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- An in-situ data based model to downscale radiometric satellite soil moisture products in
 the Upper Hunter Region of NSW, Australia
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23 Abstract

High spatial resolution soil moisture information is important for hydrological, climatic and 24 agricultural applications. The lack of high resolution soil moisture data over large areas at the 25 required accuracy is a major impediment for such applications. This study investigates the 26 feasibility of downscaling satellite soil moisture products to 1 km resolution. This study was 27 undertaken in the semi-arid Goulburn River Catchment, located in south-eastern Australia. The 28 Soil Moisture Active Passive (SMAP)-Enhanced 9 km (L3SMP-E) and Soil Moisture and 29 Ocean Salinity (SMOS) 25 km gridded (SMOS CATDS L3 SM 3-DAY) radiometric products 30 were compared with in-situ soil moisture observations and a regression tree model was 31 developed for downscaling based on thermal inertia theory. Observations from a long-term soil 32 moisture monitoring network were employed to develop a regression tree model between the 33 diurnal temperature difference and the daily mean soil moisture for soils with different clay 34 content and vegetation greenness. Moderate-resolution Imaging Spectroradiometer (MODIS) 35 land surface temperatures were used to estimate the soil moisture at high spatial resolution by 36 disaggregating the satellite soil moisture products through the regression model. The 37 downscaled SMAP-Enhanced 9 km and SMOS 25 km gridded soil moisture products showed 38 unbiased root mean square errors (ubRMSE) of 0.07 and 0.05 cm³/cm³, respectively, against 39 the in-situ data. These ubRMSEs include errors caused by measuring instrument and the scale 40 mismatch between downscaled products and in-situ data. An RMSE of 0.07 cm³/cm³ was 41 observed when comparing the downscaled soil moisture against the passive airborne L-band 42 retrievals. The findings here auger well for the use of satellite remote sensing for the assessment 43 44 of high resolution soil moisture.



47 **1. Introduction**

Soil moisture is a key variable in a number of environmental processes at both regional and 48 global scales including hydrologic, climatic and agricultural applications, such as water 49 management and irrigation scheduling (Hanson et al., 2000; Pacheco et al., 2015), weather and 50 climatic prediction (Dirmeyer et al., 2016; Huszar et al., 1999; Orth and Seneviratne, 2014), 51 52 drought monitoring (Lorenz et al., 2017; Pablos et al., 2017; Wang et al., 2011), flood forecasting (Brocca et al., 2017; Lacava et al., 2005; Norbiato et al., 2008; Tramblay et al., 53 2010) and analysing nutrient and contaminant transport potential (Dickinson et al., 2002; 54 Porporato and Rodriguez-Iturbe, 2002). Many of these applications require soil moisture data 55 at high spatial resolution, from a few kilometres to sub-kilometre scale. However, soil moisture 56 57 information is rarely available at adequate spatial and temporal scales. Soil moisture is measured at scales ranging from point (in-situ measurements) to satellite measurements at ~10s 58 of km scale. Given the limited availability of dense ground-based soil moisture monitoring 59 60 networks in most areas, satellite soil moisture products are considered a most feasible option to provide spatial and temporal soil moisture data. 61

Microwave remote sensing has been widely used to estimate global scale surface soil 62 moisture over the last three decades (Karthikeyan et al., 2017a; Kerr et al., 2016; Schmugge 63 and Jackson, 1993; Schmugge, 1976). In particular, passive microwave radiometer 64 65 measurements in the L-band frequency regime have been shown to be the best option to retrieve soil moisture (Schmugge et al., 1986). Recently, satellite soil moisture retrieval from L-band 66 sensors has been realized with the launch of the European Space Agency's (ESA) SMOS (Soil 67 Moisture and Ocean Salinity) and the National Aeronautics and Space Administration's 68 (NASA) Soil Moisture Active Passive (SMAP) satellites in 2009 and 2015, respectively. These 69 70 satellites provide global estimates of surface soil moisture at the top ~ 5 cm of the soil profile (Entekhabi et al., 2010a; Karthikeyan et al., 2017b; Kerr et al., 2010) frequently (~3-day revisit 71

period) at an expected accuracy of 0.04 v/v, but with low spatial resolution (~40 km). SMAP employs vertically polarized brightness temperature-based single-channel algorithm (SCA-V) as the current baseline retrieval algorithm for its passive soil moisture product (Chan et al., 2018). The L-band Microwave Emission of the Biosphere Model (L-MEB) is currently used as the retrieval algorithm for the SMOS products (Kerr et al., 2012; Wigneron et al., 2007). Despite their high accuracy, the satellite products cannot fully capture the spatial variability of soil moisture as required in many applications, due to their coarse resolutions.

79 Validating and downscaling satellite soil moisture products are crucial for their utilization in various applications. For example, extensive calibration and validation (cal/val) 80 activities pre- and post-launch of SMAP have been used to develop and improve the retrieval 81 algorithms using in-situ soil network measurements (Jackson et al., 2014). The quality 82 requirement of in-situ data, and the spatial mismatching between remotely sensed and in-situ 83 soil moisture, posed great challenges for the validation of satellite soil moisture products 84 85 (Colliander et al., 2017a; Crow et al., 2012; Jackson et al., 2014). The intensive cal/val phase of the SMAP mission demonstrated the SMAP radiometer based soil moisture products meet 86 their expected performance ($\sim 0.04 \text{ m}^3/\text{m}^3$) from globally selected core validation sites 87 (Colliander et al., 2017a). 88

89 Given the accuracy of passive L-band microwave remote sensing, downscaling these 90 reliable satellite soil moisture products is a logical step to estimate soil moisture at the required spatial resolution for many applications (Peng et al., 2017; Sabaghy et al., 2018). The available 91 satellite soil moisture downscaling methods can be classified as; satellite, geo-information data, 92 93 and model based approaches (Peng et al., 2017). Satellite based soil moisture downscaling methods consist of fusion of active and passive microwave retrievals (Das et al., 2011; Das et 94 al., 2014; Das et al., 2018; Leroux et al., 2012) and fusion of microwave data with optical or 95 thermal datasets (Piles et al., 2014; Piles et al., 2016; Portal et al., 2018; Sánchez-Ruiz et al., 96

2014; Piles et al., 2011; Chauhan et al., 2003). The downscaled soil moisture of the active 97 passive microwave data fusion methods provides products with a moderate resolution. Since 98 99 Carlson et al. (1994) introduced the 'universal triangle' concept between soil moisture, surface temperature and vegetation index, efforts have been made to downscale satellite soil moisture 100 products by introducing optical/thermal data. Optical/thermal based downscaling approaches 101 provide higher resolution soil moisture products and perform well in arid and semi-arid areas 102 103 with high atmospheric evaporative demand (Peng et al., 2017). Therefore, these methods have a high potential over the Australian land mass in developing a time series record of high 104 105 resolution soil moisture. In these approaches, land surface parameters (e.g., vegetation cover, land surface temperature, surface albedo) retrieved from the optical/thermal satellite sensors at 106 a high spatial resolution, have been expressed as a function of soil moisture (Carlson, 2007; 107 Chauhan et al., 2003; Merlin et al., 2010 and 2012; Peng et al., 2017; Petropolous et al., 2009; 108 Piles et al., 2011). The Disaggregation based on Physical And Theoretical scale Change 109 (DisPATCh) model proposed by Merlin et al. (2012) is one such method of downscaling 110 microwave soil moisture retrievals using optical/thermal data. In this study, MODerate-111 resolution Imaging Spectroradiometer (MODIS) products were used to derive land surface 112 temperatures (LSTs) at high spatial resolution (1 km). The MODIS-derived LSTs were 113 separated into their soil and vegetation components as in the 'universal triangle' or 'trapezoidal 114 model'. The soil evaporative efficiency (SEE) (estimated using MODIS LSTs), albedo, and 115 Normalized Difference Vegetation Index (NDVI) were related to the soil moisture variability 116 within a coarse resolution SMOS pixel (Merlin et al., 2008, 2010, 2012). The accuracy of the 117 downscaled products from DisPATCh showed a notable variation with the season, showing 118 root mean square errors (RMSEs) of 0.06 m^3/m^3 in Austral summer and 0.18 m^3/m^3 in Austral 119 winter when compared with the in-situ soil moisture, in the Murrumbidgee River catchment 120 (Merlin et al., 2012; Sabaghy et al., 2018). 121

