SSS are sparse compared to satellite measurements. For comparison at L2, in a typical year, the Aquarius satellite made 30 million L2 42 observations of surface salinity versus almost 100,000 observations from Argo floats, 43 amounting to on average over 200 Aquarius L2 satellite observations for each Argo one. 44

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One has to keep in mind here the mismatch in scale between in situ observations, which 45 are usually made at a single point in space and time, and satellite observations, which are snapshot averages over a footprint. This introduces a representation issue inherent in the comparison of satellite and in situ observations [21-24].

The details of the validation done in the numerous studies cited above differ, and the 49 results may depend on these details. One important detail the present study focuses on 50 for L2 validation is how matchups are done between individual in situ observations and 51 L2 satellite measurements for the purpose of comparison between them. That is, within 52 the validation process, how are satellite and in situ observations matched together to form 53 comparisons? [25] discussed some ways this can be done. The one we explore here is their 54 "ASD", or "all salinity difference", which averages all satellite observations within a 55 space-time window to form one comparison value for each in situ observation. Other pos-56 sibilities include taking the closest point in space, or time, or some weighted combination 57 of space/time; or computing salinity difference with all available L2 observations and no 58 averaging. Within the ASD method, the main parameters are the spatial and temporal 59 search windows used for finding and averaging matchup values. In a couple of validation 60 studies done using L2 satellite measurements and the ASD method [8,9,13] Argo float 61 measurements are compared with averages of many L2 satellite values (Table 1) but there 62 is no exploration of how differences may depend on spatial or temporal search window 63 from which these averages are computed. 64

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Table 1. Matchup criteria for three of the studies referenced.

| Reference | Comparison |
|-----------|--|
| [13] | L2 compared to Argo within 12h and 200 km |
| [8,9] | Searched for the closest point of approach (CPA) of the satellite to each Argo float. Time window +-3.5 days and space window 75 km. 11 L2 samples aver- aged with the float value. |

In this paper we do some of the exploration that [25] have started. Our main tool is a 68 high-resolution $(1/48^{\circ})$ ocean model as described below, with the assumption that the 69 model simulates the upper ocean's spatial and temporal variability well enough to make 70 valid conclusions about the matchup criteria we are studying. [26] found that the model 71 we use adequately simulated the ocean submesoscale as a part of the global heat budget. 72 Beyond that, the large advantage of using a model over real data is that there is no re-73 trieval error associated with obtaining L2 estimates from a model. That is, any differences 74 between simulated satellite and simulated float values are the result of representation er-75 ror, not errors in the corrections needed to put out actual SSS measurements as detailed 76 by, for example, [2]. Thus, to the extent that the model does simulate the real upper ocean 77 variability, the statistics we compute below can be considered as an estimate of represen-78 tation error as well. 79

So, we will examine the space-time window for doing matchups. How large should 80 that window be? Does time matter more than space? How sensitive are the comparison 81 statistics, bias and RMSD (root mean square difference), to the choices made? As the 82 space-time window decreases, and fewer L2 observations are included in the comparison, 83 the variance of the set of L2 observations increases, and thus one might expect larger de-84 viations from a comparison Argo float. On the other hand, as the space-time window in-85 creases, one would expect float measurements to depart further from the satellite meas-86 urements as there is a greater chance of the float finding itself within a larger scale SSS 87 field that varies. Thus, there may be a space-time window to use for doing validation 88 studies which minimizes the mismatch. [25] found such a result using real in situ and 89 satellite data. At the very least when considering the errors in SSS remote sensing, one 90 should be aware of these tradeoffs and how they might impact the total error. 91

The issues studied here especially pertain to potential new SSS satellite missions. For 92 new missions (or even existing ones) it is essential to not only characterize the error structure properly, but to specify how the errors are to be computed. Requirements for satellites are determined before launch (e.g. [27]). The extent to which the final mission can adhere to these requirements, as we will see in this paper, depends on the details of how 96 the errors are computed. 97

2. Data and Methods

We make use of a high-resolution numerical model to study matchup tradeoffs. This 99 is done by simulating Argo and L2 satellite observations. The model SSS field was taken 100 from the evaluation time period, 1 November 2011 to 31 October 2012. 101

2.1 *Observations*

2.1.1 L2 Aquarius

We use Aquarius L2 observations [28,29]. We used only Aquarius L2 observation 105 points with land fraction less than 0.5%, and only those that were between 68°S and 54°N, 106 according to the limits of the model. There were about 27 million Aquarius L2 observations during our one-year study period. We use mainly just the tracks, not the actual observations, though one week of real satellite observations is shown in Figure 1b. 109

