

1 **Global-scale Evaluation of SMAP, SMOS and ASCAT Soil Moisture Products using Triple**
2 **Collocation**

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10
11 **Abstract**

12 **Global-scale surface soil moisture products are currently available from multiple remote sensing platforms.**
13 **Footprint-scale assessments of these products are generally restricted to limited number of densely-**
14 **instrumented validation sites. However, by taking active and passive soil moisture products together with a**
15 **third independent soil moisture estimates via land surface modeling, triple collocation (TC) can be applied to**
16 **estimate the correlation metric of satellite soil moisture products (versus an unknown ground truth) over a**
17 **quasi-global domain. Here, an assessment of Soil Moisture Active Passive (SMAP), Soil Moisture Ocean**
18 **Salinity (SMOS) and Advanced SCATterometer (ASCAT) surface soil moisture retrievals via TC is presented.**
19 **Considering the potential violation of TC error assumptions, the impact of active-passive and satellite-model**
20 **error cross correlations on the TC-derived inter-comparison results is examined at *in situ* sites using quadruple**
21 **collocation analysis. In addition, confidence intervals for the TC-estimated correlation metric are constructed**
22 **from moving-block bootstrap sampling designed to preserve the temporal persistence of the original (unevenly-**
23 **sampled) soil moisture time-series. This study is the first to apply TC to obtain a robust global-scale cross-**

24 assessment of SMAP, SMOS and ASCAT soil moisture retrieval accuracy in terms of anomaly temporal
25 correlation. Our results confirm the overall advantage of SMAP (with a global average anomaly correlation of
26 0.76) over SMOS (0.66) and ASCAT (0.63) that has been established in several recent regional, ground-based
27 studies. SMAP is also the best-performing product over the majority of applicable land pixels (52%), although
28 SMOS and ASCAT each shows advantage in distinct geographic regions.

29

30 **1. Introduction**

31 As a key state variable in hydrological and meteorological modeling systems, the global
32 observation of soil moisture has become a major priority. Currently, several remote sensing
33 platforms provide continuous global surface (approximately 0-5 cm) retrievals: the National
34 Aeronautics and Space Administration (NASA)'s Soil Moisture Active Passive (SMAP, 2015-),
35 the European Space Agency (ESA)'s Soil Moisture Ocean Salinity (SMOS, 2009-), the European
36 Organisation for the Exploitation of Meteorological Satellites (EUMETSAT)'s Advanced
37 SCATterometers (ASCAT, 2007-), and the Japanese Aerospace Exploration Agency (JAXA)'s
38 Advanced Microwave Scanning Radiometer 2 (AMSR2, 2012-). The accuracy of the satellite
39 soil moisture retrievals is typically described via their root-mean-squared-error (RMSE; e.g.
40 Brocca *et al.* 2010; Jackson *et al.* 2010; Kerr *et al.* 2016) or de-biased/unbiased RMSE
41 (ubRMSE; e.g. Colliander *et al.* 2017) versus ground-based observations at a footprint-scale.
42 However, difficulty in obtaining viable estimates of ground truth soil moisture at the satellite
43 footprint scale has limited past validation activities to a small number of locations (e.g., SMAP's
44 core validation sites) and/or discrete time periods (e.g., field campaigns). The broader evaluation
45 of satellite soil moisture products (across regional or continental scales) is typically based on
46 comparisons with sparse ground soil moisture networks or modeled datasets (e.g., Paulik *et al.*
47 2014; González-Zamora *et al.* 2015; Piles *et al.* 2014; Al-Yaari *et al.* 2014; Polcher *et al.* 2016;

48 Kim *et al.* 2018). Naturally, such comparisons are unable to provide direct validation metrics
49 relative to the ground truth, but rather metrics against a chosen reference dataset with unknown
50 errors at the footprint-scale of satellite retrievals. For example, correlation coefficient metrics
51 obtained from comparing with point-scale ground observations have been shown to
52 underestimate the correlation between retrievals and true soil moisture values (Chen *et al.* 2017).

53 Initially designed for obtaining the calibration constants against a reference dataset in satellite
54 wind speed products, the triple collocation (TC) (Stoffelen 1998) technique provides a solution
55 to such challenge. In particular, TC can be applied to the estimate error variances of a
56 geophysical measurement system and has become an important tool for satellite soil moisture
57 assessments (e.g., Zwieback *et al.* 2012; Dorigo *et al.* 2010; Miralles *et al.* 2010; Draper *et al.*
58 2013). However, standard TC applications are limited to only providing relative error metrics. It
59 requires a reference dataset to be chosen from the three collocated data products, and the
60 resulting error variances are subject to the multiplicative and additive biases of the reference
61 dataset (Chen *et al.* 2017). Recently developed TC-based solution – the Extended Triple
62 Collocation, or ETC (McColl 2014) – for the Pearson’s correlation coefficient metric, on the
63 other hand, does not require a reference dataset and yields an absolute estimate of the temporal
64 correlation between the product under evaluation and the unknown truth. Pearson’s correlation
65 coefficient is a widely reported metric for satellite soil moisture and an appropriate metric for
66 summarizing retrieval value in a data assimilation context (Reichle *et al.*, 2008). In this analysis,
67 we adopt the ETC solution and conduct an assessment and inter-comparison of the SMAP Level
68 3, SMOS Level 3 and ASCAT Level 2 soil moisture products based on the correlation metric
69 (R). Until recently, relatively few studies have been conducted to evaluate satellite soil moisture
70 products at a continental scale (e.g. Draper *et al.* 2013; Leroux *et al.* 2013) using TC. To the best

71 of our knowledge, this study is the first attempt to apply TC to obtain the footprint-scale
72 correlation metric for SMAP observations at quasi-global scale, and compare it directly with soil
73 moisture retrievals from SMOS and ASCAT.

74

75 Our basic strategy for applying TC is to employ soil moisture data triplets comprising a passive
76 microwave product (SMAP or SMOS), an active remote sensing product (ASCAT), and a land
77 surface model product. TC is based on a fundamental assumption that each of these products
78 contain uncorrelated errors. However, recent works have identified non-negligible error
79 correlation in soil moisture products acquired from active and passive microwave sources
80 (Gruber *et al.* 2016b; Pierdicca *et al.* 2017). This suggests that it is necessary to examine the
81 impact of violating this assumption on SMAP-ASCAT and SMOS-ASCAT-based TC analyses.
82 Therefore, we also apply the least-squares quadruple collocation solution (QC, Pierdicca *et al.*
83 2015) to estimate the error cross-correlations at over 200 sparse ground observation sites to
84 further evaluate the robustness of our global TC analysis strategy.

85 This paper is organized as follows. Section 2 reviews the TC and quadruple collocation (QC)
86 methodologies and data-processing procedures as well as the use of moving-block bootstrap re-
87 sampling to obtain confidence intervals for TC-derived R . Section 3 describes the remote
88 sensing, land surface modeling and ground observation datasets used in the analysis. Section 4
89 presents the QC results at sparse network sites and discusses the sensitivity of the TC analysis to
90 both non-zero error cross-correlation between active and passive satellite soil moisture products
91 and our choice of a particular land surface model dataset. Results and discussions of global

92 comparison of SMAP, SMOS and ASCAT soil moisture via TC are presented in Sections 5 and
93 6, respectively.

94

95 **2. Methodologies**

96 **2.1 Extended Triple Collocation**

97 In soil moisture validation and comparison studies, TC has typically been applied to estimate the
98 random error variance of a particular soil moisture dataset. In contrast, the extended triple
99 collocation (ETC) approach (McColl 2014) solves for the correlation between a dataset and the
100 unknown truth. As in TC, it requires three collocated, independent measurement systems (X , Y ,
101 Z , in our case representing: a passive satellite retrieval, an active satellite retrieval and a model
102 product, respectively) that describe the same geophysical variable (in this case - average surface
103 soil moisture of the satellite grid cell, which is approximately 40 x 40 km²). ETC is based on the
104 following assumptions: 1) all three datasets are linearly related to the true state (T); 2) zero error
105 cross-correlation exists between X , Y and Z ; and 3) zero correlation exists between errors and T
106 and 4) the stationary of signal and error statistics (Gruber *et al.* 2016a; Draper *et al.* 2013;
107 Zwieback *et al.* 2012). If these assumptions hold, the correlation between X and the T can be
108 estimated as

$$109 \quad R_X = \sqrt{\frac{\sigma_{XY}\sigma_{XZ}}{\sigma_X^2\sigma_{YZ}}} \quad (1)$$

110 where σ_{XY} is the covariance of X and Y , and σ_X^2 is the variance of X . Analytical details for
111 deriving (1) from the classic TC method (Stoffelen 1998) can be found in McColl (2014).

112 To ensure consistency with the assumption listed above, seasonal signals are commonly removed
113 from the raw time-series of each product prior to the application of TC (Gruber *et al.* 2016a; Dorigo
114 *et al.* 2010; Su and Ryu, 2015). Here, anomaly time series are generated by removing the average
115 value of a 30-day moving window centered upon the data point being treated (i.e. from day -14 to
116 day +15). Given the potential temporally sparse nature of satellite retrievals, a minimum of 3
117 observations is required in each of the first and second halves of the 30-day window, in addition
118 to the data point being treated itself. This particular anomaly definition, versus the alternative
119 definition of deviations from a long-term seasonal climatology, has less stringent requirements
120 regarding the length of datasets, which is usually the limiting factor in the application of TC in
121 satellite products. While the removal of low-frequency variability has been shown to improve the
122 robustness of TC results (Chen *et al.* 2017), it renders our particular ETC approach insensitive to
123 (potentially-important) error in low-frequency and/or seasonal soil moisture dynamics. The
124 implications of this will be discussed below.

