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Olivier Merlin, Christoph Rüdiger, Al Bitar Ahmad, Philippe Richaume,

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# Disaggregation of SMOS Soil Moisture in Southeastern Australia 123 DISaggiegation of Sivios Son Iviolistule<br>23 Olivier Merlin, Christoph Rüdiger, Ahmad Al Bitar, Philippe Richaume, Jeffrey P. Walker, and Yann H. Kerr

 *Abstract***—Disaggregation based on Physical And Theoretical scale Change (DisPATCh) is an algorithm dedicated to the dis- aggregation of soil moisture observations using high-resolution soil temperature data. DisPATCh converts soil temperature fields into soil moisture fields given a semi-empirical soil evaporative efficiency model and a first-order Taylor series expansion around the field-mean soil moisture. In this study, the disaggregation approach is applied to soil moisture and ocean salinity (SMOS) data over the 500 km by 100 km AACES (Australian Airborne Calibration/validation Experiments for SMOS) area. The 40-km resolution SMOS surface soil moisture pixels are disaggregated at 1-km resolution using the soil skin temperature derived from moderate resolution imaging spectroradiometer (MODIS) data, and subsequently compared with the AACES intensive ground measurements aggregated at 1-km resolution. The objective is to test DisPATCh under various surface and atmospheric conditions. It is found that the accuracy of disaggregation products varies greatly according to season: while the correlation coefficient be- tween disaggregated and** *in situ* **soil moisture is about 0.7 during the summer AACES, it is approximately zero during the winter AACES, consistent with a weaker coupling between evaporation and surface soil moisture in temperate than in semi-arid climate. Moreover, during the summer AACES, the correlation coefficient between disaggregated and** *in situ* **soil moisture is increased from 0.70 to 0.85, by separating the 1-km pixels where MODIS temper- ature is mainly controlled by soil evaporation, from those where MODIS temperature is controlled by both soil evaporation and vegetation transpiration. It is also found that the 5-km resolution atmospheric correction of the official MODIS temperature data has a significant impact on DisPATCh output. An alternative at- mospheric correction at 40-km resolution increases the correlation coefficient between disaggregated and** *in situ* **soil moisture from 0.72 to 0.82 during the summer AACES. Results indicate that**

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O. Merlin is with the Centre d'Etudes Spatiales de la Biosphère (CESBIO), 31401 Toulouse, France (e-mail: olivier.merlin@cesbio.cnes.fr).

C. Rüdiger (e-mail: chris.rudiger@monash.edu).

A. Al Bitar (e-mail: ahmad.albitar@cesbio.cnes.fr).

P. Richaume (e-mail: philippe.richaume@cesbio.cnes.fr).

J. P. Walker (e-mail: jeff.walker@monash.edu).

Y. H. Kerr (e-mail: yann.kerr@cesbio.cnes.fr).

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**DisPATCh has a strong potential in low-vegetated semi-arid areas** 37 **where it can be used as a tool to evaluate SMOS data (by reducing** 38 **the mismatch in spatial extent between SMOS observations and** 39 **localized** *in situ* **measurements), and as a further step, to derive** 40 **a 1-km resolution soil moisture product adapted for large-scale** 41 **hydrological studies.** 42

*Index Terms***—AACES, calibration/validation, disaggregation,** 43 **Disaggregation based on Physical And Theoretical scale Change** 44 **(DisPATCh), field campaign, moderate resolution imaging spectro-** 45 **radiometer (MODIS), soil moisture and ocean salinity (SMOS).** 46

### I. INTRODUCTION 47

**EVALUATION** Disappergation hasted non-linearized And Theoretical scale Change and occur and Theoretical scale Change (Change And Theoretical scale Change Matter priority (MOIS) and Theoretical scale Change (Change Theore **P** ASSIVE MICROWAVE remote sensing has the capability 48 to provide key elements of the terrestrial hydrological 49 cycle such as surface soil moisture [1], [2] and overland pre- 50 cipitation [3], [4]. Nevertheless, due to the large discrepancy 51 between the observation scale (several tens of km) and the scale 52 of physical interactions with the land surface (one wavelength 53 or several cm), the radiative transfer models applied to passive 54 microwave remote sensing data are only semiphysically based. 55 Consequently, the retrieval process of land surface parameters 56 from microwave brightness temperatures requires ancillary data 57 for calibration and validation purposes [5]. It also requires a 58 strategy to use such ancillary data since ground-based sampling 59 is often made over a small area/point, which constrasts with 60 the large integrated extent of spaceborne passive microwave 61 observations.

The soil moisture and ocean salinity (SMOS), [6]) satellite 63 was launched on November 2, 2009. Over land, the SMOS 64 mission aims at providing  $\sim$ 5 cm surface soil moisture data 65 at a spatial resolution better than 50 km and a repeat cycle of 66 less than 3 days. The payload is a 2-D interferometer equipped 67 with 69 individual L-band antennas regularly spaced along Y- 68 shaped arms. This new concept allows observing all pixels in 69 the 1000 km wide field of view at a range of incidence angles. 70 It also allows reconstructing brightness temperatures on a fixed 71 sampling grid [7]. 22

Since the SMOS launch, various field experiments (the 73 HOBE site in Denmark [8], the Mali site in Western Africa 74 [9], the SMOSMANIA site in Southwestern France [10] just 75 to name a few) have been undertaken to validate SMOS recon- 76 structed brightness temperatures and soil moisture retrievals. 77 The AACES (Australian Airborne Calibration/validation 78 Experiment for SMOS, [11]) is one of the most compre- 79 hensive campaigns worldwide dedicated to SMOS calibra- 80 tion/validation. A series of two experiments were undertaken 81 in 2010, AACES-1 in January-February (Austral summer) and 82

 AACES-2 in September (Austral winter). The data collected in AACES include 1-km resolution airborne L-band brightness temperature mapped over a 500 km by 100 km area, 20 days of very intensive ground measurements and 20 5 km by 2 km ground sampling areas.

