

UPSCALING SPARSE GROUND-BASED SOIL MOISTURE OBSERVATIONS FOR THE VALIDATION OF COARSE-RESOLUTION SATELLITE SOIL MOISTURE PRODUCTS

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[1] The contrast between the point-scale nature of current ground-based soil moisture instrumentation and the ground resolution (typically $>10^2$ km²) of satellites used to retrieve soil moisture poses a significant challenge for the validation of data products from current and upcoming soil moisture satellite missions. Given typical levels of observed spatial variability in soil moisture fields, this mismatch confounds mission validation goals by introducing significant sampling uncertainty in footprint-scale soil moisture estimates obtained from sparse ground-based observations. During validation activities based on comparisons between ground observations and satellite retrievals, this sampling error can

be misattributed to retrieval uncertainty and spuriously degrade the perceived accuracy of satellite soil moisture products. This review paper describes the magnitude of the soil moisture upscaling problem and measurement density requirements for ground-based soil moisture networks. Since many large-scale networks do not meet these requirements, it also summarizes a number of existing soil moisture upscaling strategies which may reduce the detrimental impact of spatial sampling errors on the reliability of satellite soil moisture validation using spatially sparse ground-based observations.

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1. INTRODUCTION

[2] Soil moisture data sets are of potential value for a wide range of geophysical applications including the analysis of long-term terrestrial water cycle trends [Jung *et al.*, 2010], sources and impacts of climate variability [Seneviratne *et al.*, 2010], terrestrial contributions to the global carbon cycle [Falloon *et al.*, 2011], drought processes [Cai *et al.*, 2009], short-term weather prediction [Drusch, 2007], streamflow

generation mechanisms [Berg and Mulroy, 2006], disease vector abundance [Githeko *et al.*, 2000], and terrestrial dust emissions [Laurent *et al.*, 2008]. Unfortunately, the impact of soil moisture measurements on these applications has historically been marginalized by the relative scarcity of long-term, large-scale soil moisture data sets [Robock *et al.*, 2000]. Within the past 20 years, however, this observational gap has been progressively filled by the parallel development of remote sensing technologies and the establishment of ground instrumentation networks. In particular, the availability of soil moisture products from the recent Soil Moisture and Ocean Salinity (SMOS) and Aquarius missions and the Soil Moisture Active Passive (SMAP) mission planned for launch in 2014 will inaugurate a new era in the application of remote sensing observations to hydrology, water resource, and climate applications. These three missions are based on utilizing a variety of L band microwave radar and radiometry instrumentation to estimate volumetric soil moisture content in the top 5 cm of the soil column. Using land data assimilation techniques, these superficial

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observations can, in turn, be vertically extrapolated to constrain root zone (surface to ~ 1 m) soil moisture estimates and the impact of soil water limitations on vegetation functioning and surface energy fluxes over moderately vegetated land surfaces [Reichle *et al.*, 2008].

[3] All three missions (SMOS, Aquarius, and SMAP) are characterized by relatively coarse scale soil moisture retrievals. The SMOS mission, for example, retrieves surface soil moisture using L band radiometer observations acquired at multiple incidence angles within an average instantaneous field of view (IFOV) resolution of 43^2 km² [Kerr *et al.*, 2010; European Space Agency (ESA), 2010]. Successfully launched in November 2009, SMOS is currently producing a global surface soil moisture product with a 1 to 3 day revisit interval. Here IFOV resolution is defined as the ground-projected area within which 50% of the ground signal (integrated by the antennae) originates. Depending on the instrument type, the instrument IFOV can assume a range of shapes including ellipses (for real aperture radiometers); rhomboids (for radar retrievals based on Doppler range detection); and highly irregular, nonpolygonal shapes (for synthetic aperture sensors like SMOS).

[4] Similarly, Aquarius uses a push broom L band radiometer and real aperture radar to measure surface ocean salinity [Lagerloef *et al.*, 2008]. Because it is primarily designed to retrieve ocean salinity, Aquarius instrumentation acquires only very coarse resolution (i.e., IFOV resolution of $\sim 100^2$ km²) measurements. Nevertheless, mission plans include the retrieval of an Aquarius soil moisture product over land (T. J. Jackson, personal communication, 2012). Finally, the SMAP mission concept is based on the simultaneous acquisition of L band radar (1^2 to 3^2 km² IFOV area depending on swath position) and radiometer ($\sim 40^2$ km² IFOV area) observations from a shared conically scanning antenna to provide both a radiometer-only soil moisture product and a gridded 9^2 km² product based on the fusion of radiometer and radar information [Entekhabi *et al.*, 2010a].

[5] In addition to these three L band missions, there are other active and passive microwave instruments operated at shorter wavelengths (C and X band), including the Metop-A Advanced Scatterometer [Bartalis *et al.*, 2007], the Environmental Research Satellite Scatterometer [Naemi *et al.*, 2009], and the Advanced Microwave Scanning Radiometer (AMSR-E) [de Jeu *et al.*, 2008; Jackson *et al.*, 2010]. Although they are not optimally designed for soil moisture remote sensing and are generally based on IFOV resolutions generally greater than 30^2 km², they form an important complement to L band missions and provide the basis of existing long-term, satellite-based soil moisture data sets [Wagner *et al.*, 2007]. Validation during extensive field campaigns suggests root-mean-square errors (RMSEs) of between 0.03 and 0.07 m³ m⁻³ for these products [e.g., Jackson *et al.*, 2010; Champagne *et al.*, 2010; Brocca *et al.*, 2010a]. Note that here and throughout the review, all soil moisture values are given in volumetric soil moisture fraction units or m³ m⁻³ (i.e., the volume of soil water per total volume of soil).

[6] The accuracy of all remotely sensed soil moisture products is impacted by a range of error sources including

antennae noise, structural uncertainty in surface backscatter and emission modeling, and error in ancillary parameters required to parameterize these models. The satellite missions mentioned above are (or will be) tasked with meeting specific baseline standards for the accuracy of their soil moisture products. These standards are typically expressed via a maximum RMSE threshold for footprint-scale soil moisture retrievals. Both the SMOS and SMAP missions have a specific moisture retrieval RMSE goal of 0.04 m³ m⁻³ for land surfaces free from dense vegetation cover, frozen soil, snow cover, and complex topography [ESA, 2010; Entekhabi *et al.*, 2010a]. These RMSE thresholds are generally interpreted to reflect the accuracy of a single, near-instantaneous satellite-based retrieval and not some average in time. For this reason, all RMSE and/or standard deviations values given below should be interpreted as instantaneous values referring to a single moment in time. In addition, RMSE thresholds typically do not make allowances for the removal/correction of long-term bias in satellite products.

[7] In response to this progress, recent international activities, coordinated by the Global Energy and Water Cycle Experiment in cooperation with the Group of Earth Observation and the Committee on Earth Observation Satellites, have focused on the promotion of soil moisture as an environmental data record. A key part of this process is assuring that quality control and validation procedures for soil moisture products meet standards defined by the Quality Assurance for Earth Observation (QA4EO) initiative (<http://QA4EO.org>). Such standard are based on verifying the traceability of observations (or higher-level retrieval products) to accepted reference data sets to support credible quality control assurances. For remotely sensed soil moisture retrievals, such traceability requires establishing a robust linkage to ground-based soil moisture observations obtained at a point. While nonlinearities in microwave emission and backscatter processes are not negligible, experience in observing system simulation experiments and success in regional field campaigns suggests that they have a relatively modest impact on footprint-scale soil moisture retrievals [Drusch *et al.*, 1999a; Zhan *et al.*, 2008]. Consequently, the appropriate target variable for large-scale soil moisture retrievals is generally considered to be the linear spatial average of true surface soil conditions within the instrument IFOV. However, relative to other geophysical variables commonly retrieved from satellite instrumentation, the remote sensing of soil moisture is challenged by the particular combination of coarse instrument resolution (due to its reliance on relatively long wavelength microwave emission/backscatter) and soil moisture's notable tendency to exhibit large amounts of extremely fine scale ($<1^2$ m² to 1^2 km²) spatial variability. As a result, establishing credible ground validation approaches for soil moisture requires bridging the scale contrast between the IFOV resolution of satellite sensors and the (essentially) point-scale spatial support of current ground-based instrumentation.

[8] Ground-based soil moisture observations are increasingly available from long-term operational soil moisture measurement networks (Tables 1 and 2), and significant

TABLE 1. Current and Planned Large-Scale (>10,000 km² in Extent) Operational Soil Moisture Monitoring Network Ordered From Largest to Smallest in Areal Extent

Network Name	Country or Region	Number of Sites	Approximate Areal Extent	Average Spacing ^a
Ruswet-Grass ^b	Ukraine/Russia	122	10 ⁷ km ²	>100 ² km ²
Chinese Ecosystem Research Network	China	31	10 ⁷ km ²	>100 ² km ²
Soil Climate Analysis Network	USA	141	10 ⁷ km ²	>100 ² km ²
Climate Research Network	USA	144	10 ⁷ km ²	>100 ² km ²
National Ecological Observatory Network	USA	20	10 ⁷ km ²	>100 ² km ²
Oklahoma Mesonet	Oklahoma, USA	127	200,000 km ²	40 ² km ²
High Plains Regional Climate Center	Nebraska, USA	53	200,000 km ²	60 ² km ²
Illinois Climate Network	Illinois, USA	19	150,000 km ²	90 ² km ²
ARM-SGP ^c	Oklahoma/Kansas, USA	31	140,000 km ²	70 ² km ²
Mumbridgee Basin ^{d,e}	Australia	73	80,000 km ²	33 ² km ²
Upper Danube Basin ^f	Germany	10	80,000 km ²	90 ² km ²
SMOSMANIA ^{f,g}	France	12	40,000 km ²	60 ² km ²
Mongolia Validation	Mongolia	14	14,000 km ²	30 ² km ²

^aAverage spacing is calculated as the ratio of areal extent/number of sites.

^bSee <http://www.ipf.tuwien.ac.at/insitu/> for historical data and network information.

^cAtmospheric Radiation Measurement Southern Great Plains.

^dSee <http://www.oznet.org.au>.

^eInclusive of the Yanco, Kyeamba, and Adelong Creek subnetworks within the Mumbridgee Basin.

^fSMOS validation site.

^gSoil Moisture Observing System–Meteorological Automatic Network Integrated Application.

efforts have been made to unify observations from various networks into a common database [Robock *et al.*, 2000; Dorigo *et al.*, 2011]. However, the spatial characteristics of these networks are not ideal for the evaluation of coarse-scale satellite soil moisture products (or to construct continuous, coarse-resolution soil moisture products in general). As shown in Table 1, “large-scale” networks (i.e., ones with spatial coverage greater than several SMOS or SMAP footprints or ~10,000 km²) typically lack required sampling densities to provide multiple measurements per footprint. For instance, one of the densest networks listed in Table 1, the Oklahoma Mesonet, provides (on average) a single point-scale soil moisture observation per 40² km² area. This density equates to an average of about one observation per 40² km² SMAP IFOV (or ~43² km² SMOS IFOV) and considerably less than one observation within each grid of the merged 9² km² SMAP active/passive product. Since the subfootprint spatial standard deviation of point-scale soil moisture observations often exceeds the 0.04 m³ m⁻³ RMSE accuracy goal set for SMOS and SMAP [Famiglietti *et al.*, 2008], significant sampling errors are likely when estimating an instantaneous footprint-scale mean via such sparse sampling of the underlying surface soil moisture distribution. The presence of such errors and their potential impact on satellite validation RMSE goals motivate the development of soil moisture upscaling methods to more effectively translate information derived from sparse point-scale ground-based sensors to satellite footprint resolutions.