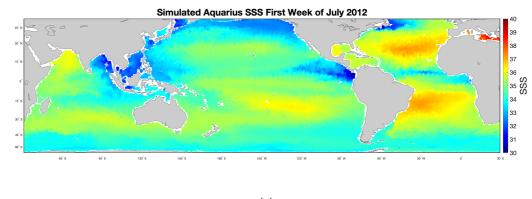
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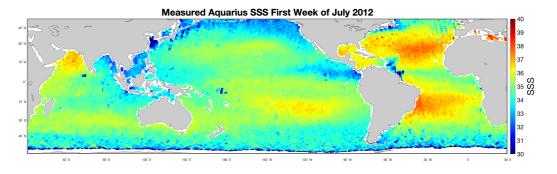
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(b)

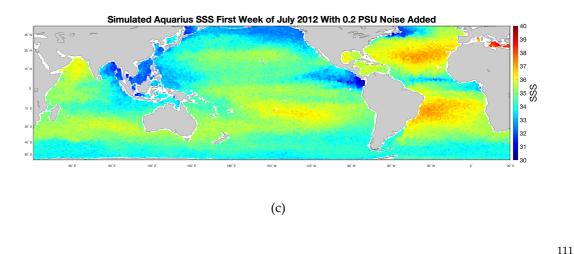


Figure 1. Aquarius L2 SSS observations during the first full week of July 2012. a) Simulated values from the model. b) Measurements from the Aquarius satellite. c) Simulated values from the model with gaussian random noise added with a standard deviation of 0.2. Color scale is at right for each panel.

Aquarius had 3 parallel beams along the satellite track [28,30], sampled every 1.44 113 seconds. Figure 2a shows a single Argo float observation and a set of matching Aquarius 114 tracks and L2 samples. A single ascending satellite pass, with three beams, is seen going 115 southwest-northeast in the figure, with the float observation situated between two of the 116 beams. The total coverage in 7 days, and 2 days, surrounding a float observation is in-117 cluded in the figure. Also seen are the observations within 2 days and a 200 km radius. It 118 is the green points in the figure that would be averaged together to get a single value to 119 compare with the float observation at the 2 day / 200 km search window. The particular 120 float observation shown, from the North Atlantic poleward of the subtropical SSS maxi-121 mum, is in a region where SSS increases to the north by about 0.2-0.4 within the 200 km 122 sample radius (Figure 2b). The distribution of SSS within the 200 km radius has a typical 123 long low tail and sharp cutoff on the high side (Figure 2c; [31]). The (ASD) mean value of 124 SSS from those L2 observations (black line in Figure 2c) is lower than the float value (red 125 line) by about 0.1. The same computation can be done with all the available simulated 126 Argo floats and combined to get an RMS difference as will be displayed below. 127

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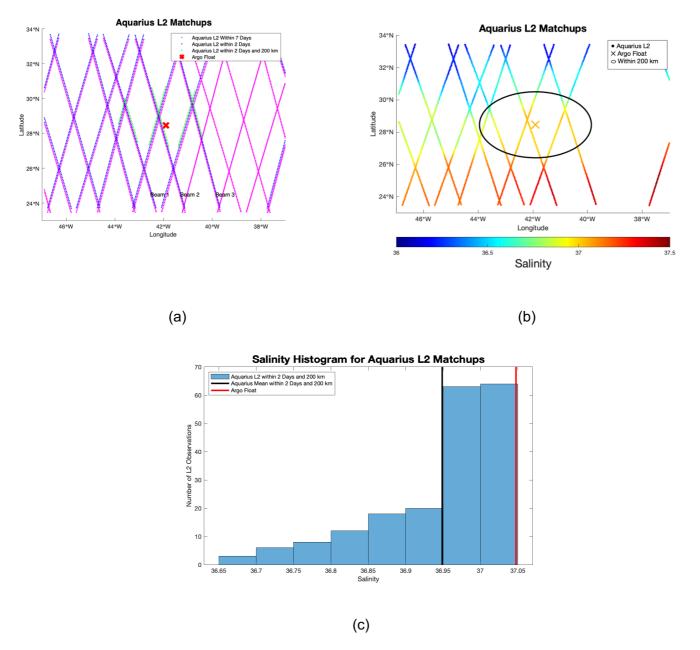
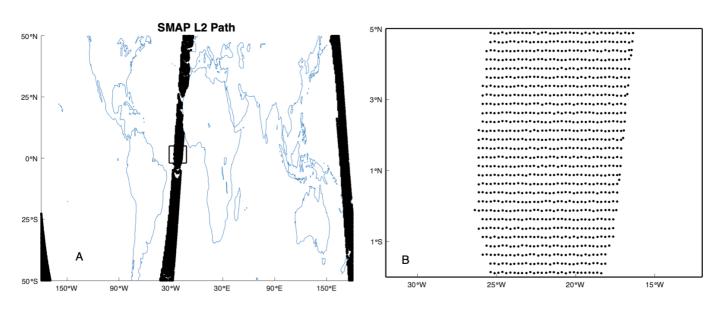