Fang et al. (2013) and Fang and Lakshmi (2014) proposed a regression model to downscale 122 the SMOS and the Advanced Microwave Scanning Radiometer for the Earth Observing System 123 (AMSR-E) soil moisture products. This downscaling approach is based on the thermal inertia 124 relationship between the diurnal soil temperature difference (ΔT) and the daily mean soil 125 moisture ($\theta\mu$). Model derived soil moisture and soil temperature estimates from North 126 American Land Data Assimilation System (NLDAS), NDVI data from MODIS, Satellite Pour 127 128 l'Observation de la Terre (SPOT) and Advanced Very High Resolution Radiometer (AVHRR) along with the MODIS LST products were used to demonstrate the capability of the proposed 129 130 downscaling model over Oklahoma, Midwest region of the United States. The downscaled soil moisture showed RMSEs ranging from 0.02 to 0.06 m^3/m^3 over the Little Washita Watershed 131 in Oklahoma (Fang and Lakshmi, 2014), and unbiased RMSEs (ubRMSE) of 0.042 m³/m³ and 132 $0.026 \text{ m}^3/\text{m}^3$ against ground observations from the soil monitoring networks (Fang et al., 2013). 133 The spatial data gaps due to cloud cover and impact of vegetation on optical/thermal 134 observations are two major limitations in the optical/thermal data based downscaling methods 135 (Peng et al., 2017; Sabaghy et al., 2018). 136

The study presented in this paper investigates the feasibility of developing a time series 137 record of high spatial resolution soil moisture by downscaling satellite soil moisture products 138 using an in-situ data based model. The regression tree method developed here is similar to Fang 139 140 et al. (2013, 2018) and Fang and Lakshmi (2014), but based on in-situ observations with additional factors. Fang et al. (2013) and Fang and Lakshmi (2014) developed monthly lookup 141 regressions using model derived ΔT and $\theta\mu$ modulated by the NDVI, and then used this 142 regression tree method to downscale AMSR-E and SMOS soil moisture products using MODIS 143 LSTs. Since global scale land surface models are not fully calibrated to specific sites, these 144 products can be associated with high uncertainties caused by scaling issues, accuracy of the 145 input data and the model-algorithms (Chen et al., 2014). For arid or semi-arid landscapes with 146

the extreme climate variability and the complex ecosystem, global land surface modelled data 147 can be subjected to high prediction errors and they may not be reliable reference data for 148 representing actual soil conditions without rigorous calibration and validation. To avoid the 149 uncertainties and errors associated with the model-derived estimates, the study presented here 150 employed a high quality, reliable in-situ observations of soil moisture and temperature over a 151 long period from well-designed and maintained monitoring sites (described in section 2.2.1) to 152 153 develop the downscaling model. Also, the downscaling model was generalized over the study catchment area, i.e., relative soil moisture variability to mean catchment soil moisture 154 155 condition, considering site-specific soil characteristics as a modulating factor to explain the spatial variability and temporal stability of surface soil moisture in a semi-arid region (Cosh et 156 al., 2008; Chen et al., 2014). 157

As the first step, SMAP-Enhanced 9 km and SMOS 25 km gridded soil moisture 158 products were compared with in-situ soil moisture observations and then a regression tree 159 model was developed to downscale the satellite soil moisture products to 1 km resolution based 160 on thermal inertia theory. Finally, the reliability of the downscaled products was assessed using 161 ground observations and an airborne soil moisture retrieval. The study presented in this paper 162 was undertaken in the Goulburn River Catchment, located in the south-eastern region of 163 Australia, where significant efforts have been made to measure soil moisture through 164 continuous in-situ soil moisture monitoring network, field-based studies, and remote sensing 165 (Chen et al., 2014; Martinez et al., 2007; Panciera et al., 2008; Rüdiger et al., 2007). 166

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171 **2.** Study area and data

172 *2.1. Description of the study area*

The Goulburn River catchment is located approximately 150 km northwest of Sydney, 173 extending from 31°46 'S to 32°51 'S and from 149°40 'E to 150°36 'E (Fig. 1). The Goulburn 174 River is a tributary of the Hunter River in south-eastern Australia. The catchment size is ~7000 175 km² and its elevation varies from 100 m on the floodplains to 1300 m in the northern and 176 southern mountain ranges. The northern and southern halves of the catchment can be 177 distinguished both geologically and on the basis of land use/land cover. The northern half of 178 the catchment is dominated with basalt derived soils while the southern part is dominated with 179 sandstone, conglomerate and shale derived soils. The northern part has been cleared mainly for 180 181 cropping and grazing, whereas the southern part consists of dense vegetation with forests. The distribution of clay, silt and sand contents of the top soils in the catchment is shown in Fig. 2. 182 The area exhibits a semi-arid climate with a mean annual precipitation of 700 mm. However, 183 184 the study catchment shows an increasing gradient in precipitation towards higher altitudes resulting in a range from 500 mm to 1100 mm. The monthly mean temperatures vary from 16° 185 C to 30°C in the summer and from 3°C to 17°C in the winter (Rüdiger et al., 2003). This region 186 has experienced a range of climatic events during the last 15 years, including the millennium 187 drought from 2001 to 2009 (Van Dijk et al., 2013), strong La Niña conditions in 2010/11 188 (Boening et al., 2012) and an extreme storm event with a 100-year return period (Pasha Bulker 189 storm) in 2007 (Mills et al., 2010). 190

The study site has been thoroughly studied in order to develop a better understanding of the land surface processes driving soil moisture variability. Under the Scaling and Assimilation of Soil Moisture and Streamflow (SASMAS) project, the study site has been heavily instrumented for soil moisture, rainfall, and runoff since 2002 (Rüdiger et al., 2007). The monitoring stations were established to provide in-situ data to validate AMSR-E soil Fig. 1

Fig. 2

moisture retrievals, develop downscaling algorithms for coarse resolution satellite soil
moisture products, assimilate remotely sensed soil moisture data to retrieve soil moisture
profile and to improve streamflow forecasting (Rüdiger et al., 2003). National Airborne Field
Experiment 2005 (NAFE'05) airborne campaign was conducted in this area using L-band
radiometers to provide simulated SMOS observations for soil moisture while validating the
AMSR-E near-surface soil moisture products (Panciera et al., 2008).

202 This study is focused on two sub-catchments, the Krui (562 km²) and Merriwa (651 km²) River, located in the northern half of the Goulburn River catchment. These sub-203 204 catchments include a dense soil moisture monitoring network (Fig. 1) and have been mostly cleared for cropping and grazing (Fig. 3a). Figure 3b shows the average seasonal vegetation 205 density in 2015 as inferred by the MODIS NDVI composites over these two sub-catchments. 206 The dense vegetation in the north and south-most parts of the two sub-catchments is evident in 207 Fig. 3b. The temporal dynamics of NDVI in the Krui River catchment SASMAS monitoring 208 stations retrieved from the MODIS 16-day NDVI composites are shown in Fig. 4. A high 209 variability of NDVI can be observed at stations in croplands (i.e. K1 and K3), compared to the 210 other stations which are in grazing areas. K6 shows a consistently high NDVI value, possibly 211 due to the high vegetation growth driven by the higher rainfall. 212

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214 *2.2. Data*

This section discusses details on in-situ soil moisture observations, the satellite soil moisture products, and other geospatial data used for developing the downscaling algorithm. Table 1 provides a summary of the datasets used in this study.

218

219

Fig. 3

Fig. 4

Table 1

220 2.2.1. In-situ soil moisture observations

Twenty-six soil moisture and temperature monitoring stations were established from 2002 221 Goulburn 222 over the River catchment under the SASMAS project (http://www.eng.newcastle.edu.au/sasmas/SASMAS/sasmas.htm). 223 The SASMAS soil moisture monitoring stations were established in the representative, 'time stable' locations of 224 their surrounding landscape, so that they could adequately represent the watershed as whole 225 226 and the footprint scale radiometric satellite soil moisture products after upscaling (Grayson and Western, 1998; Rüdiger et al., 2003; Rüdiger et al., 2007; Crow et al., 2012). These sites were 227 228 carefully chosen by selecting mid-slope locations with representative vegetation, soil type, elevation, aspect, etc. (Rüdiger et al., 2003; Rüdiger et al., 2007). During the NAFE'05, an 229 intensive field campaign had been carried out to support the L-band airborne soil moisture 230 observations. This ground sampling had been conducted from very high resolutions (6.25 and 231 12.5 m spacing) to intermediate resolutions from 125 m to 250 m spacing and coarse 232 resolutions from 500 m and/or 1 km spacing. The NAFE'05 data analysis showed the potential 233 of using the SASMAS dataset to validate coarse resolution satellite soil moisture products such 234 as SMOS over the Goulburn River catchment area (Panciera et al., 2008). The sites have been 235 instrumented with three vertically inserted Campbell Scientific CS616 water content 236 reflectometers at soil depths of 0-30, 30-60 and 60-90 cm, at each station. Stevens Water 237 HydraProbes were later installed to measure soil temperature at 25 mm and soil moisture of 238 the top 5 cm soil layer at the monitoring stations (Rüdiger et al., 2007). Six monitoring stations 239 were established in the Krui River catchment (K1 to K6) and seven in the Merriwa River 240 catchment (M1 to M7). In addition, seven monitoring stations (S1 to S7) were established over 241 a densely monitored micro-catchment, "Stanley" (with a catchment size of 175 ha) located 242 within the Krui River catchment (Martinez et al., 2007) (Fig. 1). These monitoring stations are 243 located over a range of soil types, varying from sandy to clayey soils. The land cover and soil 244