 Even though the AACES ground measurements are very extensive, it is not feasible to cover the whole extent of a SMOS pixel by ground sampling alone. This is the reason why most validation strategies of spaceborne passive microwave data using *in situ* measurements have been based on the as- sumption that local observations are representative of a much larger spatial extent (i.e., the size of a microwave pixel). In the heterogeneous case where this assumption does not hold, up- scaling approaches [12], [13] have been developed to relate the available ground observations to satellite scale soil moisture. Such approaches are very useful over sites which have been monitored for a long time and where extensive measurements have been made over a range of spatial scales. However, aggre- gation rules are difficult to build over sites which have been set up recently, or where no extensive field campaigns have been undertaken.

 This study develops a methodology to facilitate the cali- bration and validation of SMOS data using localized ground measurements, such as those collected during AACES. The methodology combines upscaling (aggregation) and downscal- ing (disaggregation) approaches to make remote sensing and *in situ* observations match at an intermediate spatial resolution of 1 km. The key step in the procedure is a disaggregation algorithm of passive microwave soil moisture using kilometric optical data [14]–[16]. Disaggregating SMOS soil moisture can solve the disparity of spatial scales between satellite and *in situ* observations. However, the validation of spaceborne data by means of a disaggregation approach requires the uncertainties and potential error sources in downscaled data to be assessed. Generally speaking, disaggregation is a compromise between downscaling resolution and accuracy. The higher downscaling resolution, the more disaggregated values are spatially repre- sentative of ground observations, but typically have a lower accuracy and vice versa [17]. In this context, a disaggrega- tion algorithm named Disaggregation based on Physical And Theoretical scale Change (DisPATCh) is applied to 40-km resolution SMOS soil moisture over the AACES area using 1- km resolution Moderate resolution Imaging Spectroradiometer (MODIS) data. The objective is to test DisPATCh under various surface and atmospheric conditions. Specifically, the impact of climatic (evaporative demand), meteorologic (presence of clouds), and vegetation (cover and water status) conditions on 1-km resolution disaggregated soil moisture is evaluated both qualitatively by visual assessment of disaggregation images and quantitatively by comparing DisPATCh output with AACES intensive ground measurements.

 The AACES, SMOS, and MODIS data used in this study are first described. Next, the disaggregation methodology is presented followed by a step-by-step description of the Dis- PATCh algorithm. Results of the comparison between disag- gregated SMOS soil moisture and *in situ* measurements are then reported. To test DisPATCh under various surface and atmospheric conditions, the algorithm is run during AACES-1

and AACES-2 in different modes, by including (or not) a 141 correction for vegetation and atmospheric effects. Finally, some 142 perspectives in the use of DisPATCh for validating SMOS data 143 using ground-based sampling are given. 144

### II. DATA COLLECTION AND PREPROCESSING 145

The AACES experiments were planned to provide ground 146 and airborne soil moisture data over an area of approximately 147 500 km by 100 km during the two main seasons in the 148 Murrumbidgee river catchment, in southeastern Australia. The 149 first AACES campaign (AACES-1) was undertaken in summer 150 2010 from January 18 to February 21, and the second campaign 151 (AACES-2) was undertaken in the following Austral winter 152 from September 11 to September 24 [11]. Fig. 1 presents the 153 study area including the 20 5 km by 2 km ground sampling 154 focus areas. The background image is the MODIS 250-m res- 155 olution 16-day normalized difference vegetation index (NDVI) 156 product of February 2, 2010. The climate of the Murrumbidgee 157 catchment area ranges from semi-arid in the west to alpine in 158 the east, with a strong rainfall and potential evapotranspiration 159 gradient in the west-east direction. Land use is extensive graz- 160 ing in the west, cropping in the center, and mostly grazing/forest 161 in the east (refer to [11] for a detailed account of AACES). 162

*A. HDAS* 163

If over sites when they been studied that increases the C attention and the search that increases the MODIS 250-m respective measurements focus areas. The background image is the MODIS 250-m respective measurements focus During both AACES-1 and AACES-2, a spatially enabled 164 platform (Hydraprobe Data Acquisition System, HDAS) was 165 used to collect extensive measurements of near-surface soil 166 moisture. HDAS is a handheld system combining a soil dielec- 167 tric sensor (Hydraprobe) and a pocket PC with GPS receiver, 168 allowing for direct storage of location and measurement within 169 the GIS software. HDAS measurements were calibrated using 170 the approach presented in [18] with a root mean square error 171 of point estimate of about  $0.03 \text{ m}^3/\text{m}^3$ . The sampling coverage 172 was two 5 km by 2 km farms per day during AACES-1 and one 173 5 km by 2 km farm per day during AACES-2. Within each farm, 174 a total of six adjacent 5 km long transects separated by 330 m 175 were walked to cover each area of  $10 \text{ km}^2$ , and three separate 176 HDAS measurements were made along transects every 50 m. 177