125 ETC-based estimates of correlation are considered viable when: 1) the collocated triple time series
126 is comprised of at least 50 data points; 2) positive correlation is found between each of the three
127 input anomaly time-series, and 3) ETC correlation outputs are real and positive for each of the
128 three datasets. All other ETC correlation estimates are masked. The positive correlation
129 requirement between input datasets (#2 above) is necessary to avoid ambiguity since ETC is unable
130 to resolve the sign of the output R values (McColl 2014). This limitation results in the exclusion
131 of pixels in certain regions where active and passive soil moisture retrievals are negatively
132 correlated (see additional discussion in Section 5).

133 **2.2 Estimation of error cross-correlation: Quadruple collocation**

134 As noted above, a potential source of error for the TC analysis is the presence of error cross-
135 correlation (ECC) between the soil moisture datasets, especially between active and passive
136 remote sensing products. Non-zero ECC violates the underlying TC assumptions and can lead to
137 biased TC results. In past studies, ECC was typically assumed to be zero between all products
138 (e.g., Leroux *et al.* 2013). However, recent works have revealed the presence of non-zero ECC
139 between active and passive soil moisture retrievals (Gruber *et al.* 2016b; Pierdicca *et al.* 2017).
140 Therefore, it is prudent to re-examine ECC levels in SMAP-ASCAT and SMOS-ASCAT soil
141 moisture data pairs utilized here.

142 The TC algorithm can be extended to include a fourth dataset (i.e., quadruple collocation, or QC)
143 and the error variances can be estimated with a least squares solution (Pierdicca *et al.* 2015) with
144 the same TC assumptions. Furthermore, the zero ECC assumption can be relaxed, and – on the
145 condition that only one pair within of the four datasets have non-zero ECC – estimates of ECC
146 can be obtained from the least-squares solution (Zwieback *et al.* 2012; Gruber *et al.* 2016b).

147 Here we adopt the formulation in Gruber *et al.* (2016b) to estimate the error cross-correlation
148 between the active (ASCAT) and passive (SMAP, SMOS) soil moisture datasets and assess the
149 impact of such cross-correlation on TC results. The QC analysis is conducted at sparse soil
150 moisture network sites where ground observations can serve as the fourth soil moisture dataset.
151 The QC formulation also provides estimates of the error variances of each dataset. In certain
152 cases, such estimates will be more accurate than those obtained from TC since QC can account
153 for the presence of non-zero ECC within a particular pair of collocated datasets (Yilmaz and
154 Crow, 2014).

155 Given four soil moisture measurement systems X, Y, Z, W , representing a passive remote sensing,
 156 an active remote sensing, a model and point-scale ground observation, respectively, the least-
 157 squares solution for the QC problem is given by

$$\begin{aligned}
 158 \quad y = & \begin{bmatrix} \sigma_X^2 \\ \sigma_Y^2 \\ \sigma_Z^2 \\ \sigma_W^2 \\ \sigma_{XY} \\ \sigma_{XZ}\sigma_{XW}/\sigma_{ZW} \\ \sigma_{YZ}\sigma_{YW}/\sigma_{ZW} \\ \sigma_{XZ}\sigma_{ZW}/\sigma_{XW} \\ \sigma_{YZ}\sigma_{ZW}/\sigma_{YW} \\ \sigma_{XW}\sigma_{ZW}/\sigma_{XZ} \\ \sigma_{YW}\sigma_{ZW}/\sigma_{YZ} \\ \sigma_{XZ}\sigma_{YW}/\sigma_{ZW} \\ \sigma_{XW}\sigma_{YZ}/\sigma_{ZW} \end{bmatrix} A = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} x = \begin{bmatrix} \beta_X^2 \sigma_\Theta^2 \\ \beta_Y^2 \sigma_\Theta^2 \\ \beta_Z^2 \sigma_\Theta^2 \\ \beta_W^2 \sigma_\Theta^2 \\ \beta_X \beta_Y \sigma_\Theta^2 \\ \sigma_{\varepsilon_X}^2 \\ \sigma_{\varepsilon_Y}^2 \\ \sigma_{\varepsilon_Z}^2 \\ \sigma_{\varepsilon_W}^2 \\ \sigma_{\varepsilon_X \varepsilon_Y} \end{bmatrix} \quad (2)
 \end{aligned}$$

159 where Θ is the true soil moisture signal, and β is the multiplicative bias of a given dataset as in
 160 $X = \alpha_X + \beta_X \Theta + \varepsilon_X$, and ε is the zero-mean random error.

161 And the least squares solution for the parameters in x is given as

$$162 \quad \hat{x} = (A^T A)^{-1} A^T y \quad (3)$$

163 Note that this solution enables the TC approach described in section 2.1 to be slightly relaxed. In
 164 particular, non-zero ECC is now allowed in one data pair (here between X and Y , where X is
 165 SMAP or SMOS, and Y is ASCAT). ECC between any other data pairs are still required to be
 166 zero (i.e., $\sigma_{\varepsilon_X \varepsilon_Y} \neq 0$, and $\sigma_{\varepsilon_X \varepsilon_Z} = \sigma_{\varepsilon_X \varepsilon_W} = \sigma_{\varepsilon_Y \varepsilon_Z} = \sigma_{\varepsilon_Y \varepsilon_W} = \sigma_{\varepsilon_Z \varepsilon_W} = 0$). As in Gruber *et al.*
 167 (2016b), we consider these conditions generally satisfied in the active-passive-LSM-*in situ* data
 168 quadruples in this study.

169 **2.3 Confidence interval from moving block bootstrapping**

170 Using collocated surface soil moisture retrievals from passive (SMAP or SMOS) and active
171 (ASCAT) sensors and a land surface modeling product, the correlation metric of the three
172 satellite products (versus an unknown truth) can be estimated via TC at a quasi-global scale.
173 However, considerable sampling errors are expected in TC results, especially when the length of
174 the analysis is shortened to accommodate new satellite products (e.g., the two years of SMAP
175 considered here). Therefore, it is critical to account for sampling uncertainties when making
176 comparisons between the satellite products.

177 Here, such uncertainties are quantified via bootstrap re-sampling at each pixel to construct the
178 confidence interval (CI) of TC estimates. As noted earlier, auto-correlation in time-series will
179 reduce the effective sample size and thus underestimate the probability that the original bootstrap
180 confidence interval contains the true statistical property (Zwiers, 1990; von Storch and Zwiers,
181 1999). Since soil moisture time series typically contain large amounts of temporal auto-
182 correlation, this effect should be considered when generating boot-strapped errors estimates for
183 soil moisture TC results. Although mean 30-day signals have been removed from the original
184 time-series, our analysis suggests the resulting anomaly time-series still contains significant first-
185 order autocorrelation (not shown). This impact also applies for correlation estimated by ETC
186 techniques since the latter is essentially an expansion upon the Pearson's correlation coefficient
187 formula from two to three time series members (McColl, 2014). A solution is proposed in
188 Mudelsee (2002, 2010) where a pair-wise moving block bootstrap (MBB) re-sampling technique
189 is applied to obtain a robust estimate of the confidence intervals for Pearson's correlation
190 coefficient in serially-correlated time-series.

191 Here, we have adapted the MBB method introduced in Ólafsdóttir and Mudelsee (2014) for the
 192 bi-variate correlation problem to the triple collocation problem to construct the confidence
 193 interval of the ETC correlation results. In each iteration of the re-sampling procedure, MBB is
 194 applied to draw blocks of data triplets from the original time series samples to form samples that
 195 preserve the temporal persistence of the original data. Block length is determined from the
 196 equivalent autocorrelation coefficient of the three anomaly time-series (i.e., ETC inputs) which is
 197 calculated from individual persistence time, τ , of the three time-series. Persistence times are then
 198 estimated by minimizing the sum of squares:

$$199 \quad S(\tau_X) = \sum_{i=2}^n [x(i) - \exp\{-[t(i) - t(i-1)]/\tau_X\} \cdot x(i-1)]^2 \quad (4)$$

200 where n is the length of the time-series, $x(i)$ is the i th data point (i.e. soil moisture anomaly) and
 201 $t(i)$ is the linear time point (in unit of day) with uneven spacing, which is typical of satellite
 202 retrievals. Note that although the land surface model time-series are evenly spaced with sub-daily
 203 frequency, only the data points that temporally matched to the satellite retrievals are considered
 204 and thereby treated as an unevenly-spaced time series. The equivalent AR(1) autocorrelation
 205 coefficient is given by $a_X = \exp(-d/\tau_X)$, where $d = [t(n) - t(1)]/(n - 1)$ is the average time
 206 spacing. The autocorrelation coefficient is then bias-corrected to approximate the AR(1) process
 207 with an even time-spacing:

$$208 \quad a'_X = [a_X \cdot (n - 1) + 1]/(n - 4). \quad (5)$$

209 A joint, bias-corrected equivalent autocorrelation coefficient for the triple collocation analysis is
 210 given by

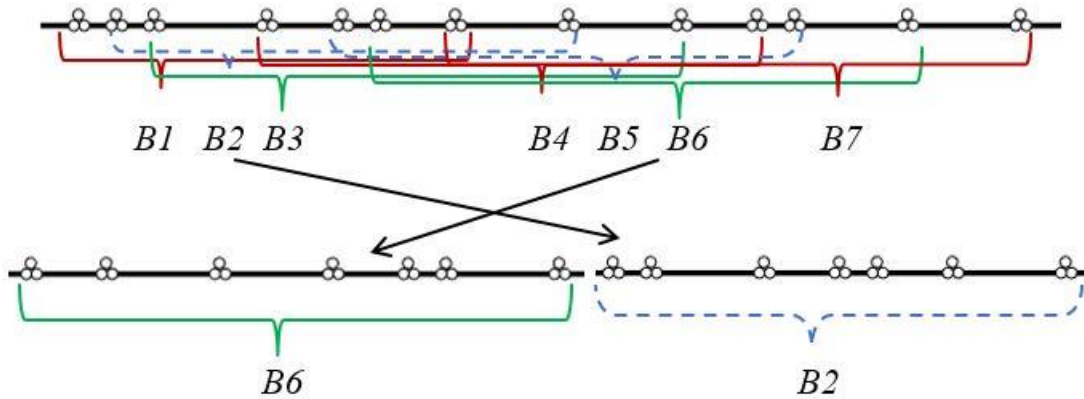
$$211 \quad a'_{XYZ} = (a'_X \cdot a'_Y \cdot a'_Z)^{1/3}. \quad (6)$$

