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Relating satellite gravimetry data to global soil moisture products via data harmonization and correlation analysis

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Abstract

Due to limited in-situ data global soil moisture products should also be validated with respect to independent global data sets. Our study investigates possibilities and benefits of relating soil moisture products from remote sensing and hydrological modeling to information on total water storage change from satellite gravimetry. We use soil moisture data from the active satellite sensor ASCAT and the hydrological model WGHM as well as satellite gravity field observations from the GRACE mission. First we apply a data harmonization procedure to equalize the distinct data representations and formats of those data sets. Then we perform a correlation analysis. The results show correlations close to one between GRACE and soil moisture data specifically for humid and temperate regions. A comparison of correlation coefficients from different data pairs highlights that in arid environments total water storage from GRACE corresponds better to surface soil moisture captured by ASCAT than to total soil moisture from WGHM. In humid and temperate regimes the observation is reversed. Furthermore regions could be identified where the input data of the WGHM might be of low quality, producing higher correlations between ASCAT and GRACE than between ASCAT and WGHM. We therefore conclude that GRACE data can deliver valuable information for the quality assessment of soil moisture products and provide a link to their contribution to continental water storage.

Key words: soil moisture, correlation analysis, data harmonization, GRACE, WGHM, ASCAT

1. Introduction

High-quality global or small-scale soil moisture products are of great interest to various sectors, dealing for example with agricultural development, disaster management (drought and flood forecast), or water supply (Bolten et al. 2010). Comprehensive and continuous measurements of soil moisture on site in direct contact with the medium are currently not available on global scale (Wang & Qu, 2009). Only some continental areas start to be well covered by The International Soil Moisture Network (www.ipf.tuwien.ac.at/insitu/). Therefore recent small-scale soil moisture maps are either derived indirectly from satellites or from the outputs of hydrological models. Examples of satellite sensors and models which are used for the generation of soil moisture maps are given in Table 1.

Table 1: Examples of satellite sensors and models, delivering data for global soil moisture maps.

Satellite Sensors				**Models**		
Sensor	**Satellite Platform**	**Type**	**Operation Time**	**Name**	**Type**	**Operation Time**
ASCAT (Advanced SCATterometer)	METOP	Active Scatterometer (C-Band)	2006 - present	WGHM (WaterGAP Global Hydrology Model)	Hydrological water balance model	1901 - present
AMSR-E (Advanced Microwave Scanning Radiometer for EOS)	AQUA	Passive Radiometer (X-Band and C-Band)	2002 - 2011	GLDAS (Global Land Data Assimilation System)	Land Surface Model	1979 - present
MIRAS (Microwave Imaging Radiometer using Aperture Synthesis)	SMOS	Passive Radiometer (L-Band)	2010 - present	ERA-Interim (ECMWF global atmospheric reanalysis)	Atmospheric Reanalysis	1989 - present

For creating or improving global data sets on soil moisture four main research targets can be identified:

1. Understanding the nature of soil moisture and associated processes
2. Understanding the nature of satellite data that are used to indicate soil moisture
3. Developing methods for the generation of soil moisture products based on this understanding
4. Developing methods for the validation of the generated soil moisture products and with it doing a quality assessment on Research Targets 1 to 3.

This study focuses on Research Target 4.

Most commonly the validation of global soil moisture products is performed by choosing one or more local study sites where satellite or modeled data are compared against in-situ measurements. The lessons learnt from these local sites are then projected to larger regions. Major in-situ validation sites for AMSR-E are located in the United States. As part of the Soil Moisture Experiments (SMEX) they are situated for example in the Walnut Creek Watershed, Iowa (Cosh, 2004) and the little Washita river watershed, Oklahoma (Cosh et al. 2006). For ASCAT various studies have been done within Europe. An example is the extensive work of Brocca et al. (2011), comparing ASCAT and AMSR-E data with measurements of 17 in-situ stations in Italy, Spain, France, and Luxembourg. Another extensive study of Albergel et al. (2012) evaluates data from 200 stations, located in Africa, Australia, Europe, and the United States for ASCAT and SMOS. Specifically for the verification of SMOS data the field campaign "Surface Monitoring Of the Soil Reservoir EXperiment" (SMOSREX) has been established in Mauzac near Toulouse, France (De Rosnay et al., 2006). An example of respective validation studies on models is the work of Kato et al. (2007) comparing soil water content of the three GLDAS land surface models NOAH, MOSAIC and CLM with globally distributed in-situ data from thirty field measurement stations from the Global Energy and Water Cycle Experiment (GEWEX).

Due to the sparse distribution of operating field measurement stations, the comparison of satellite or modeled data with in-situ data is limited to regional scales. Therefore comprehensive global validation studies are mainly done by the mutual comparison of different global soil moisture products, using various mathematical approaches such as statistical analysis (Dirmeyer et al. 2004), triple collocation method (Dorigo et al., 2010; Scipal et al. 2008; Leroux et al. 2011) or correlation analysis (Jeu et al., 2008; Reichle et al. 2004). Subject to those validation studies are mostly different remote sensing products from active and passive satellite sensors and various models providing hydrological information, as listed in Table 1.

Based on global validation studies of soil moisture products the following statements were for example made:

- High foliage density contaminates the microwave signal of soil moisture specifically for radiometers (Dirmeyer et al., 2004; Scipal et al., 2008; Dorigo et al., 2010; Jeu et al., 2008)
- Over dense forest no retrieval is possible, applying for both active and passive microwave data (Jeu et al., 2008)
- In desert areas microwave scatterometers are prone to volume scattering effects of dry sand and systematic surface roughness effects (Scipal et al., 2008; Dorigo et al., 2010; Jeu et al., 2008)
- Radio Frequency Interference artificially lowers soil moisture values (Jeu et al., 2008)
- Regions of snow and ice are susceptible to signal contamination for passive microwave sensors (Dirmeyer et al., 2004)
- Poor or absent snow-melt modeling degrades the quality of soil moisture products from models (Dirmeyer et al., 2004)

Furthermore information on data quality is used to produce merged global soil moisture products from different sensors (Liu et al., 2012; Liu et al., 2011) and to assimilate satellite soil moisture data into models (Reichle et al., 2013; Draper et al., 2012; Dharssi et al., 2011).

Reflecting on these results one can conclude that inter-comparisons of independent data sets on global scale have been helpful to identify and locate problems arising from the mapping of soil moisture from space or by modeling. In addition to direct comparisons with in-situ data they provide valuable information for global quality control.

Considering the fundamental importance of quality control for global soil moisture products and recognizing previous findings of inter-comparison studies, this paper investigates the possibilities and benefits of relating data from satellite gravimetry to global soil moisture products. Specifically satellite data from the GRACE (Gravity Recovery And Climate Experiment) mission are used. Those data have already been subject to several studies focusing on the quality control or calibration of model outputs in terms of total continental water storage (Güntner, 2008; Werth et al., 2009; Werth & Güntner, 2010; Mueller et al. 2011; Houborg et al., 2012). However, a specific analysis with respect to soil moisture data has not been performed yet. In our research we compare GRACE data against surface soil moisture products from ASCAT and total soil moisture and total water storage data from WHGM. For the comparison we perform a correlation analysis.