In this study, HDAS soil moisture data are aggregated at 178 1-km resolution by averaging all measurements made within 179 each pixel of the MODIS resolution grid. Out of concern for 180 spatial representativeness of *in situ* observations, only the 1-km 181 pixels whose ground sampling covers more than two third of 182 its surface area are kept for comparison with disaggregation 183 results. The 1-km average of HDAS measurements is denoted 184  $\langle SM_{\rm HDAS} \rangle$  and the standard deviation of *in situ* measurements 185 (denoted  $\sigma_{\text{HDAS}}$ ) computed to estimate the subpixel variability 186 at 1-km resolution. 187

*B. SMOS* 188

The version-4 SMOS level-2 soil moisture product is used. 189 This product (released on March 24, 2011) was produced from 190 the reprocessed level 1C data, and the version-4 level-2 soil 191 moisture algorithm. SMOS has a 6 am (ascending) and 6 pm 192



Fig. 1. Overview of the study area. During AACES, ten 100 km by 50 km patches were overflown by an airborne L-band radiometer. Within each patch, two 5 km by 2 km subareas were sampled to collect spatial soil moisture measurements. In this study, DisPATCh is run over a 640 by 240 km area including the whole AACES area, and disaggregation results are evaluated over the ground sampling areas.

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The samp (descending) equator crossing time. The sampling grid of the SMOS level-2 soil moisture product is called DGG or discrete global grid [19], [20] and has a node separation of about 15 km. The DGG provides a discretization that is higher than the SMOS natural pixel size, which is 40 km on average, ranging from 30 km at boresight to 90 km at high incidence angles. In this study, the disaggregation procedure takes advan- tage of the oversampling of SMOS data to potentially reduce (and provide an estimate of) random errors in disaggregated SMOS data. Instead of using a single snapshot SMOS im- age, DisPATCh uses four (overlapping) independent snapshots, which are generated by: 1) sliding a 40-km resolution grid; and 2) extracting the DGG nodes approximately centered on each 40 km pixel. The extraction of SMOS DGG nodes is presented in [21]. The DGG node(s) that fall(s) near the center of the 208 40-km resolution pixels with a  $+/-10$ -km tolerance are se- lected. If more than one DGG is selected, the associated soil moisture values are averaged to produce a single value for each 40-km resolution pixel. The 40-km resolution grid that fits the study area corresponds to what is termed here Resampling 1. Similarly, Resampling 2, 3, and 4 are performed by sliding the 214 40-km resolution grid to coordinates  $(+20 \text{ km}, 0), (0, -20 \text{ km}),$  and ( +20 km, −20 km), respectively. The four 40-km resolu- tion SMOS data sets are then used independently as input to DisPATCh.

### 218 *C. MODIS*

219 The MODIS data used in this paper are composed of:

220 • Version-5 MODIS/Terra land surface temperature and

221 emissivity daily level-3 global 1-km grid product 222 (MOD11A1) and version-5 MODIS/Aqua land surface

temperature and emissivity daily level-3 global 1-km grid 223 product (MYD11A1). The land surface temperature data 224 set is the main component of DisPATCh. It is used to 225 estimate 1-km resolution soil evaporative efficiency at 226 10 am (Terra data) and 1 pm (Aqua data) [22]. 227

- Version-5 MODIS/Terra vegetation indices 16-day level-3 228 global 1-km grid product (MOD13A2). The NDVI data set 229 is used in DisPATCh to estimate the fractional vegetation 230 cover at 1-km resolution [23].
- Version-5 MODIS/Terra+Aqua albedo 16-day level-3 232 global 1-km grid product (MCD43B3). The surface albedo 233 data set is used in DisPATCh to estimate the vegetation 234 temperature at maximum water stress from the space land 235 surface temperature albedo [24]. The MCD43B3 product 236 provides 1-km data describing both directional hemispher- 237 ical reflectance (black-sky albedo) at local solar noon 238 and bihemispherical reflectance (white-sky albedo). In this 239 study, surface albedo refers to the MODIS shortwave white 240 sky albedo. 241
- MODIS/Terra level-1B calibrated radiances swath 1-km 242 grid product (MOD021KM) and MODIS/Aqua level- 243 1B calibrated radiances swath 1-km grid product 244 (MYD021KM). The radiance data set is used to derive 245 a land surface temperature data set that differs from the 246 official MOD11A1 and MYD11A1 products with respect 247 to atmospheric correction. 248

Products MOD11A1, MYD11A1, MOD13A2, and 249 MCD43B3 were downloaded through the NASA Warehouse 250 Inventory Search Tool (WIST http://wist.echo.nasa.gov/) and 251 products MOD021KM and MYD021KM were downloaded 252 through the NASA Level 1 and Atmosphere Archive and Dis- 253 tribution System (LAADS http://ladsweb.nascom.nasa.gov). 254

TABLE I SCALE AND OFFSET VALUES USED TO CONVERT TERRA (AND AQUA ) MODIS RADIANCE DATA TO PHYSICAL RADIANCE VALUES OVER THE AACES AREA

Thermal band	Scale (W m <sup><math>-2</math></sup> sr <sup><math>-1</math></sup> )	Offset $(-)$
	$8.4002 \cdot 10^{-4}$ $(6.5081 \cdot 10^{-4})$   1577 (2036)	
	$7.2970 \cdot 10^{-4}$ (5.7100 $\cdot 10^{-4}$ ) 1658 (2119)	

255 All products were projected in UTM 55 South with a sampling 256 interval of 1000 m using the MODIS reprojection tool.