212

213 The optimal block length is then estimated as

214
$$l_{opt} = \text{NINT} \left\{ \left[\sqrt{6} \cdot a'_{XYZ} / (1 - a'^2_{XYZ}) \right]^{2/3} \cdot n^{1/3} \right\} \quad (7)$$

215 where NINT denotes rounding to the nearest integer. Overlapping blocks of data triplets with the
216 length of l_{opt} are then extracted from the match-up anomaly time-series and then randomly
217 drawn with replacement to be concatenated until the original data length is reached (see Figure 1
218 for an illustration of this procedure). Extra data points in the end of the newly-formed bootstrap
219 sample are trimmed. The re-sampling procedure is repeated 1000 times in each grid pixel.
220 Estimated 95% confidence intervals for each correlation coefficient are defined as the range
221 between 2.5th and 97.5th percentile of the bootstrapped sampling distribution.



222

223 **Figure 1.** Schematic diagram of moving block bootstrapping for the case $l_{opt} = 7$ applied to a temporally
224 sporadic time series of available soil moisture triplets. Overlapping data blocks from the original time
225 series (top) are drawn randomly with replacement and then concatenated to generate a new bootstrap
226 resample (bottom).

227

228 **3. Data**

229 As discussed above, three satellite surface soil moisture products (acquired between March 31,
230 2015 and March 31, 2017) are evaluated in this analysis: Level 3 SMAP passive radiometer
231 retrievals (L3_SM_P, v4-R14010), Level 3 SMOS radiometer retrievals (v300), and Level 2
232 ASCAT scatterometer retrievals. All three retrieval time series contain retrievals obtained from
233 both ascending and descending orbits. Details of each product are given below.

234 **3.1 Soil Moisture Active Passive (SMAP)**

235 Launched in January 2015, NASA's SMAP satellite began continuous science data acquisition
236 on March 31, 2015 with its L-band (1.41 GHz) radiometer (Entekhabi et al., 2010). The SMAP
237 L3 data is in the format of global gridded maps of daily composites of the SMAP Level 2 Passive
238 Soil Moisture (L2_SM_P) ascending/descending swath data, and is posted on a global cylindrical
239 36 km Equal-Area Scalable Earth, version 2 (EASEv2) grid. The validated SMAP L2/3 soil
240 moisture product is based on the V-polarization single-channel (SCA-V) retrieval algorithm
241 (Chan *et al.* 2016). Data screening is based on the soil moisture retrieval quality flag and only
242 those flagged as "recommended for retrieval" are considered in this analysis. The retrieval
243 quality flag is determined from a number of surface and retrieval conditions which can be found
244 in Chan *et al.* (2016) and Chan and Dunbar (2015). Soil moisture retrievals from the ascending
245 (6 PM LST) overpasses are now included in the SMAP Level 2/3 passive version 4 data
246 products. Validation of the ascending (PM) retrievals indicate that it also meets the mission
247 requirement of $0.04 \text{ m}^3/\text{m}^3$ unbiased root mean square error (ubRMSE), but with a small
248 degradation compared to the descending (AM) retrievals (Jackson *et al.* 2016).

249 **3.2 Soil Moisture Ocean Salinity (SMOS)**

250 ESA's SMOS satellite was launched in November 2009 and measures L-band microwave
251 emission (1.400-1.427 GHz) with equatorial ascending/descending overpasses at 6 AM/PM local
252 solar time and a 3-day revisit period at the equator (Kerr *et al.* 2001). The SMOS soil moisture
253 retrieval algorithm can be found in Kerr *et al.* (2013). The SMOS Level 3 (v300) soil moisture
254 product used here is generated on a 25-km EASEv2 grid (Brodzik and Knowles, 2002) available
255 through the Centre Aval de Traitement des Données (CATDS) (<http://www.catds.fr>). In this
256 study, the SMOS L3 soil moisture data was re-gridded to the SMAP 36 km-EASEv2 grid by
257 bilinear interpolation. Data were screened primarily by the SMOS Data Quality index (DQX),
258 which takes into account the error in the retrieval parameters and the Level 1 brightness
259 temperatures (Kerr, *et al.* 2013). DQX has been applied to screen SMOS soil moisture retrievals
260 in several studies with thresholds varying between 0.045 and 0.07 (e.g. Polcher *et al.* 2016; Al-
261 Yaari *et al.* 2014; Pierdicca *et al.* 2013). Here, pixels with $DQX > 0.07 \text{ m}^3/\text{m}^3$ or covered by
262 snow or ice were removed. A stricter screening threshold of $0.04 \text{ m}^3/\text{m}^3$ for DQX is also applied
263 to examine the impact on the overall performance SMOS relative to SMAP and ASCAT (see
264 Section 5). The impact of varying this threshold on key results will be discussed below.
265 However, unless otherwise noted, satellite comparison results shown below are based on the 0.07
266 m^3/m^3 DQX threshold to maximize the temporal and spatial coverage of the analysis.

267 **3.3 Advanced Scatterometer**

268 The Advanced Scatterometer (ASCAT) sensor onboard the Meteorological Operational-B
269 (MetOp-B) satellite measures C-band (5.3 GHz) radar backscatter since September 2012, with
270 25-34 km spatial resolution and equatorial ascending/descending overpasses at 9:30 PM/AM
271 local solar time and a revisit frequency of 3 days. The ASCAT Level 2 (v5) soil moisture index
272 product utilized here is based on the change-detection algorithm developed by Vienna University

273 of Technology (TU Wien; see Wagner *et al.* 1999; Naeimi *et al.* 2009) obtained from
274 EUMETSAT Earth Observation Portal (EOP). As conversion to volumetric soil moisture unit is
275 not required in calculation of correlation coefficient, potential error due to inaccurate global
276 porosity dataset is avoided here. Pixels were masked if the probability of snow, frozen ground
277 and estimated retrieval error are greater than 50%. The ASCAT L2 soil moisture index data are
278 available at 12.5-km grid resolution and were re-sampled onto the SMAP 36 km-EASEv2 grid
279 through inverse-distance-weighting interpolation.

280 **3.4 Land surface modeling products**

281 Two operational global land surface modeling (LSM) soil moisture datasets are used in this
282 analysis. The first is the operational analysis layer-1 (0-7 cm) volumetric soil moisture field from
283 the European Centre for Medium Range Weather Forecasts (ECMWF) H-TESEL (Hydrology-
284 Tiled ECMWF Scheme for Surface Exchanges over Land) land-surface scheme (Balsamo *et al.*
285 2009). The operational soil moisture analysis product data is produced by ECMWF's Land Data
286 Assimilation System by the assimilation of 2-m air temperature and relative humidity
287 observations (Drusch *et al.* 2009; de Rosnay *et al.* 2012). The ECMWF soil moisture analysis
288 data is available at 00, 06, 12 and 18Z hours and in a N640 reduced Gaussian grid. Here, it was
289 re-gridded to the nearest 36-km EASEv2 grid using a nearest neighbor approach.

290

291 The second LSM soil moisture product utilized here is the so-called SMAP Nature Run, version
292 3 (NRv3), available at 3-hourly interval and 9-km EASEv2 grid and were aggregated to 36-km
293 EASEv2 grid by spatial averaging. The NRv3 data were generated with an early version of the
294 SMAP Level 4 Surface and Root Zone Soil Moisture (L4_SM) algorithm by the NASA Goddard

295 Space Flight Center (GSFC) Global Modeling and Assimilation Office (Reichle *et al.* 2016),
296 which was applied in a model-only configuration using a single ensemble member, without
297 perturbations, and without the assimilation of SMAP observations.

298
299 The re-sampling methods for the satellite and LSM datasets were each chosen considering the
300 features of both source and target grids (i.e. SMAP EASEv2 grid). For ECMWF, the average
301 grid size is close to the target grid size and therefore nearest-neighbor type simple grid
302 transformation is appropriate given that it avoids potential interpolation artifacts. For NRv3 the
303 source grid is perfectly nested within the target grid so simple averaging is ideal. The choice of
304 re-sampling method for SMOS and ASCAT has been made with close attention to limiting
305 factors and after discussion with data providers. A bilinear interpolation was found to produce
306 fewest artifacts for SMOS with its 25-km EASEv2 grid. ASCAT's grid resolution is higher (12.5
307 km) and the original data was provided in time-ordered format; an inverse-distance-weighting
308 interpolation was found to be most accurate.