texture of the SASMAS stations in the Krui and Merriwa River catchments are shown in Table 245 2. The in-situ soil moisture data were measured at 1 min interval and averaged using 20 min 246 247 time window. The SASMAS dataset is available from 2003 to 2015, but contains a number of data gaps. These data gaps are caused mainly due to failure of sensors/telemetry, and erroneous 248 readings caused by extremely dry weather conditions that resulted in soil cracking, especially 249 250 dominate in the clay soils in the northern parts of the sub-catchments. Erroneous readings were 251 recorded at some of the stations during this time due to sensors not remaining in contact with soils during dry periods and the cracks getting filled with water during wet periods. The 252 253 SASMAS datasets are available up to 2015. The daily mean soil moisture data and hourly soil temperature data of the 0-5 cm soil profile from 2003 to 2014 were employed in this study to 254 develop the regression algorithms. The daily mean soil moisture data in 2015 from the Krui, 255 Merriwa and Stanley stations were employed in the validation of satellite and downscaled soil 256

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259 2.2.2. Satellite soil moisture products

moisture products (details discussed in Section 3).

The ESA's SMOS mission launched in 2009 (Barré et al., 2008; Kerr et al., 2010) and the 260 NASA's SMAP launched in 2015 (Chan et al., 2016; Entekhabi et al., 2010a) are two L-band 261 missions which use 1.4 GHz radiometer frequencies with approximately 3-day revisit times. 262 Both SMAP and SMOS provide near surface soil moisture (~0-5 cm) based on the L-band 263 penetration depth. One major objective of the SMAP mission was to fuse the coarse resolution 264 (~40 km) radiometric measurements with fine resolution (1-3 km) radar measurements (1.26 265 266 GHz) to produce soil moisture products at intermediate resolution (9 km) (Entekhabi et al., 2014). However, only the radiometric soil moisture products of SMAP are available following 267 the failure of the SMAP radar on 7th July 2015. SMAP radar-based products are available for 268 the first three months prior to the failure involving its high-power amplifier (HPA) (Neeck, 269

Table 2

2015). Combining Sentinel-1 radar data with SMAP radiometric data is an approach employed 270 as a solution to the SMAP radar failure (Das and Dunbar, 2018). The target accuracy of both 271 SMAP and SMOS is 0.04 cm³/cm³. The accuracy of SMAP derived soil moisture has been 272 demonstrated as 0.04 cm³/cm³ for both 36 km and 9 km gridded products (Chan et al., 2016; 273 Chan et al., 2017; Colliander et al., 2017a). SMOS has demonstrated its expected accuracy of 274 0.04 m³/m³ at some of the sites (Al Bitar et al., 2012; Jackson et al., 2012). However, higher 275 276 uncertainties in SMOS products have been observed in a number of other studies (Djamai et al., 2015; Pacheco et al., 2015; Niclòs et al., 2016). Despite their identical L-band frequencies 277 278 and spatial and temporal resolutions, there are notable differences between SMAP and SMOS. SMOS measures surface emissions from a large number of view angles from 0 to 55° whereas 279 SMAP measures surface emissions only at a 40° angle (Entekhabi et al., 2014; Karthikeyan et 280 al., 2017b). Moreover, SMAP measures brightness temperatures with a better sensitivity with 281 a noise-equivalent delta temperature (NEDT) < 1 K for 17-ms samples (Piepmeier et al., 2017) 282 compared to SMOS, which has a sensitivity of ~2-4.5 K (Corbella et al., 2011). Furthermore, 283 the SMAP and SMOS soil moisture products use different retrieval algorithms, model 284 parameters, some of the ancillary datasets (e.g. land cover maps) and assumptions (Al-Yaari et 285 al., 2017; Karthikeyan et al., 2017b). 286

For downscaling, two different satellite products have been used in this study (Fig. 5). First, 287 the SMAP Enhanced L3 Radiometer Global Daily 9 km EASE-Grid Soil Moisture, Version 2 288 (L3SMP-E) products over the Goulburn River catchment from April 2015 to September 2016 289 were obtained from the National Snow and Ice Data Center (NSIDC) (http://nsidc.org/). Here, 290 Backus-Gilbert optimal interpolation techniques, the classical inversion method in microwave 291 radiometry (Chaubell et al., 2016), have been used to retrieve maximum information from 292 SMAP antenna temperatures and then converted into brightness temperatures (Chan et al., 293 2018; O'Neill et al., 2016). This interpolation process allows the preservation of the spatial 294

Fig. 5

resolution of the antenna gain function associated with the sampled radiometer data (Poe, 295 1990). The brightness temperatures have been resampled onto the 9-km Equal-Area Scalable 296 Earth Grid, Version 2.0 (EASE-Grid 2.0) in a global cylindrical projection. Herein this dataset 297 will be called as SMAP-E. The SMAP-E 9 km grid over the study area is shown in Fig. 5b. 298 Secondly, the SMOS CATDS L3 SM 3-DAY, Release 4 soil moisture products (Product code: 299 MIR CLF33A and MIR CLF33D) of 25 km grid size (CATDS, 2016; Al Bitar et al., 2017) 300 301 were obtained from the Centre Aval de Traitement des Données SMOS (CATDS) (https://www.catds.fr). The CATDS Level 3 soil moisture products include daily ascending 302 303 and descending multi-orbit retrievals, and their average was taken as the daily mean soil moisture in this study. The SMOS 3-day aggregation generates global L3 soil moisture on a 3-304 day sliding window at daily basis by performing a temporal aggregation of the L3 CATDS 305 306 daily product. The soil moisture retrievals were resampled onto a 25-km Global Equal-Area Scalable Earth Grid (EASE grid) (Kerr et al., 2013). The SMOS 25 km grid is shown in Fig. 307 5c. It is noteworthy to mention that the spatial resolutions of the SMAP and SMOS soil 308 moisture products stated in this article, i.e. SMAP-E 9 km and SMOS 25 km, are their grid 309 posting resolutions, not the actual observation resolutions. 310

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312 2.3. Other geospatial data

313 2.3.1. MODIS-derived NDVI and LST products

NDVI data over the Krui and Merriwa River catchments from 2003 to 2015 were obtained from MODIS/Aqua Vegetation Indices 16-Day L3 Global 1 km Grid V005 (MYD13A2) products (Didan, 2015) in order to classify the downscaling model based on different NDVI classes. MODIS/Aqua Land Surface Temperature and Emissivity (LST/E) Daily L3 Global 1 km Grid V006 (MYD11A1) (Wan et al., 2015) dataset (1 km spatial resolution) was used in this study to derive daily night and day time LSTs over the Krui and
Merriwa River catchments in 2015 and for the period of NAFE'05 (in 2005).

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322 2.3.2. Soil and Landscape Grid National Soil Attributes Maps

The clay content in the 0-50 mm soil profile over the Krui and Merriwa River 323 catchments was extracted from the National Soil Attributes Maps of the Soil and Landscape 324 Grid of Australia (Grundy et al., 2015). This is a new soils database for Australia released in 325 late 2014, as a part of the GlobalSoilMap initiative. It provides quantitative soil properties on 326 a 90 m grid for all of Australia. The Australian site data and spectroscopic estimates were used 327 to develop the Soil and Landscape Grid dataset. The site data had been collected from 1931 to 328 329 2013 by the state and territory government agencies and Commonwealth Scientific and Industrial Research Organisation's (CSIRO) National Soil Archive and National Soil Database 330 (NatSoil) to develop the National Soil Site Data Collection (NSSDC). The spectroscopic 331 estimates were made with the National soil visible-near infrared database (NSVNIRD) to 332 estimate soil properties, by using the soil samples collected for the National Geochemical 333 Survey of Australia (Rossel et al., 2015). The clay content at 0-5 cm soil profile was used in 334 this study for the regression tree as a modulating parameter of $\Delta T - \theta \mu$ relationship. Data from 335 15192 NSSDC sites and 1113 NSVNIRD sites were used to develop the clay content maps in 336 337 the Soil and Landscape Grid of Australia (Rossel et al., 2015). The uncertainties of the clay content of the top 5 cm soil layer is 18.5% with 14.1% and 23.0% at lower and upper 90% 338 confidence limits, respectively (Rossel et al., 2015). The dataset was obtained from the 339 Commonwealth Scientific and Industrial Research Organisation (CSIRO) data access portal 340 (https://data.csiro.au). 341