257 The level-1B calibrated radiance data ( $R_{31}$  and  $R_{32}$  for bands 258 31 and 32, respectively) were converted from digital number 259 (DN) to radiance in W m<sup>-2</sup> sr<sup>-1</sup> using the radiance scales and 260 offsets provided with each MODIS granule as listed in Table I

$$
R_{\lambda} = \text{Scale}_{\lambda} \times (\text{DN}_{\lambda} - \text{Offset}_{\lambda}) \tag{1}
$$

261 The radiance values were then converted to brightness temper-262 ature in K using the inverse of the Planck function [25]

$$
Tb_{\lambda} = \frac{c_2}{\lambda \ln\left(1 + \frac{c_1}{R_{\lambda}\lambda^5}\right)}\tag{2}
$$

263 with  $c_1 = 1.19107 \times 10^8$   $\mu$ m<sup>5</sup> W m<sup>-2</sup> sr<sup>-1</sup> and  $c_2 =$ 264  $1.43883 \times 10^4 \mu$ m K, for center wavelength of the given band 265 (11.0186  $\mu$ m and 12.0325  $\mu$ m for 31 and 32 band, respectively).

### 266 *D. Overlapping HDAS, SMOS, and MODIS Data and* 267 *Generating an Input Data Set*

 As indicated in Table II, HDAS soil moisture, SMOS soil moisture, and cloud-free MODIS land surface temperature data have overlapped on five days during AACES-1 (on January 28 and 30 and February 15, 18, and 20) and on five days during AACES-2 (on September 11, 13, 21, 22, and 24). On each sampling day, two farms were sampled during AACES-1 (except on February 18 when three farms were sampled), and one farm was sampled during AACES-2, so that disaggregation results can be evaluated for ten date-farm units during AACES-1 and five date-farm units during AACES-2.

 DisPATCh is applied to an input ensemble composed of the different combinations of available SMOS (ascending orbit at 6 am and/or descending orbit at 6 pm) and MODIS (onboard Terra platform at 10 am and/or Aqua platform at 1 pm) data. To increase the quantity of input data sets, the MODIS data col- lected on the day before and the day after the SMOS overpass date are also included. For SMOS data on day of year (DoY) 51, the clear sky MODIS data collected on DoY 54 are used. Note that one implicitly assumes that no rainfall occurs between MODIS and SMOS overpasses, and that the spatial variability captured by MODIS is relatively similar to the actual variabil- ity of surface soil moisture at the time of SMOS overpass. Moreover, the SMOS data oversampling is used to generate four (overlapping) 40-km resolution SMOS grids on which DisPATCh is run independently, thus increasing the number of downscaled data that could be used in the validation. It is reminded that the spacing (about 15 km) between neighboring SMOS DGG nodes is smaller than the SMOS resolution (about

40 km). By combining the four SMOS grids, the two potential 296 SMOS data sets (two orbits in one day) and the six potential 297 MODIS data sets (three days including two overpasses each), 298 the maximum number of input data sets is 48. The generation 299 of input data sets is shown in Fig. 2 and the number of daily 300 input data sets is indicated for each date-farm unit in Table II. 301

### III. DISAGGGREGATION ALGORITHM 302

DisPATCh converts 1-km resolution MODIS-derived soil 303 temperature fields into 1-km resolution surface soil moisture 304 fields given a semi-empirical soil evaporative efficiency model 305 [26] and a first-order Taylor series expansion around the 306 40-km resolution SMOS observation. DisPATCh is an im- 307 proved version of the algorithms in [16] and [27], and mainly 308 differs with regard to the representation of the vegetation water 309 status. In previous versions [16], [27], the soil temperature was 310 derived from MODIS land surface temperature by assuming 311 that vegetation was unstressed so that vegetation temperature 312 was uniformly set to the minimum surface temperature ob- 313 served within the SMOS pixel. In this study, the approach in 314 [28] is implemented to take into account vegetation water status 315 in the estimation of soil temperature. 316

### *A. Disaggregation Methodology* 317

DN<sub>A</sub> - Offsets, (1) differs with regard to the representation of the vegatition water<br>states. In previous versions [16], [27], the soil temperature with<br>certain and states. In previous versions [16], [27], the soil tempe The disaggregation procedure decouples the soil evaporation 318 from the 0–5 cm soil layer and the vegetation transpiration 319 from the root-zone soil layer by separating MODIS surface 320 temperature into its soil and vegetation components as in the 321 triangle or trapezoidal method [28], [29]. MODIS-derived soil 322 temperature is then used to estimate soil evaporative efficiency, 323 which is known to be relatively constant during the day on clear 324 sky conditions. MODIS-derived soil evaporative efficiency is 325 finally used as a proxy for surface (0–5 cm) soil moisture 326 variability within the SMOS pixel. The link between surface 327 soil moisture and soil evaporative efficiency at different scales 328 is ensured by a downscaling relationship and a soil evapo- 329 rative efficiency model, as described below in more detail. 330 The originality of DisPATCh relies on a dynamical land cover 331 classification (based on the hourglass approach in [28]) that 332 takes into account the subpixel variability of the sensitivity of 333 soil evaporative efficiency to surface soil moisture. 334