Figure 2. a) Red "X": Argo float that surfaced at the indicated point on 28 Nov 2011 at 10:10:33. Magenta symbols: Aquarius L2 129 observations within 7 days and 5° of the float. Blue symbols: Aquarius L2 observations within 2 days and 5° of the float. Green 130 symbols: Aquarius L2 observations within 200 km and 2 days of the float. Beams are indicated with black text. Blue and green 131 symbols are shifted slightly for clarity. b) "X": The same Argo float colored by model salinity with the scale at the bottom of the 132 plot. Small circular symbols: Aquarius L2 observations within 2 days and 5° of the float, colored by salinity with the scale at the 133 bottom of the plot. Black ellipse shows the area within 200 km of the float. c) Histogram of simulated Aquarius L2 salinity within 2 134 days and 200 km of the Argo float from panel a). The mean of the simulated Aquarius L2 values is shown in black and the s 135 lated float SSS value is shown in red. 136

2.1.2 L2 SMAP

We also extracted the L2 observation points from the SMAP data [32]. SMAP was not139launched until 2015. Since our evaluation time period was 2011-2012 -- that is the period140model output was available for -- we simply subtracted 4 years from the time of each141SMAP L2 observation to match the time span of the model. We do not use the actual sat-142ellite SMAP L2 observations in this study, only their locations and times. Thus, the SMAP143tracks we used were from the 1 November 2015 - 31 October 2016 time frame. There were144

about 142 million observations. The SMAP L2 dataset is much larger than Aquarius one 145 because it is collected in a different way. SMAP data are averaged onto an approximately 146 25 km X 25 km grid that surrounds the nadir point of the satellite track (Figure 3). There 147 are two standard versions of the SMAP data, the JPL (Jet Propulsion Laboratory) and RSS 148 (Remote Sensing Systems), with differently structured L2 grids. We chose to use the RSS 149 version [32], shown in Figure 3. Similar to Aquarius, we used only observation points with 150 land fraction <0.5% and between 68°S and 56°N. (The limits are slightly different for 151 SMAP than for Aquarius because of the way the L2 simulation is done.) 152



(a)

(b)

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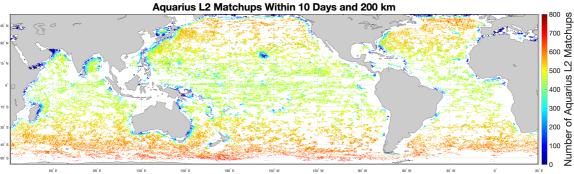
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Figure 3. a) A sample path of the SMAP satellite showing the locations of L2 observations for one swath. b) A zoomed in view showing the L2 observation grid from a small box near the equator indicated in panel a).

2.1.2 Argo

The Argo data we used were downloaded from the Argo data assembly center at the 159 National Centers for Environmental Information for the evaluation time period. We used 160 only the locations and times of the float surfacings, not the measurements themselves. 161 However, to make sure we had a good dataset, we only made use of Argo data where the 162 salinity quality flag had a value of "1", and the shallowest observation was at 10 dbars 163 pressure or less. The Argo dataset has about 98,000 observations (Figure 4). 164



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2.2 The MITgcm

The model we use is the MITgcm, the ocean general circulation model from the Mas-170 sachusetts Institute of Technology. The model is on a latitude-longitude polar cap (LLC) 171 grid, between the latitudes of 70°S and 57°N. We use the LLC4320 version with a nominal 172 horizontal spacing of 1/48° forced by 6-hourly surface atmospheric fields from the 173 ECMWF (European Centre for Medium-Range Weather Forecasting) operational atmos-174 pheric analysis [26]. There are about 14 months of model output available, but we use 175 exactly one year, the evaluation time period, 1 November 2011 to 31 October 2012. Our 176 analysis is with hourly output, though the model has a shorter time step than that. The 177 model is free-running: it does not assimilate any ocean data. 178

Figure 4. Locations of float observations used in this study. Colors indicate the number of Aquar-

ius L2 observations within 10 days and 200 km of each float with scale at right.