The comparison of GRACE data with global soil moisture products has some advantages. Firstly GRACE data are available on global scale from 2002 until present with a temporal resolution of one month. Secondly the derived information on changes in total water storage are based on the measurement of mass changes and are therefore totally independent of any other remote sensing technique or hydrological modeling method. Also the topographic complexity or land cover do not play any role for data quality (as it does for example for scatterometers).

Other characteristics of GRACE are rather challenging when it comes to the comparison with global soil moisture products. For example several assumptions have to be made in order to link changes in total water storage to changes in soil moisture, which are in fact two different kinds of parameters. Also

GRACE data, which are usually provided in spherical harmonic coefficients, have to be corrected for signals related to the satellite's orbit characteristics and short-term mass changes using specific algorithms and filters (see Section 2.2). Consequently the soil moisture data have to be treated in the same way to achieve a harmonized representation of all data sets for the comparison. Relating soil moisture products to products from GRACE is therefore not straight forward.

Focusing on the integration of GRACE data into the validation of soil moisture products via correlation analysis this study addresses three main research questions:

1. Is the correlation of GRACE and soil moisture data feasible with respect to the harmonization steps:
    a. Conversion of soil moisture data into spherical harmonics
    b. Filtering
2. Can we observe in certain regions of the world correlations between the different data sets and with it identify where GRACE data may be useful for the understanding of soil moisture products?

3. What is the benefit of correlating GRACE data with soil moisture data sets?

For seeking the answers to those research questions the chapters of this study are structured in the following way. In Chapter 2 on "Methodology" we first focus on the assumptions we make in order to link changes in total water storage to changes in soil moisture (2.1). Afterwards we point out our approach for harmonizing soil moisture products and data from satellite gravimetry and describe the subsequent correlation analysis (2.2). In Chapter 3 on "Materials" we introduce the data sets of GRACE, ASCAT and WGHM. In the fourth chapter we present the results of the correlation analysis with respect to the first two research questions. We demonstrate how correlation results are impacted if the input soil moisture products are converted into spherical harmonics and filtered using a standard Gauss-filter (Research Question 1). Furthermore we show world maps, highlighting the correlation coefficients for different data combinations for the time period September 2006 to August 2011 (Research Question 2). The correlation results and the benefits of relating GRACE data to soil moisture products (Research Question 3) are discussed in the fifth Chapter. Finally we draw conclusions in the last chapter.

2. Methods

2.1 Assumptions

Putting the signal from GRACE in relation to soil moisture is not directly possible. This is mainly based on the fact that GRACE is not only sensitive to signals of soil moisture but to all sources of mass changes on the Earth's surface and its interior. Changes of atmospheric and oceanic masses as well as signals from solid Earth tides are removed from the signal already during pre-processing using background-models (Flechtner, 2007). This implies that over non-polar continental regions GRACE provides information predominantly on mass changes within the continental hydrology, that entail the largest remaining effect on temporal variations of the gravity field on seasonal time scales. On first sight we compare two different parameters in our analysis: soil moisture and terrestrial masses. Figure 1 illustrates that soil moisture is (together with surface water, ground water, canopy storage and snow and ice) part of the total continental water storage (TWS). The mass of TWS sums up together with changes of non-hydrological masses (e.g. within the solid Earth's body due to mantle convection and post-glacial rebound) to the total terrestrial mass variation that is sensed by GRACE. Soil moisture is one component out of the terrestrial mass. If it changes, the terrestrial mass changes as well.

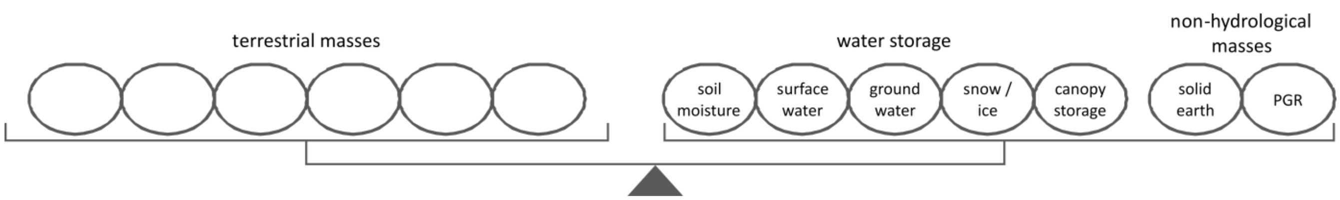

Figure 1: Balance illustrating main mass components on earth, adding up to the terrestrial masses as sensed by GRACE. PGR refers to post-glacial rebound.

In order to put variations in soil moisture in direct relation to changes in terrestrial masses we make several assumptions:

1. We assume that solid earth does not change in the time span of our study and that consequently a change in the gravity field is only related to changes in terrestrial water masses. Therefore we

refer to change in total water storage when mentioning GRACE data.

2. For assumption 1 we only make one exception: as post-glacial rebound (PGR) is also visible over shorter time periods (Geruo et al., 2012; Purcell et al., 2011), we neglect correlation values of regions affected by post glacial rebound in our study (Alaska, Canada, Greenland, Scandinavia, Antarctica).
3. We only focus on areas, where snow and ice can be neglected. In this way we can exclude these contributions to total water storage.
4. We do not focus on regions with high foliage density due to the low precision of ASCAT data in these regions. Therefore we neglect the small contribution of canopy storage to continental water storage.
5. Considering the prior assumptions we are only left with three components that make up the change in continental water storage, namely surface water, ground water and the target parameter soil moisture. We assume that correlations between change in soil moisture and change in total water storage are high if:
    a. the change in soil moisture is much larger than the change of ground water and surface water combined.
    b. soil moisture changes proportionally with ground water and surface water.

Assumption 4a) we consider possible, as surface water is rather a point-like (lake) or line-like (river) phenomenon, while soil moisture changes over large areas. Furthermore groundwater does not show strong short-term variation (recharge ≤ 5mm/year), unless excessively impacted by humans for example through irrigation (Taylor et al., 2012). Assumption 4b) is based on the idea that soil moisture serves as transition zone between surface and ground water and therefore may show similar variations.

Accounting for assumptions 1 to 4 we assume that under certain circumstances changes in soil moisture can be put in relation to changes in total water storage as sensed by GRACE.