[9] In addition to the large-scale networks described in Table 1, there are a number of smaller-scale (<10,000 km²) networks actively measuring surface soil moisture at much higher spatial densities (Table 2). While the restricted coverage of these local networks limits their effectiveness as the basis of any large-scale validation effort, they provide an excellent source of validation information over a range of land cover types and an opportunity to examine sub-footprint-scale soil moisture spatial scaling. In particular,

comparisons against independent soil moisture observations acquired during intensive field campaigns suggests that if acquired at sufficient spatial densities, observations from these networks can be spatially aggregated to provide basin-scale (1000 to 10,000 km²) soil moisture estimates at RMSE accuracies (~0.01 m³ m⁻³) which are small relative to validation goals imposed for current and future satellite missions [Cosh *et al.*, 2006, 2008].

[10] As noted above, multiscale soil moisture data sets have also been periodically made available by short-term, intensive field campaign activities. Within North America, these activities include the Southern Great Plains (SGP) hydrology experiments in 1997 and 1999 (SGP97 and SGP99)

TABLE 2. Current and Planned Local- to Regional-Scale (>100 km² and <10,000 km² in Extent) Operational Soil Moisture Networks Ordered From Largest to Smallest in Areal Extent

Network Name	Country or Region	Number of Sites	Approximate Areal Extent	Average Spacing ^a
Goulburn ^{b,c}	Australia	20 ^c	6500 km ²	18 ² km ²
Valencia Anchor Site ^d	Spain	11	2500 km ²	50 ² km ²
Yanco ^b	Australia	37	3600 km ²	10 ² km ²
Saskatchewan	Canada	16	1600 km ²	10 ² km ²
Ontario	Canada	26	1600 km ²	8 ² km ²
REMEDHUS ^d	Salamanca, Spain	23	1250 km ²	7 ² km ²
Little Washita ^e	Oklahoma, USA	20	600 km ²	5 ² km ²
Kyeamba ^b	Australia	14	600 km ²	7 ² km ²
Fort Cobb ^e	Oklahoma, USA	15	340 km ²	5 ² km ²
Little River ^e	Georgia, USA	33	330 km ²	3 ² km ²
Reynolds Creek ^e	Idaho, USA	15	240 km ²	3 ² km ²
Walnut Gulch ^e	Arizona, USA	9	150 km ²	4 ² km ²
Adelong Creek ^b	Australia	5	145 km ²	5 ² km ²
Kenaston	Canada	24	100 km ²	2 ² km ²

^aAverage spacing is calculated as the ratio of areal extent/number of sites.

^bSee <http://www.oznet.org.au>.

^cThe Goulburn network actually has 26 soil moisture stations in total, but 7 stations within a 1² km² focus farm are counted as a single site here.

^dSMOS validation site.

^eU.S. Department of Agriculture Agricultural Research Service Experimental Watersheds [Jackson *et al.*, 2010].

[Jackson *et al.*, 1999, 2002]; the 2002 Soil Moisture Experiment (SMEX) in Iowa (SMEX02) [Jackson *et al.*, 2003]; the multisite SMEX03 experiment in Alabama, Oklahoma, and Georgia [Jackson *et al.*, 2005]; the SMEX04 experiment in Arizona [Jackson *et al.*, 2008]; and the Canadian Experiment for Soil Moisture 2010 [Magagi *et al.*, 2012]. Likewise, the National Airborne Field Experiments (NAFE) were a series of large-scale field campaigns in southeastern Australia with the primary aim of collecting airborne and ground observations of soil moisture for development of algorithms and techniques for SMOS soil moisture products. NAFE'05 was conducted during fall 2005 in the Goulburn catchment [Panciera *et al.*, 2008], and NAFE'06 was conducted during fall 2006 in the Yanco area [Merlin *et al.*, 2008]. More recent Australian field campaigns in 2010 include the Australian Airborne Cal/val Experiment for SMOS [Peischl *et al.*, 2012] and the Soil Moisture Active Passive Experiments aimed at prelaunch SMAP validation activities. Extensive soil moisture sampling in North Africa was also conducted as part of the African Monsoon Multidisciplinary Analysis (AMMA) project [Redelsperger *et al.*, 2006; de Rosnay *et al.*, 2009b]. This sampling included both a ground-based soil moisture measurement network installed in 2004 within the Gourma region of Mali and a series of high-intensity ground sampling periods during the 2005 and 2006 monsoon seasons [de Rosnay *et al.*, 2009a].

[11] Leveraging soil moisture data sets acquired from both the small-scale (but high-density) soil moisture measurement networks listed in Table 2 and intensive field campaigns listed above, this review characterizes the magnitude of the soil moisture upscaling problem and assesses the feasibility of potential solutions. Following a summary of sources for surface soil moisture spatial variability, the current literature characterizing the magnitude of the soil moisture upscaling problem is reviewed, and expected measurement density requirements for ground-based surface soil moisture measurement networks are defined. The paper concludes by summarizing a range of existing soil moisture upscaling strategies for reducing the impact of spatial sampling error on satellite soil moisture validation activities.

2. SOURCES OF SOIL MOISTURE VARIABILITY

[12] The soil moisture upscaling problem follows directly from the presence of extensive horizontal variability in surface soil moisture fields. Such variability is generated through complex interactions between pedologic, topographic, vegetative, and meteorological factors [Reynolds, 1970; Sharma and Luxmoore, 1979; Loague, 1992; Charpentier and Groffman, 1992; Rodriguez-Iturbe *et al.*, 1999; Mohanty and Skaggs, 2001]. While these factors are generally difficult to isolate and measure, a general understanding of their magnitude is useful background for discussing the viability of soil moisture upscaling strategies. Therefore, this section briefly summarizes the role of these factors in generating and sustaining soil moisture spatial variability.

2.1. Soil

[13] Soil heterogeneity affects the distribution of soil moisture through variations in texture, organic matter content, porosity, structure, and macroporosity. Significant soil moisture variations may therefore exist over small spatial distances due to variations in soil particle and pore size distributions and their subsequent impact on local hydrologic processes impacting soil moisture. In addition, soil color can influence albedo and thus the rate of evaporative drying for bare or lightly vegetated soil. Numerous studies have demonstrated the impact of soil hydraulic conductivity on components of the soil water balance and subsequent soil moisture spatial patterns [e.g., Moore *et al.*, 1998; Grote *et al.*, 2010]. Likewise, soil heterogeneity has been shown to affect soil water balance processes. For example, where evapotranspiration is limited by percolation through a lower boundary, soil heterogeneity increases the spatially averaged evapotranspiration relative to a uniform soil [Kim *et al.*, 1997]. In a related study, Kim and Stricker [1996] showed the stronger effect of soil spatial heterogeneity on components of the water budget for a loamy soil as compared to a sandy soil. They suggested that soil heterogeneity has a great influence for loamy soil because most of the variation of the water budget is present at finer field ($\sim 800^2$ m²) scale. Conversely, most of the water budget variation for sandy soil occurs at coarser scales correlated with antecedent rainfall variations.

[14] The impact of soil texture heterogeneity on soil moisture spatial structure has also been well documented in large-scale data sets acquired from soil moisture field campaigns. Soil moisture patterns derived from airborne remote sensing and ground-based soil moisture sampling during field campaigns in the south-central United States have revealed large-scale patterns corresponding to known variations in soil texture [Mattikalli *et al.*, 1998; Kim *et al.*, 2002]. Similarly, Panciera [2009] used data from the NAFE'05 in situ monitoring network and regional sampling during the experiment period (31 October to 25 November) to investigate land surface controls on soil moisture spatial distributions at the satellite footprint scale ($\sim 40^2$ km²). They found that soil moisture variability within a satellite footprint could be related to spatial patterns of land cover type and soil texture. Soils with higher sand content exhibited persistently drier soil moisture conditions than soils with lower sand content.

2.2. Topography

[15] Topography also plays an important role in the spatial organization of soil moisture at different scales. Variations in slope, aspect, curvature, upslope contributing area, and relative elevation all affect the distribution of soil moisture near the land surface. At the small catchment and hillslope scales, soil moisture varies as a result of water-routing processes, radiative (aspect) effects, and heterogeneity in vegetation and soil characteristics. Charpentier and Groffman [1992] studied the effects of topography and the overall magnitude of moisture content on the variability of soil moisture within fine-scale pixels during the First International

Satellite Land Surface Climatology Project field experiment. They showed that within a 66^2 m^2 pixel, soil moisture variability increased with increased topographic heterogeneity. A flat pixel had significantly lower standard deviations and fewer outlier points than a sloping or a valley pixel.

[16] *Mohanty et al.* [2000a] showed the dominance of a slope effect on the diurnal soil moisture distribution in a gently sloping agricultural field within the Little Washita agricultural watershed. Likewise, for the SMEX02 campaign, *Jacobs et al.* [2004] demonstrated the significance of slope positions in locating the time-stable points for mean soil moisture in four agricultural fields in Iowa. Several other studies also showed that relative slope position is important in determining soil moisture variation, suggesting that a simple averaging of soil moisture values over the slope may lead to errors at different time scales. In West Africa, *de Rosnay et al.* [2009a] found a stable inverse correlation between soil moisture and hillslope position within the Gourma research site (i.e., lower soil moisture at higher hillslope positions and vice versa). In Australia, *Western et al.* [1999] showed systematic or organized spatial variation in soil moisture, particularly saturated areas associated with topographic convergence. Conversely, *Western et al.* [2003] concluded that although topographic control of soil moisture patterns does occur in some landscapes for part or all of the time, terrain is a relatively poor indicator of soil moisture patterns and variability. They suggested that during soil moisture drying events (mid-moisture range), soil and vegetation properties dominate the control in several watersheds. Similar findings have been reported by other studies including *Kim and Barros* [2002], *Bindlish and Barros* [2002], *Chang and Islam* [2003], and *Ryu and Famiglietti* [2005].

2.3. Vegetation

[17] Land cover characteristics are also important for understanding soil moisture regimes as they directly affect soil water processes (e.g., infiltration and evapotranspiration) which determine soil moisture levels. Vegetation type, density, and uniformity have all been shown to contribute to soil moisture variation at different space and time scales. Furthermore, the influence of vegetation on spatial variation in soil moisture is more dynamic as compared to soil and topographic factors. *Hawley et al.* [1983] demonstrated that various vegetation-topography-soil combinations lead to temporal persistence (clustering) of soil moisture patterns in complex terrains with mixed vegetation. They also suggested that the presence of vegetation tends to diminish the magnitude of soil moisture variations caused by topography. During the NAFE'05 field campaign in Australia, land cover was found to have a strong influence on soil moisture distribution at the satellite footprint [*Panciera, 2009*]. Specifically, cropped areas exhibited persistently wetter-than-average conditions, and forested areas exhibited drier-than-average conditions, while grassland sites were more representative of the area average soil moisture conditions (the NAFE'05 study area was 70% grassland).