309

310 **3.5 Sparse network ground observations**

311

312 In order to verify aspects of our ETC analysis (see Section 4), two years (3/31/2015 – 3/31/2017)
313 of ground soil moisture measurements were obtained from various sparse networks (Table 1) and
314 applied in a QC analysis (see Section 4 below). These networks typically provide one point-scale
315 measurement per satellite footprint at approximately 5-cm depth, except for the COsmic-ray Soil
316 Moisture Observing System (COSMOS) and PBO H₂O/GPS networks. The cosmic-ray neutron
317 detectors (Zreda *et al.*, 2008; 2012) in the COSMOS network measure soil moisture have a

318 footprint radius varying between ~130 to 240 meters and a dynamic penetration depth of
 319 between ~15 to 83 centimeters (Köhli *et al.* 2015). The PBO H₂O/GPS network utilizes Global
 320 Positioning System (GPS) receivers that record temporal changes in the signal-to-noise
 321 characteristic of GPS reflectometry data to estimate changes in soil moisture with a sensing
 322 depth of 2.5 cm or less (Chew *et al.* 2014) and a sensing area of approximately 120 m² per
 323 satellite track (Larson and Nievinski, 2013). Multiple tracks are combined to produce a daily
 324 average soil moisture value with the aggregate sensing area of approximately 1000 m². Except
 325 for the GPS network, hourly soil moisture measurements are generally available for all networks.

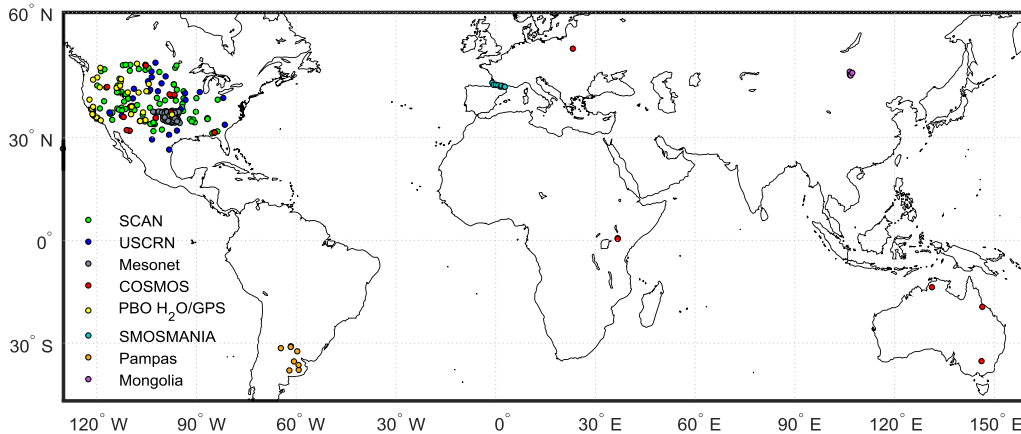
326

327 Table 1. Sparse networks providing ground measurements of soil moisture.

Network	Instrument	Region	Number of stations	Reference
Soil Climate Analysis Network (SCAN)	Hydra Probe	USA	71	Shafer <i>et al.</i> 2007
U.S. Climate Reference Network (USCRN)	Hydra Probe II	USA	44	Bell <i>et al.</i> 2013
Oklahoma Mesonet	Campbell Scientific 229-L	Oklahoma, USA	84	Illston <i>et al.</i> 2008; Scott <i>et al.</i> 2013
COSMIC-ray Soil Moisture Observing System (COSMOS)	cosmic-ray soil moisture probe	USA, Europe, Africa, Australia	23	Zreda <i>et al.</i> , 2008, 2012
PBO H ₂ O (GPS)	Global Positioning System (GPS) receivers	Western USA	28	Larson <i>et al.</i> 2008
SMOSMANIA	ThetaProbe ML2X	France	8	Calvet <i>et al.</i> 2007
Pampas	ThetaProbe ML2X	Argentina	8	
Mongolia Grasslands	Time Domain Reflectometry (TDR) probes	Mongolia	5	Kaihotsu <i>et al.</i> 2009

328

329 Figure 2 shows the location of the ground observation sites used in this study. Note that some of
330 the stations were missing in certain subsequent figures due to the limited availability of
331 collocated satellite observations.



332

333 Figure 2. Location of ground observation sites (N=271) from sparse networks.

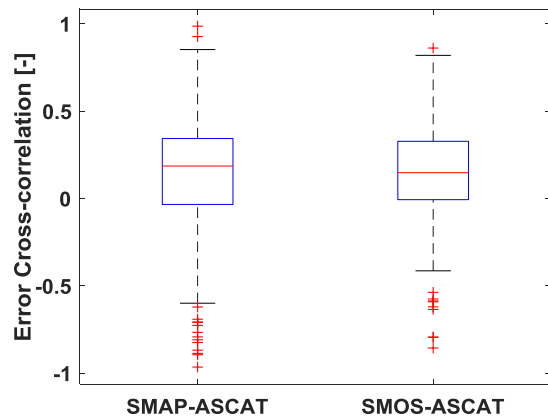
334

335 4. Validation of global TC approach

336 Prior to the global application of TC, we will validate aspects of the approach using ground-
337 based observations acquired at the sparse networks shown in Figure 2. For example, it is often
338 assumed that satellite retrievals obtained from active and passive sensors are free from error
339 cross-correlation (ECC). As a result, the data triplets applied here consist of an active product
340 (ASCAT), a passive product (SMOS or SMAP) and a land surface model product (ECMWF or
341 NRv3). However, given the active-passive ECC discovered in a recent studies, it is necessary to
342 investigate the ECC between the proposed SMAP-ASCAT and SMOS-ASCAT combinations in
343 TC and its potential impacts on the TC-based satellite comparisons.

344 This investigation is made possible by adding point-scale (pts) soil moisture observations
345 obtained at sparse networks sites (Fig. 2) into the data triplets, to obtain the data quartets [pts,
346 SMAP, ASCAT, ECMWF] and [pts, SMOS, ASCAT, ECMWF]. Applying the least-square
347 solution for quadruple collocation in (3) to these quartets, and assuming that non-zero ECC
348 exists only between the active and passive soil moisture retrievals, allows us to calculate the
349 SMAP-ASCAT and SMOS-ASCAT ECC's across the ground sites. As shown in Fig. 3 these
350 two distributions are quite similar. That is, most sampled ECC's are positive with a median of
351 0.19 [-] (SMAP-ASCAT) and 0.15 [-] (SMOS-ASCAT) and an interquartile range between 0 and
352 ~0.35 [-].

353 Once estimated, the impact of using of such non-zero ECC on TC results can be assessed. To this
354 end, ASCAT R values obtained from both SMAP- and SMOS-based QC or TC analyses are
355 averaged across all sparse sites. Since QC-generated R value takes into account the possibility of
356 non-zero SMAP-ASCAT and SMOS-ASCAT ECC's, it is taken as a reference to evaluate the
357 TC results. On average, TC-estimated R exhibited a slight positive bias compared with
358 corresponding QC results, with average bias values of 0.06 and 0.05 [-] for SMAP and SMOS,
359 respectively. Average bias for ASCAT R is 0.07 (obtained by SMAP-based TC) and 0.12
360 (SMOS-based TC). However, since this bias is comparable and positive for all three products,
361 the transition from QC to TC is expected to have small net global impact on product-to-product
362 differences. See below for additional discussion.



363

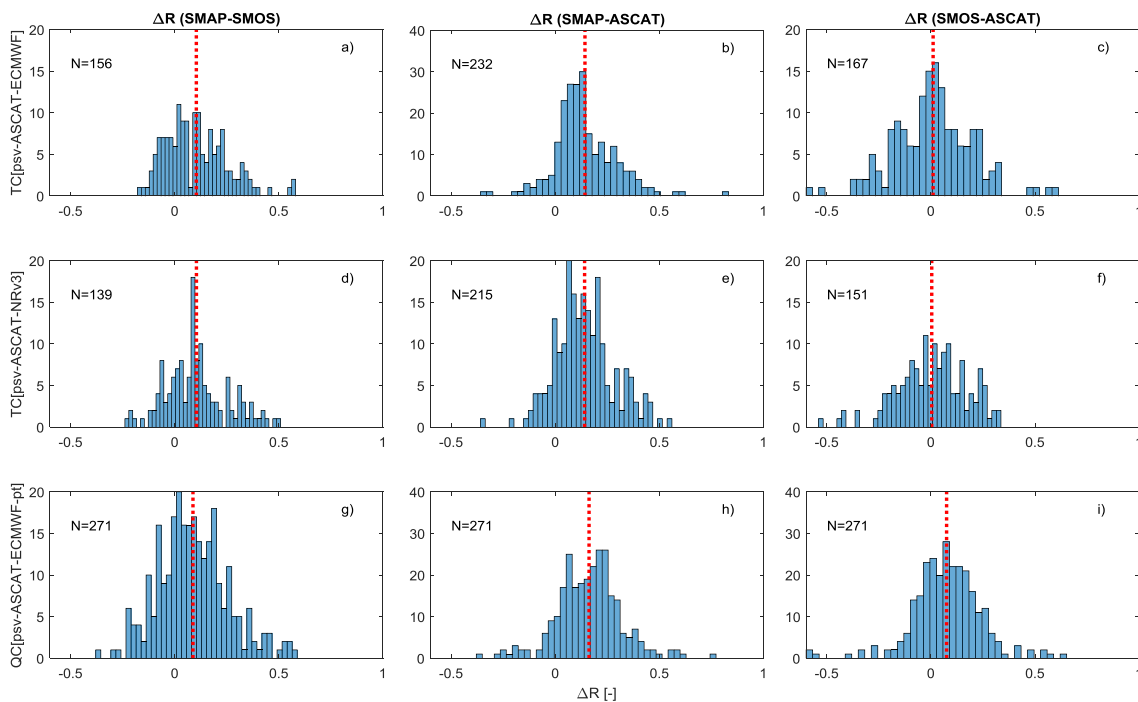
364 **Figure 3.** Distribution of ECC between SMAP-ASCAT and SMOS-ASCAT pairs estimated via the
 365 application of QC at sparse sites listed in Fig. 2. The upper and lower bounds of the boxes indicate 25th
 366 and 75th percentiles respectively and the red line in the box indicates the median. Whiskers extending
 367 from the 25th and 75th percentiles to represent 1.5 times the interquartile range.