*1) Downscaling Relationship:* The downscaling relation- 335 ship can be written as 336

$$
SM_{1 \text{ km}} = SM_{SMOS} + \frac{\partial SM_{mod}}{\partial SEE} \times (SE_{MODIS,1 \text{ km}} - \langle SEE_{MODIS,1 \text{ km}} \rangle_{40 \text{ km}})
$$
(3)

with **SM<sub>SMOS</sub>** being the SMOS soil moisture (for clarity, 337 the variables defined at SMOS scale are written in bold), 338  $SEE_{\text{MODIS}}$  the MODIS-derived soil evaporative efficiency (ra- 339) tio of actual to potential evaporation),  $\langle$ SEE<sub>MODIS</sub> $\rangle$ <sub>40 km</sub> its 340 average within a SMOS pixel and ∂**SMmod**/∂**SEE** the partial 341 derivative evaluated at SMOS scale of soil moisture with re- 342 spect to soil evaporative efficiency. Note that the linearity of (3) 343 implies that a possible bias in SMOS data would produce the 344

### TABLE II

LIST OF OVERLAPPING HDAS, SMOS, AND MODIS (MOD11A1 AND MYD11A1) DATA DURING AACES-1 AND AACES-2. ONLY THE SMOS DATA COLLECTED ON THE SAME DAY AS GROUND SAMPLING HAVE BEEN CONSIDERED. THE MODIS DATA CONSIDERED AS INPUT TO DISPATCH HAVE BEEN COLLECTED WITHIN PLUS OR MINUS ONE DAY EITHER SIDE THE GROUND SAMPLING (AND SMOS OVERPASS) DATE. ON EACH SAMPLING DATE, THE RESULTANT NUMBER OF INPUT DATA SETS TO DISPATCH IS ALSO INDICATED





Fig. 2. Schematic diagram presenting the combination of SMOS and MODIS to generate an ensemble of input data to DisPATCh. The output data are composite d at 1-km resolution by computing the average  $(SM_{1 \text{ km}})$  and standard deviation  $(\sigma_{SM,1 \text{ km}})$  of disaggregated SMOS soil moisture.

 same bias in disaggregated data [30]. Consequently, although the possible presence of a bias in SMOS data limits the accuracy in the disaggregated soil moisture, it is not a limiting factor to the applicability of DisPATCh. MODIS derived soil evaporative efficiency is expressed as a linear function of soil temperature

$$
SEE_{\text{MODIS},1 \text{ km}} = \frac{\mathbf{T}_{\mathbf{s},\mathbf{max}} - T_{\mathbf{s},1 \text{ km}}}{\mathbf{T}_{\mathbf{s},\mathbf{max}} - \mathbf{T}_{\mathbf{s},\mathbf{min}}} \tag{4}
$$

350 with  $T<sub>s</sub>$  being the MODIS-derived soil skin temperature,  $T_{s, max}$  the soil skin temperature at  $SEE = 0$  and  $T_{s, min}$ 352 the soil skin temperature at  $SEE = 1$ . The linearity of the relationship between soil evaporative efficiency and surface soil temperature was verified using the physically based dual source energy budget model in [31] using a synthetic data set composed of a range of surface soil moisture values and differ- ent atmospheric conditions (results not shown). End-members **T s** ,**min** and **T s** ,**max** are estimated from the polygons obtained

by plotting MODIS surface temperature against MODIS NDVI 359 and MODIS albedo as in [24]. Derivation of soil temperature is 360 based on a linear decomposition of the surface temperature into 361 its soil and vegetation components as a good approximation of 362 the relationship with fourth power for temperatures [32], [33] 363 and consistent with the triangle method. MODIS-derived soil 364 skin temperature is expressed as  $365$ 

$$
T_{\rm s,1\ km} = \frac{T_{\rm MODIS} - f_{\rm v,1\ km} T_{\rm v,1\ km}}{1 - f_{\rm v,1\ km}}
$$
(5)

with  $T<sub>MODIS</sub>$  being the 1-km resolution MODIS land sur-366 face temperature,  $f_v$  the MODIS-derived fractional vegetation 367 cover, and  $T_v$  the vegetation temperature. In this study, vegeta- 368 tion temperature is estimated using the approach proposed by 369 [28]. In (5), fractional vegetation cover is written as  $370$ 

$$
f_{\rm v,1\ km} = \frac{\rm NDVI_{MODIS} - NDVI_{s}}{\rm NDVI_{v} - NDVI_{s}} \tag{6}
$$

 with NDVI<sub>MODIS</sub> being the 1-km resolution MODIS NDVI, **NDVI <sup>s</sup>** the NDVI corresponding to bare soil, and **NDVI <sup>v</sup>** the NDVI corresponding to full-cover vegetation. Minimum and maximum NDVI values are set to 0.15 and 0.90, respectively. In [16], the accuracy and robustness of the disaggregation methodology were tested using three different formulations of soil evaporative efficiency [26], [34], [35]. Results based on the NAFE'06 data set [36], which was collected over a 60 km by 40 km area in the AACES area, indicated that the model in [26] was better adapted for conditions where soil properties are unknown at high resolution. Consequently, the partial derivative in (3) is computed using the soil evaporative efficiency model 383 in [26]

$$
SEE_{\text{mod}} = \frac{1}{2} - \frac{1}{2}\cos(\pi \cdot SM / SM_{\text{p}})
$$
 (7)

 with **SM <sup>p</sup>** being a soil parameter (in soil moisture unit). In [26], **SM <sup>p</sup>** was set to the soil moisture at field capacity. In DisPATCh, **SM <sup>p</sup>** is retrieved at 40-km resolution from SMOS and aggregated MODIS data [16]. By inverting (7), one obtains

$$
SM_{\text{mod}} = \frac{SM_{\text{p}}}{\pi} \cos^{-1}(1 - 2 \text{SEE})
$$
 (8)