Soil moisture retrievals from the NAFE'05 (Panciera et al., 2008) were used in this 344 study to validate the downscaling algorithms. The NAFE'05 was conducted in November 2005 345 in the Goulburn River catchment to provide simulated SMOS observations from an L-band 346 radiometer along with the soil moisture and other relevant ground observations. The objectives 347 348 of the experiment were to develop the SMOS soil moisture retrieval algorithms, the SMOS downscaling approaches, and the assimilation of SMOS into land surface models for root zone 349 soil moisture estimations. The regional airborne data collection was carried out in four 350 consecutive Mondays starting from 31^{st} October 2005 over a 40 km \times 40 km area in the northern 351 part of the catchment (Fig. 5 a). The long drying period followed by the heavy rainfall on 352 October 31st and November 1st allowed the NAFE'05 campaign to observe near surface soil 353 moisture observations ranging from fully-saturated conditions to very dry conditions (Panciera 354 et al., 2008). This covered the area cleared for cropping and grazing in the Krui and Merriwa 355 River catchments where the SASMAS monitoring stations were concentrated, while the south-356 most part of the NAFE'05 study area included forested areas with dense vegetation. The 357 Polarimetric L-band Multibeam Radiometer (PLMR) was employed for the regional NAFE'05 358 airborne data collection. The 1 km NAFE'05 soil moisture products were derived from PLMR 359 brightness temperatures using a two channel inversion of the L-MEB model (Panciera et al., 360 2009). Although the nominal ground resolution of the dataset is 1 km, the pixel size varied 361 from 860 to 1070 m due to the constant altitude of the flights above the median elevation over 362 the varying terrain. The average flight altitude was 3000 m Above Ground Level (AGL) and 363 the data was acquired in the morning between 6:00 hrs to 10:00 hrs along north-south orientated 364 flight lines. Herein the term 'NAFE'05' is used in this paper to refer to this regional airborne 365 campaign. 366

368 3. Methods

Fig. 6

SMOS products with in-situ data; (2) developing the regression tree model for downscaling;
and (3) evaluation of the downscaled soil moisture data with SASMAS in-situ and NAFE'05
airborne observations. The overall approach is summarized in the flowchart shown in Fig. 6.

The methodology section consists of: (1) evaluation and inter-comparison of SMAP and

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374 3.1. Evaluation and inter-comparison of SMAP-E and SMOS soil moisture products with in375 situ data

The SASMAS in-situ soil moisture data from the top 5 cm soil profile was employed to 376 evaluate near surface soil moisture measurements from SMAP-E and SMOS. Fig. 5 shows the 377 378 distribution of SMAP-E 9 km and SMOS 25 km grids, as well as the SASMAS in-situ monitoring stations over the study area. Location details of the pixels used in this evaluation 379 380 process are given in Table 3. The average of available in-situ observations of the top 5 cm over the SMAP and SMOS satellite foot prints were used in this comparison. Note that the spatial 381 averaging of limited in-situ observations can also contribute to the potential error in this 382 comparison. This comparison was conducted over one SMAP-E 9 km pixel (X, Fig. 5b) and 383 one SMOS 25 km pixel (R, Fig. 5c). Average soil moisture of three SASMAS monitoring 384 stations over the nominal 33 km contribution domain (Fig. 5b) of the SMAP-E 9 km pixel X 385 and two stations on SMOS 25 km pixel R (Fig. 5c) were employed in this comparison (Chan 386 et al., 2018). Colliander et al. (2018) has employed a similar approach to validate SMAP-E 387 products with core validation sites. 388

Then, the SMOS and SMAP-E soil moisture products over the Krui and Merriwa River catchments in 2015/16 were compared against each other over the four SMOS 25 km pixels, P, Q, R and S (Fig. 5c) by interpolating SMAP-E soil moisture to the SMOS 25 km grid centres. Table 3

This interpolation of SMAP-E into SMOS grid centres allows to capture a near approximationof average soil moisture from the actual contributing domain of SMAP-E.

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395 3.2. Developing the downscaling model

The downscaling method presented in this paper is based on the soil thermal inertia relationship between ΔT and $\theta\mu$, which has been demonstrated by Fang et al. (2014, 2018) for multiple sites in United States. We first discuss the thermal inertia theory, and then present details on the regression tree model developed for this study.

Thermal inertia is a measure of the resistance of an objects temperature to the changes in its surrounding temperature (Sellers, 1965). The objects with high thermal inertia show a lower temperature change compared to the objects with low thermal inertia. Therefore, a low thermal inertia of soil shows a high variation in the diurnal temperature and vice versa. Accordingly, the relationship between the thermal inertia (*TI*) and ΔT can be given as (Engman, 1991):

$$\Delta T = f(1/TI), \tag{1}$$

$$\Delta T = T_{PM} - T_{AM} , \qquad (2)$$

408 where T_{PM} and T_{AM} are the afternoon and early morning soil surface temperatures.

409 *TI* can also be defined as (Wang et al., 2010):

410
$$TI = \sqrt{\rho kc},\tag{3}$$

411 where ρ is the bulk density (kg m⁻³), k is the specific heat capacity (J kg⁻¹ K⁻¹) and c is the 412 thermal conductivity (W m⁻¹ K⁻¹) of the material. Water has a high specific heat capacity 413 compared to the dry soil. Therefore, the thermal inertia of wet soil is significantly higher than dry soil and exhibits lower diurnal temperature fluctuation. When the moisture content of the soil is increasing, the thermal inertia of the soil increases proportionally. Therefore, wet soils exhibit low diurnal soil temperature difference compared to dry soils (Verstraeten et al., 2006).

The relationship between the diurnal soil temperature difference and the daily mean 417 soil moisture is complex and modulated by the season, vegetation density and the soil texture 418 (Engman, 1991; Farrar et al., 1994; Peng et al., 2017; Sandholt et al., 2002). A regression tree 419 model was used to represent this complex relationship. A basic regression tree algorithm 420 typically produces a set of rules in a decision tree format, which can be used to represent the 421 correlation between the independent variable and the predictor variables under different 422 conditions (De'ath and Fabricius, 2000). This approach does not require the assumption of a 423 globally linear relationship, nor a priori knowledge of the mathematical form of nonlinear curve 424 fitting methods (Breiman et al., 1984). 425

The downscaling method employed here is similar to the NLDAS product-based 426 regression model developed by Fang et al. (2013, 2018) and Fang and Lakshmi (2014), but 427 with in-situ data and additional factors. In this study, continuous long term in-situ observations 428 of soil moisture and temperature were used together with a time series of remotely sensed 429 NDVI data to develop the regression tree models by season. The in-situ data from the SASMAS 430 431 network provided details on surface soil moisture change under different climatic conditions 432 over the range of soil types. Soil texture information was also considered in the regression tree models, given the spatial variation in edaphic characteristics for this semi-arid study site and 433 its implication for the spatio-temporal surface soil moisture dynamics (Chen et al., 2014; Cosh 434 435 et al., 2008). In particular, a large portion of the study area is covered by vertisols, extensively swelling soils with high clay content. This type of soil shows large structural and volumetric 436 changes during wetting, and this directly affects the soil water retention characteristics and near 437 surface soil moisture (Rüdiger et al., 2005). The soils were classified into two classes as heavy 438

clays (clay content >35%) and other soils (Bonan, 2015). The soil clay content was considered
as a modulating factor based on the effect of soil texture on the thermal conductivity, with
thermal conductivity directly proportional to the thermal inertia (Engman, 1991).

The $\theta\mu$ and ΔT values of the top 5 cm soil profile at each monitoring station were calculated from the SASMAS in-situ dataset between 2003 and 2014. The ΔT values ($\Delta T = LST_{AM} - LST_{PM}$) were computed by using the LST difference between early morning and afternoon based on the approximate MODIS Aqua day and night overpass times over the study area, i.e. 01:30 (*LST*_{AM}) and 13:30 hours (*LST*_{PM}). The NDVI (Tucker, 1979) was used in the regression tree model, to account for the impact of vegetation density in modulating soil temperature and soil moisture. The *NDVI* is defined as:

449
$$NDVI = (NIR - RED)/(NIR + RED)$$
 (4)

where NIR and RED are the reflectance values from infrared and red bands respectively. NDVI 450 451 values vary from -1 to +1, with negative values representing water, near zero values no vegetation cover (e.g., bare lands and urban areas), and values closer to +1 dense vegetation. 452 Three NDVI classes were defined for the classification of the ΔT - $\theta\mu$ regression model based 453 on the vegetation density, i.e., NDVI<0.4 (grasslands or no vegetation), 0.4<NDVI<0.6 454 (abundant and vigorous vegetation), and NDVI>0.6 (dense and vigorous vegetation) (de 455 456 Alcântara Silva et al., 2016). The NDVI values at each station over the period of 2003 to 2014 were estimated by using MODIS 16-day NDVI composites (MYD13A2) (1 km resolution). 457

Lastly, the four Austral seasons, spring (from September to November), summer (from December to February), autumn (from March to May), and winter (from June to August), were used to classify the regression tree in view of the seasonal impact to the ΔT - $\theta\mu$ relationship. In summary, the entire ΔT - $\theta\mu$ regression model was classified into 24 classes, i.e. three NDVI 462 classes, two soil classes and four seasonal classes. Fig. 7a shows the regression tree developed463 for the Austral spring. The regression tree for the other seasons were similarly developed.