2.2 Data Set Harmonization and Correlation Analysis

In our study we relate fundamentally different data sets from satellite gravimetry, remote sensing, and hydrological models via correlation analysis. From satellite gravimetry we obtain the change in total water storage. From remote sensing data and hydrological modeling we receive information on soil moisture. The data sets do not only differ in the observed parameter as discussed in the previous chapter, but also show different characteristics in terms of spatial and temporal resolution, units, representation and processing. In order to best possibly avoid an impact of the different data structures on the correlations between the data sets, we harmonize all data sets before correlating them. The different steps that are taken for data harmonization are shown in Figure 2.

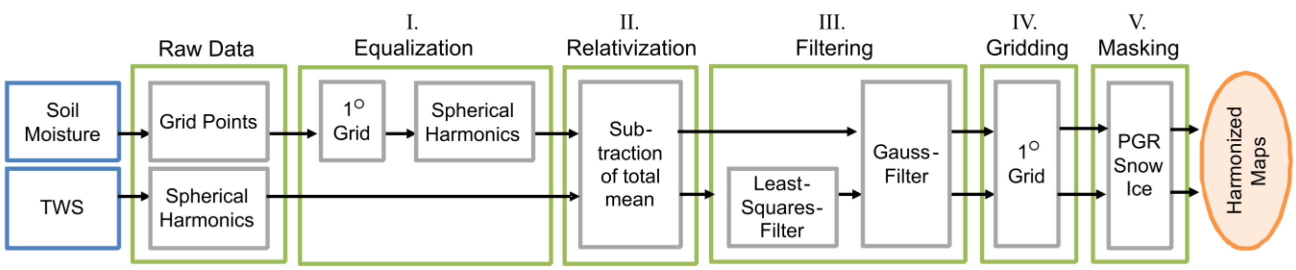

Figure 2: Flowchart describing the data harmonization process for equalizing soil moisture products and satellite gravimetry data on total water storage (TWS).

The monthly change in continental water mass from GRACE is commonly derived from spherical harmonic coefficients of the Earth's gravity field (Wahr et al., 1998). Soil moisture products are usually provided in different grid formats of for example 25 km x 25 km or 0.5° x 0.5°. To equalize the representation of all data sets the gridded soil moisture data from remote sensing and hydrological modeling are first brought to a 1° x 1° grid by computing the simple average of all data points falling within a 1° grid cell. Then the grid points are converted into spherical harmonics up to the same degree and order as the data from GRACE (here we apply data sets of degree and order 70). Research Question 1a) addresses, how this first change of representation influences the correlation between the two soil moisture data sets.

Since we restrict our analysis of GRACE data to changes of continental water storage we reduce the spherical harmonic coefficients from GRACE by their long-term mean over the overlapping time period of all compared products. Likewise the spherical harmonic coefficients of the soil moisture products (obtained from the conversion of the grids by spherical harmonic analysis) were reduced by their mean values. Consequently we end up with information on changes in TWS (GRACE) and changes in soil moisture (ASCAT and WGHM). Proceeding with values relative to the mean and not absolute values implies that we will relate information on hydrologic anomalies from different data sets.

As third processing step the data are filtered. GRACE Level-2 data (spherical harmonic coefficients) contains specific errors resulting from measurement principle and orbit characteristics of the twin-satellite mission (Wahr et al., 1998). So-called correlated errors are due to the mission's inability to resolve spherical harmonic coefficients at all degrees and orders. Furthermore mass fluctuations on sub-monthly timescales that are not captured by the applied background models of atmosphere and oceans cause high frequency aliasing. These errors would show up as meridional stripes in maps of gravity field variations if not treated accordingly. Here we follow the widely used procedure by applying (a) a least-squares polynomial filter for the reduction of the correlated errors in the coefficients ("destriping") (Swenson & Wahr, 2006) and (b) an isotropic Gaussian smoothing filter (Wahr et al., 1998) with 300km half-wavelength for the reduction of noisy short wavelength components. The latter is applied in the course of the conversion of spherical harmonic coefficients into monthly fields of Equivalent Water

Heights (EWHs).

The least-squares filter is only applied to GRACE data. It has been demonstrated by Swenson and Wahr (2006) that this filter only marginally influences data sets, which are not affected by correlated errors (like our converted fields of ASCAT and WGHM). In contrast it is well-known that the Gaussian smoothing filter does not only remove the unwanted noise but also (depending on the filter wavelength) a significant part of the desired signal. Therefore it is necessary to filter all data sets with this filter in order to obtain comparable data. Without applying this common filter the soil moisture products would show much finer patterns than the GRACE data. In Research Question 1b) we focus on the impact of Gaussian filtering on the correlations between two soil moisture data sets.

As forth step we convert the spherical harmonic coefficients of all data sets back into geographical grids of 1°. We do not scale the data, as Liu et al. (2011) have shown that correlation values are not impacted by scaling. As a last step we mask areas influenced by snow, ice or PGR. The snow mask is derived from the hydrological model, excluding areas where the absolute value of all variation in snowfall over the observed time span is bigger than 20mm EHW and therefore might influence our filtered GRACE fields (Wahr et al., 2006). Respectively we also mask areas where (according to Geruo et al., 2012) PGR-rates exceed +/-5mm EWH per year (Gaussian-filter with 200km radius, maximum degree and order 60). The resulting harmonized maps are then used as input for the correlation analysis. We correlate the values of two data sets for each 1° grid cell over time. The correlation is simply assessed by computing the Pearson product-moment correlation coefficient (Rodgers & Nicewander, 1988), whereby the correlation coefficient between the two variables is equal to the covariance of both variables divided by their standard deviations. By computing the correlation coefficients we intend to identify regions where GRACE data corresponds well with soil moisture data (Research Question 2). Finally we interpret the results and conclude if there are benefits of including GRACE data into studies on soil moisture products (Research Question 3).

3. Data Sets

Within our study we compare gravimetric data from GRACE, remote sensing data on surface soil moisture (< 5cm) from the active sensor ASCAT and total soil moisture (simulated for the entire soil column) and TWS from the hydrological model WGHM. Table 2 gives an overview on the individual characteristics of each data set. The last column emphasizes the data specifications that we implemented for all data sets in the course of the data harmonization as described in Chapter 2.2. We focus on the time period September 2007 to October 2011 to allow the computation of mean values over complete annual cycles.