368

369 In the TC and QC analyses above we also assume no error cross-correlation between the model
 370 and satellite products, which may not be true in all cases. For example, the SMOS soil moisture
 371 retrieval algorithm uses the ECMWF forecast temperature fields as dynamic auxiliary data input
 372 to obtain the effective soil temperature (Kerr *et al.* 2013), leading to potential ECC between the
 373 two soil moisture products. Likewise, the NASA GEOS-5 soil temperatures used in the SMAP
 374 L2_SM_P soil moisture retrieval algorithm are derived using the same GEOS-5 forward
 375 processing system that also provides the surface meteorological forcing (except precipitation) for
 376 generating NRv3. Therefore, potential ECC between SMAP and NRv3 is also of concern. An
 377 earlier study suggests small amounts of anti-correlation may exist between SMAP and NRv3 soil
 378 moisture errors that could cause slight underestimation of SMAP R when both datasets are used
 379 in a TC analysis (Chen *et al.* 2017). To fully address the impact of this issue on our current

380 study, the impact of ECC on the relative evaluation of the three satellite products is examined
 381 here via both QC and TC.

382 Figure 4 summarizes these results. In particular, the first and second rows of Figure 4 plot the
 383 difference in correlation values (ΔR) between the satellite pairs obtained from TC using both
 384 ECMWF (a-c) and NRv3 (d-f) at the sparse sites. The third row (g-i) shows the ECMWF-based
 385 QC results of ΔR . Strong similarity in the shape of the histogram, and the values of mean ΔR (see
 386 dashed vertical lines) suggest that the net mean impact of potential ECC between model and
 387 passive soil moisture products is small. Furthermore, while non-zero active-passive ECC impacts
 388 absolute TC-based R slightly, it has very little net impact on relative R differences observed
 389 between SMAP, SMOS and ASCAT (compare the first and second rows against the third row in
 390 Fig. 4).



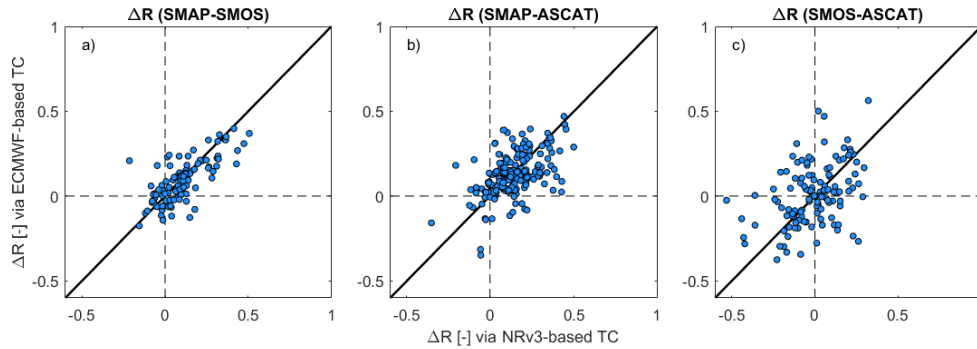
391

392 **Figure 4.** Comparison of differences in SMAP, SMOS and ASCAT correlation coefficients (ΔR) obtained
393 from TC (a-f) and QC (g-i) at ground locations shown in Fig. 2. In the vertical axes, “psv” refers to
394 passive satellite products, (SMAP or SMOS), “pt” refers to point-scale ground observations. The vertical
395 dashed lines indicate the mean ΔR for each histogram. “N” refers to the number of stations used in each
396 subplot.

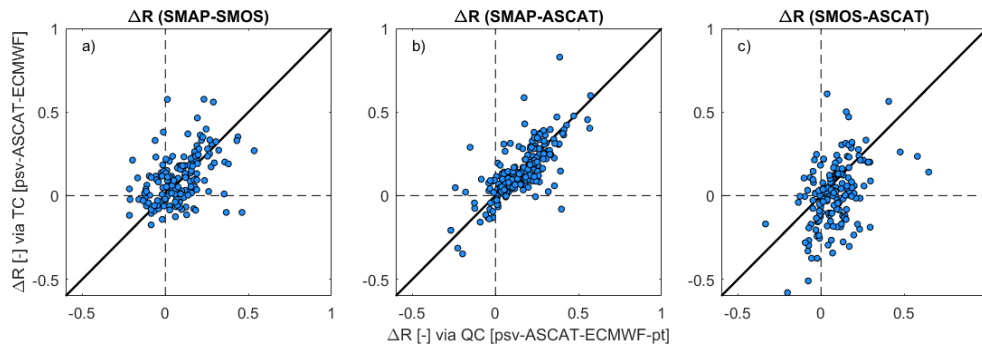
397
398 In addition to assessing the impact of ECC on the relative global bias of TC-based R distributions
399 (as in Fig. 3), it is useful to assess its impact on the spatial pattern of R differences observed
400 between satellites (ΔR). Since sparse network observations are not spatially dense enough to
401 yield continuous imagery (even after interpolation), we are restricted to the use of scatter plots
402 when examining spatial consistency.

403 The spatial robustness of ΔR is examined via scatterplots comparing results obtained when
404 utilizing different source of LSM soil moisture (Fig. 5) and QC versus TC analysis (Fig. 6).
405 While significant sampling noise is evident, the general one-to-one correspondence suggested in
406 Figures 5 and 6 suggest that spatially patterns present in ΔR are relatively robust to the use of
407 competing LSM soil moisture products and the presence of ECC (accounted for in QC results but
408 neglected in TC). While good agreement in the SMAP-SMOS ΔR and SMAP-ASCAT ΔR is
409 observed in both cases (Fig. 5, 6), larger scatter is present in SMOS-ASCAT ΔR (Fig. 5c and 6c).
410 This is likely due to the tendency for SMOS and ASCAT soil moisture products to exhibit
411 relatively lower R , and thus relatively higher sampling uncertainty effects for ΔR differences,
412 than SMAP-based results (see additional discussion in Section 5).

413 Therefore, across the sparse site locations in Fig. 2, relative inter-comparisons between various
 414 satellite-based soil moisture products are generally insensitive to both our choice of the
 415 collocation method (QC vs. TC) and a particular land model (ECMWF vs. NRv3).
 416



417
 418 **Figure 5.** Comparison of R differences (ΔR) between SMAP, SMOS and ASCAT soil moisture retrievals
 419 obtained from NRv3- and ECMWF-based TC analyses. Subplots a), b) and c) include common data
 420 points shown above in Fig. 4a and 4d, Fig. 4b and 4e, and Fig. 4c and f, respectively.

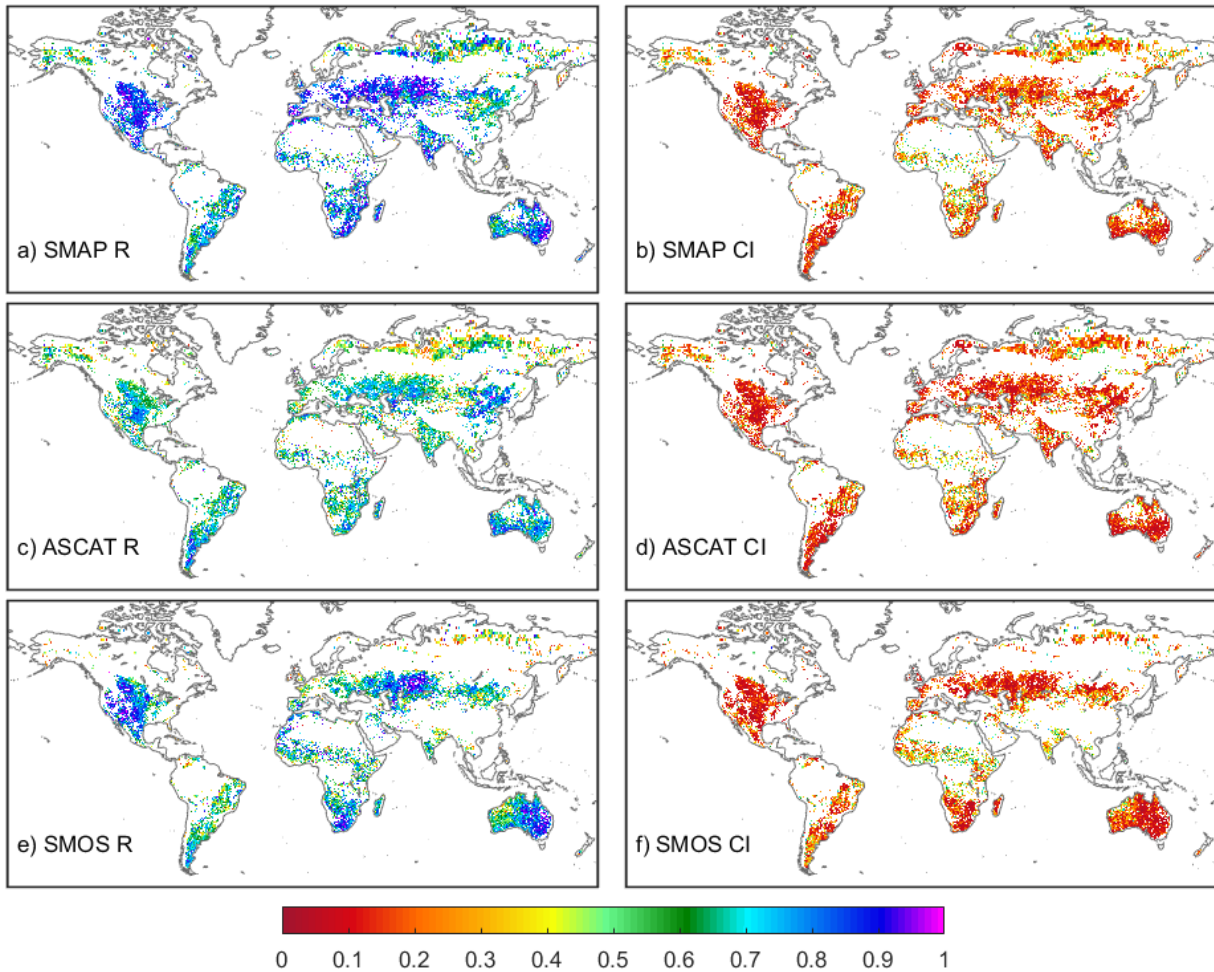


421
 422 **Figure 6.** Comparison of R differences (ΔR) between SMAP, SMOS and ASCAT soil moisture retrievals
 423 obtained from TC and QC analyses. Subplots a), b) and c) include common data points shown above in
 424 Fig. 4a and 4g, Fig. 4b and 4h, and Fig. 4c and i, respectively.