2.3 Simulation Data

The satellite and Argo observations were simulated from the model using the track and float surfacing data described above.

2.3.1 Simulated Satellite L2

The model was sampled as if the satellite were flying over it. We took the L2 tracks 185 from the Aquarius and SMAP satellites (e.g. Figures 2 and 3) and superimposed them on 186 the model. For Aquarius, the footprint is about 100 km in diameter [30], and each L2 observation is a weighted average with half-power point at 50 km radius from the center of 188 the footprint. SMAP SSS L2 values are similar, with a 20 km footprint radius [2].

At every point in time and space where there was a satellite L2 observation of SSS, 190 we created a simulated one at the closest hourly model time step. This was done by looking at a 100 km (40 km for SMAP) distance surrounding each L2 observation, the light and dark blue areas in Figure 5. We took all of the model grid points within that area (the "evaluation region") and computed a Gaussian-weighted average of those points, 194

$$S_{L2} = \frac{\sum_{C} w_i S_i}{\sum_{C} w_i} \tag{1}$$

where Si is the set of gridded model SSS values (located at the red dots in Figure 5)195within 100 km (40 km for SMAP) of the L2 observation point. Si2 is the simulated L2196value at the same point (yellow dot). The summation, C, is done over the set of model197grid points within the evaluation region, i.e. the red dots within the light and dark blue198areas in Figure 5. The wi are weights given by199

$$w_i = e^{-\ln(2)(d_i/d_0)^2},$$
(2)

where d_i is the distance between the L2 observation point and each model grid node and d_0 is 50 km (20 km for SMAP), the footprint radius. The weighting function is such that its value is 0.5 at a distance equal to the footprint radius. 202

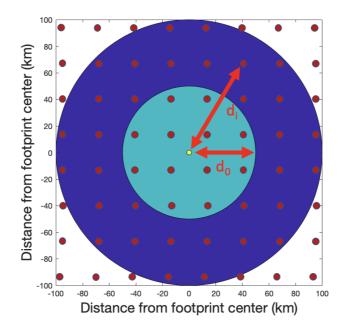


Figure 5. Diagram showing how the L2 simulation is done for the Aquarius satellite. The yellow dot in the center is the location of an L2 observation. The red circles are example model grid nodes - the ones from the actual model are much more densely packed. do is the footprint radius, 50 km. 206 d_i is the distance from the evaluation point to a sample model grid node used in the computation 207 of w_i in equation (2). The light blue region is the 100 km diameter footprint. The darker blue region 208 contains more model grid nodes used in the computation of the simulated value. The summation, 209 C, in equation (1) is over all model grid nodes within the light and dark blue regions. 210

Figure 1a and b compare one week of model output with one week of real Aquarius 211 observations. One can see there are differences in the details - there is no expectation that 212 these would match exactly as no ocean data are assimilated by the model. The simulated 213 fields are smoother and less noisy, especially at high latitudes. However, the basic features 214 of the real data are reflected in the simulated data, the high SSS subtropical regions in each 215 ocean basin, the eastern Pacific fresh pool, the contrast in SSS between Atlantic and Pacific 216 basins, etc. The high SSS subtropical regions in all the ocean basins are saltier in the meas-217 ured values than the model, as well as fresh regions such as the eastern Pacific fresh pool, 218 western Pacific, South China Sea and Bay of Bengal. A big difference between the panels 219 is that the low SSS signature of the Amazon outflow in the real observations is almost 220 absent in the model. This is likely because the model uses monthly climatological runoff 221 values from [33] for river input [34] which may be very different from the actual discharge 222 of the Amazon in July 2012. 223

2.3.2 Simulated Argo

In addition to the simulated satellite data, we put together a simulated Argo dataset. 226 We took all the Argo data described above and sampled the model as if the float had 227 popped up to the surface at its designated time and location. That is, we sampled the 228 model at the closest grid node and hourly value to that of each float. 229