[18] *Vinnikov et al.* [1996] noted differences in soil moisture evolution for three catchments at Valdai, Russia, with different vegetation. Likewise, *Mohanty et al.* [2000b] examined the evolution of the soil moisture spatial structure in a wheat/grass (mixed vegetation) remote sensing footprint during the Southern Great Plains 1997 (SGP97) hydrology field campaign. Their results showed that the vegetation dynamics (growth/decay), land management (tillage), and precipitation events controlled the intraseasonal soil moisture spatial structure for the pixel with flat topography and uniform soil texture. During the Soil Moisture Experiment 2002 (SMEX02) in Walnut Creek agricultural watershed in Iowa with corn and soybean crops, *Jacobs et al.* [2004], *Cosh et al.* [2004], and *Joshi and Mohanty* [2010] all noted the impact of land cover variations on the spatial distribution of soil moisture in the region.

2.4. Meteorological Forcing

[19] Solar radiation, wind, and humidity variations all contribute to the space-time dynamics of soil moisture. However, precipitation is the single most important meteorological forcing for soil moisture content and its distribution. As shown by *Sivapalan et al.* [1987], the dominant runoff producing mechanism may vary with storm characteristics and antecedent soil moisture conditions resulting in the spatiotemporal variability in soil moisture. During the SGP97 hydrology campaign, *Famiglietti et al.* [1999] found a distinct trend in mean soil moisture for Little Washita (in southern Oklahoma), El Reno (in central Oklahoma), and the U.S. Department of Energy Atmospheric Radiation Measurement Central Facility (in north Oklahoma) locations along a north/south precipitation gradient. Within an analytical framework, *Kim and Stricker* [1996] showed the significance of rainfall pattern on partitioning of water over the budget terms for different climatic conditions. Likewise, *Salvucci* [2001] showed the conditional dependence of soil moisture storage, drainage, runoff, and evapotranspiration with amount of precipitation in Illinois. A multiscale analysis by *Crow and Wood* [1999] using SGP97 data revealed a qualitatively different relationship between soil moisture means and soil moisture spatial variances when variability is sampled at fine ($<1^2 \text{ km}^2$) versus coarse ($>10^2 \text{ km}^2$) spatial scales. The threshold between these two scale regimes may represent a transition between organized coarse-scale spatial heterogeneity imposed by the land surface response to rainfall and disorganized fine-scale variability produced by local variations in soil, topography, and vegetation.

2.5. Summary of Spatial Variability Sources

[20] In general, it is difficult to draw broad conclusions regarding the impact of soil, topography, land cover, and meteorological forcing on multiscale soil moisture variability from the above mentioned water balance/soil moisture studies. In most cases examined above, one or more of these contributing factor(s) was either neglected or assumed to be spatially homogenous across the study area. Moreover, the impact of various environmental factors on soil moisture spatial patterns appears to vary significantly over time with

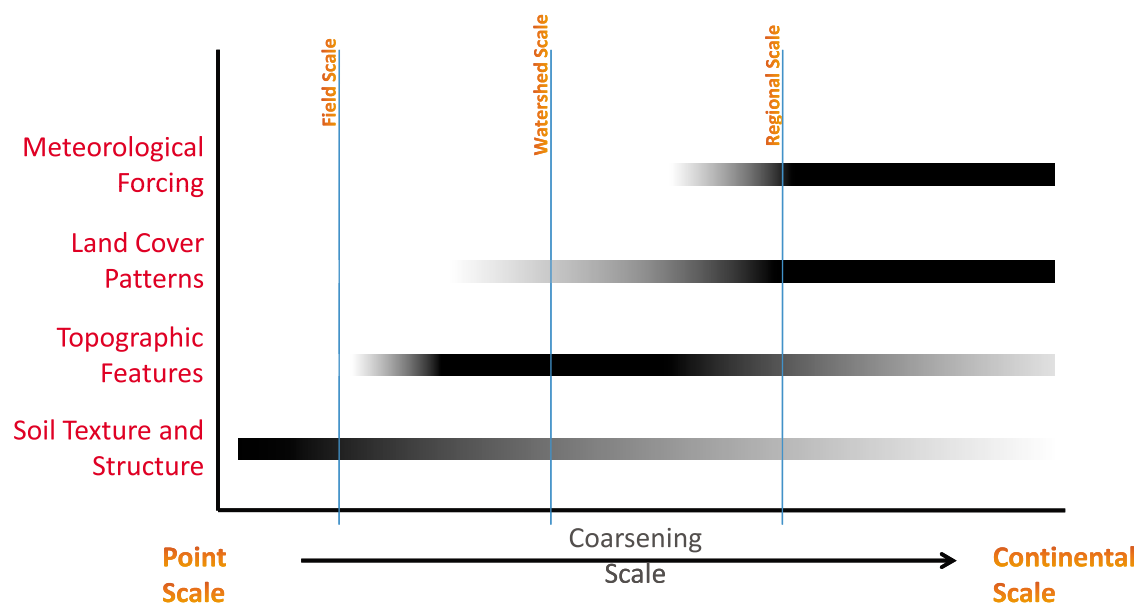


Figure 1. Dominant physical controls on soil moisture spatial variability as a function of scale. The gray shading of bars reflects the relative importance of each control at various scales with increasing intensity according to importance. (Modified from *Jana* [2010].)

various relationships emerging at different points during wet-up and dry-down cycling [*Pancierera*, 2009] and/or the annual seasonal cycle [*Western et al.*, 2003]. Nevertheless, the above research can be generalized to produce a rough conceptual model of various environmental factors inducing surface soil moisture variability over a set of overlapping scales [*Jana*, 2010]. This model, first proposed by *Vinnikov et al.* [1996] and summarized in Figure 1, predicts that large-scale soil moisture variability (observed at watershed to continental scales) is generally dominated by meteorological forcing (e.g., rainfall patterns) and land cover patterns with topographic and soil factors gaining predominance at finer spatial scales.

3. SCOPE OF THE SOIL MOISTURE UPSCALING PROBLEM

[21] The interaction of environmental factors discussed in section 2 produces complex spatial patterns in surface soil moisture. The statistical properties of these patterns, in turn, determine the magnitude of the soil moisture upscaling problem. Using data sets gleaned from recent soil moisture field experiments, this section reviews recent literature describing the magnitude of multiscale soil moisture variability (section 3.1) and sampling requirements for obtaining footprint-scale soil moisture averages with predefined accuracies (section 3.2). When discussing the relationship between soil moisture variability and scale we conform to *Western and Blöschl* [1999] and use the term “support” to refer to the area (or volume) integrated by an individual soil moisture measurement, “extent” to refer to the overall area within which individual soil moisture measurements are sampled to estimate a spatial statistic, and “spacing” to refer to the typical distance between samples. Note that the

apparent variability of soil moisture increases at larger extent scales [*Hills and Reynolds*, 1969] and decreases at larger support scales [*Hawley et al.*, 1982]. Individual ground observations will be treated as a point support sample, although it should be noted that traditional ground-based measurements at a “point” actually sample slightly different soil volumes [*Robinson et al.*, 2008].

[22] All “surface” soil moisture data sets referenced here are assumed to possess vertical support equal to the ~5 cm penetration depth expected of L band soil moisture retrievals. During field campaign and ground validation activities, this 5 cm surface depth is commonly assumed to start at the air/soil interface present after clearing of vegetation detritus (T. J. Jackson, personal communication, 2012). The exact elevation of this interface (and thus the bottom of the 5 cm surface layer) can vary spatially due to microtopography. In addition, note that a wide variety of ground instrumentation can be applied to provide soil moisture measurements at such depths. For data sets discussed here, the most common techniques are gravimetric sampling (where soil samples are oven-dried to determine soil water weight) and the use of handheld time domain reflectivity sensors to measure the soil dielectric constant. Note that both approaches require additional ancillary information/assumptions in order to convert their direct measurements into volumetric soil moisture. A full description of these techniques and associated measurement errors is outside the scope of this review but has been addressed extensively in previous reviews [*Walker et al.*, 2004; *Evelt et al.*, 2008; *Robinson et al.*, 2008].

3.1. Observed Soil Moisture Spatial Variability

[23] Soil moisture spatial statistics are known to vary with the spatial extent of sampling domain and mean soil moisture [*Western and Blöschl*, 1999; *Western et al.*, 2002].

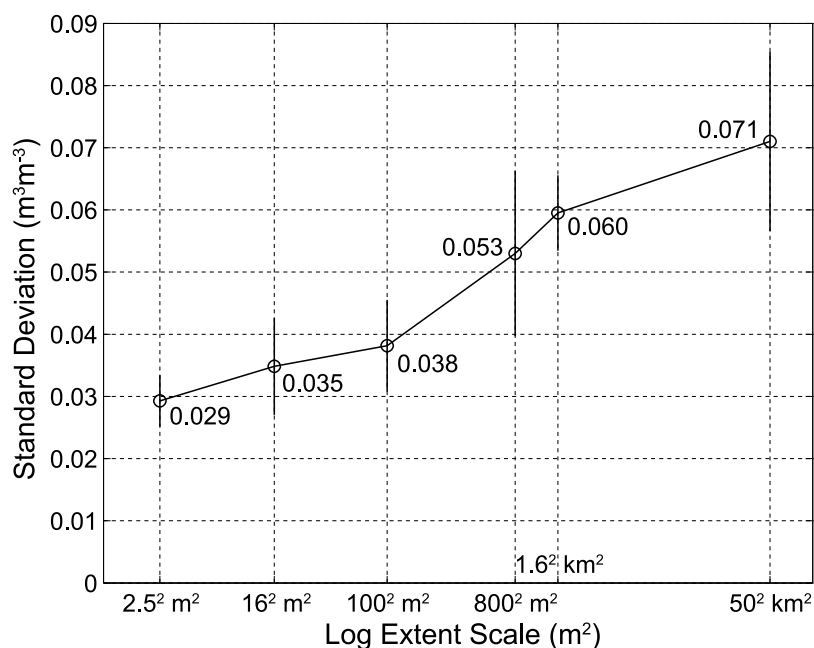


Figure 2. Summary of the instantaneous spatial standard deviation for point-scale, surface soil moisture samples obtained within sampling extents ranging from 2.5^2 m^2 to 50^2 km^2 for ground data collected under a range of land surface conditions during SGP97, SGP99, SMEX02, and SMEX03. The circles represent the sample mean of soil moisture standard deviation, and the whiskers are the one-standard deviation ranges. (Modified from Famiglietti *et al.* [2008].)

Moreover, multiscale structure of soil moisture variability can be characterized by several typical types of semivariogram or power spectral density from local [Western and Blöschl, 1999; Western *et al.*, 2002] to regional scales [Kim and Barros, 2002; Oldak *et al.*, 2002; Ryu and Famiglietti, 2006]. This implies that the surface soil moisture can be regarded as a second-order stationary random variable [Yaglom, 1987] whose second-order moment changes with mean soil moisture.