 *2) Vegetation Temperature:* Vegetation temperature in (5) is estimated at 1-km resolution with the "hourglass" approach in [28]. By plotting the diagonals in the quadrilateral in Fig. 3, four areas are distinguished in the space defined by surface temperature and fractional vegetation cover. In zone A, land surface temperature is mainly controlled by soil evaporation leading to optimal sensitivity to surface soil moisture. In zone D, land surface temperature is mainly controlled by vegetation transpiration with no sensitivity to surface soil moisture. In zones B and C, land surface temperature is controlled by both soil evaporation and vegetation transpiration with intermediate (average) sensitivity to surface soil moisture. Based on this un- derstanding, vegetation temperature is estimated in a different manner in each zone.

402 For a given data point located in Zone A, vegetation temper-403 ature is

$$
T_{\mathbf{v},1 \text{ km}} = (\mathbf{T}_{\mathbf{v},\mathbf{min}} + \mathbf{T}_{\mathbf{v},\mathbf{max}})/2
$$
 (9)

404 with  $T_{v,min}$  and  $T_{v,max}$  being the vegetation temperature 405 at minimum and maximum water stress, respectively. End-406 members  $T_{v,min}$  and  $T_{v,max}$  are estimated from the poly-407 gons obtained by plotting MODIS surface temperature against 408 MODIS NDVI and MODIS albedo as in [24].

409 For a given data point located in Zone B, vegetation temper-410 ature is

$$
T_{\mathbf{v},1 \text{ km}} = (T_{\mathbf{v},\text{min},1 \text{ km}} + \mathbf{T}_{\mathbf{v},\text{max}})/2 \tag{10}
$$

411 with  $T_{\rm v,min,1\ km}$  being the vegetation temperature associated 412 with  $\text{SEE} = 0$  ( $T_s = \mathbf{T}_{s,\text{max}}$ ).

413 For a given data point located in Zone C, vegetation temper-414 ature is

$$
T_{\rm v,1\ km} = (\mathbf{T}_{\mathbf{v},\mathbf{min}} + T_{\rm v,max,1\ km})/2 \tag{11}
$$



Fig. 3. Polygon defined in the land surface temperature-fractional vegetation cover space contains four distinct zones A, B, C, and D. In Zone A (soildominated area), the estimated vegetation temperature is constant leading to optimal sensitivity of estimated soil temperature to surface soil moisture. In Zone D, the estimated soil temperature is constant with no sensitivity to surface soil moisture. In Zone B and C (mixed surface), surface temperature is both controlled by soil evaporation and vegetation transpiration with intermediate (average) sensitivity of estimated soil temperature to surface soil moisture. DisPATCh can be run in the Zone A+B+C mode or in the Zone A only mode.



Fig. 4. Temperature end-members  $T_{s,min}$ ,  $T_{s,max}$ ,  $T_{v,min}$ , and  $T_{v,max}$  are estimated from the surface temperature-fractional vegetation cover space and the surface temperature-surface albedo space within two given SMOS pixels. In (b), the pixel corresponding to the largest MODIS albedo has a fractional vegetation cover larger than 0.5, so that  $T_{v, max}$  is set to its surface temperature. In (d), the pixel corresponding to the largest MODIS albedo has a fractional vegetation cover lower than 0.5, so that  $T_{\mathbf{v},\mathbf{max}}$  is set to  $T_{\mathbf{v},\mathbf{min}}$ .

415 with  $T_{v, \text{max}, 1 \text{ km}}$  being the vegetation temperature associated 416 with  $\text{SEE} = 1$  ( $T_s = T_{s,\text{min}}$ ).

417 For a given data point located in Zone D, vegetation temper-418 ature is

$$
T_{\rm v,1\ km} = (T_{\rm v,min,1\ km} + T_{\rm s,max,1\ km})/2 \tag{12}
$$

 *3) End-Members:* End-members **T s** ,**min** , **T s** ,**max** , **T v** ,**min** and **T v** ,**max** are estimated by combining the spatial information provided by the surface temperature-fractional vegetation cover space and the surface temperature-albedo space plotted using MODIS data collected in a 40-km resolution SMOS pixel. An illustration is provided in Fig. 4 for two given SMOS pixels.