Fig. 7

The MODIS Aqua LST (MYD11A1) values over the Krui and Merriwa stations showed a 464 strong linear relationship with the SASMAS observations in 2015 with a R² value of 0.74 at 465 day time and 0.76 at night time. The day and night time MODIS Aqua LST (MYD11A1) values 466 467 over SASMAS in-situ stations were compared against the top 5 cm SASMAS in-situ soil temperature values at approximate MODIS overpass times (13:30 hrs at day time and 01:30 468 hrs at night time). Consequently, MODIS day time and night time LST values were bias 469 corrected using a linear calibration with the SASMAS observations and subsequently used to 470 calculate ΔT values at 1 km spatial resolution. The MODIS derived ΔT values were input into 471 the regression tree to calculate respective $\theta\mu$ estimates at 1 km spatial resolution. The NDVI 472 and soil clay content values at each 1 km ΔT pixel were extracted from the MODIS 16-day 473 NDVI composites and the Soil and Landscape Grid National Soil Attributes Maps respectively. 474

The coarse resolution soil moisture products (θ_{SAT}) were thereafter downscaled to 1 km pixel $p(\theta_{ds, p})$ as:

477
$$\theta_{ds,p} = \theta_{est,p} + \left[\theta_{SAT} - \frac{1}{n} \sum_{1}^{n} \theta_{est,p}\right], \tag{5}$$

where $\theta_{est, p}$ is soil moisture content estimated by the regression tree at the 1 km pixel p, θ_{SAT} the satellite soil moisture product where p is laid within its foot print, and n is the total number of 1 km pixels (p=1..n) within the coarse resolution satellite pixel.

481

482 *3.3. Evaluation of the downscaled products*

483 Evaluation of the downscaled soil moisture products and algorithms consisted of two parts:484 (1) assessing the accuracy of the downscaled products against the SASMAS in-situ

observations during 2015; and (2) evaluating the consistency in spatial patterns between high
resolution L-band airborne soil moisture retrievals and the downscaled soil moisture estimates
derived from the upscaled airborne soil moisture retrievals.

- 488
- 489

3.3.1 Validating the downscaled products with SASMAS in-situ observations

The downscaled soil moisture products were compared with the SASMAS in-situ 490 observations of the top 5 cm soil profile from K3, M6 and S3 stations in 2015. Due to the 491 492 limited data availability, only a single station per downscaled pixel was compared; hence, subgrid-scale spatial variability of soil moisture within a downscaled pixel could not be 493 assessed. However, in-situ soil moisture observations, albeit the limited availability, were 494 495 assumed to be a reasonable representation of downscaled soil moisture products with the following reasons. First, SASMAS soil moisture monitoring sites are able to represent their 496 surrounding landscape since they were established at carefully chosen 'time stable' locations 497 (see Section 2.2.1). It is noteworthy to mention that the intensive field sampling conducted at 498 the NAFE'05 and the careful positioning of stations supported the potential of using SASMAS 499 500 data for upscaling to a large spatial extent to validate coarse resolution satellite soil moisture products without significant errors (Crow et al., 2012; Panciera et al., 2008; Rüdiger et al., 501 2003; Rüdiger et al., 2007). Second, subgrid spatial variability within the downscaled pixel 502 503 deemed to be rather small. There existed very little difference in environmental factors (e.g., land cover, vegetation, soil type, topography, meteorological factors) that could contribute to 504 large uncertainties in soil moisture within the spatial extent of downscaled pixel. Indeed, a 505 506 multiscale analysis by Martinez et al. (2007) demonstrated very little soil moisture variability at a fine $(< 1 \text{ km}^2)$ spatial scale based on intensive field campaigns conducted in this area during 507 NAFE'05. Lastly, Chen et al. (2014) showed the temporal stability of the SASMAS network 508

sites using the HYDRUS-1D soil water model. The sensitivity analyses revealed soil type and 509 leaf area index as the key parameters affecting soil moisture variability through time. The 510 calibrated model to a single site was able to simulate soil water storage for closely located 511 monitoring sites as well as for distant sites (up to 30 km) if spatially variable rainfall was 512 allowed. Chen et al. (2014) demonstrated the potential usefulness of continuous time, point-513 scale SASMAS in-situ observations and simulations for predicting the soil wetness status over 514 a catchment of significant size (up to 1000 km²) across scales. Note that relative metrics (see 515 Section 3.3.3) were used in this validation process, due to the low density of in-situ soil 516 517 moisture monitoring stations.

518

519 3.3.2 Validating the downscaling algorithms using NAFE'05 airborne observations

One major problem in validating downscaled soil moisture products with sparse in-situ 520 networks is the large spacing between the monitoring stations. When in-situ observations are 521 used as reference observation to assess downscaled products, several problems could arise from 522 resolution cell representation, station-to-station biases, and consistency of data records 523 524 (Colliander et al., 2017b). Use of high spatial resolution airborne soil moisture observations as reference observations has been considered as a robust, alternative approach to validate spatial 525 downscaling methods (Colliander et al., 2017b; Merlin et al., 2008; Piles et al., 2009; Wu et 526 al., 2017). Due to unavailable resources, the field experiment to collect a set of high resolution 527 airborne soil moisture observations could not be conducted during the study period. Instead, 528 our downscaling algorithms were further tested with the NAFE'05 airborne soil moisture 529 530 dataset over the 40 km × 40 km study area covering Krui and Merriwa River catchments as follows. This is the only high resolution airborne soil moisture dataset available in our study 531 area. The ~1 km resolution airborne soil moisture data were first upscaled by taking the spatial 532

mean over the study area to simulate a coarse resolution satellite soil moisture pixel. The 533 aggregated soil moisture data were then downscaled to 1 km using the developed regression 534 tree models (Eq. 5) with MODIS-derived NDVI and LST datasets. If the LST datasets had 535 significant spatial data gaps due to the clouds on the NAFE'05 campaign days, the LST data 536 prior to or just after the campaign days were used assuming no significant variation in the daily 537 soil moisture between adjacent dates. Then, the spatial patterns of the downscaled soil moisture 538 were compared against the NAFE'05 1 km resolution airborne soil moisture data and the 539 absolute difference between the two datasets was calculated for each day. The region covered 540 541 by the dense vegetation along the southern border of the NAFE'05 study area was masked and excluded from this analysis (Fig. 8a). The data from 31st October 2005 was not considered in 542 this comparison due to the large data gaps caused by the cloud cover. 543

544

545 3.3.3 Performance Metrics

The RMSE, ubRMSE, coefficient of determination (R²), Pearson's correlation coefficient
(R) and coefficient of variation (CV) were used as metrics in data comparisons. These metrics
are computed as (Entekhabi et al., 2010b; Colliander et al., 2018):

549
$$\operatorname{RMSE} = \sqrt{\frac{\sum_{i=1}^{n} \left(\theta_{ds,i} - \theta_{obs,i}\right)^{2}}{n}}, \qquad (6)$$

550 ubRMSE =
$$\sqrt{\frac{\sum_{i=1}^{n} \left(\left(\theta_{ds,i} - \overline{\theta_{ds}} \right) - \left(\theta_{obs,i} - \overline{\theta_{obs}} \right) \right)^{2}}{n-1}}$$
, (7)

where $\theta_{obs,i}$ is the *i*th value of soil moisture observations (in-situ or airborne) used in these comparisons as the true values, $\theta_{ds,i}$ the *i*th value of the downscaled 1 km soil moisture products Fig. 8

and *n* is the number of observations. $\overline{\theta_{obs}}$ and $\overline{\theta_{ds}}$ are the means of observed and downscaled soil moisture, respectively.