[24] Famiglietti *et al.* [2008] combine over 36,000 ground-based measurements of surface soil moisture collected during the SGP97, SGP99, SMEX02, and SMEX03 field campaigns to generalize the spatial variability of point support surface soil measurements sampled within spatial extents ranging between 2.5^2 m^2 to 50^2 km^2 . The temporal extent of these campaigns ranged between about 2 weeks to 1 month and most captured at least one complete wet-up/dry-down cycle. Figure 2 shows the mean soil moisture standard deviations sampled within six separate extent scales (circles) and the one-standard deviation range (whiskers) of soil moisture standard deviations sampled within six separate extent scales. All plotted values are calculated using only (near-instantaneous) spatial standard deviations sampled when mean soil moisture varies between $0.1 \text{ m}^3 \text{ m}^{-3}$ and $0.3 \text{ m}^3 \text{ m}^{-3}$; thus, the quantities in Figure 2 can be assumed to be typical values of soil moisture variability for intermediate soil moisture conditions. Relatively short whiskers at the 2.5^2 m^2 , 16^2 m^2 , 100^2 m^2 , and 1.6^2 km^2 extent scales are associated with a limited number of samples at those scales, collected only during the SGP99 field campaign. Mean soil moisture variability gradually

increased from a mean standard deviation of $0.029 \text{ m}^3 \text{ m}^{-3}$ within a 2.5^2 m^2 scale extent to $0.071 \text{ m}^3 \text{ m}^{-3}$ within a 50^2 km^2 extent, and relative to other scale ranges, soil moisture variability increased steeply between 100^2 m^2 and 1.6^2 km^2 .

[25] While it is generally acknowledged that the scaling behavior of soil moisture varies as a function of large-scale wetness, past studies are divided on whether soil moisture variability generally increases [Bell *et al.*, 1980; Hawley *et al.*, 1983] or decreases [Famiglietti *et al.*, 1999; Hupet and Vanclooster, 2002] with mean surface wetness. Naturally, the relationship between the mean and spatial standard deviation of a soil moisture field is partially dependent on the spatial characteristics of the particular rainfall events sampled during a field experiment. However, ground observations from the SGP and SMEX field campaigns display a robust concave pattern of soil moisture variability with peak variability found at intermediate soil moisture levels. Figure 3 shows mean soil moisture versus spatial variability empirically derived from the data used by Famiglietti *et al.* [2008] at four selected scales: 2.5^2 m^2 (SGP99), 100^2 m^2 (SGP99), 800^2 m^2 (SGP97, SGP99, SMEX02, and SMEX03), and 50^2 km^2 (SMEX02 and SMEX03). In spite of the diverse climatic and land surface conditions of the sites (e.g., subhumid and rolling topography in Oklahoma sites for SGP97, SGP99, and SMEX03 and humid and low-relief topography in Iowa sites for SMEX02), ground data show quite similar ranges of variability. This pattern of maximum spatial variability during periods of intermediate soil wetness is also found in NAFE'06 results when soil moisture variability is sampled

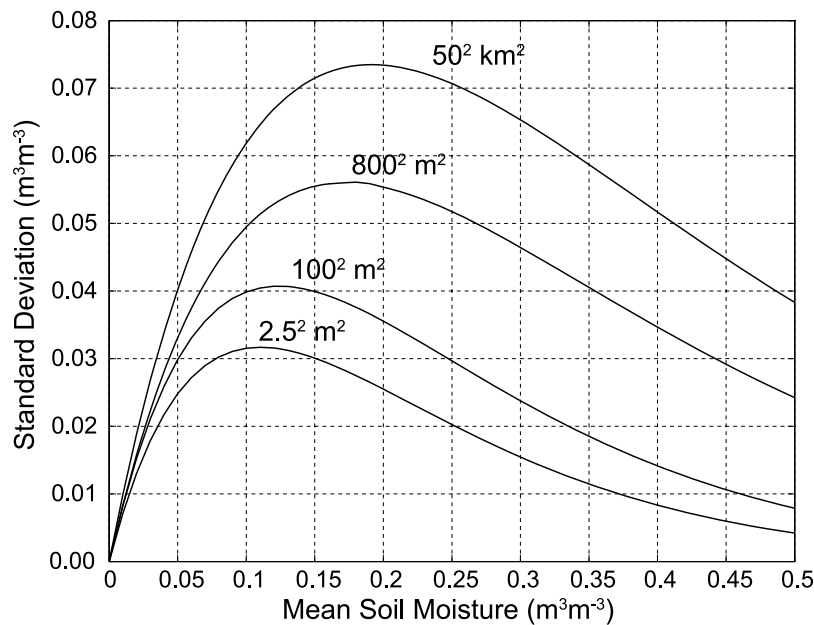


Figure 3. Empirical relationships between the mean soil moisture and point-scale soil moisture standard deviation sampled within four selected spatial extents (2.5^2 , 100^2 , 800^2 , and 50^2 km²) during the SGP97, SGP99, SMEX02, and SMEX03 field experiments. (Modified from *Famiglietti et al.* [2008].)

using both point-scale and field-scale supports within a 40^2 km² extent [Merlin *et al.*, 2008].

3.2. Derived Spatial Sampling Requirements

[26] The most direct way to upscale a set of sparse ground-based soil moisture measurements is calculating their sample mean and assigning it as the average soil moisture within the total extent of the ground-based measurements. Uncertainty in this coarse-scale soil moisture estimate can then be estimated from spatial variability of the point measurements assuming that the surface soil moisture content is a stationary random variable [Ryu and Famiglietti, 2005; Famiglietti *et al.*, 2008]. The rationale behind this uncertainty estimation is that according to the central limit theorem, the sampling distribution of a sample mean has a normal distribution when the sample size is sufficiently large. This theorem holds even when the population is not normally distributed. When the number of samples is not sufficiently large, the Student *t* distribution is used in place of the normal distribution to describe the distribution of a sample mean. In

either case, the spatial variability of the point-scale soil moisture offers a basis for estimating the uncertainty associated with upscaling a single ground-based observation to a given coarser-scale footprint.

[27] Figure 2 predicts that the standard deviation of point-scale soil moisture samples within extent scales corresponding to the footprint resolution of SMOS and SMAP footprint resolutions will tend to be greater than both missions' RMSE accuracy goals. Therefore, if validated directly against a single instantaneous, point-scale ground measurement, even an error-free footprint-scale retrieval would be interpreted as exceeding validation mission RMSE targets. In the absence of a more complex upscaling approach, such high levels of variability require that multiple sites be sampled within each footprint to dampen the impact of spatial sampling error on footprint-scale averages.

[28] In such cases, a critical design issue becomes the minimum number of sampling sites required (or, stated differently, the maximum spacing distance allowable) to

TABLE 3. Reported Number of Point-Scale Measurements Necessary to Characterize Instantaneous Mean Soil Moisture Within a Field-Scale Extent ($\sim 800^2$ m²) to Within a Predetermined Accuracy

Study	Accuracy (Absolute Error)	Minimum/Maximum Required Measurements	Location and Depth of Measurements
<i>Brocca et al.</i> [2010b]	$0.02 \text{ m}^3 \text{ m}^{-3}$	4–15	central Italy (0–15 cm depths)
<i>Brocca et al.</i> [2007]	$0.02 \text{ m}^3 \text{ m}^{-3}$	15–35	central Italy (0–15 cm depths)
<i>Jacobs et al.</i> [2004]	$0.02 \text{ m}^3 \text{ m}^{-3}$	3–32	Iowa, USA (0–6 cm depths)
<i>Wang et al.</i> [2008]	$0.05 \text{ m}^3 \text{ m}^{-3}$	41	Gansu province, China (0–20 cm depth)
<i>Famiglietti et al.</i> [2008]	$0.03 \text{ m}^3 \text{ m}^{-3}$	7–17	Oklahoma and Iowa, USA (0–6 cm depth)
<i>Famiglietti et al.</i> [1999]	$0.02 \text{ m}^3 \text{ m}^{-3}$	34	Oklahoma, USA (0–6 cm)
<i>Western et al.</i> [2004]	$0.02 \text{ m}^3 \text{ m}^{-3}$	14	multiple sites in Australia and New Zealand (0–30 cm)
<i>Hupet and Vanlooster</i> [2002]	$0.025 \text{ m}^3 \text{ m}^{-3}$	1–12	Belgium (depths are 0–20 cm)

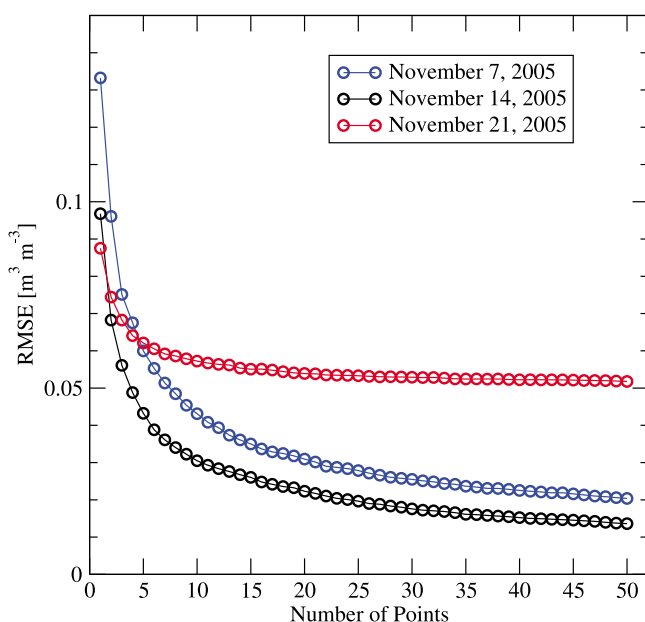


Figure 4. For a dry-down event in the Goulburn catchment during the NAFE’05 field campaign, the RMSE between a random sample of point-scale measurements and 40^2 km^2 footprint-scale average soil moisture. The data for 7 November capture wet conditions ($0.38 \pm 0.14 \text{ m}^3 \text{ m}^{-3}$) in the aftermath of a rainfall event, while the data for 14 and 21 November represent drier conditions ($0.18 \pm 0.11 \text{ m}^3 \text{ m}^{-3}$ and $0.16 \pm 0.1 \text{ m}^3 \text{ m}^{-3}$, respectively).

capture an instantaneous footprint-scale average with sufficient accuracy. Table 3 summarizes recent work aimed at quantifying the number of point-scale soil moisture sampling sites necessary to characterize mean field-scale ($\sim 800^2 \text{ m}^2$) soil moisture to within a specified accuracy. Results in Table 3 suggest that around 10–20 point support observations per field are generally required to obtain field-scale means to within a 1σ accuracy of $0.02 \text{ m}^3 \text{ m}^{-3}$.

[29] Since soil moisture variability increases when sampled within progressively larger spatial extents [Hills and Reynolds, 1969; Western and Blöschl, 1999], the number of sampling locations necessary to estimate footprint-scale means is likely to exceed the field-scale requirements reported in Table 3 [Famiglietti et al., 2008]. Examining a $\sim 60^2 \text{ km}^2$ catchment in central Italy, Brocca et al. [2010b] found that up to 40 samples were necessary to estimate instantaneous catchment mean soil moisture to within an absolute error of $0.02 \text{ m}^3 \text{ m}^{-3}$. Likewise, Famiglietti et al. [2008] and Hansen [2007] found that between 20 and 30 samples were necessary to estimate the mean of a 50^2 km^2 extent to within an accuracy of $0.03 \text{ m}^3 \text{ m}^{-3}$ for field sites in Oklahoma (USA), Iowa (USA), and New South Wales (Australia).