Table 2: Specifications of the original data sets and the targeted harmonized specifications for all data sets for the correlation analysis**.**

	Satellite Gravimetry	**Remote Sensing**	**Hydrological Model**	**Harmonized Specifications**
Source	GRACE	ASCAT	WGHM	
Product	Level 2, RL04, German Research Centre for Geosciences (GFZ)	Level 2 Soil Moisture at 25 km Swath Grid EUMETSAT, Vienna University of Technology (TU Wien)	2.1f, German Research Centre for Geosciences (GFZ)	
Reference	(Flechtner et al., 2010)	(Bartalis et al., 2007)	(Döll et al., 2003)	this paper
Parameter	change in total water storage	surface soil moisture	total soil moisture, change in total water storage	only changes can be compared, further assumptions are needed
Availability	2002 - present	2007 - present	1901 - present	Sep. 2007 - Aug. 2011
Temporal Resolution	monthly	daily	monthly	monthly
Spatial Resolution	~ 1°	25 km	0.5°	1°
Coverage	global	global	global	global
Unit	millimeter Equivalent Water Height (mm EWH)	% (0% dry, 100% wet)	millimeter Equivalent Water Height (mm EWH)	scaling to millimeter Equivalent Water Height (mm EWH)
Representation	spherical harmonics (SH)	ascending and descending tracks	0.5° world map	spherical harmonics (SH)
Post-Processing	least-squares-filtering, Gauss-filtering	-	-	least-squares-filtering only for GRACE, Gauss-filtering for ALL

ASCAT data provided by EUMETSAT contain additional information on quality control (Bartalis et al., 2008). Table 3 points out the criteria which we apply to exclude soil moisture data based on this information. The soil moisture error is derived from error propagation of the backscatter noise, and we exclude data if this error exceeds 10%. For the non-scatterometer based output variables containing information on topographic complexity, snow cover fraction, frozen land surface fraction, and inundation and wetland fraction a common threshold of 50% is applied. Furthermore all data are excluded where processing flags are set. Those flags account for limitations of the instrument (such as noise levels and sensitivity) and the amount of land in the scene. Correction flags indicate data that allow for the calculation of soil moisture but might be of reduced quality based on the choice of references for minimum and maximum saturation level of soil and backscattering. We do not take into account those flags as they limit data availability significantly; in contrast we aim at a better understanding of the quality of those data through the comparison with GRACE observations.

Table 3: Quality control information for ASCAT data as provided by EUMETSAT and respective exclusion criteria applied for this study.

Flags ASCAT	Exclusion Criteria
Soil moisture error	> 10%
Topographic complexity	> 50%
Snow cover fraction	> 50%
Frozen land surface fraction	> 50%
Inundation and wetland fraction	> 50%
Processing Flags	on
Correction Flags	off

The WaterGAP Global Hydrology Model (WGHM) is a state of the art water balance model, developed for the assessment of water resources and water balances in river basins. It simulates change in total continental water storage, accounting for the hydrological compartments groundwater, soil moisture, snow, canopy storage, and surface water in rivers, lakes, reservoirs, and wetlands. With it more compartments are included than for example in the Land Dynamics (LaD) World model (accounting for snow, soil and groundwater) or the Global Land Data Assimilation System (GLDAS) (accounting for canopy, snow and soil moisture). Solutions are provided in daily time steps at a spatial resolution of 0.5 degree. The model is calibrated for river discharge by over 1200 gauging stations worldwide. For the selected time period of this study the climate forcing data (temperature, cloudiness and number of rainy days per month) are provided by the operational forecasts of the European Centre for Medium-Range Weather Forecasts (ECMWF) (Werth & Güntner, 2010). Furthermore precipitation input from the Global Precipitation Climatology Centre (GPCC) is used. Soil moisture is modeled for one layer with spatially varying thickness, depending on the rooting depth of vegetation. The land cover dependent rooting depth is multiplied with the total available water capacity in the first uppermost meter of soil to compute the maximum available soil water capacity (Döll et al., 2003). Global TWS variations from WGHM have been compared in various studies to those from GRACE (Forootan et al., 2012; Crossley et al., 2012; Papa et al., 2008; Schmidt et al., 2006 and 2008).

4. Results

4.1 Data Harmonization

Regarding data harmonization we first pose the question how the conversion of gridded data into spherical harmonics (step I in Figure 2) changes the correlation values between two different data sets (Research Question 1a). Figure 3a shows the correlation coefficients for the mean- reduced ASCAT and WGHM data, when being brought to a 1° grid (we omit step I and III in Figure 2). Figure 3b displays the correlation of the same data sets with the sole difference that this time the data have been converted into spherical harmonics up to degree and order 70 and then brought back onto a 1° grid (we only skip step III in Figure 2). The impact of this equalization step is pointed out in Figure 3c, where the values of Figure 3b have been subtracted from the values of Figure 3a. Two major observations can be made from the plots: firstly data points are gained over the Sahara desert when applying spherical harmonics. Secondly correlations increase from Figure 3a to Figure 3b in a uniform manner, as Figure 3c shows an almost consistent difference between 0 and -0.2 in the correlation coefficients. A large difference of -1 is only observed around the Sahara desert.

The gain in data points over the Sahara is caused by the spherical harmonic conversion of the WGHM data. Prior to the conversion for extended regions over the Sahara the standard deviation of soil moisture change provided by the model is equal to zero. Therefore no correlation value can be calculated (denominator becomes zero). Due to the conversion in spherical harmonics the standard deviation becomes unequal zero (and with it also the denominator of the correlation coefficient), leading to additional correlation coefficients on the map. In arid environments, e.g. in the Arabian and Taklimakan desert, variations in soil moisture are very close to zero. Those extreme low values are also artificially increased by the transformation into spherical harmonics. With it standard deviations very close to zero become biased and generate (as shown in Figure 3c) large correlation differences of -1 (between Figure 3a and 3b) in hyper-arid environments with low soil moisture variation (< 5% of the data range).

Since ASCAT does not provide absolute soil moisture but percentage values (0% = lowest and 100% = highest inverted dielectric constant obtained over an extended observation period), the variation in soil moisture in hyper-arid regions is relatively high compared to WGHM. Consequently we do not identify any significant impact of the spherical harmonic conversion on the standard deviations of the ASCAT data. However, for change in TWS from WGHM the same bias for approximately the first 5% of the data range is observed. Based on these findings we avoid artifacts from spherical harmonic conversion in the following processing steps by excluding for all maps pixels where the standard deviation is smaller than 5% of the data range. The respective map of the correlation coefficients between ASCAD and WGHM after the conversion in spherical harmonics (still omitting step III in Figure 2) and the masking is shown in Figure 3d.