555 The R^2 value, R and CV are estimated as:

556
$$R^{2} = 1 - \frac{\Sigma(\theta_{i} - \theta_{reg,i})^{2}}{\Sigma(\theta_{i} - \overline{\theta})^{2}},$$
(8)

557
$$\mathbf{R} = \frac{1}{(n-1)} \sum_{i=1}^{n} \left(\frac{\theta_{ds,i} - \overline{\theta_{ds}}}{s_{ds}} \right) \left(\frac{\theta_{obs,i} - \overline{\theta_{obs}}}{s_{obs}} \right), \tag{9}$$

558
$$CV = \frac{s}{\overline{\theta}},$$
 (10)

where $\theta_{reg,i}$ is the predicted soil moisture from a regression fit between θ_{ds} and θ_{obs} . s_{ds} and sobs are the standard deviations of downscaled and observed soil moisture values,

respectively. The standard deviation (s) is estimated by:

562
$$\mathbf{S} = \sqrt{\frac{\sum_{i=1}^{n} \left(\theta_i - \overline{\theta}\right)^2}{n - 1}} \,. \tag{11}$$

Here, θ_i is the soil moisture estimate at the *i*th observation (*i*= 1:*n*) and $\overline{\theta}$ is the spatial or temporal mean of the soil moisture estimates.

565

566 **4. Results**

567 *4.1. Comparison of coarse resolution satellite soil moisture products*

The comparisons between the in-situ observations and satellite soil moisture products are shown in Fig. 9. Fig. 9a shows the agreement between SMAP-E products and the SASMAS in-situ data at SMAP-E pixel X (Fig. 5b), along with the daily precipitation measured at the K3 station. The response of SMAP soil moisture to the precipitation is evident in Fig. 9. The

Fig. 9

SMAP-E soil moisture product showed a good agreement with the in-situ data at pixel X 572 showing an ubRMSE value of 0.051 and R² values of 0.73 (Fig. 9a). However, a slight 573 underestimation was observed from the SMAP products when compared with the in-situ data, 574 particularly during the drying stage. Chen et al. (2017) also explain an underestimation bias in 575 SMAP data, especially in drying conditions, possibly caused by the mismatch between the 576 measuring depths of in-situ sensors and L-band penetration depths. The SMOS soil moisture 577 578 products showed a notable underestimation when compared against SASMAS in-situ observations (Fig. 9b) at pixel R (Fig. 5c). The temporal pattern of soil moisture (i.e. 579 580 climatology) was reasonably captured by the SMOS products (Fig. 9b). An ubRMSE of 0.056 cm³/cm³ with R² value of 0.64 was found between SMOS 25 km gridded product and in-situ 581 data at this pixel. The limited in-situ observations along with the errors in spatial averaging 582 and instrument errors in in-situ data were also potential error sources in these comparisons 583 between satellite soil moisture products and in-situ observations. The underestimation is less 584 evident in SMAP compared to SMOS soil moisture products. A number of studies have 585 observed the same behaviour of a general under-estimation with SMOS (Al Bitar et al., 2012; 586 Dall'Amico et al., 2012; Gherboudj et al., 2012; Cui et al., 2018; Dente et al., 2012, Pacheco 587 et al., 2015, Niclòs et al. 2016). Some of the possible reasons for the SMOS underestimation 588 can be identified as; the L-band penetration depth being less than 5 cm for wet soils (Ulaby et 589 al., 1986), inability to represent spatial heterogeneity at the coarser resolution, in-situ 590 591 measurements overestimating the soil moisture, systematic bias created by the retrieval algorithm and the erroneous ancillary data such as soil texture and land use (Al Bitar et al., 592 2012). The improved instrument design and algorithm of SMAP (Karthikeyan et al., 2017b) 593 can also contribute to the better accuracy of SMAP. 594

The comparison between SMOS and SMAP-E soil moisture products over the SMOS
pixels P, Q, R and S shows a reasonably good agreement with RMSEs of 0.089, 0.075, 0.072

and 0.072 cm³/cm³ (R^2 = 0.58, 0.57, 0.69 and 0.68, p-values < 0.001 for all cases) over the SMOS 25 km pixels P, Q, R and S, respectively (Fig. 10).

599

600 *4.2. Development of the downscaling model*

The regression fits developed for the class with clay < 35% and 0.4<NDVI<0.6 for Austral summer and winter are shown in Fig. 7 (i) and (ii). Around 20,000 (ΔT , $\theta\mu$) data pairs obtained from ten SASMAS stations from 2003 to 2014 were used to develop the regression tree model, based on the availability of reliable near surface (0-5 cm) datasets. The large sample size collected over different climate conditions was sufficient to capture the variability as required by the regression tree classification.

607

608 *4.3. Validating the downscaled products with in-situ data*

Fig. 11a shows the comparison of the downscaled soil moisture products of SMAP-E 609 km, and SMOS, with the in-situ observations at K3, M6, and S3 stations. The top 5 cm soil 610 611 moisture data were unavailable at the other SASMAS stations in 2015. Therefore, the only option was to compare the downscaled data with the available in-situ measurements, although 612 these three monitoring stations are laid within seperate 1 km pixels. The downscaled soil 613 moisture estimates of the satellite products, SMAP-E and SMOS, have captured the temporal 614 variability of soil moisture with a good accuracy at all stations (Fig. 11a). At the M6 monitoring 615 station, the downscaled products showed a general underestimation compared to the in-situ 616 record. Lack of spatial representativeness of M6 station and instrument errors can be possible 617 causes for this mismatch. Fig. 11b shows the agreement between the in-situ data and 618 downscaled soil moisture estimates of SMAP-E and SMOS products. These downscaled 619

Fig. 11

620 SMAP-E and SMOS soil moisture products showed average ubRMSE values of 0.068 and 621 $0.051 \text{ cm}^3/\text{cm}^3$ (with average R² values of 0.40 and 0.61), respectively.

Table 4 shows a summary of the agreement between the SASMAS in-situ observations 622 and the downscaled soil moisture product at stations K3, M6, and S3. Downscaled SMOS 623 products show better ubRMSE values and high R² against in-situ data, compared to the 624 downscaled SMAP-E products. Fig. 12 illustrates the spatial variability of soil moisture over 625 the Krui and Merriwa River catchments, as captured by the SMAP-E and SMOS soil moisture 626 products and their downscaled counterparts on 28th June 2015. This epoch was selected due to 627 little cloud cover of the MODIS LST scene. When compared to the coarse resolution soil 628 moisture products, it is evident that the downscale products have captured the sub-catchment 629 level spatial variability of soil moisture at a much finer scale. It can be seen that the wet pixels 630 in the middle of the Krui River catchment and the northern half of the Merriwa River catchment 631 (Fig. 12) are closely related to the clay content of the soils (Fig. 2a). The increasing soil 632 633 moisture gradient towards north, driven by the precipitation patterns and soil texture, is visible in the downscaled products. The subpixel scale spatial patterns of SMOS and SMAP soil 634 moisture are similar, since these patterns are based on the soil moisture estimates derived from 635 MODIS LSTs. 636

637

4.4. Validating the downscaling algorithms with the NAFE'05 airborne observations

Fig. 13a shows the distribution of the NAFE'05 soil moisture data of the regional airborne campaign on 7th November, 14th November and 21st November 2005, with corresponding downscaled soil moisture estimates. Soil moisture variability of 31st October 2005 was excluded in this figure due large data gaps caused by clouds. The NAFE'05 regional soil moisture datasets of the four subsequent campaign days showed spatial means of 0.44, 0.36, 0.16 and 0.14 cm³/cm³ with CVs of 0.32, 0.37, 0.63 and 0.60 respectively over the 40 × 40 km Table 4

Fig. 12

Fig. 13

study area. This clearly showed a drying trend from 7th November to 21st November 2005. The SMAP-E soil moisture products show a mean value of 0.20 cm³/cm³ (standard deviation of 0.07 cm³/cm³) over the NAFE'05 study area during 2015 and 2016. The spatial average of the NAFE soil moisture data in the 40 km × 40 km study area over the 4 days showed a mean value of 0.27 cm³/cm³ (standard deviation = 0.15 cm³/cm³). This shows that the NAFE'05 data shows slightly high soil moisture content compared to the soil moisture content as measured by the SMAP over the two years, yet displaying the typical soil moisture conditions of the area.