[30] Given the known relationship between soil moisture variances and means (Figure 3), it is not surprising that such sampling requirements vary as a function of large-scale soil moisture conditions. For instance, results from extensive NAFE soil moisture sampling within a 40^2 km^2

footprint shown in Figure 4 suggest that at least 15 point-scale measurements are required to estimate the footprint average soil moisture to within $0.04 \text{ m}^3 \text{ m}^{-3}$ during wet conditions (7 November) but as few as 5 are sufficient in intermediate-dry conditions (i.e., mean soil moisture less than $0.20 \text{ m}^3 \text{ m}^{-3}$) on 14 November [Azcurra and Walker, 2006]. However, this conclusion is only valid provided that the distribution of the measurements is capable of providing an unbiased estimate of footprint-scale soil moisture. If this condition is not satisfied, then sampling errors may not reduce below $0.04 \text{ m}^3 \text{ m}^{-3}$ regardless of the number of measurements taken (see, e.g., the 21 November results in Figure 4).

4. SOIL MOISTURE UPSCALING STRATEGIES

[31] At the SMOS, Aquarius, or SMAP footprint scale, sampling density requirements identified above can only be met during extensive field campaigns or within isolated, small-scale sites encompassing a very small number of satellite footprints (Table 2). Larger-scale soil moisture networks listed in Table 1 sample surface soil moisture at significantly lower sampling densities. Therefore, unless effective upscaling and site selection strategies can be implemented, section 3 suggests that the value of these networks for satellite soil moisture validation activities will be limited.

[32] This section details several different potential strategies for addressing this problem. The following simple framework is used to classify these approaches. Assume that the vector θ_{POINT} contains a set of N point-scale soil moisture observations sampled within a given remotely sensed footprint. This set of measurements can be resampled to provide a scalar estimate of mean footprint-scale soil moisture via the upscaling function F_{\uparrow} :

$$\theta_{\text{UPSCALE}} = F_{\uparrow}(\theta_{\text{POINT}}). \quad (1)$$

See Figure 5 for an illustration of the case $N = 4$. Strictly speaking, error in θ_{UPSCALE} can arise from two separate sources: random ground-based measurement error impacting elements of the θ_{POINT} vector and upscaling error introduced by a lack of knowledge concerning the appropriate functional form for F_{\uparrow} . Here, our primary focus is on the latter source of error, but it is not always clear that ground measurement errors can (or should) be neglected or treated separately from upscaling errors. We will return to this issue during the evaluation of various upscaling approaches.

[33] Nevertheless, if error in θ_{UPSCALE} is independent of retrieval error impacting the remotely sensed product θ_{RS} , then the mean square difference (MSD) between a hypothetical representation of true soil moisture (θ_{TRUE}) and θ_{RS} can be written as

$$\begin{aligned} \text{MSD}(\theta_{\text{TRUE}}, \theta_{\text{RS}}) &= \text{MSD}(\theta_{\text{UPSCALE}}, \theta_{\text{RS}}) \\ &\quad - \text{MSD}(\theta_{\text{UPSCALE}}, \theta_{\text{TRUE}}), \end{aligned} \quad (2)$$

which states that the measurable quantity $\text{MSD}(\theta_{\text{UPSCALE}}, \theta_{\text{RS}})$ is spuriously inflated relative to the actual validation quantity of interest $\text{MSD}(\theta_{\text{TRUE}}, \theta_{\text{RS}})$ by the uncertainty in

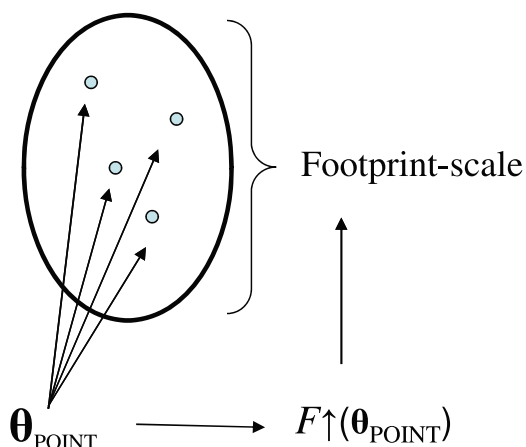


Figure 5. Schematic for the configuration of the upscaling problem summarized in (1). The upscaling function F_{\uparrow} is used to link a set of $N = 4$ point-scale ground observations to a spatial mean corresponding to the footprint scale of a satellite-based surface soil moisture retrieval.

our ability to estimate θ_{UPSCALE} from ground-based observations or $\text{MSD}(\theta_{\text{UPSCALE}}, \theta_{\text{TRUE}})$.

[34] It is also useful to further decompose each θ time series into a static, long-term mean ($\bar{\theta}$) and a times series of anomalies relative to this mean (θ'). Based on this decomposition, the upscaling error term in (2) can be expanded as

$$\text{MSD}(\theta_{\text{UPSCALE}}, \theta_{\text{TRUE}}) = (\bar{\theta}_{\text{UPSCALE}} - \bar{\theta}_{\text{TRUE}})^2 + \text{MSD}(\theta'_{\text{UPSCALE}}, \theta'_{\text{TRUE}}). \quad (3)$$

Here the term $(\bar{\theta}_{\text{UPSCALE}} - \bar{\theta}_{\text{TRUE}})^2$ reflects long-term bias in (1) and $\text{MSD}(\theta'_{\text{UPSCALE}}, \theta'_{\text{TRUE}})$ describes the magnitude of random error in anomalies relative to a long-term mean.

[35] Taken together, (1)–(3) provide a framework for classifying various soil moisture upscaling strategies. The most direct strategies are based on minimizing (3) through either optimizing the geographic location of point-scale observations (see section 4.1) or improving the formulation of F_{\uparrow} in (1) (see sections 4.2–4.4). An alternative approach lies in accepting nonnegligible values for the bias and random error terms in (3) and instead seeking techniques for accurately estimating their magnitude and then correcting RMSE-based error estimates for the impact of sampling errors (see section 4.5).

[36] Note that the footprint-scale evaluation in (1)–(3) implies that the spatial support of θ_{RS} can be associated with a finite, uniformly sampled domain. In reality, the antennae gain pattern for microwave observations is a nonlinear two-dimensional surface and does not conform to either of these characteristics [Drusch et al., 1999b]. However, here we will follow the typical convention of defining a footprint scale as the fixed IFOV boundary within which 50% of the integrated antennae signal originates and neglect variations in antennae weighting within such a region. Also, note that (1)–(3) can be applied either to microwave swath products or to a gridded product based on resampling of a swath product into a fixed

grid. However, in the later case, additional retrieval error may be introduced by such resampling.

4.1. Enhanced Upscaling Using Time Stability Concepts

[37] One approach for minimizing upscaling errors is locating soil moisture measurement sites at particular landscape locations in order to minimize subsequent upscaling errors. In particular, time stability approaches are based on the assumption that soil moisture patterns tend to be persistent in time within a particular landscape [Vachaud et al., 1985]. The temporally persistent patterns are mainly functions of static vegetation type, soil type, and topography [Grayson et al., 1997; Mohanty and Skaggs, 2001; Cosh et al., 2004; Martínez-Fernández and Ceballos, 2005; Brocca et al., 2007; de Lannoy et al., 2007]. A number of studies have been devoted to study the phenomena of soil moisture time stability and its application to soil moisture validation activities. For instance, Cosh et al. [2006] and Starks et al. [2006] demonstrated that distributed soil moisture monitoring networks within the 611 km² Little Washita watershed are temporally stable and accurately represent the watershed as a whole.

[38] Figure 6 shows an example of a time stability analysis taken from Cosh et al. [2004] for 2 months of soil moisture observations within the 100 km² Walnut Creek watershed in central Iowa. The plot shows comparisons between true watershed-scale soil moisture (here assumed to be equal to the spatial average of 12 separate soil moisture measurement sites within the Walnut Creek watershed) and each individual measurement, i.e., the case of $N = 1$ when applying the trivial upscaling function $\theta_{\text{UPSCALE}} = \theta_{\text{POINT}}$ in (1). Individual measurement sites within the Walnut Creek basin are aligned along the x axis. Open circles and error bars represent the sampled temporal mean and standard deviations, respectively, of relative error or $(\theta_{\text{POINT}} - \theta_{\text{TRUE}})/\theta_{\text{TRUE}}$ when using any single station to characterize the entire watershed. While many sites provide a poor representation of coarse-scale dynamics, soil moisture measurements at certain sites (e.g., WC06 in Figure 6) can be effectively upscaled to represent dynamics at a coarser watershed scale. While Figure 6 is based on a relatively short time period of data (~ 2 months), similar time stability results have been obtained using multiyear data sets. For instance, Cosh et al. [2006] have been able to identify “time-stable” sampling sites using multiple years of ground measurements acquired within the Walnut Gulch watershed in Arizona. Likewise, Wagner et al. [2008] found time-stable locations within the REMEDHUS network (see Table 2) in Spain by analyzing 4 years of synthetic aperture radar data.

[39] At these sites, even trivial upscaling of point-scale observations leads to relatively low values of both the bias and time-varying error terms in (3). Within the Walnut Creek watershed, Cosh et al. [2004] demonstrated that a single soil moisture measurement at the WC06 site captures watershed-scale dynamics to within a RMSE of 0.029 m³ m⁻³. The existence of time-stable locations can therefore be leveraged to reduce spatial sampling requirements for ground-based soil

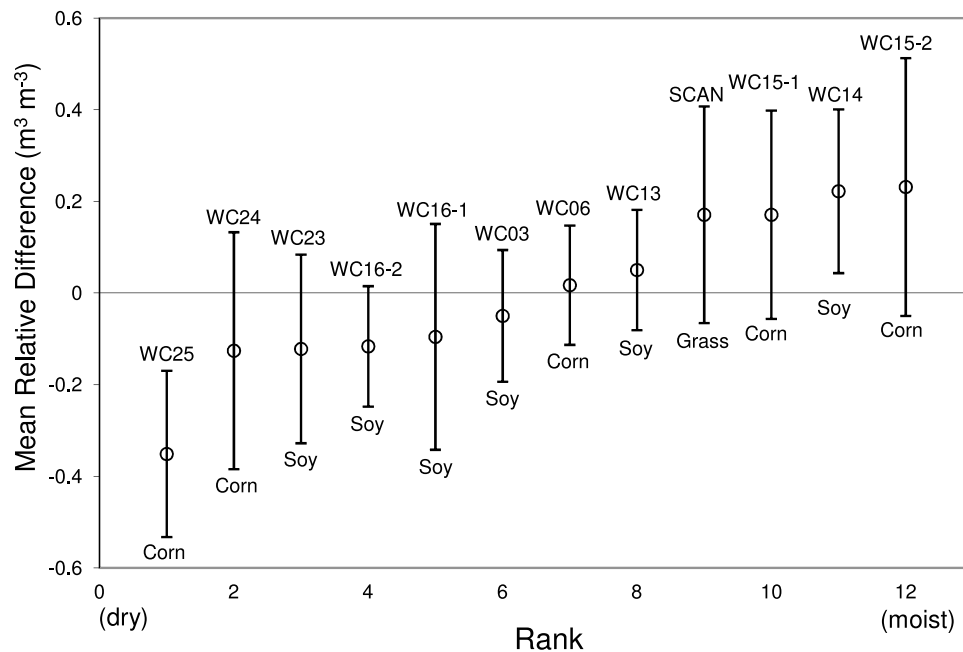


Figure 6. For the Walnut Creek watershed in central Iowa, the mean relative difference ($\theta_{\text{POINT}} - \theta_{\text{TRUE}})/\theta_{\text{TRUE}}$ between individual point-scale soil moisture measurements obtained at various sites (see listed site names and land covers) and true soil moisture defined as the spatial average of measurements at all watershed sites. Plotted error bars capture 1σ variation in the relative differences. (Modified from Cosh *et al.* [2004], copyright 2004, with permission from Elsevier.)

moisture observations. For example, over the extent of an AMSR-E satellite footprint (75^2 km^2), Cosh *et al.* [2006] demonstrated that only six sampling sites were necessary to adequately represent the footprint-scale soil moisture.