425

426 **5 Global triple collocation**

427 QC results at ground measurement sites in Section 4 indicate that neither ECC between
428 SMAP/SMOS and ASCAT nor ECC between the land surface model and SMAP or SMOS has a
429 discernible impact on the inter-comparison of R results for SMAP, SMOS and ASCAT. Hence
430 our strategy for a quasi-global application of TC using either a [SMOS-ASCAT-ECMWF] or
431 [SMAP-ASCAT-ECMWF] triplet is believed to be robust. Figure 7a plots estimated R against
432 true footprint surface soil moisture for SMAP, SMOS and ASCAT obtained from a TC[SMAP-
433 ASCAT-ECMWF] (Fig.7 a, c) and TC[SMOS-ASCAT-ECMWF] (Fig. 7e) analysis. In
434 particular, note that ASCAT results in Figure 7c are based on a TC[SMAP-ASCAT-ECMWF]
435 analysis. Similarity of the ASCAT R results between the SMAP-based and SMOS-based TC
436 analyses is shown in Fig. 8. Figures 7b, 7d and 7c show the total width of the corresponding 95%
437 confidence interval generated from a 1,000-member moving-block bootstrap re-sampling (see
438 Section 2.3). The global distributions of TC-based R results are also summarized in Fig. 8.



439

440 **Figure 7.** Quasi-global image of TC-based R [-] (single run, without bootstrap re-sampling) for SMAP,
 441 ASCAT and SMOS (left column: subplots a, c, e) and total width of the 95% confidence interval ('CI',
 442 right column: subplots b, d, f) derived from a 1,000-member bootstrap sampling. Subplots a) – d) are
 443 based on a [SMAP-ASCAT-ECMWF] triplet. Subplots e) - f) are based on a [SMOS-ASCAT-ECMWF]
 444 triplet.

445

446 Among the three satellite products, SMAP demonstrates the best overall performance, achieving
 447 excellent (> 0.8 [-]) R over the mid-latitudes of North America and Europe, as well as in
 448 southeastern Africa, India and the eastern half of Australia. Relatively good correlations (> 0.5

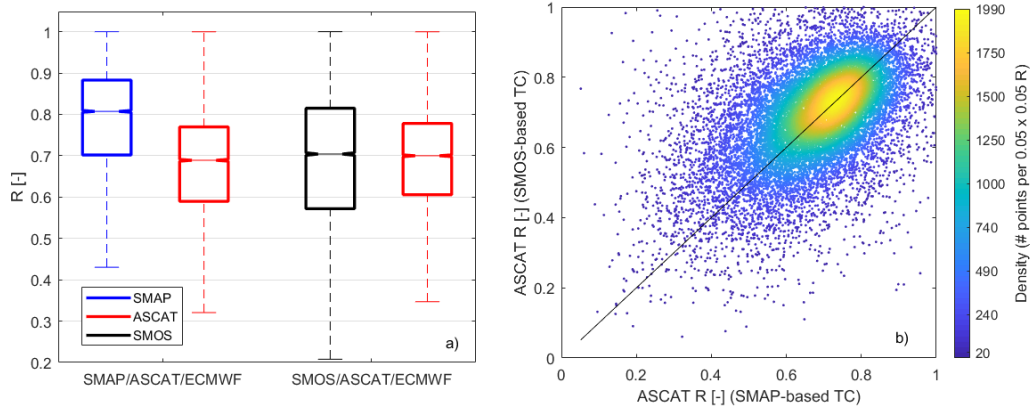
449 [-]) are found mostly elsewhere, except for parts of northern China/Mongolia and high-latitude
450 areas of Russia where retrievals are temporally scarce due to the extended cold season.

451

452 Also retrieving from a passive radiometer, SMOS demonstrates a similar R pattern as SMAP, but
453 the area of high correlation shrinks considerably in North America, Europe and Africa. SMOS
454 also has less coverage than SMAP in the high latitudes of northern hemisphere and Asia, where
455 correlations are relatively poor. On the other hand, SMOS has better spatial coverage and
456 exhibits good correlations across Australia.

457

458 ASCAT presents moderate ($\sim 0.5 - 0.8$ [-]) correlations in most available land pixels, and
459 achieves higher values only in limited regions. However, higher ASCAT R are found in
460 Northeastern China, where both SMAP and SMOS are out-performed by ASCAT. The 95%
461 confidence interval (CI) (Fig. 7b, d, f) indicate relatively narrow (mostly < 0.2 [-]) ranges from
462 Monte-Carlo simulation (i.e., small uncertainty in North America, Europe and Australia for
463 SMAP, ASCAT and SMOS). Larger uncertainties are found in the high latitudes, tropical Africa
464 and India, where retrieval is hindered by frequently frozen ground or high biomass. Uncertainties
465 for SMOS are overall greater than SMAP and ASCAT over Argentina, but are smaller in South
466 Africa.



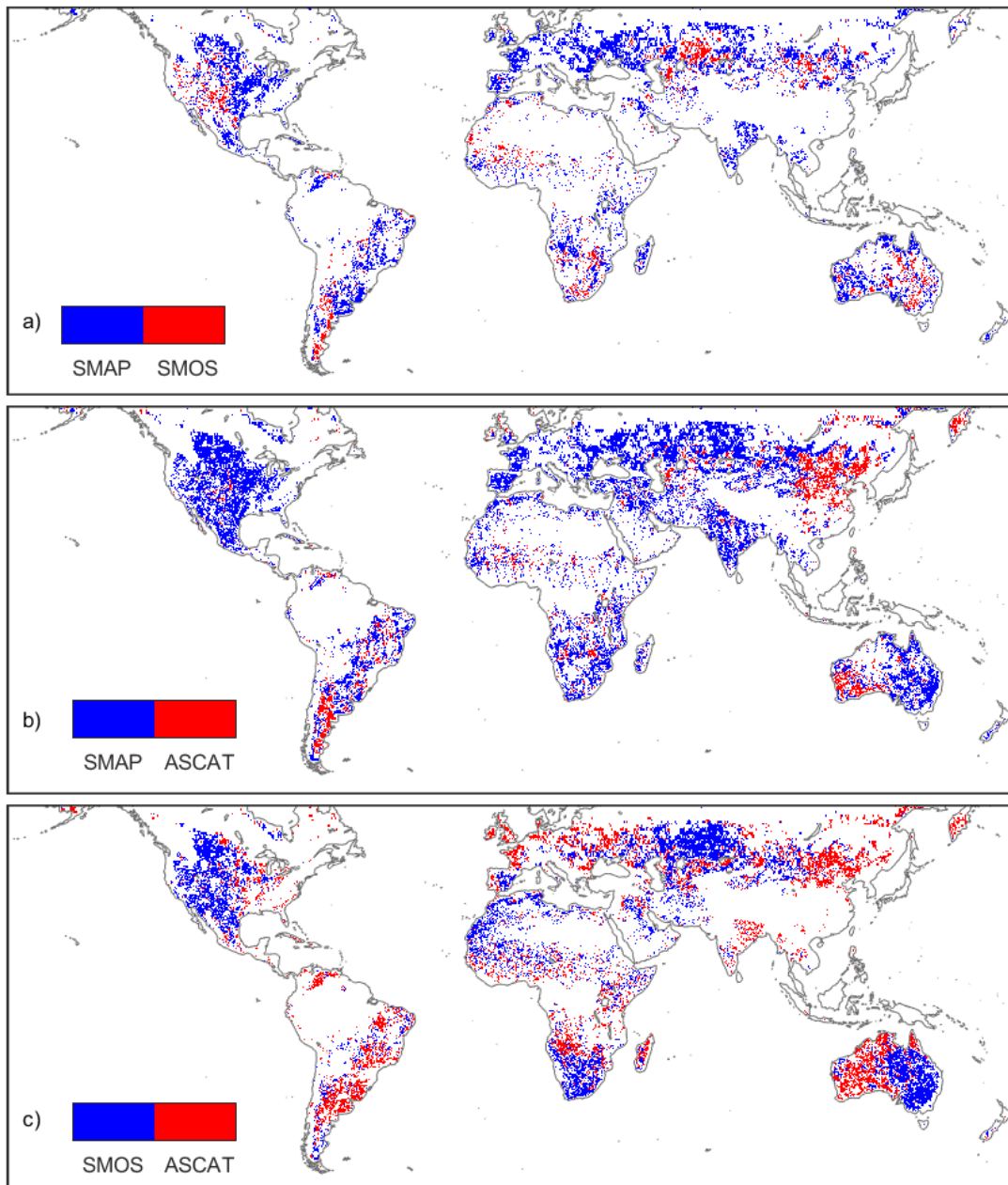
467

468 **Figure 8.** a) Distribution of correlation coefficients in common grid pixels ($N=16,332$) where both sets of
 469 single-run TC analyses (i.e., [SMAP/ASCAT/ECMWF] and [SMOS/ASCAT/ECMWF]) are available.
 470 See Fig. 3 caption for boxplot descriptions. b) Scatterplot comparison of ASCAT R obtained via SMAP-
 471 and SMOS-based TC.