The downscaled data showed mean soil moisture values close to the NAFE'05 652 observations, but with less variability (Fig. 14). The response from the saturated clay soils and 653 the surface runoff, caused by the early morning precipitation events is a probable reason for 654 the high variability in NAFE'05 datasets. The SASMAS in-situ data shows precipitation of ~20 655 mm at S2 on 30th and 31st October 2005. This included light precipitation events (~12 mm) in 656 the early morning of 31st October, i.e., a couple of hours before the flight time. This resulted 657 in wet conditions on 31st October 2005 observed from the NAFE'05 dataset. In addition, the 658 precipitation events on 31st October 2005 (Table 5) caused large data gaps in the MODIS LST 659 due to the dense cloud cover on this day. A 12 mm precipitation event was also recorded at S2 660 on 5th November 2005 which explains the higher mean soil moisture values observed from the 661 NAFE'05 dataset compared to the average of the SMAP soil moisture products over this area 662 during 2015/16. Furthermore, Table 5 shows a general gradient of precipitation towards north 663 across the NAFE'05 study area. This can be a possible reason for the higher soil moisture 664 values in the northern part of the NAFE'05 area compared to the southern part. The response 665 from surface runoff and soil saturation can also be identified as possible reasons for the extreme 666 wet pixels in the NAFE'05 dataset. 667

Fig 13 shows a good agreement in the spatial patterns between NAFE'05 data anddownscaled soil moisture products. The lower soil moisture values resulting from the high sand

Fig. 14

Table 5

content in the southern part of the 40 km \times 40 km NAFE'05 area (i.e. the southern parts of the 670 Krui and Merriwa River catchments) and the high soil moisture values resulting from the high 671 clay content in the mid-regions of the two sub-catchments (Fig. 8b) were evident in both 672 downscaled and NAFE'05 maps, especially during the dry conditions on 21st November 2005 673 (Fig. 13a). This highlights soil texture as a dominant factor regulating spatial patterns of soil 674 moisture in the study area. This is compatible with the findings of Martinez et al. (2007) at the 675 676 Stanley catchment, explaining that the wettest areas of the catchment are dominated by the clay soils. 677

The error maps shown in Fig. 13b illustrate the absolute error between observed and 678 downscaled datasets of the NAFE'05. The two datasets have a reasonable agreement showing 679 an error $< 0.1 \text{ cm}^3/\text{cm}^3$ for more than 80% of the area on 7th and 14th November 2005. Over 680 95% of the area shows an error less than 0.1 cm³/cm³ on 21st November 2005 under the dry 681 conditions. Higher error values (> $0.1 \text{ cm}^3/\text{cm}^3$) can be seen in the wetter pixels, possibly 682 caused by higher precipitation in the northern part of the study area. A better agreement can be 683 seen between the two datasets with increasing catchment dryness (Fig. 13 and 14). Overall, the 684 comparison between NAFE'05 and downscaled soil moisture datasets show an average RMSE 685 of 0.07 cm^3/cm^3 (with R value of 0.4). 686

687

688 5. Discussion and conclusion

This paper explored the feasiblity of generating a time record of soil moisture at high spatial resolution (1 km) using SMAP-E 9 km and SMOS 25 km gridded satellite soil moisture products over two semi-arid river catchments in the Upper Hunter Region of New South Wales, Australia. The soil moisture and soil temperature dataset for the top 5 cm soil layer, obtained from the in-situ soil moisture network (SASMAS) over the Goulburn River catchment, was used to develop a thermal inertia based regression tree model between ΔT and $\theta\mu$. The regression tree model was classified based on the modulating factors; season, vegetation density and soil texture. The MODIS LST products were then used to estimate soil moisture at 1 km resolution from the coarse satellite products using the rule-based regression tree model. The accuracy of the downscaled soil moisture products was evaluated by using the SASMAS in-situ and the NAFE'05 airborne datasets.

Both SMAP-E and SMOS soil moisture products showed a temporal change consistent 700 with the precipitation. SMAP-E soil moisture showed an agreement with the in-situ data of 701 $0.051 \text{ cm}^3/\text{cm}^3$ ubRMSE (R² = 0.73), which is slightly higher than the accepted SMAP accuracy 702 of 0.04 cm³/cm³. The SMOS 25 km gridded product showed ubRMSE of 0.056 cm³/cm³ ($R^2 =$ 703 0.64) against in-situ data. The unavailability of evenly and densely distributed in-situ stations 704 over the SMAP-E footprint are a major limitation of this comparison. Beside the measurement 705 errors from the in-situ sensors (~0.03 cm³/cm³), soil cracking over the clay soils was a serious 706 issue for the near surface (0-5 cm) soil moisture monitoring. In the dry periods, the cracks 707 caused sensors to be not in contact with the soils, whereas after precipitation, the soils get 708 flooded and swelled. This creates a challenge for maintaining near surface sensors and assuring 709 710 the data quality for in-situ observations. The limited availability of in-situ observations and the error in spatial averaging of in-situ data over the satellite footprints are the main sources of 711 errors in this comparison. Because of the limited availability of the top 5 cm soil moisture 712 observations, Senanayake et al. (2017) tested the proposed downscaling approach with the in-713 situ data of 0-30 cm soil layer. Soil moisture and temperature data from five Krui River 714 catchment monitoring stations in 2015 (~1700 data pairs) were employed in this work, based 715 on the premise that the daily mean of the near surface soil moisture (0-5 cm) was closely related 716 to the daily mean soil moisture of the 0-30 cm soil layer in the study area (Martinez et al., 717

2007). This study showed an RMSE of 0.14 cm³/cm³ when the downscaled data were compared
against the in-situ observations.

720 The downscaled soil moisture products of the SMAP-E and SMOS showed ubRMSEs of 0.068 and 0.051 cm³/cm³, respectively, with the SASMAS in-situ observations. The accuracy 721 of the coarse resolution satellite soil moisture products directly affects the accuracy of their 722 723 downscaled counterparts. It is noteworthy to mention that, the average of the downscaled soil moisture products within a coarse resolution satellite footprint was the same as the original 724 value of the coarse resolution satellite soil moisture product (see Eq.5). The errors in MODIS 725 LSTs (Wan, 2008) and the uncertainties in clay content values (Rossel et al., 2015) can also be 726 identified as possible sources of errors. 727

728 Lack of in-situ network sites within 1 km pixel was a major limitation in validating the downscaled soil moisture products. Therefore, presenting metrics for absolute soil moisture 729 (i.e. RMSE and bias) is invalid. Accordingly, relative metrics were used in presenting the 730 731 results of this validation (i.e. ubRMSE and correlation). In addition, NAFE'05 data was also used in this study as a solution to lack of ground measurements for validation. The downscaled 732 soil moisture showed a good agreement with the spatial patterns shown by NAFE'05 airborne 733 campaign. Both NAFE'05 and downscaled data shows the spatial patterns driven by soil 734 texture. The clay-rich mid-catchment areas of the Krui and Merriwa River (Fig. 8b) can be 735 736 distinguished from the north and south-most regions in the soil moisture maps (Fg.13a). This agrees with the findings of the previous studies (Cosh et al., 2008; Cantón et al., 2004; Gómez-737 Plaza et al, 2000) that have shown soil properties and vegetation as the main factors affecting 738 soil moisture variability in semi-arid regions. The results show that the algorithms work well 739 over both spatially and temporally dry conditions compared to wet conditions. Another major 740 limitation of this downscaling method is the data gaps in MODIS LST occurred due to the 741 cloud cover. One possible approach to address this problem is by using the LST products from 742

geostationary satellites (Oyoshi et al., 2014; Yamamoto and Ishikawa, 2018). Although their 743 spatial resolution is slightly coarser than MODIS LST products, the high temporal resolution 744 of the geostationary LST data allows the retrieval of close representations of T_{AM} and T_{PM}. The 745 4 km spatial and one-hour temporal resolution of Multi-functional Transport Satellite 746 (MTSAT)-1R (Himawari-6) LSTs can be shown as an example dataset of LST. However, use 747 of geostationary satellites do not completely ensure to avoid data gaps along a day due to the 748 749 presence of clouds. Piles et al. (2016) have proposed a technique to improve the spatiotemporal resolution of soil moisture from the synergy of SMOS and Meteosat Second 750 751 Generation (MSG) Spinning Enhanced Visible and Infrared Imager (SEVIRI) observations. SEVIRI is a geostationary orbit optical imaging radiometer on-board the MSG satellite. Soil 752 moisture retrievals from SMOS with LST and Fractional Vegetation Cover (FVC) products 753 from the SEVIRI have been employed in this approach. In addition, Djamai et al. (2016) 754 proposed a method to estimate soil moisture at high resolution on cloudy days, by combining 755 the Canadian Land Surface Scheme (CLASS) with DisPATCh model. This involves 756 interpolating the input data of CLASS at high resolution by kriging and subsequent near surface 757 soil moisture simulation and calibrating the CLASS using the downscaled soil moisture from 758 DisPATCh model. Another potential way of filling these data gaps caused by the cloud cover 759 is using the persistent spatial patterns of soil moisture. A number of researchers have studied 760 the temporal persistence of soil moisture patterns (Vanderlinden et al., 2012; Brocca et al., 761 2009; Gómez-Plaza et al., 2000; Cosh et al., 2008). However, the spatial pattern of catchment 762 soil moisture can be changed based on the factors such as precipitation pattern, seasonal 763 vegetation dynamics and mean catchment wetness (Famiglietti et al., 2008; Chen et al., 2014). 764 Therefore, comprehensive studies on time stability of soil moisture is required prior to such 765 766 approach.

The methodology introduced in this study shows a good potential in producing a time series record of high-resolution soil moisture over arid and semi-arid regions. Future studies should be directed on further refining the regression algorithms by combining model-derived datasets and other forcing factors.

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Highlights

The SMAP and SMOS soil moisture products were compared against in-situ observations.