2.4 Matchups

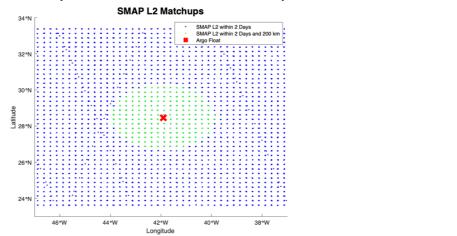
To study matchup criteria, we used an ASD approach as described above [25]. That 232 is, we matched each individual float measurement with some set of L2 observations. The 233 L2 observations were taken within a given time and space window and averaged to form 234 one value for comparison. For example, Figure 2a shows the set of matchup satellite ob-235 servations for one particular float at a distance of 200 km and a time of 2 days - the green 236 symbols. Figure 6 shows a similar set of matchup values for SMAP. The time window 237

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indicates a total before and after difference. That is, a time window of 5 days indicates all 238 data from 5 days before the float observation to 5 days after. 239

Figure 6. Red "X": Argo float depicted in Figure 2. Blue symbols: SMAP L2 observations within 2241days and 5° of the float. Green symbols: SMAP L2 observations within 200 km and 2 days of the242float.243

Figure 4 shows the number of matchups for each Argo float for the loosest criterion 245 (10 days and 200 km). This is the number of L2 observations averaged together to form a 246 comparison value for each float. The number mainly depends on latitude, and is smaller 247 at low latitudes. Near coastlines and islands, the number is lower. This is due to the land 248 fraction criterion used to filter the L2 observations - the closer one is to land, the fewer 249 valid L2 observations there are. At high latitudes there are more matchups per float. This 250 is because the satellite tracks tend to get closer together and denser with increasing lati-251 tude. 252

The averages were used to compute statistical measures of offset: RMSD (root mean square difference) and bias (mean difference). That is, the RMSD is the RMS of the differences between the ~98,000 individual Argo measurements and the matched set of averaged L2 satellite measurements. 256

The median number of satellite L2 observations averaged together per float as a func-257 tion of search radius and time window is shown in Figure 7a and b. As expected, the 258 number increases with both distance and time from about 600 (2400) for Aquarius (SMAP) 259 to near zero at short time and space windows. Comparing the color scales for Figure 7a 260 and b, it is seen that the number of L2 observations per float for SMAP is 4-5 times that 261 for Aquarius. This is a result of the different sampling strategies of the two satellites 262 shown by comparing Figures 2 and 6. The rotating antenna and trochoidal sampling pat-263 tern of SMAP yields more samples than the fixed antenna swath of Aquarius [4]. 264

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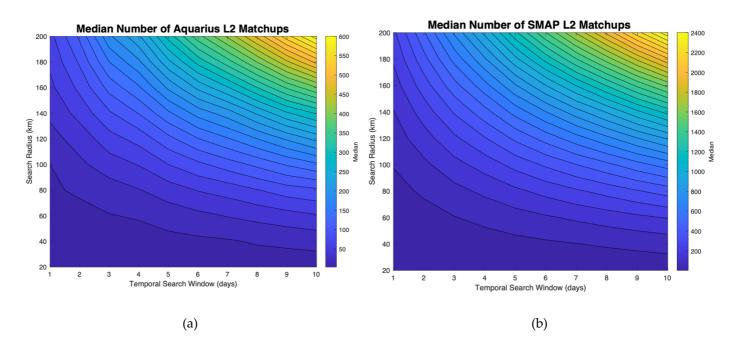
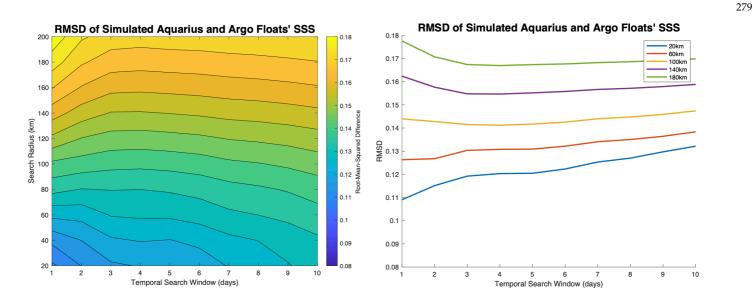


Figure 7. a) Median number of Aquarius L2 observations per Argo float for a given temporal search window (x-axis) and search radius (y-axis). Contour lines are drawn at intervals of 20, with the lowest one having a value of 20. b) Same for SMAP but with contour lines drawn at intervals of 75, with the lowest one having a value of 75. Note different color scales for each panel.