472 The distribution of TC-estimated correlation values obtained globally illustrates the overall
 473 superiority of SMAP (median of ~ 0.8 [-]) to SMOS and ASCAT (median of ~ 0.7 [-]) (Fig. 8a).
 474 SMAP also presents the narrowest spread with most of its R values above 0.40 [-]. SMOS shows
 475 the largest spread and relatively greater number of lower values compared to SMAP and
 476 ASCAT. Note the ASCAT R values obtained from SMAP- and SMOS-based TC analyses are
 477 highly consistent in terms of both statistical distributions (Fig. 8a) and point-by-point
 478 comparisons (Fig. 8b). This consistency lends further support on the overall robustness of our TC
 479 approach. In particular, it suggests that the impact of non-zero ECC is nearly identical for
 480 ASCAT R results derived from the [SMAP-ASCAT-ECMWF] and [SMOS-ASCAT-ECMWF]
 481 triplets, and it is appropriate to simply average ASCAT R estimated from each triplet for
 482 comparison against SMAP and SMOS. This approach is applied later when the three remote
 483 sensing products are compared at the same time. Global-averaged R obtained for SMAP, SMOS

484 and ASCAT (averaged from SMAP- and SMOS-based TC) retrievals over common pixels are
485 0.76, 0.66 and 0.63, respectively.

486



487

488 **Figure 9.** Comparison of TC-estimated correlation coefficients between the satellite retrieval products.

489 Color shade indicates the product that obtains higher R in more than 95% of the bootstrap re-sampling

490 runs in a given grid cell. All areas of non-significant differences are masked. Plotted results are based on
491 the following triplets: a) [SMAP-ASCAT-ECMWF] (for SMAP) vs. [SMOS-ASCAT-ECMWF] (for
492 SMOS); b) [SMAP-ASCAT-ECMWF] (for SMAP and ASCAT); and c) [SMOS-ASCAT-ECMWF] (for
493 SMOS and ASCAT).

494

495 As noted in Section 4, it is likely that R values in Figures 8 and 9 are uniformly biased high (on
496 the order of 0.05 to 0.10 [-]) due to low amounts of ECC in SMAP-ASCAT and SMOS-ASCAT
497 pairs. However, relative R comparisons between products are expected to be more robust.

498 Qualitative comparisons between the satellite products are presented in Fig. 9, in which only
499 pixels with 95% significance of comparison are shown. Superiority at 95% significance is
500 achieved when one product has higher R value in more than 95% of the bootstrap re-samples.
501 Each bootstrap replicate is treated as an independent sample and the i th sample TC result for
502 SMAP is compared with the i th sample result for SMOS. In this way, approximately two-thirds
503 of the pixel-wise R differences are identified as being significant (see Table 2).

504 The two L-band passive soil moisture products are compared in Fig. 9a. SMOS out-performs
505 SMAP in areas of the Western United States, Southern Argentina, Central Asia and Eastern
506 Australia, but ‘SMAP better’ pixels dominate the rest of the globe. Globally, the SMAP
507 correlation is significantly higher than SMOS in 47% of the land pixels where comparisons are
508 available, while SMOS is significantly higher in 14% of the pixels (Table 2). In areas of
509 generally strong RFI pollution (e.g., Europe), the aggressive RFI mitigation efforts applied to
510 SMAP retrievals (Mohammed *et al.* 2016; Johnson *et al.* 2016; Piepmeier *et al.* 2017) may
511 explain their superior performance versus SMOS.

512 The relative performance of SMAP versus SMOS could conceivably be impacted by (somewhat
513 arbitrary) decisions regarding data flagging and threshold for estimated quality measure. Here,
514 the sensitivity of TC results to the SMOS data screening rules is examined by experimenting
515 with a stricter DQX threshold ($0.04 \text{ m}^3/\text{m}^3$). Currently a less-stringent SMOS DQX threshold (\leq
516 $0.07 \text{ m}^3/\text{m}^3$) is applied in order to include more retrievals and increase the sample size for TC. As
517 suggested in Table 2, more than 5000 pixels (or 14.4%) were removed by applying a DQX =
518 $0.04 \text{ m}^3/\text{m}^3$ threshold in the TC[SMOS-ASCAT-ECMWF] analysis. Results show that the
519 default threshold (DQX = $0.07 \text{ m}^3/\text{m}^3$) leads to a slight increase in the 'SMAP better' pixel
520 classification relative to the DQX = $0.04 \text{ m}^3/\text{m}^3$ case (which favors SMAP in ~7% of all the
521 commonly available pixels); however, it does not reduce the frequency of 'SMOS better' pixels
522 as much (only ~2% pixels affected). In addition, only 0.3% of the common pixels change from a
523 'SMOS better' to a 'SMAP better' category when the DQX threshold is relaxed from $0.04 \text{ m}^3/\text{m}^3$
524 to $0.07 \text{ m}^3/\text{m}^3$. Therefore, our default DQX threshold results in only a small negative impact on
525 SMOS performance relative to SMAP.

526 C-band active scatterometer retrievals from ASCAT are out-performed by SMAP in most areas
527 except for Northeastern China, Southern Argentina and Southwestern Australia, where ASCAT
528 retrievals demonstrate higher R (Fig. 9b). ASCAT R is significantly higher than SMAP R in only
529 14% of the pixels where TC results are available, while SMAP is significantly better than
530 ASCAT at more than 50% of the available global land pixels. Note that both SMOS and ASCAT
531 data used here were subject to processing errors due to grid transformation (to the SMAP native
532 grid), which may cause slight under-performance and benefit SMAP in these comparisons.
533 However, the slight global superiority of SMAP relative to SMOS is consistent with SMAP
534 validation results at core validation sites (Chan *et al.* 2016).

535 The SMOS-ASCAT comparison shows a relatively even number of pixels being superior.
536 SMOS correlation is significantly higher in most of United States, Central Asia and eastern
537 Australia, whereas ASCAT is better in most of Northeastern China, Western Europe (areas
538 SMOS suffers severely from RFI contamination), Argentina, and Western Australia. Considering
539 both products being extensively validated and relatively mature, the comparison in Fig. 9c
540 suggests that distinctive strength in each product has been firmly established in specific regions.
541 The spatial pattern of these comparisons is largely consistent with Al-Yaari *et al.* (2014), which
542 compared SMOSL3 and ASCAT with the Modern-Era Retrospective analysis for Research and
543 Applications (MERRA-Land) surface soil moisture, except in Western Australia and Argentina
544 where SMOS is found to correlate better with MERRA-Land than ASCAT.

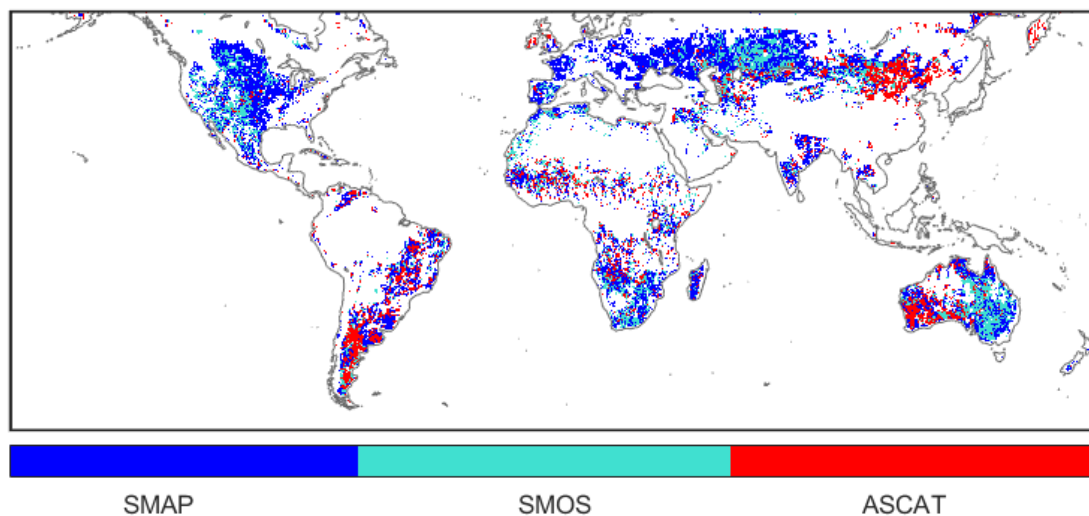
545 **Table 2.** Pair-wise comparisons between TC-estimated correlation coefficients for various satellite
546 products. The significance of differences is assessed using a 95% confidence threshold and the boot-
547 strapping approach described in Section 2.3. Percentages are out of all global land pixels with viable TC
548 estimates (see Section 2.1).