Satellite soil moisture products were downscaled using thermal inertia theory.

A regression tree was developed for downscaling, based on in-situ soil moisture data.

Downscaled SMAP and SMOS products showed ubRMSEs of 0.07 and 0.05 cm^3/cm^3 .

Downscaled airborne soil moisture retrievals showed an accuracy of $0.07 \text{ cm}^3/\text{cm}^3$.









(b)

















Fig 10

















1	Fig. 1. The location of the Goulburn River catchment, and the distribution of the monitoring
2	stations established under the SASMAS project.
3	
4	Fig. 2. Soil (a) clay, (b) silt, and (c) sand contents of the top 5 cm soil profile in the Goulburn
5	River catchment (Source: National Soil and Landscape Grid, Australia).
6	
7	Fig. 3. (a) Land use/land cover of Krui and Merriwa River catchments. (Source: The
8	Department of Environment and Climate Change, NSW). (b) Seasonal average NDVI maps in
9	2015 of Krui and Merriwa River catchments calculated by using MODIS 16-day NDVI
10	composites.
11	
12	Fig. 4. The temporal variability of vegetation in Krui River catchment SASMAS monitoring
13	stations as captured by the MODIS 16-day NDVI composites (MYD13A2).
14	
15	Fig. 5. The location of (a) NAFE'05 study area, (b) SMAP-Enhanced 9 km, and (c) SMOS 25
16	km grids over the Goulburn River catchment. The pixels used for validation are marked with
17	letters (X for SMAP-E and P-S for SMOS).
18	
19	Fig. 6. Flow chart of the approach used to validate and downscale the satellite soil moisture
20	products and to assess the reliability of the downscaled soil moisture products.
21	
22	

Fig. 7. (a) The regression tree developed for the Austral spring. The ΔT and $\theta\mu$ values were classified based on the season, soil clay content and the NDVI value as shown in the regression tree. (b) Regression Models developed for the class of clay< 35% and 0.4< NDVI<0.6 for (i) Austral summer, and (ii) Austral winter seasons.

27

Fig. 8. (a) Land use/land cover, and (b) soil clay content over the NAFE'05 study area. The dense vegetation belt across the southmost region of the NAFE'05 study area can also be identified as a divide of soil texture.

31

Fig. 9. Comparison of the temporal patterns and agreement between SASMAS in-situ
observations at top 5 cm soil profile and (a) SMAP-E, and (b) SMOS soil moisture products.
The daily precipitation shown in the figure is based on the in-situ observations at SASMAS K3
monitoring station.

36

Fig. 10. Comparison and correlation between SMOS and SMAP-E soil moisture products over
Krui and Merriwa River catchments in 2015/16.

39

Fig. 11. (a) Temporal variability of soil moisture as captured by the downscaled SMAP-E 9
km, and SMOS 25 km gridded products with respect to SASMAS in-situ data at stations K-3,
M-6, and S-3. (b) The agreement between the downscaled SMAP-E, and SMOS soil moisture
products with SASMAS in-situ data.

45	Fig. 12. The spatial variability of soil moisture as captured by the coarse resolution satellite
46	soil moisture products and their downscaled counterparts of (a) SMAP-E 9 km, and (c) SMOS
47	25 km gridded products on 28th June 2015 over the Krui and Merriwa River catchments.

48

49	Fig. 13. (a) Comparison of the downscaled soil moisture products with NAFE'05 airborne
50	dataset. The downscaled products of the closest date to the NAFE'05 regional airborne data
51	collection were used in this comparison based on the cloud effect on MODIS LSTs. (b) The
52	absolute difference between the soil moisture of NAFE'05 airborne dataset and downscaled
53	products on 7th November, 14th November and 21st November 2005 over the NAFE'05 study
54	area. Data from 31st October 2005 was excluded in this figure due to high cloud cover.

55

Fig. 14. The distribution of NAFE'05 and downscaled soil moisture with the absolute error
between the two datasets over the 40 km × 40 km study area on 7th November, 14th November
and 21st November 2005.

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Dataset	Data type	Data source	Spatial resolution/ grid size	Temporal resolution	Accuracy	Period used in the study
SMAP 9 km enhanced radiometric soil moisture products (L3SMP-E)	Satellite	National Snow and Ice Data Center (NSIDC)	9 km	Daily global composites	0.04 v/v	2015/16
SMOS 25 km soil moisture products (CATDS L3 SM 3-DAY)(Product code: MIR_CLF33A and MIR_CLF33D)	Satellite	Centre Aval de Traitement des Données SMOS (CATDS)	25 km	Daily global composites	0.04 v/v	2015/16
MODIS Aqua LSTs (MYD11A1)	Satellite	Land Processes Distributed Active Archive Center (LP DAAC)	1 km	daily	±1 K (Wan, 2008)	2005, 2015
MODIS Aqua 16- day NDVI composites (MYD13A2)	Satellite	Land Processes Distributed Active Archive Center (LP DAAC)	1 km	16-day	±0.020	2003- 2015
The National Airborne Field Experiment 2005 (NAFE'05) soil moisture data	Airborne	http://www.n afe.monash.e du/	1 km	Four consecutive Mondays	0.04-0.05 v/v (Gao et al., 2018)	31 st Oct, 7 th Nov, 14 th Nov and 21 st Nov 2015
SASMAS in-situ data (0-5 cm soil profile) i. soil moisture ii. soil temperature	In-situ	http://www.e ng.newcastle. edu.au/sasma s/SASMAS/s asmas.htm	Point scale	20-min	$\pm 0.01 -$ $\pm 0.03 \text{ v/v}$ for fine textured soils $\pm 0.3^{\circ}\text{C}$	2015. 2003- 2015
National Soil and Landscape Grid (Soil Grid) i. clay content	Modelled	Commonwea lth Scientific and Industrial Research Organisation (CSIRO)	90 m	-	-	-

Summary of the datasets used in this study.

Station	Land cover	Soil type	Clay%	Silt%	Sand%
K1	Crop/fallow	Loam	23	32	45
К2	Native pasture	Loamy sand	12	14	75
КЗ	Crop/fallow	Clay	71	16	13
К4	Native pasture	Clay	55	30	15
К5	Native pasture	Clay	64	20	16
К6	Improved Pasture	Clay loam	38	40	22
M1	Native pasture	Sandy loam	7	11	83
M2	Native pasture	Sand	0	0	100
M3	Native pasture	Clay loam	40	34	26
M4	Native pasture	Loam	29	41	30
M5	Native pasture	Clay	73	20	7
M6	Native pasture	Clay	72	20	8
M7	Improved Pasture	Clay loam	41	32	26
S1	Improved Pasture	Clay	55	35	10
S2	Native pasture	Clay loam	43	27	30
S3	Native pasture	Clay			
S4	Native pasture	Clay			
S5	Native pasture	Clay	47	34	19
S6	Native pasture	Clay	53	28	19
S7	Native pasture	Silt loam	19	41	40

The land cover and soil texture of the SASMAS monitoring stations in Krui and Merriwa River catchments (modified from Kunkel et al., 2016).

Dataset	Pixel	Longitude	Latitude
SMAP-E 9 km grid	Х	150°15′ 52″ E	31° 59′ 50″ S
SMOS 25 km grid	Р	150° 2′ 36″ E	31° 53′ 27″ S
SMOS 25 km grid	Q	150°18′09″ E	31° 53′ 27″ S
SMOS 25 km grid	R	150° 02′ 36″ E	32° 07′ 17″ S
SMOS 25 km grid	S	150°18′ 09″ E	32° 07′ 17″ S

Locations of the centroid of pixels used in the data validation process.

Downscaled	SASMAS monitoring station					
product	K-3	5	M-	6	S-3	3
	ubRMSE	R ²	ubRMSE	\mathbb{R}^2	ubRMSE	R ²
	(cm^3/cm^3)		(cm ³ /cm ³		(cm ³ /cm ³	
D/s SMAP-E	0.066	0.44	0.074	0.36	0.063	0.40
D/s SMOS	0.044	0.72	0.054	0.59	0.055	0.53

Agreement between SASMAS in-situ data and downscaled satellite soil moisture data at monitoring stations K3, M6 and S3.

Week			Precipi	tation (mi	n)	
	Kru	i River	Merriwa River			
	catchment			catchment		
	S2	K4	M1	M3	M4	M5
25 Oct - 31 Oct	17.0	18.2	22.0	11.8	19.0	16.6
1 Nov - 7 Nov	14.4	18.2	12.4	23.2	23.2	35.4
8 Nov - 14 Nov	11.0	8.4	1.4	5.0	11.2	8.8
15 Nov - 21 Nov	0	0	0.2	0	0	0

Weekly precipitation data recorded at the SASMAS monitoring stations during the period of NAFE'05 regional airborne campaign.