[40] The challenge in exploiting the potential of time stability lies in identifying and deploying instrumentation at landscape locations possessing desirable stability characteristics over multiannual time scales [Loew and Schlenz, 2011]. Direct identification of time-stable sites typically requires very dense spatial sampling of a coarse-scale area over an extended period [Brocca *et al.*, 2010b]. In locations where such sampling is impractical, time-stable sites might be identifiable based on observable land surface characteristics. To this end, Mohanty and Skaggs [2001], Jacobs *et al.* [2004], Cosh *et al.* [2006], and Joshi *et al.* [2011] conducted analyses of ground and remote sensing soil moisture data collected during the SGP and SMEX field campaigns (see section 1) and concluded that characteristic differences were observed in the space-time dynamics of soil moisture within selected remote sensing footprints with various combinations of soil texture, slope, vegetation, and precipitation. Mohanty and Skaggs [2001] showed similar time-stable locations within different remote sensing footprints at multiple sites and related them to different physical controls such as soil, topography, vegetation, and precipitation patterns. Jacobs *et al.* [2004] examined the potential for the a priori selection of time-stable sites through an analysis of daily surface sampling locations conducted at over 90–140 landscape locations across a $\sim 1 \text{ km}^2$ field. They concluded that appropriate locations are most likely on mild slopes, and

hilltops and steep slopes were found to consistently underestimate the field mean. However, they found that knowledge of soil parameters could not be used to select time-stable locations within the field. Recent work [Joshi and Mohanty, 2010; Joshi *et al.*, 2011] has also made progress on defining land surface characteristics typically associated with time-stable behavior within coarser spatial domains. For example, Figure 7 indicates that time-stable measurement locations within the 30^2 km^2 Little Washita watershed in Oklahoma are mostly located on loamy soil type with moderate to high slope values [Joshi *et al.*, 2011]. These generalizations, however, are based on relatively short (~ 1 month) field campaign data sets and must be verified over longer observation periods.

4.2. Enhanced Upscaling Using Block Kriging

[41] A second viable upscaling strategy is deriving an improved form for the upscaling function F_{\uparrow} in (1). Required sampling densities reported in Table 3 are generally based on assuming a simple linear averaging form for F_{\uparrow} :

$$\theta_{\text{UPSCALE}} = F_{\uparrow}(\theta_{\text{POINT}}) = N^{-1} \sum_{i=1}^N \theta_{i,\text{POINT}}, \quad (4)$$

where all point-scale observations are given equal weighting. However, for cases in which the underlying soil moisture field is autocorrelated, block kriging can be used to derive optimal (and nonequal) weights w for each particular θ_{POINT} measurement, and therefore improve estimates of θ_{UPSCALE} , without increasing the spatial density of measurements sites [Vinnikov *et al.*, 1999].

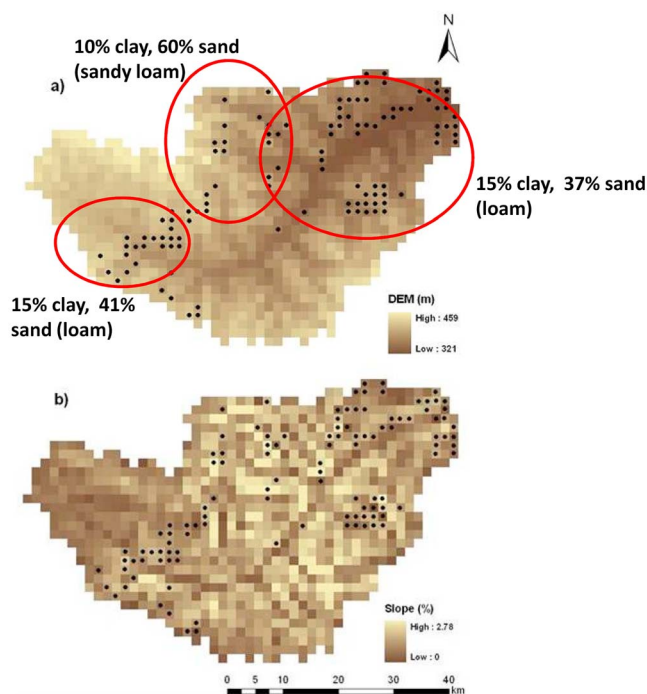


Figure 7. The (a) elevation and (b) slope of time-stable 800^2 m^2 soil moisture pixels (identified with small black dots) acquired from airborne remote sensing during the SGP97 and SGP99 remote sensing field campaigns in the Little Washita (Oklahoma, USA) watershed [Joshi *et al.*, 2011]. Large red circles identify variations in soil texture within the basin. (Modified from Joshi and Mohanty [2010].)

[42] In block kriging, θ_{UPSCALE} is acquired from

$$\theta_{\text{UPSCALE}} = F_{\uparrow}(\theta_{\text{POINT}}) = \sum_{i=1}^N w_i \theta_{i,\text{POINT}} = \frac{1}{\hat{w}} \theta_{\text{POINT}}^T \mathbf{C}^{-1} \mathbf{D}, \quad (5)$$

where \mathbf{C} is an $N \times N$ matrix containing the correlations among the N point measurements contained in the vector θ_{POINT} and \mathbf{D} is the $N \times 1$ vector containing correlations between elements of θ_{POINT} and θ_{TRUE} . The scalar factor \hat{w} is required to ensure that all weights sum to unity. The soil moisture autocorrelation information required to construct \mathbf{C} and \mathbf{D} is typically parameterized from a time series of observations at each of the N measurement sites. Such sampling is viable for the small-scale networks listed in Table 2, but low measurement densities in large-scale networks (Table 1) make it difficult to accurately parameterize \mathbf{C} and \mathbf{D} in many instances.

[43] One possible alternative is obtaining soil moisture autocorrelation information within a densely instrumented region and assuming its suitability for similar (and/or nearby) areas. To this end, several studies have attempted to generalize the multiscale autocorrelation characteristics of soil moisture fields. At the field scale, soil moisture correlation lengths have been calculated between 30 and 60 m [Western *et al.*, 2004; Wang *et al.*, 2008], although these estimates are dependent upon sample spacing [Western and Blöschl, 1999]. Reflecting the inherent multiscale nature of

soil moisture patterns, other researchers have also reported correlation structure at much larger spatial scales. For instance, Entin *et al.* [2000] report a 500 km correlation length in soil moisture variations due to meteorological forcing. This discrepancy suggests the need for use of a nested correlation structure to reflect variability driven by different land surface processes (see Figure 1). For instance, to estimate soil moisture correlation lengths at 50^2 km^2 scales, Ryu and Famiglietti [2006] analyzed semivariograms constructed from satellite data over Oklahoma as part of the Southern Great Plains 1997 experiment. Their results suggest a nested spatial correlation structure with correlation lengths of 10–30 km related to soil texture and vegetation spatial patterns and a larger 60–100 km correlation length related to atmospheric effects. Recently, Joshi and Mohanty [2010] presented a range of correlation lengths for soil moisture across hierarchical spatial sampling scales, from field, to watershed, to region in the agricultural belt of Iowa.

4.3. Enhanced Upscaling Using Field Campaign Data

[44] In addition to block kriging, other empirical approaches exist to optimize F_{\uparrow} . For instance, short-term field data collection can be leveraged to characterize site-specific soil moisture upscaling functions. An example of this is provided by soil moisture sampling studies conducted as part of the AMMA project [Redelsperger *et al.*, 2006]. These studies were based on a ground-based soil moisture measurement network installed in 2004 within the Gourma region of Mali [de Rosnay *et al.*, 2009a]. The network was designed to obtain multiscale estimates of surface soil moisture for remote sensing validation purposes. Over all, 10 stations were located within the Gourma supersite with a concentration of three sites located at Agoufou, Mali, along a single small-scale (100 m) hillslope transect (top, middle, and bottom). Of the 10, 8 stations were located on coarse-textured soils (sandy to sandy loam) that represent 65% of the mesoscale site area.

[45] As a first step, soil moisture scaling properties were investigated based on a time stability analysis similar to Figure 6. This method allowed investigators to identify the most representative station in terms of soil moisture temporal variability at a satellite footprint scale [Gruhier *et al.*, 2008; de Rosnay *et al.*, 2009a]. In addition, transect measurement campaigns were performed in 2005 and 2006 to address surface soil moisture upscaling properties at the 1 km transect scale for permanent soil moisture stations, particularly those stations exhibiting stable relationships with footprint-scale soil moisture variations. Transect measurements consisted of measuring surface soil moisture at 100 locations every 10 m along a transect located in the vicinity of each ground station. Each transect measurement was considered to be instantaneous. Therefore, transect mean and spatial standard deviation values of surface soil moisture at the time of the transect measurement can be considered to give a snapshot of surface soil moisture value and spatial variability. Defined transects were measured on a regular basis for different soil moisture conditions at different stages of the 2005 and 2006 monsoon seasons. Linear regressions

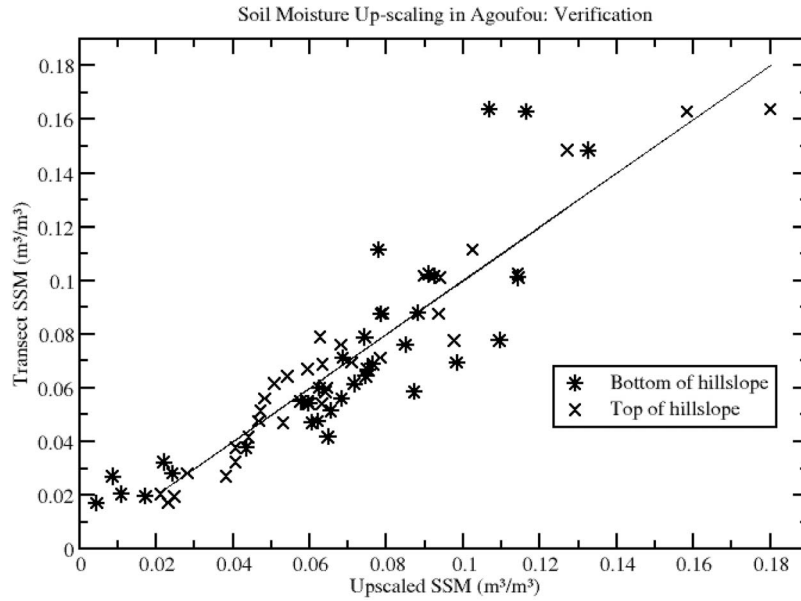


Figure 8. Surface soil moisture (SSM) estimated at the 1 km scale from transect measurements (vertical axis) and from the local Agoufou top and bottom of hillslope measurements transformed via a static, linear upscaling equation. (Reprinted from *de Rosnay et al.* [2009a], copyright 2009, with permission from Elsevier.)

between transects and local station measurements were then shown to be stable (1) across the Gourma supersite for all sandy sites of the area and (2) at the interannual scale (2005–2006). For instance, Figure 8 demonstrates the ability of linear upscaling functions to reliably map point-scale observations acquired at the top and bottom of the Agoufou transect site to transect-averaged soil moisture. This apparent stability of linear regressions between local and transect measurements demonstrates the possibility of using short-term field campaigns to define local F_{\uparrow} functions capable of providing continuous coarse-scale soil moisture estimates derived from sparse, point-scale observations.