- 425 • **T v** ,**min**: the vegetation temperature at minimum vegeta-426 tion water stress is set to the minimum MODIS surface 427 temperature in the SMOS pixel [see Fig. 4(a) and (c)].
- 428 • **T v** ,**max**: the vegetation temperature at maximum vegeta-429 tion water stress is set to the MODIS surface temperature 430 of the pixel with the maximum value of MODIS albedo in 431 the SMOS pixel [see Fig. 4(b)]. If the fractional vegetation 432 cover of that pixel is lower than 0.5 [see Fig. 4(d)], the veg-433 etation temperature at maximum vegetation water stress 434 is alternatively set to **T v** ,**min**, meaning that vegetation is 435 unstressed within the SMOS pixel. The condition based 436 on fractional vegetation cover is lower than 0.5 aims to 437 increase the robustness of the determination approach of

**T v** ,**max**, particularly in the SMOS pixels where all surface 438 conditions are not met. 439

- $T_{\rm s,min}$ : the soil temperature at SEE = 1 is extrapolated 440 along the wet soil edge at  $f_v = 0$ . The wet soil edge 441 is defined as the line passing through  $(1, \mathbf{T}_{\mathbf{v},\mathbf{min}})$  and 442 through the data point such that all the data points with 443  $f_{\rm v}$  < 0.5 are located above the wet soil edge [see Fig. 4(a) 444 and (c)].  $445$
- $\mathbf{T}_{\mathbf{s},\mathbf{max}}$ : the soil temperature at SEE = 0 is extrapolated 446 along the dry soil edge at  $f_v = 0$ . The dry soil edge 447 is defined as the line passing through  $(1, T_{\mathbf{v},\mathbf{max}})$  and 448 through the data point such that all the data points with 449  $f_{\rm v}$  < 0.5 are located below the dry soil edge [see Fig. 4(a) 450 and (c)].  $451$

### *B. Atmospheric Correction* 452

In MOD11A1 and MYD11A1 products, the land surface 453 temperature is derived from MODIS thermal radiances using 454 the split window algorithm [37] 455

$$
T_{\text{MODIS}} = C + \left(A_1 + A_2 \frac{1 - \epsilon}{\epsilon} + A_3 \frac{\Delta \epsilon}{\epsilon^2}\right) \frac{Tb_{31} + Tb_{32}}{2} + \left(B_1 + B_2 \frac{1 - \epsilon}{\epsilon} + B_3 \frac{\Delta \epsilon}{\epsilon^2}\right) \frac{Tb_{31} - Tb_{32}}{2} \tag{13}
$$

456 with  $T b_{31}$  and  $T b_{32}$  being the brightness temperatures mea-457 sured in the MODIS bands 31 and 32, respectively,  $\epsilon_{31}$  and  $\epsilon_{32}$  the surface emissivities estimated in the respective bands, and  $A_1$ ,  $A_2$ ,  $A_3$ ,  $B_1$ ,  $B_2$ ,  $B_3$ , and C regression coefficients. These coefficients are available during algorithm execution via a look up table stratified by subranges of near surface air temperature and total column water vapor. These input field are obtained at a 5-km resolution from the MODIS07\_L2 product.

 Given that regression coefficients in (13) are provided at 5-km resolution, the atmospheric corrections on the MODIS land surface temperature product are actually made at 5-km resolution. To test whether atmospheric corrections on MODIS temperature have an impact on disaggregation results, a differ- ent procedure is proposed to obtain another temperature data set whose atmospheric corrections are operated at the scale of a SMOS pixel, i.e., at 40-km resolution (instead of 5-km resolution for the official MODIS temperature product). The approach is to normalize the mean MODIS radiance-derived brightness temperature at the SMOS resolution. Normalization is done by adjusting the minimum and maximum mean MODIS brightness temperature to the minimum and maximum value of the official MODIS land surface temperature product within the SMOS pixel, respectively. The new temperature noted  $T_{\text{MODIS}}^{\text{unif. corr.}}$  (uniform atmospheric corrections) is written

$$
T_{\text{MODIS}}^{\text{unif. corr.}} = T_{\text{MODIS,min}} + (T_{\text{MODIS,max}} - T_{\text{MODIS,min}})
$$

$$
\times \frac{Tb_{31} + Tb_{32} - \text{Min}(Tb_{31} + Tb_{32})}{\text{Max}(Tb_{31} + Tb_{32}) - \text{Min}(Tb_{31} + Tb_{32})} \quad (14)
$$

 with T**MODIS** ,**min** and T**MODIS** ,**max** being the minimum and maximum MODIS land surface temperature within the SMOS pixel, and **Min**() and **Max**() the function that returns the mini- mum and maximum value within the SMOS pixel, respectively. Note that the underlying assumptions of (14) are:

- 485 near surface air temperature and column water vapor vary
- 486 at scales larger than 40 km (size of a SMOS pixel).
- 487 surface emissivity is close to 1.

### 488 *C. Algorithm*

 The steps used in applying DisPATCh include: 1) select- ing the SMOS pixels with at least 90% (clear sky) MODIS- retrieved land surface temperature coverage; 2) computing soil evaporative efficiency over nominal MODIS pixels with (4); 3) estimating soil evaporative efficiency over non-nominal MODIS pixels; 4) retrieving parameter **SM <sup>p</sup>**; 5) applying the downscaling relationship of (3); 6) correcting disaggregated soil moisture by the SMOS pixel weighting function; and 7) compositing on a daily basis the disaggregation output en- semble [21]. The input and output data and their link within DisPATCh are summarized in Fig. 5.