3. Results

The RMSD between simulated float and Aquarius (Figure 8a,b) shows the tradeoff between time and space search windows. For search radius less than 60 km, RMSD increases continuously as a function of time window (blue and red curves in Figure 8b). 272 However, for search radius greater than 60 km, there is a small decrease in RMSD as a 273 function of time window until the RMSD reaches a minimum somewhere around 3 days 274 (yellow, purple and green curves in Figure 8b). The RMSD then increases again. Another 275 way of saying this is that above 60 km search radius contour lines in the figure slope up-276 ward for a short time window, and then downward for a time window longer than 3 days. 277 This characteristic becomes clearer with increasing search radius. 278



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(a)

Figure 8. a) RMS difference between simulated Argo float and average of simulated Aquarius L2 280 observations for a given temporal search window (x-axis) and search radius (y-axis). b) The same 281 RMS difference plotted as a function of temporal search window for 5 given search radii. 282

(b)

This minimum RMSD at about three-day time window is the result of a tradeoff. With 284 a short time window there are fewer measurements to average together to make reliable 285 estimates. For a long time window there is time variability in the SSS field that generates 286 differences between in situ and satellite values [25]. The three-day time frame appears to 287 be just close enough to a snapshot with enough satellite measurements to make a reliable 288 average. There is no such ideal window in space. At every time window, RMSD increases 289 as a function of search radius. The search radius with the smallest RMSD is the one that is 290 as small as possible. This analysis shows how the value of RMSD between satellite L2 and 291 in situ data can vary depending on the search windows chosen. 292

The RMSD for SMAP (Figure 9a,b) shows similar values as for Aquarius - the color 293 scales are the same for both figures - though the RMSD values at short spatial window are smaller for SMAP. The main difference for SMAP is that the minimum RMSD is at 2 days instead of 3 (yellow, purple, and green curves in Figure 9b), and is not as strong a 296 minimum as for Aquarius. One would guess that the shorter time window for this mini-297 mum for SMAP is simply a result of having more data to produce reliable averages.

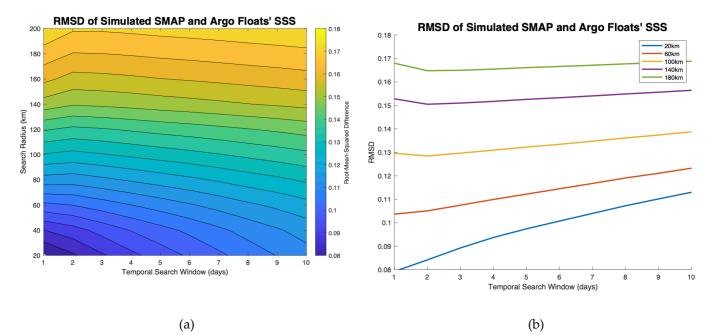


Figure 9. a) As in Figure 8a, but for SMAP. b) As in Figure 8b, but for SMAP.

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We computed bias for all the observations. The numbers were consistently negative, 302 meaning floats tend to take on higher values than the satellites on average. Though nega-303 tive, the bias was very small, generally less in absolute value than 0.002. We omit these 304 plots for brevity. The fact that float SSS tends to be greater than satellite values is a conse-305 quence of the common negatively skewed distribution of SSS (e.g. Figure 2c; [31]) as ex-306 plained at length by [24]. 307

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As another approach, we computed the RMSD in a different way. Given the short 308 spatial scales of SSS [35] we computed the ASD comparison mean L2 satellite value using 309 a weighted average instead of a simple one. The weighting is given by a Gaussian drop-310 off with distance from the comparison Argo float, 100 km for Aquarius and 40 km for 311 SMAP, the same function shown in equation (2). The RMSD for Aquarius (Figure 10a) 312 shows a different pattern than the non-weighted one for larger spatial window. At dis-313 tances beyond about 100 km, the RMSD shows little dependence on spatial window size. 314 For a window less than 100 km, the RMSD is very similar to that computed with no 315 weighting (Figure 8a). For SMAP, the results are a little different (Figure 10b). The 316 weighted RMSD is much smaller than the non-weighted (Figure 9a,b), and dependence 317 on spatial window size almost disappears. 318