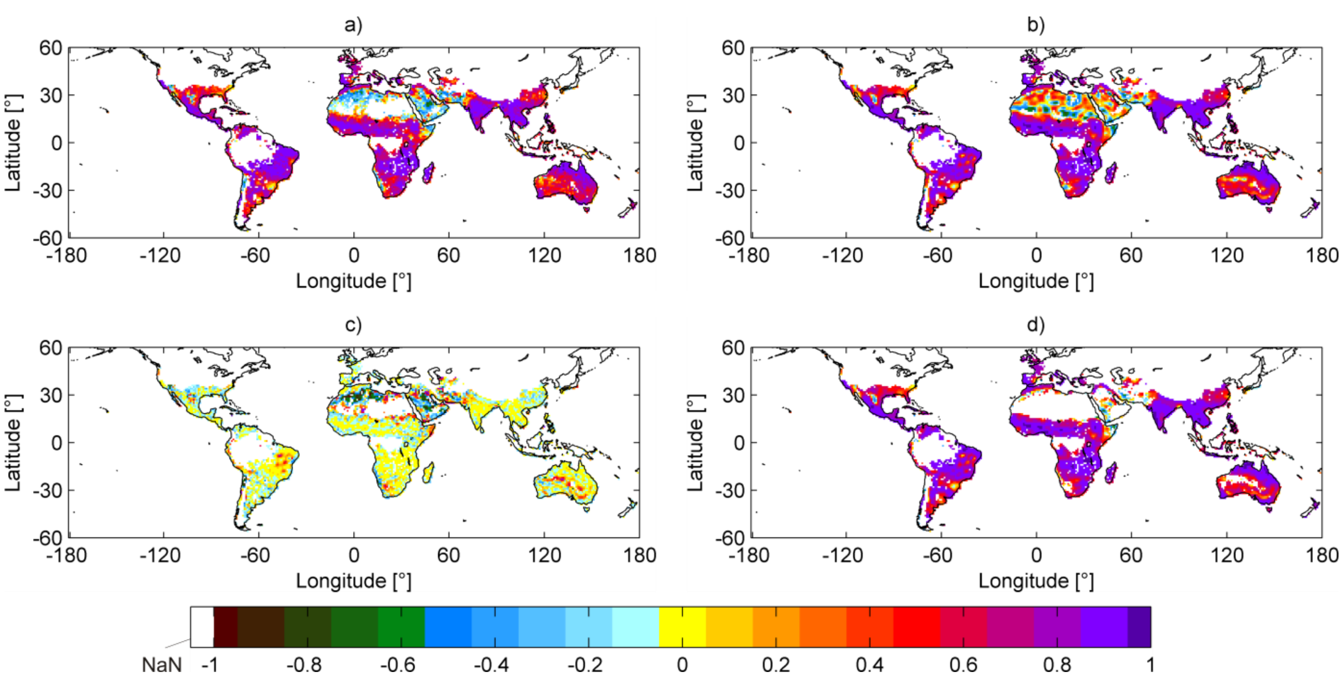

Figure 3: Correlation coefficients for change in soil moisture from WGHM and ASCAT, showing a) results for the original data when being brought to a 1° grid, b) results for the data from a) after spherical harmonic conversion of maximal degree and order 70 and c) the difference between the map from a) and the map from b). In d) we see the map of b) where regions with high negative differences (mainly in the Sahara) as shown in c) and artificial variations from b) are masked out.

Next, the impact of Gauss-filtering on the correlation coefficients of ASCAT and WGHM data is studied (step III in Figure 2, Research Question 1b). Figure 4a shows the correlation coefficients of soil moisture data from ASCAT and WGHM after spherical harmonic conversion and Gauss-filtering (all steps in Figure 2 are implemented). Figure 4b shows the difference between the filtered (Figure 4a) and unfiltered correlation coefficients. For filtered data the correlation coefficients are almost consistently higher.

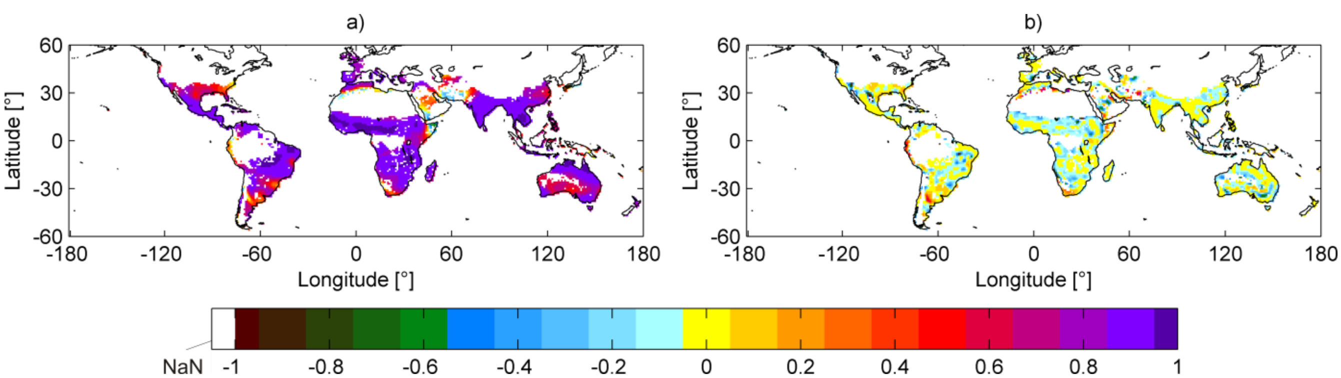

Figure 4: Correlation coefficients for change in soil moisture from WGHM and ASCAT, showing a) results from Figure 3d) after Gauss-filtering with 300km radius and b) the difference between the map from Figure 3d) and the map from Figure 4a).

Figure 5 shows impacts of the conversion in spherical harmonics and Gauss-filtering for time series of soil moisture variation (mean is subtracted) from ASCAT (Figure 5a, c, and, e) and WGHM (Figure 5b, d, and, f) at three selected locations. The data gaps in January 2011 and June 2011 appear as for these months GRACE data is not available. For the first location in India at 16°Latitude and 77°Longitude the correlation between ASCAT (Figure 5a) and WGHM (Figure 5b) increases from 0.7 to 0.9 due to data harmonization. In the case of the second location (Figure 5c and d) in Africa at 24.5°Latitude and

30.5°Longitude the original data from WGHM gives constantly values of zero (calculation of correlation is not possible). Those values are then artificially increased by the harmonization process leading to a correlation coefficient of 0.3. The time series for the third location in Africa at 27°Latitude and 0.5°Longitude (Figure 5e and f) shows a very small standard deviation for the original WGHM data with only one event during winter 2008/2009. The correlation coefficient with the original ASCAT data is -0.5 due to the well-known volume scattering effects of ASCAT in hyper-arid environments (see Chapter 1). It is then increased to 0.4 in the course of the conversion into spherical harmonics and Gauss-filtering. The faulty correlation results from the last two locations are not taken into account in the following correlation analysis due to the prior mentioned masking.