4.4. Enhanced Upscaling Using Land Surface Modeling

[46] In cases where field campaign data are not available, it may also be possible to parameterize F_{\uparrow} using distributed land surface modeling. The application of land surface modeling is based on the assumption that spatially distributed soil, topographic, and meteorologic forcing data fed into the model and subsequent model physics which act upon these forcings can accurately capture processes generating spatial soil moisture variability (see section 2). If this assumption holds, then the land surface model (LSM) can help define an appropriate functional form for F_{\uparrow} .

[47] *Crow et al.* [2005a] tested this assumption using a detailed LSM during the SMEX02 field experiment in central Iowa. Using a set of field-scale ($\sim 800^2 \text{ m}^2$) surface soil moisture observations (θ_{FIELD}) obtained from spatially intensive ground sampling within a 2 week period, they binned all possible paired combination of soil moisture measurements according to the spatial distance between observations and calculated the semivariance (i.e., one half the mean squared difference between pairs) for each distance

bin. Plots of semivariance versus distance are commonly referred to as semivariograms. Figure 9 shows semivariograms for several days during SMEX02 for both the spatial distribution of soil moisture ground observations and an analogous distribution obtained by subtracting field-scale soil moisture model predictions from observations. Results in Figure 9 demonstrate that subtracting off the model-based soil moisture predictions results in a spatial field that is less spatially variable and contains less large-scale spatial structure than the original field-scale soil moisture observations. This reduction occurs because the land surface model has nonnegligible skill in simulating the temporal evolution of soil moisture spatial patterns.

[48] As a result of this apparent skill, *Crow et al.* [2005a] suggest running a distributed LSM within a single remote sensing footprint to obtain both field-scale model predictions at a discrete set of N ground sampling sites (θ_{LSM}) and a model-based prediction of mean soil moisture for the entire remote sensing footprint $\theta_{\text{FP,LSM}}$ (obtained by averaging distributed LSM soil moisture predictions within the entire footprint). They then upscaled soil moisture using the discrete set of observations contained in the vector θ_{FIELD} via

$$\theta_{\text{UPSCALE}} = F_{\uparrow}(\theta_{\text{FIELD}}) = \theta_{\text{FP,LSM}} + N^{-1} \sum_{i=1}^N (\theta_{i,\text{FIELD}} - \theta_{i,\text{LSM}}). \quad (6)$$

The schematic diagram in Figure 10 is an illustration of applying (6) to the case $N = 4$. The basis of (6) is the assumption that since model/observations differences $\theta_{\text{FIELD}} - \theta_{\text{LSM}}$ are less spatially variable than raw θ_{FIELD} (Figure 9), they can be more reliably upscaled to the footprint scale. In this way, they propose an alternative formulation of F_{\uparrow} which leverages modeling skill to reduce the

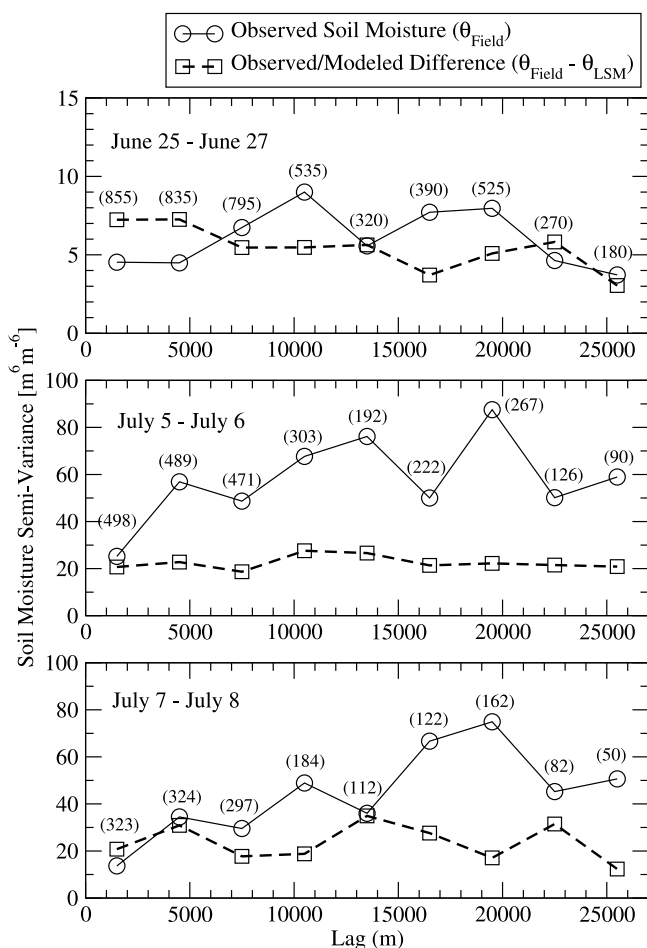


Figure 9. Spatial semivariogram for soil moisture observations (circles) and the differences between such observations and a spatially distributed land surface model (squares) during various periods of the SMEX02 field experiment. (Reprinted from *Crow et al.* [2005a], copyright 2005, with permission from Elsevier.)

spatial variability of the sampled variable and create a less challenging upscaling problem. Conceptually similar approaches can also be based solely on static land surface characteristics commonly used as LSM input. For example, *Ceballos et al.* [2005] note substantially reduced spatial variability after the subtraction of soil moisture wilting points from ground-based soil moisture observations. In a manner analogous to (6), this transformation compensates for known variations in the impact of soil texture on soil moisture and results in a less variable spatial field which is more amenable to spatial averaging.

[49] By applying (6) during SMEX02 for the case $N = 1$, *Crow et al.* [2005a] were able to demonstrate reduced error in θ_{UPSCALE} relative to a simple form for F_{\uparrow} based on (4). However, the approach was markedly less effective for $N = 1$ when the spatial support of the ground-based observations was shrunk from the field scale to the point scale [*Crow et al.*, 2005a]. In addition, the approach is limited to reducing upscaling errors and provides no benefit for the case of large random error in ground-based measurements themselves.

[50] Work by *Loew and Mauser* [2008] provides another example of parameterizing a stable F_{\uparrow} relationship using a distributed LSM. Based on a 10 year high-resolution (1^2 km^2) soil moisture simulation of a hydrological catchment in southern Germany, they regressed 1^2 km^2 soil moisture time series against the soil moisture dynamics of large-scale soil moisture fields (40^2 km^2) and found statistically significant stable linear relationships between field and footprint-scale soil moisture dynamics. This suggests that simple model-based F_{\uparrow} relationships can be derived to link field and footprint-scale soil moisture variability.

4.5. Estimating the Magnitude of Upscaling Errors

[51] All strategies described to this point have addressed the soil moisture upscaling problem by attempting to minimize the magnitude of upscaling error terms on the right-hand side of (3). An alternative approach is accepting inevitable non-negligible upscaling errors and instead attempting to estimate their magnitude.

[52] Given the known impact of land cover characteristics on soil moisture it seems likely that such characteristics can be used to estimate the bias term in (3). Numerous field campaign results have demonstrated that local topographic, vegetation, and soil variation conditions have a predictable impact on the relative bias of local soil moisture conditions versus a larger-scale areal average (see discussion in section 2). Ongoing advances in the spatial mapping of these fine-scale land surface characteristics suggest that known variations in local topographic, land cover, and soil characteristics can be leveraged to estimate the bias error term in (3). Once estimated, its impact on validation results could be minimized.

[53] In addition to correction for bias effects associated with local conditions, viable strategies also exist for estimating (and subsequently correcting for) the random MSD component of (3). Triple collocation (TC) is a statistical tool for leveraging three independently acquired estimates of a given geophysical variable to determine the RMSE of each estimate [*Scipal et al.*, 2008]. *Miralles et al.* [2010] applied TC to the soil moisture upscaling problem by acquiring independent representations of footprint-scale soil moisture based on coarse-scale LSM output (θ_{LSM}), a remote sensing observation (θ_{RS}), and the trivial upscaling of a single point-

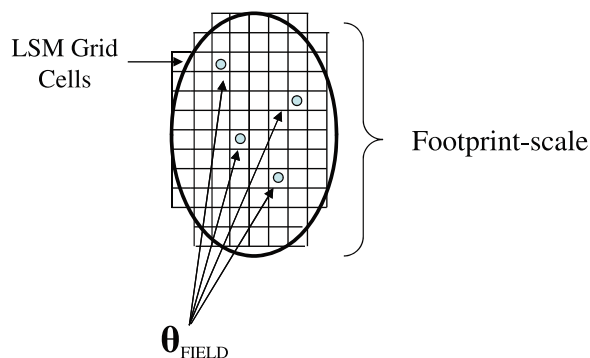


Figure 10. Schematic for the application of the upscaling approach summarized in (6) for the case $N = 4$. Note that the LSM grid cell size is not to scale and has been coarsened for display purposes.

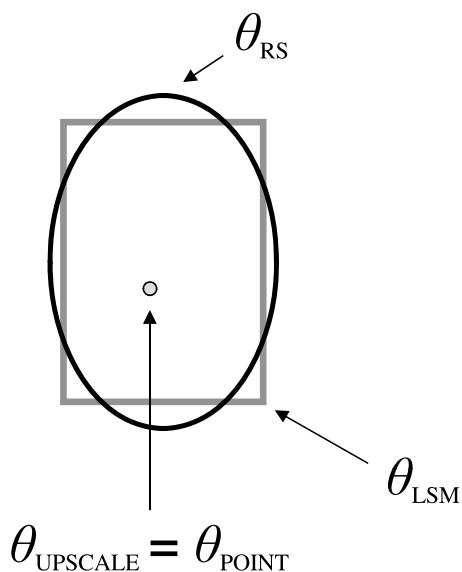


Figure 11. Schematic for the acquisition of the three independent soil moisture estimates required as input by (7).

scale soil moisture observations up to the footprint scale ($\theta_{\text{UPSCALE}} = \theta_{\text{POINT}}$). Figure 11 provides the schematic for this case. Prior to the application of TC, *Miralles et al.* [2010] also remove a 31 day moving average climatology from each soil moisture product to produce a time series of scaled soil moisture anomalies (θ').

[54] If errors in all three soil moisture anomaly products are mutually independent, then the random error term in (3) can be estimated from

$$\text{MSD}(\theta'_{\text{UPSCALE}}, \theta'_{\text{TRUE}}) = \overline{(\theta'_{\text{UPSCALE}} - \theta'_{\text{LSM}})(\theta'_{\text{UPSCALE}} - \theta'_{\text{RS}})}. \tag{7}$$

Note that (7) holds even if all three of the anomaly soil moisture products are degraded by random errors.