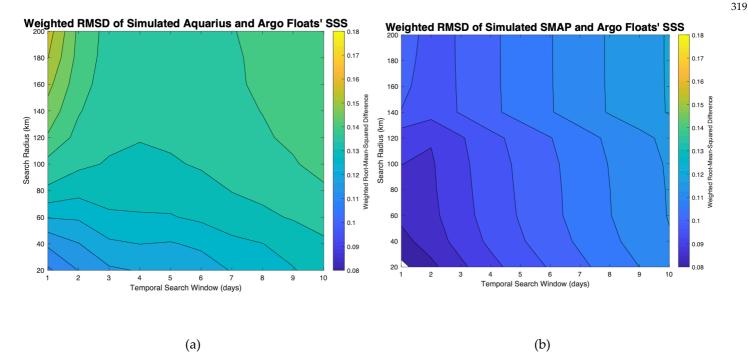


Figure 10. a) As in Figure 8a, but using gaussian weighting as described in the text. b) The same as panel a) but for SMAP. 321

The simulated L2 satellite values we have been using come with no "retrieval error". 322 That is, the real satellite observation includes all the errors associated with converting raw 323 brightness temperatures into a value of SSS, roughness corrections, galactic noise, etc. 324 [2,3,30] The simulated values do not contain any of that, only representation error as dis-325 cussed above. For that reason, we wanted to see what impact adding noise to the input 326 data would do to the computed RMSD. Two experiments were carried out, one with nor-327 mally-distributed noise with zero mean and standard deviation of 0.1 and another with 328 standard deviation of 0.2 (Figure 11). That is, in computing the matchup RMSD, we first 329 added noise to all of the L2 values used to formulate the ASD average. The simulated 330 Aquarius SSS field for the first week of July 2012 with 0.2 noise added (Figure 1c) looks 331 visually more like that of the real Aquarius data than does the no-noise version (Figure 332 1a,b). 333

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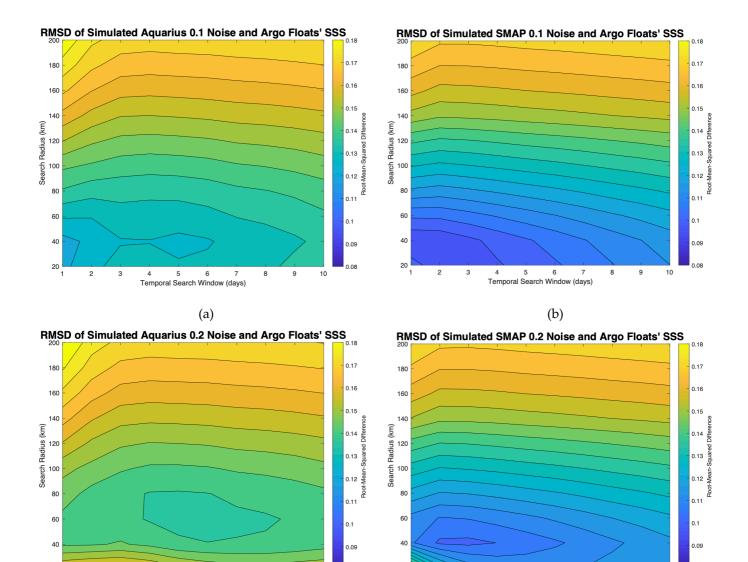
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(c)

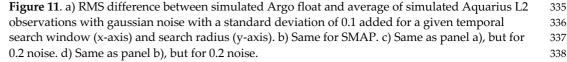
Temporal Search Window (days)



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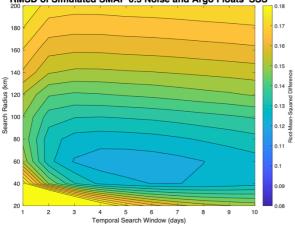
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Comparing Figures 11a and 11c with Figure 8a, we see that the added noise intro-339 duces a minimum in RMSD at 40 km for 0.1 noise and 60 km for 0.2 noise. For spatial 340 window larger than 100 km, the addition of noise makes little difference. This again high-341 lights the tradeoff between number of observations and variability of the underlying SSS 342 field. The ideal spatial window for the trade-off depends on the amount of noise inherent 343 in the field. The results for SMAP (Figures 11b,d) show no minimum in RMSD for 0.1 344 noise, and a minimum at 40 km for 0.2 noise. We did one more experiment with the SMAP 345 data only with 0.5 noise (Figure 12). The spatial minimum moves further out to 60 km. 346

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0.05



RMSD of Simulated SMAP 0.5 Noise and Argo Floats' SSS

Figure 12. As in Figure 11b, but with 0.5 noise.