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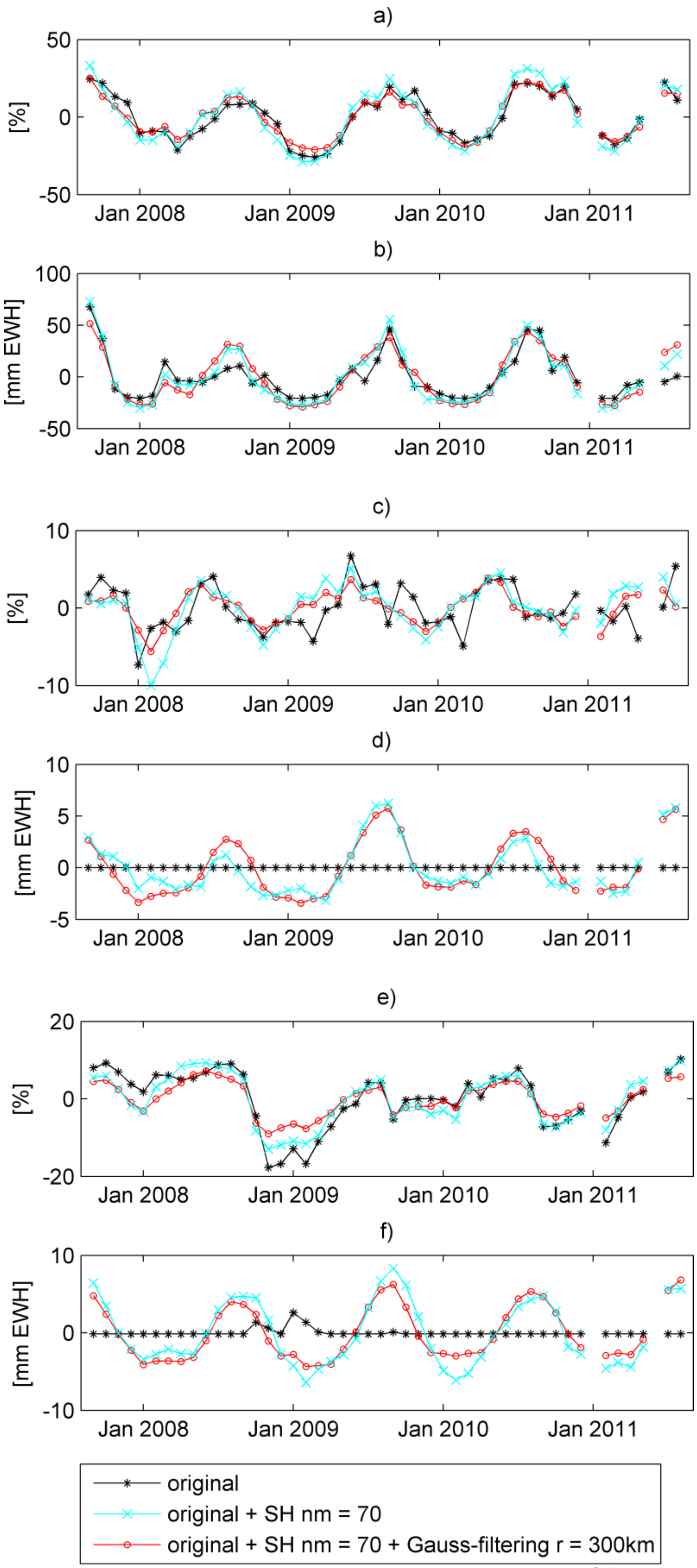

a)
b)
c)
d)
e)
f)
[%]
[mm EWH]
Jan 2008
Jan 2009
Jan 2010
Jan 2011
original
original + SH nm = 70
original + SH nm = 70 + Gauss-filtering r = 300km

Figure 5: Time series showing impacts of data harmonization (conversion in spherical harmonics of degree and order 70, and Gaussian-filtering with 300km radius) on data in India at 16°Latitude and 77°Longitude for soil moisture variation from a) ASCAT and b) WGHM, on data in Africa at 24.5°Latitude and 30.5°Longitude for soil moisture variation from c) ASCAT and d) WGHM, and on data in Africa at 27°Latitude and 0.5°Longitude for soil moisture variation from e) ASCAT and f) WGHM.

4.2 Correlation Analysis

In the following we focus on the actual correlation values that can be observed for two harmonized data sets (all steps in Figure 2 are implemented). First we focus on pairs of the same parameter. The correlation coefficients between change in total water storage as sensed by GRACE and modeled by WGHM are shown in Figure 6a. Over extended regions the correlation coefficient exceeds 0.6. In dry climate regimes rather low correlations (for example in Patagonia) or most often no values are available (Sahara desert, Arabia). This is due to the fact that the data were masked out based on the low standard deviation of WGHM data. In Figure 6b correlation coefficients for change in soil moisture derived from ASCAT and WGHM are displayed. Even higher correlation values than for the two data sets on total water storage are visible, indicating that both data sets are in good agreement.

Secondly we focus on pairs of two different parameters. Figure 6c shows the correlation values between change in soil moisture from WGHM and change in total water storage from GRACE. This time the correlation coefficients are lower than in Figure 6a and Figure 6b, especially in dry climate regimes. In humid climate zones, e.g. the Amazonian region and East Asia, correlation is close to 1. In Figure 6d the correlation coefficients for change in soil moisture from ASCAT and change in total water storage from GRACE are displayed. Again high correlation values close to 1 are visible in humid climate regimes, specifically in East Asia. Also in temperate regions, including parts of Europe and Western US, correlation values of about 0.5 are reached. Negative values are again found in dry climate zones with the exception of the Australian desert.