[55] Using dense soil moisture observations acquired at four separate U.S. Department of Agriculture Experimental Watersheds listed in Table 2 (the Little River watershed in Georgia (LR), the Little Washita watershed in Oklahoma (LW), the Reynolds Creek watershed in Idaho (RC), and the Walnut Gulch watershed in Arizona (WG)), *Miralles et al.* [2010] tested (7). Each watershed has been instrumented with a spatially dense distributed soil moisture network as part of satellite validation work described by *Jackson et al.* [2010]. Using all available soil moisture observations, high-quality watershed-scale estimates of θ'_{TRUE} were obtained for verifying the accuracy of (7).

[56] The y axis of Figure 12 shows the square root of MSD ($\theta'_{\text{UPSCALE}}, \theta'_{\text{TRUE}}$) obtained by acquiring θ'_{TRUE} from the average of all surface soil moisture observations available within each watershed. while the x axis shows the same value obtained by (7) assuming access to data from only a single ground-based measurement site. Each point in the graph represents the use of this single measurement location as an error-prone estimate of θ_{UPSCALE} (i.e., applying a trivial F_{\uparrow} of $\theta_{\text{UPSCALE}} = \theta_{\text{POINT}}$). Despite requiring only

the availability of a single ground-based sampling location, (7) is able to accurately predict the magnitude of the square root of the MSD($\theta'_{\text{UPSCALE}}, \theta'_{\text{TRUE}}$) term in (2) to within $0.006 \text{ m}^3 \text{ m}^{-3}$ (Figure 12). Once known, this term can be subtracted from the directly observed quantity MSD($\theta'_{\text{UPSCALE}}, \theta'_{\text{RS}}$) in (2) to obtain corrected estimates of MSD($\theta'_{\text{TRUE}}, \theta'_{\text{RS}}$) [*Miralles et al.*, 2010]. One appealing aspect of this approach is that TC-based estimates of MSD($\theta'_{\text{TRUE}}, \theta'_{\text{RS}}$) should also reflect the impact of all random errors on θ_{UPSCALE} and not simply those associated with upscaling. Therefore, unlike other upscaling approaches presented here, it can be used to compensate for the impact of random measurement error on ground-based observations.

[57] There are, however, some clear limitations to the TC-based approach. First, (7) holds only for soil moisture anomaly time series in which a mean or seasonal climatology has first been removed. As a result, the approach is of no value for estimating the bias component of (3). In addition, *Miralles et al.* [2010] found degraded results for cases in which the climatological seasonal cycle of soil moisture differed between various soil moisture products. Therefore, the approach is most effective for the calculation of error in soil moisture anomalies *after* a seasonal climatology has been removed. Finally, *Miralles et al.* [2010] utilized a relatively long sampling period (5 years) for the averaging in (7) to obtain a single temporally fixed value of MSD($\theta'_{\text{UPSCALE}}, \theta'_{\text{TRUE}}$).

[58] Some of these shortcomings have recently been addressed by *Loew and Schlenz* [2011]. Following *Miralles*

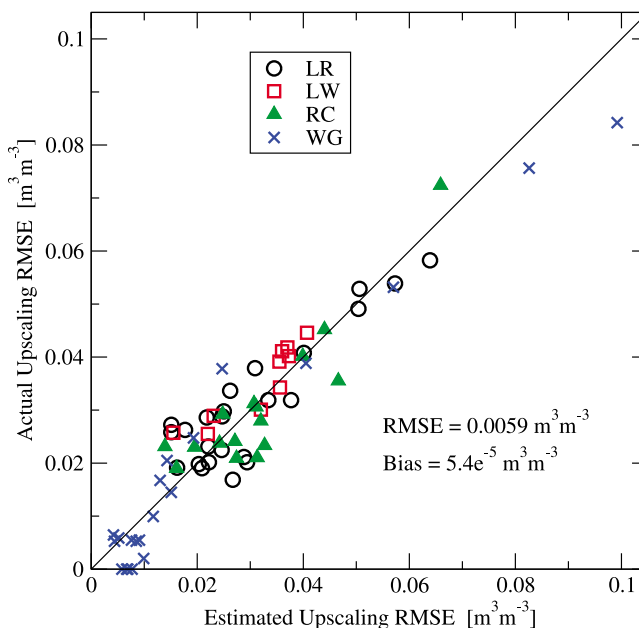


Figure 12. Using all available ground-based observations at each site within the Little River (LR), Little Washita (LW), Reynolds Creek (RC), and Walnut Gulch (WG) watersheds, the RMSE of soil moisture when using a single site to characterize the entire basin (“actual upscaling RMSE”) versus the RMSE calculated using only a single point-scale soil moisture measurement and TC (“estimated upscaling RMSE”). (Modified from *Miralles et al.* [2010].)

et al. [2010], they applied the TC technique to a triplet of soil moisture estimates obtained from sparse in situ observations, a coarse-scale LSM, and satellite observations and verified the theoretical basis of their approach by comparing TC-based estimates $\text{MSD}(\theta'_{\text{UPSCALE}}, \theta'_{\text{TRUE}})$ to estimates of upscaling error obtained independently within densely instrumented watersheds. However, unlike *Miralles et al.* [2010], they also examined the dependency of TC results on the length of the averaging period in (7) by subsampling their 2 year data set into a series of shorter time periods. They found that even without removal of the seasonal cycle, TC provides useful estimates of $\text{MSD}(\theta'_{\text{UPSCALE}}, \theta'_{\text{TRUE}})$ when applied to time series as short as 50 days in duration, provided that sampled cross correlations between data sets were still statistically significant at 95% confidence. This implies that the effectiveness of TC as an upscaling tool can be realized using relatively short data sets and/or applied to realistic cases in which $\text{MSD}(\theta'_{\text{UPSCALE}}, \theta'_{\text{TRUE}})$ varies in time. This is particularly important given the known impact of soil moisture wet-up and dry-down dynamics on the magnitude of observed spatial soil moisture variability (Figure 3).

5. DISCUSSION AND CONCLUSIONS

[59] The proposed QA4EO strategy (<http://QA4EO.org>) is based on deriving appropriate quality indicators for remote sensing retrieval products. In order to be credible, such assurances must be based on traceable comparisons to standard reference measurements that can be obtained at error levels which are small relative to stated validation goals. For remotely sensed soil moisture, rectifying the scale contrast between remotely sensed retrievals and ground-based reference measurements obtained at a point represents a key challenge for establishing such traceability. Extensive observations from soil moisture field campaigns suggest that upscaling via simple spatial averaging of soil moisture data acquired from randomly distributed measurement sites results in unacceptable upscaling errors unless high sampling densities are maintained (section 3). Such high spatial densities are not likely to be available outside of local, data-rich test bed sites and/or time periods of extensive field investigations (Tables 1 and 2). Therefore, more sophisticated upscaling strategies are required to fully leverage large-scale soil moisture network observations for SMOS, SMAP, and Aquarius soil moisture validation activities. Fortunately, a number of viable soil moisture upscaling strategies already exist (section 4). This review summarizes viable ground sampling strategies, modeling approaches, and statistical tools that can potentially contribute to this traceability. As a number of these approaches are based on the application of models and/or assumptions concerning the nature of soil moisture variability, these approaches must be independently verified before they can be applied with confidence. However, taken in their totality, results reviewed here suggest that currently available upscaling techniques offer a viable approach toward addressing this gap and greatly expanding the geographic and temporal scope of soil moisture ground validation activities.

[60] It is also worth noting that strategies reviewed here tend to target different aspects of the upscaling problem and,

as such, can be readily combined. For instance, site selection based on time stability attributes (section 4.1) is particularly useful for minimizing the bias component of (3) but of less value for reducing the random error term in (3) since temporal variations will likely be driven by time-varying precipitation patterns. Conversely, the triple collocation approach in section 4.5 provides estimates for the magnitude of the time-variable term in (3), but it is of no value for addressing the bias term. Therefore, the two approaches are mutually complementary in their ability to correct both aspects of the soil moisture upscaling problem. Likewise, strategies for minimizing (3) via optimal site selection can be readily combined with optimized function forms for F_{\uparrow} . This particular strategy is illustrated in the work by *de Rosnay et al.* [2009b], where investigators *first* down-select measurement sites using a time stability analysis and *then* acquire linear upscaling functions to match measurements at time-stable locations to coarse-scale soil moisture averages. Finally, many approaches appear mutually compatible with regard to scale. For instance, upscaling based on stable patterns gleaned from sporadic intensive sampling (section 4.3) has been validated for point- to field-scale upscaling, while model-based upscaling approaches (section 4.4) appear more amenable to field-to-footprint upscaling. It is therefore likely that the most effective and robust upscaling approaches will be based on applying two or more different upscaling strategies in tandem.

[61] While the demonstrated viability of upscaling approaches suggests that current ground instrumentation is adequate for satellite mission validation needs, it is also possible that new ground measurement technologies could significantly expand the spatial support of soil moisture observations derived from ground-based instrumentation. Examples of such new technologies include the possibility of making roughly $\sim 15^2$ m² resolution measurements using ground-based GPS receivers [*Larson et al.*, 2008] or $\sim 500^2$ m² resolution measurements using passive cosmic ray sensors [*Desilets et al.*, 2010]. In addition, the use of fiber optic cables for continuous two-dimensional soil moisture estimation along long transects (>1 km) has also been demonstrated [*Sayde et al.*, 2010; *Steele-Dunne et al.*, 2010]. While these new technologies might not completely eliminate the need for effective upscaling strategies, they would significantly ease the severity of the challenge by reducing the contrast between the spatial support of ground-based observations and satellite-based soil moisture retrievals.

[62] Finally, it is worth considering broader questions concerning appropriate validation strategies for remotely sensed surface soil moisture retrievals. While forming the basis for most current soil moisture validation goals, RMSE-based evaluation metrics in (1) and (2) do not always provide a true proxy for the ultimate value of a remotely sensed product for specific applications [*Crow et al.*, 2005b]. This has motivated recent attempts to develop alternative evaluation metrics which explicitly account for the relationship between soil moisture and target prediction variables (e.g., crop yield, drought indices, or evapotranspiration) for users of remotely sensed soil moisture products [*Entekhabi et al.*,

2010b]. The use of these alternative metrics often eases the severity of the soil moisture upscaling problem. For example, the development of land data assimilation systems allows for the evaluation of surface soil moisture retrievals based on their ability to enhance forecast skill for related land surface and lower atmospheric variables. In many cases, such alternative variables (e.g., streamflow from a hydrologic model or precipitation forecasts from a numerical weather prediction model) are much easier to validate at coarse spatial scales than surface soil moisture. Consequently, quantifying the ability of soil moisture retrievals to enhance the prediction of these variables (within the context of a data assimilation system) represents a large-scale measure of skill in remotely sensed soil moisture products that can be used to supplement direct soil moisture validation activities [see, e.g., Crow *et al.*, 2010]. While these techniques lack the ability to provide RMSE-based evaluation metrics required for strict validation, they can be used for more general, and potentially more relevant, assessments of overall utility in remotely sensed soil moisture products.

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