With noise added, the size of the time window becomes more of an issue. Rather than having almost no time dependence (Figure 8) for short space windows, the RMSD reaches 350 a minimum at 6 days for Aquarius, vs. 2-3 days for no noise, and 3 days for SMAP (Figure 351 12d) for 0.2 noise, vs. no minimum at all for no noise (except at large space window). For 352 0.5 noise, the minimum RMSD for SMAP is at 5-6 days. The change in time window de-353 pendence seems to be a result of the number of observations to average over. 354

4. Discussion

In this work we have looked at the way SSS is sampled by remote sensing and how 356 that sampling is validated by comparison with in situ data at L2. We have focused on the 357 Aquarius and SMAP missions in generating the L2 comparison values from the model. 358 These missions provide a relatively straightforward sampling pattern and footprint size. 359 Further work in this area will focus on SMOS using a similar set of methods. The SMOS 360 mission has a variable footprint size [4] and presents more of a challenge to simulating 361 the L2 values. 362

[25] do a very similar calculation to what we have done here, with a final recommen-363 dation to use the same "all salinity difference" method we have used. Their recommenda-364 tion to use a 50 km search window matches closely with the minimum RMSD seen in 365 Figure 11. As SMAP is so much more heavily sampled and has a smaller footprint, a 366 smaller search window than for Aquarius would be appropriate. As for the time window, 367 Schanze et al. recommend using +-3.5 days, i.e. 3.5 days as done here. This recommenda-368 tion seems about right for SMAP given the results of Figure 11, though the window might 369 be relaxed a little bit, to 5-7 days, for Aquarius. 370

Keep in mind that there are many ways of validating SSS remote sensing data besides 371 the simple one used here, as was discussed at length by Schanze et al. (2020). One could 372 validate at L3 instead of L2; or compare L3 values with gridded in situ products, which 373 have their own issues of representation error [12,36], instead of individual measurements; 374 or do the matchups a different way than the simple block averages we computed here, 375 e.g. Figure 10. All of this is to say there is no perfect way of doing validation, only many 376 possibilities, each with its own set of tradeoffs. 377

This work has been carried out entirely with model data as an exercise in understand-378 ing the choices involved in doing matchups using in situ point measurements and L2 sat-379 ellite values combined in a particular way. The RMSD values shown in Figures 8 and 9 380 should not be considered any kind of overall error value for the satellite measurements. 381 They are associated only with representation error, i.e. temporal aliasing and subfootprint 382 variability (SFV). They do not contain any of the main sources of error inherent in satellite 383 measurement of SSS [2]. The numbers indicated in those figures, 0.08-0.18, could be 384

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considered estimates of representation error, assuming the variability in the model is sim-385ilar to that of the real surface ocean [26]. [24] and [37] computed very similar numbers for386representation error from in situ data at two sites in the subtropical North Atlantic and387eastern tropical North Pacific at 100 km scale. [23] made a global map of variability at 100388km scale from in situ data (their Figure 9a) with numbers a little bit larger than ours. Their389values of variability at <100 km scales are about 0.1-0.25 in mid-ocean, but larger in certain</td>390areas like western boundaries.391

The main lesson to be taken from the work we have done here is that the error involved in satellite measurement of SSS depends strongly on how the evaluation is carried out. If minimizing the error is an important goal, then techniques like that demonstrated in Figure 10, give some guidance as to ways to do that.

One item we explored here is the tradeoff between time and space window in formu-396 lating the comparison L2 averages. The clear conclusion is that for the representation error 397 there is only a small dependence on time in the range we examined but a strong depend-398 ence on space (e.g. Figure 8). This is a result of the unique nature of the SSS field. It has a 399 short spatial decorrelation scale due to the influence of rainfall and submesoscale varia-400 bility [23], but is dominated in time scale by the seasonal cycle in many areas [35,38,39]. 401 This can give those doing validation studies ways to formulate their space/time search 402 criteria for optimum results (i.e. minimum error). 403

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- Aquarius L2. DOI:10.5067/AQR50-2IOCS
- SMAP L2. DOI:10.5067/SMP40-2SOCS
- Argo profiles. https://www.nodc.noaa.gov/argo/index.htm
- MITgcm SSS. https://catalog.pangeo.io/browse/master/ocean/LLC4320/LLC4320_SSS/ 418

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