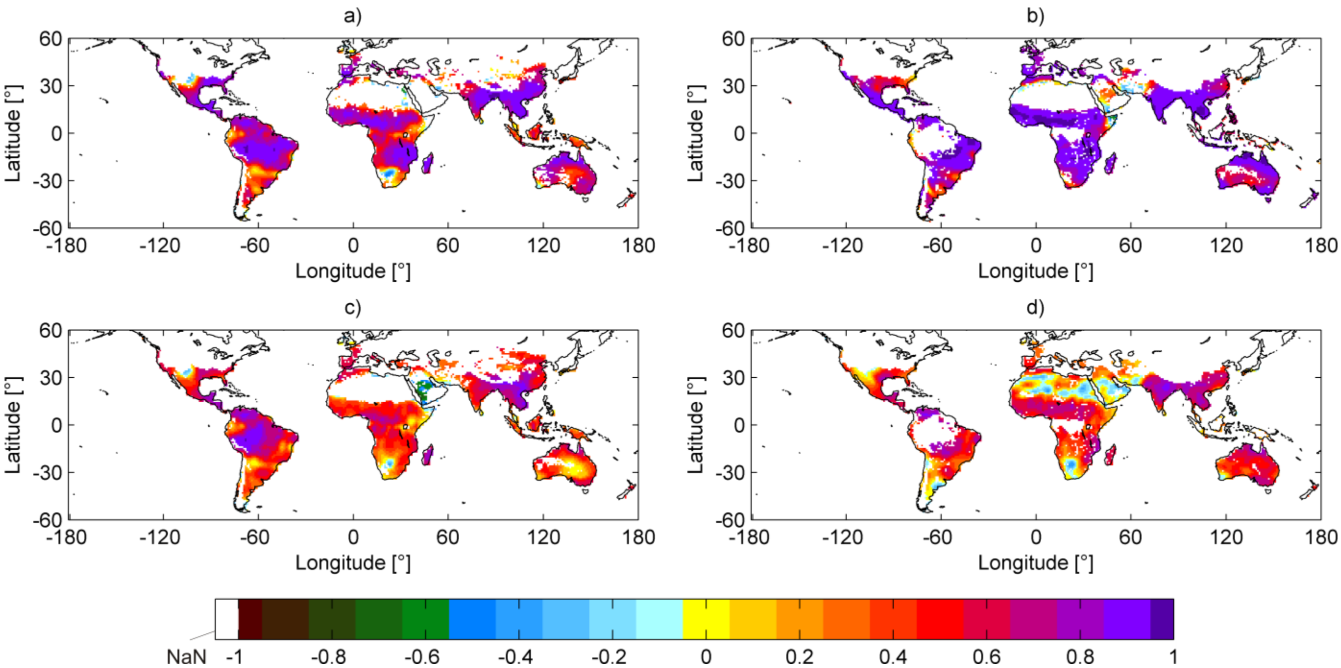

Figure 6: Correlation coefficients for a) total water storage changes from GRACE and WGHM, b) soil moisture changes from ASCAT and WGHM, c) soil moisture changes from WGHM and total water storage changes from GRACE, d) soil moisture changes from ASCAT and total water storage changes from GRACE.

5. Discussion

The results from Chapter 4.1 emphasize two major effects that are connected with the data harmonization process described in Figure 2 (Research Question 1): first, the conversion into spherical harmonics and the Gauss-filtering smooth the signal, and detail is lost on spatial scale. Also the temporal resolution is decreased by downscaling from daily to monthly values. The comparison of soil moisture products with GRACE data can therefore only be integrated in studies focusing on phenomena of a coarse spatial and temporal resolution. Studies on the scale of small catchments, as usually performed for the validation of soil moisture products, are not feasible with GRACE. Smoothing or filtering impact the correlation coefficients mainly in a uniform way. By losing detail and reducing noise correlation increases. This indicates that the analyzed products differ almost uniformly on spatial scale in the high frequencies. This could be due to the diverse acquisition and interpolation techniques that are used to generate the grid points of the different data sets.

But spherical harmonics do not in all cases smooth the signal. For very small variations in the signal (as in the Sahara desert) a reverse effect can be seen: the signal itself is not smoothened but its variation increases artificially. Such artifacts impact the correlation with other data sets or generate new correlation coefficients in regions where the standard deviation of the original data was equal to zero. We therefore suggest masking out areas that show artificial variations after the spherical harmonic conversion and exclude them from correlation studies.

Results from Chapter 4.2 provide information on absolute correlation values for different data set combinations (Research Question 2). Highest correlation values occurred when either soil moisture data from WGHM and ASCAT or total water storage data from WGHM and GRACE were correlated. This result is expectable since in both cases the data sets contain information on the same parameter. It can also be concluded that WGHM agrees very well with data from remote sensing and gravimetry.

When two different parameters are correlated, the coefficients are generally lower. Higher correlation values can be found in humid climate regimes than in arid ones. Three possible explanations may be given for this phenomenon: firstly the data on TWS from GRACE can be viewed as highly uncertain in arid regimes as the accuracy of GRACE is restricted to several tens of mm EWH (Wahr et al., 2006). Secondly modeled data on soil moisture might have lower quality, since there are fewer in-situ data from river gauges available to calibrate the WGHM. Also it has been shown that ASCAT data correlate negatively with other soil moisture products in deserts (Liu et al., 2011). Thirdly it is possible that the assumptions above (Chapter 2.1) do not hold in areas of low correlation. This would imply that either soil moisture is not the dominant component in the water balance, or total water storage and soil moisture do not change proportionally.

Based on the results of the correlation analysis the benefits of correlating changes in total water storage from GRACE with changes in soil moisture from ASCAT and WGHM shall be discussed (Research Question 3). Therefore absolute correlation values of different product pairs are put in relation. Figure 7 shows in which regions ASCAT correlates better, worse or similar with total water storage from GRACE than with soil moisture data from WGHM. Only in very few regions GRACE correlates better with ASCAT, e.g. in the South-East of the US or in Japan. GRACE data is therefore not able to deliver comparable information than WGHM. However, GRACE may help to identify areas where WGHM needs to be improved. For example the dark areas in South America may correspond to river catchments, where the model is not reliable.

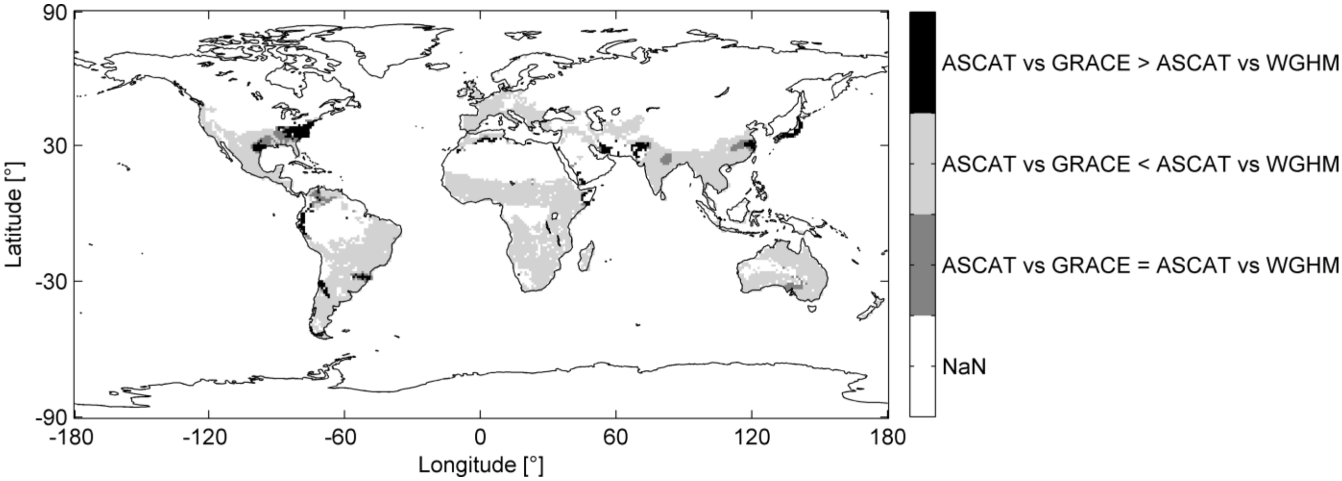

Figure 7: Map indicating in which regions of the world ASCAT correlates better, worse or similar with total water storage from GRACE than with soil moisture data from WGHM

Figure 8 shows in which regions of the world total water storage from GRACE correlates better, worse or similar with soil moisture data from ASCAT than with soil moisture data from WGHM. Clear patterns are visible: to a large extent those can be related to the soil moisture regimes map, provided by the United States Department of Agriculture (Source: Soil climate map, USDA-NRCS, Soil Science Division, World Soil Resources, Washington D.C., Production Date: April, 1997). Comparing both maps, we find that in most cases:

1. ASCAT correlates better than WGHM with GRACE in
    - ustic regimes (Semi-arid climate): Great Plains, USA; North-East Brazil; Africa's savanna, scrub and woodland; India
    - aridic regimes (Arid climate): world deserts
2. ASCAT correlates worse than WGHM with GRACE in
    - udic regimes (Humid or subhumid climate): Eastern USA; Brazil; China
    - xeric regimes (Mediterranean climate): Western USA; Mediterranean countries; Western Australia
3. ASCAT correlates similar than WGHM with GRACE in

- the transitions zones between different regimes

In summary there is a higher agreement between ASCAT and GRACE in arid and semi-arid environments, and a higher agreement between WGHM and GRACE in humid and Mediterranean environments.