	SMAP higher		SMOS higher		No. pixels
	sig.	non-sig.	sig.	non-sig.	
SMAP vs. SMOS*	47%	21%	14%	17%	28294
SMAP vs. SMOS**	40%	23%	17%	20%	24614
	SMAP higher		ASCAT higher		
SMAP vs. ASCAT	53%	19%	14%	14%	39181
	SMOS higher		ASCAT higher		
SMOS* vs. ASCAT	35%	18%	29%	18%	36520
SMOS** vs. ASCAT	41%	19%	23%	17%	31264

549 * $DQX \leq 0.07 \text{ m}^3/\text{m}^3$; ** $DQX \leq 0.04 \text{ m}^3/\text{m}^3$

550

551



552

553 **Figure 10.** The satellite product (SMAP, SMOS or ASCAT) with the highest single-run TC-based
554 correlation coefficient.

555

556 A map showing the best-performing satellite product is presented in Fig. 10. Note that regions
557 with dense vegetation are largely masked due to a lack of successful retrievals. Likewise, in arid
558 regions such as the Sahara Desert and Great Basin Desert, earlier studies have revealed poor or
559 even negative correlation between active and passive products (de Jeu *et al.* 2008; Pierdicca *et*
560 *al.* 2013; Burgin *et al.* 2017). This limits the area over which TC can be performed due to the
561 masking of pixels where negative mutual correlation exists among the input datasets (see Section
562 2.1). As indicated above, ASCAT R values obtained from SMAP- and SMOS-based TC analyses
563 are averaged for comparison. Overall, SMAP and SMOS are superior to ASCAT in most areas of
564 North America, Europe, Southern Asia and Eastern Australia. The significant overlap of

565 geographic regions where both passive satellites excel is generally consistent with the high level
566 of correlation between SMAP and SMOS found earlier by Burgin *et al.* (2017). ASCAT
567 generally performs better than SMAP and SMOS across high-latitude areas of Eastern Asia, parts
568 of South America (mainly Argentina) and Southwestern Australia. As in Fig. 9, SMOS has
569 higher R than SMAP in the Western United States, Central Asia and most inland pixels of
570 Eastern Australia. Overall, SMAP ranks highest in 52% of the pixels with viable TC results (see
571 Section 2.1) whereas SMOS and ASCAT each does in 24% of these pixels.

572

573 **6. Summary**

574 In this analysis, a global assessment and comparison of SMAP (L2 passive), SMOS (L3) and
575 ASCAT (L2) surface soil moisture products is performed based on the correlation metric (R)
576 obtained via triple collocation (TC). In order to produce robust TC results, R is estimated
577 following removal of low-frequency variability in the soil moisture time series and therefore
578 reflects the R of soil moisture anomalies relative to a 30-day moving temporal average. Given
579 that low-frequency error sources have been previously identified in certain remotely-sensed soil
580 moisture products (Wagner *et al.*, 2014), this focus on solely high-frequency noise represents a
581 limitation in our approach. Nevertheless, sensitivity experiments suggest that our global TC
582 results are relatively insensitive to changing the size of the moving window from 30 to 60 days
583 (not shown).

584 In addition, when comparing satellite products, it is critical to account for the sampling
585 uncertainties due to sparse temporal availabilities or suboptimal retrieval conditions. To this end,
586 a moving-block bootstrap re-sampling approach, with emphasis on preserving the temporal

587 properties of the original soil moisture time series, was applied at each grid pixel to construct the
588 confidence interval for TC estimates. The re-sampled distribution of correlation estimates is then
589 used to obtain the significance of TC-based R differences between SMAP, SMOS and ASCAT
590 soil moisture retrieval products.

591 Concern about the violation of TC assumption due to error cross-correlations between active-
592 passive observations and between satellite and model products is addressed via a quadruple
593 collocation (QC) analysis conducted within available sparse network sites (Fig. 2). Slight
594 positive error cross-correlation is found to exist between ASCAT and both SMAP and SMOS
595 which suggests that TC-estimated R for the three satellite-based products may be positively
596 biased. However, since this bias is small and approximately equal for all three products, the
597 relative evaluation against each other changes only slightly from QC to TC. Results also indicate
598 limited impact associated with potential satellite-model error cross-correlations. Recent findings
599 by Pierdicca *et al.* (2017) using a novel extended QC algorithm and 15 months of satellite and
600 model data reveals weak SMAP-SMOS ECC that is lower than the SMAP-ASCAT ECC found.
601 Such findings suggest the further potential of using SMAP and SMOS together in TC in future
602 analyses. Finally, the sensitivity of SMOS TC results to the specification of the DQX threshold is
603 shown to be low.

604 To the best of our knowledge, this study is the first to present a global-scale triple collocation
605 analysis that compares the footprint-scale correlation metric of SMAP with SMOS and ASCAT
606 soil moisture products. Results suggest that, out of these three products, SMAP has the highest
607 global average R (0.76, SMOS: 0.66, ASCAT: 0.63) and is the superior product for the majority
608 (52%) of global land pixels with a viable TC result. This finding is consistent with several recent
609 validation studies (e.g. Kumar *et al.* 2017; Montzka *et al.* 2017; Pierdicca *et al.* 2017; Kim *et al.*

610 2018). For example, using information theory-based metrics, SMAP has also been found to
611 provide higher information content than other microwave satellite soil moisture products (Kumar
612 *et al.* 2017). Likewise, in a validation study applying both standard validation methods and triple
613 collocation at footprint-scale soil moisture measurements from the Cosmic Ray Neutron Probes
614 (CRNP, including some of the COSMOS stations used here) across five continents, SMAP
615 outperformed other satellite products including AMSR2, SMOS and ASCAT (Montzka *et al.*
616 2017). Nevertheless, each of the three satellite retrieval products (SMAP, SMOS and ASCAT)
617 were found to be superior (to the other two) in specific global land regions. Therefore, the global
618 inter-comparison maps in Figures 9 and 10 provide useful information for regional-scale
619 applications such as the choice of dataset for assimilation into rainfall-runoff models.

620 In closing, it should be noted that all products considered here are subject to frequent re-
621 processing and algorithm improvements. For example, a new global daily SMOS SM product --
622 the SMOS-INRA-CESBIO (SMOS-IC) product was recently released and shown to yield
623 generally higher correlations versus ground observation versus the v300 SMOS Level 3 soil
624 moisture product considered here (Fernandez-Moran *et al.*, 2017). Comparable enhanced SMAP
625 soil moisture products are likely to arise in the foreseeable future. Therefore, the cross evaluation
626 efforts described here are, in reality, an on-going effort requiring updating as improved products
627 are released.

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636

637

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829 **List of Figure Captions**

830 **Figure 1.** Schematic diagram of moving block bootstrap sampling on collocated, temporally uneven
831 triple-soil-moisture-product time series with an l_{opt} of 7. Overlapping data blocks from the original time
832 series (top) are drawn randomly with replacement and then concatenated to generate a new bootstrap
833 resample (bottom).

834 **Figure 2.** Location of ground observation sites (N=271) from sparse networks.

835 **Figure 3.** Distribution of ECC between SMAP-ASCAT and SMOS-ASCAT pairs estimated via the
836 application of QC at sparse sites listed in Fig. 2. The upper and lower bounds of the boxes indicate 25th
837 and 75th percentiles respectively and the red line in the box indicates the median. Whiskers extending
838 from the 25th and 75th percentiles to represent 1.5 times the interquartile range.

839 **Figure 4.** Comparison of differences in SMAP, SMOS and ASCAT correlation coefficients (ΔR) obtained
840 from TC (a-f) and QC (g-i) at ground locations shown in Fig. 2. In the vertical axes, “psv” refers to
841 passive satellite products, (SMAP or SMOS), “pt” refers to point-scale ground observations. The vertical
842 dashed lines indicate the mean ΔR for each histogram. Number of stations used in each subplot is shown
843 as “N”.

844 **Figure 5.** Comparison of ΔR (same as in Fig. 4) obtained from NRV3- and ECMWF-based TC analyses.
845 Subplots a), b) and c) include common data points in Fig. 4a and 4d, Fig. 4b and 4e, and Fig. 4c and f,
846 respectively.

847 **Figure 6.** Comparison of ΔR (same as in Fig. 4) obtained from TC and QC analyses. Subplots a), b) and
848 c) include common data points in Fig. 4a and 4g, Fig. 4b and 4h, and Fig. 4c and i, respectively.

849 **Figure 7.** Quasi-global image of TC-based R [-] (single run, without bootstrap re-sampling) for SMAP,
850 ASCAT and SMOS (left column: subplots a, c, e) and total width of the 95% confidence interval (‘CI’,
851 right column: subplots b, d, f) derived from a 1,000-member bootstrap sampling. Subplots a) – d) are
852 based on a [SMAP-ASCAT-ECMWF] triplet. Subplots e) - f) are based on a [SMOS-ASCAT-ECMWF]
853 triplet.

854 **Figure 8.** a) Distribution of correlation coefficients (from single triple collocations runs) in common grid
855 pixels (N=16,332) where both sets of TC analyses [SMAP/ASCAT/ECMWF and
856 SMOS/ASCAT/ECMWF] are available (see Fig. 2 caption for boxplot descriptions); b) comparison of
857 ASCAT R obtained via SMAP- and SMOS-based TC analyses.

858 **Figure 9.** Comparison of TC-estimated correlation coefficients between the satellite retrieval products.
859 Color shade indicates the product that obtains higher R in more than 95% of the bootstrap re-sampling
860 runs in a given grid cell. All areas of non-significant differences are masked. Plotted results are based on
861 the following triplets: a) [SMAP-ASCAT-ECMWF] (for SMAP) vs. [SMOS-ASCAT-ECMWF] (for

862 SMOS); b) [SMAP-ASCAT-ECMWF] (for SMAP and ASCAT); and c) [SMOS-ASCAT-ECMWF] (for
863 SMOS and ASCAT).

864 **Figure 10.** The satellite product (SMAP, SMOS or ASCAT) with the highest TC-based correlation
865 coefficient (\bar{R} , bootstrap mean).