This observation is in concordance with the characteristics of each soil moisture data set. ASCAT delivers information on soil moisture for the soil surface, as the signal only penetrates a few centimeters into the ground. On a daily basis it is able to capture short term variations. This functionality is favorable for arid environments. Soil moisture changes quickly and mainly at the surface, as precipitation evaporates rapidly due to high solar radiation. In addition, surface soil moisture is more likely to present the moisture in the whole soil column as the soil layer is shallow and its water holding capacity is low. Also soil moisture has a proportionally large impact on the whole water balance as there are fewer surface water bodies and there are only low variations in (fossil) ground water, unless excessively used by humans. It is therefore expectable that surface soil moisture from ASCAT shows similar variations in arid climate regimes as TWS from GRACE. In contrast, the hydrological model shows lower correspondence since it is more difficult to model fast changes in those highly sensible environments, where often less data from river gauges are available for the calibration of the model.

In humid climate regimes it is expected that deeper soil layers have a larger correspondence to TWS, since the water holding capacity is high and the soil profile reaches several meters into the ground. Consequently, changes in surface soil moisture are less representative for changes in total soil moisture, and along with this also for changes in TWS. This behavior is also reflected in the result of the correlation analysis, where surface soil moisture from ASCAT showed lower correlations with GRACE than total soil moisture from WGHM.

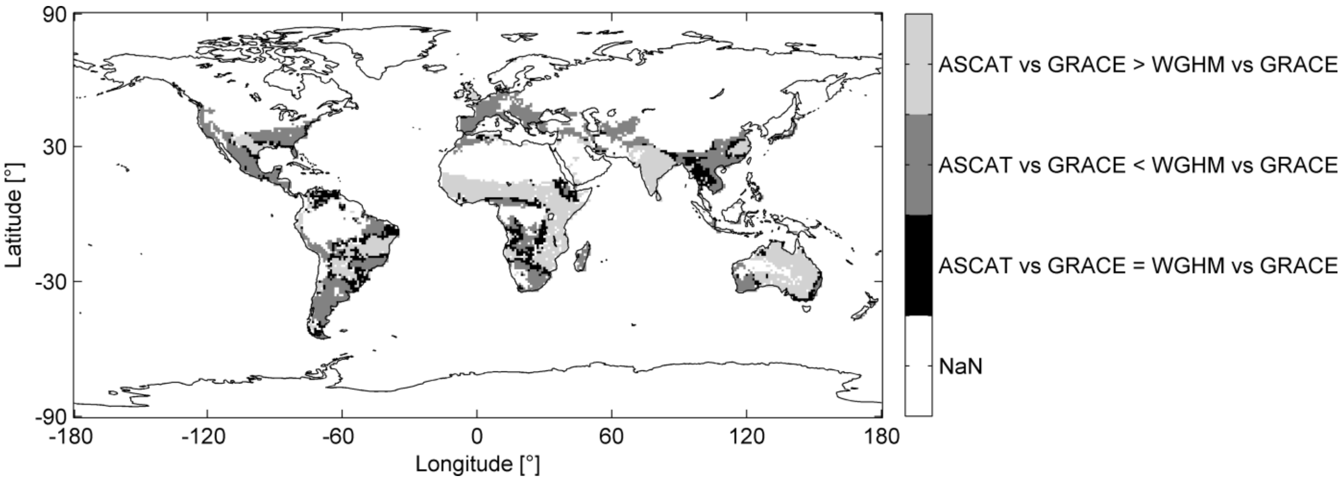

Figure 8: Map indicating in which regions of the world total water storage from GRACE correlates better, worse or similar with soil moisture data from ASCAT than with soil moisture data from WGHM.

6. Summary and Conclusions

In this paper we investigated possibilities and benefits of relating data from satellite gravimetry to global soil moisture products. Specifically we performed a correlation analysis between gravimetric data from the satellite mission GRACE and two soil moisture products from the active satellite sensor ASCAT and the hydrological model WGHM. In order to equalize the otherwise distinct representations and formats of each data set, they were harmonized previous to the correlation analysis. It is assumed that changes in total water storage can be linked to changes in soil moisture, if either soil moisture is the dominating compartment of continental hydrology or if soil moisture changes proportionally with total water storage. Therefore areas of intensive snowfall, ice coverage and post-glacial rebound effects were excluded from our study.

We raised three main research questions. First it was analyzed how the data harmonization process influences the correlation results between different data sets. It has been demonstrated that it does not impact the correlation coefficients with three exceptions: (a) Gauss-filtering and spherical harmonic conversion smooth the data spatially. Thereby the correlation coefficients increase uniformly, so that they cannot be directly compared with the absolute correlation values of other studies. (b) Smoothing decreases the level of detail, making the data not suitable for studies on small catchments. (c) The correlation results were not reliable in regions where the soil moisture data showed variations equal or very close to zero. Therefore we had to exclude hyper-arid environments like the Sahara desert from our study.

Secondly, we focused on the results of the correlation analysis and posed the question whether regions can be identified where GRACE data shows similar variations as soil moisture data. It was found that in most regions with high precipitation the correlation coefficients are close to one, while in arid regions they can be lower than 0.5 or even negative. This indicates that GRACE data is specifically linked to soil moisture data in humid and temperate climate zones.

Finally the benefit of correlating GRACE data with soil moisture data sets has been investigated. Therefore the correlation results of different data pairs were put in relation. As expected, in general soil moisture products correlated better with each other than with GRACE. However, also some regions were found where the soil moisture product of ASCAT correlates better with total water storage from GRACE than with soil moisture from WGHM. In these areas the hydrological model might be of low quality. Furthermore the results showed in most cases that in arid environments daily surface soil moisture from ASCAT maps better the overall situation on total water storage than the hydrological model. In contrast, the hydrological model performs better in humid and temperate regions, where the soil moisture in the whole soil column is more representative for changes in total water storage.

Therefore our results indicate that GRACE data can indeed help to validate soil moisture products and increase the understanding on surface and total soil moisture as well as their link to total water storage.

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