 *1) Selecting Clear Sky SMOS Pixels:* A threshold of 90% cloud-free MODIS coverage is used to select the SMOS pix- els to be disaggregated. In the official MODIS land surface temperature product (MOD11A1 for Terra and MYD11A1 for Aqua), the data affected by the presence of clouds are already masked. Hence, selection of the 90% clear sky SMOS pixels is



Fig. 5. Schematic diagram presenting the input and output data of DisPATCh.

directly based on the MODIS land surface temperature product 506 masking. 507

It resolution (instead of  $\theta$ -final control instead of the same of the same of the same of the correction and maximum mean MODIS and maximum means and maximum means and maximum means are corrections) is written<br>  $\lim_{n \to \$ *2) Non-Nominal Pixels:* Nominal MODIS pixels are de- 508 fined as the 1-km resolution pixels that do not include open 509 water and where land surface temperature is actually retrieved. 510 Open water pixels are flagged in the algorithm when MODIS 511 NDVI retrievals yield negative values. The soil evaporative 512 efficiency of open water pixels is set to 1. The emerged pixels 513 where land surface temperature is not retrieved (due to the 514 presence of some clouds within the SMOS pixel) are processed 515 as pixels with mean surface conditions. In practice, the soil 516 evaporative efficiency of cloudy pixels (which represent less 517 than 10% of the surface area within the SMOS pixel) is set to 518 the mean soil evaporative efficiency calculated over the clear 519 sky MODIS pixels. Allocating a soil evaporative efficiency 520 value to non-nominal pixels allows DisPATCh to be run over a 521 wider range of SMOS pixels, including those partially covered 522 by clouds. However, non-nominal 1-km resolution pixels are 523 flagged and discarded from the disaggregation output ensemble. 524

> *3) Forested Areas:* In this study, DisPATCh is applied to all 525 the SMOS pixels where the soil moisture retrieval is successful, 526 even those including forest class, as long as the 1 km MODIS 527 pixels are in Zone A, B or C (see Fig. 3). This choice is 528 relevant here because the AACES extensive data were almost 529 exclusively collected in agricultural areas (cropping/grazing), 530 so forests for this study are not an issue. In the case of a 531 mixed SMOS pixel including a significant fraction of forest, 532 DisPATCh should be applied to the surface area of the dominant 533

534 class, thus excluding the surface area of the minority land cover 535 classes.

536 *4) Calibration:* The soil moisture parameter **SM <sup>p</sup>** used to 537 compute ∂**SMmod**/∂**SEE** in (3) is estimated by inverting the 538 SEE model in (7) at SMOS resolution

$$
SM_{p} = \frac{\pi \cdot SM_{SMOS}}{\cos^{-1} \left(1 - 2\langle SEE_{MODIS,1 \text{ km}}\rangle_{40 \text{ km}}\right)} \tag{15}
$$

 A value of **SM <sup>p</sup>** is obtained for each SMOS pixel and each input data set. Note that the main assumption limiting validity of the calibration approach is the soil evaporative efficiency model [26] itself. The soil evaporative efficiency model in [26] was chosen for its simplicity (one parameter) and its ability to represent the general behavior of soil evaporative efficiency over the full range of soil moisture: particularly the null deriva- tive at zero and at maximum soil moisture, and an inflexion point in between [38]. However, it has some inconsistencies. In particular, [38] have indicated that 1) potential evaporation is physically reached at soil saturation and not at field capac- ity; therefore the model in [26] should be (strictly speaking) parameterized by the soil moisture at saturation and not by the soil moisture at field capacity, and 2) soil evaporative efficiency varies with potential evaporation, meaning that the soil moisture parameter (set to the soil moisture at field capacity in [26]) should theoretically vary in time with atmospheric evaporative demand. Consequently, the **SM <sup>p</sup>** retrieved from SMOS and MODIS data using the model in [26] is definitely not the soil moisture at field capacity as in [26], although it could be in part related to it. In this study, **SM <sup>p</sup>** is therefore considered to be a fitting parameter self-estimated by DisPATCh.

 *5) Weighting Function:* A SMOS pixel WEighting Function (WEF) is used to take into account the impact of soil mois- ture distribution on the SMOS scale soil moisture as seen by SMOS radiometer. A centrosymmetric analytical approxima-tion MEAN\_WEF is provided in [19], [20]

$$
MEAN\_WEF(\rho) = C_{\text{MWEF2}} + WEF_A \left( \frac{\rho}{C_{\text{MWEF1}}} \cdot \frac{\pi}{C_{\text{WEF1}}} \right)
$$
\n(16)

566 with  $\rho$  being the distance from the SMOS pixel center, and 567  $C_{\text{MWEF1}} = 40 \text{ km}, C_{\text{MWEF2}} = 0.027, C_{\text{WEF1}} = 73.30 \text{ and}$ 

$$
WEF_A(\rho') = \frac{\left[\operatorname{sinc}(C_{WEF1} \cdot \rho')\right]^{C_{WEF2}}}{1 + C_{WEF3} \cdot \rho'^{C_{WEF4}}} \tag{17}
$$

568 with  $\rho'$  being the distance in the director cosines coordinates, 569 sinc $(x) = \sin(x)/x$ , and  $C_{\text{WEF2}} = 1.4936$ ,  $C_{\text{WEF3}} = 524.5$ 570 and  $C_{\text{WEF4}} = 2.103$ .

571 A correction is applied to disaggregated soil moisture in (3)

$$
SM_{1 \text{ km}}^{\text{wef corr.}} = SM_{1 \text{ km}} + \frac{\sum \text{MEAN\_WEF}(\rho) \cdot SM_{1 \text{ km}}(\rho)}{\sum \text{MEAN\_WEF}(\rho)} - SM_{\text{SMOS}} \quad (18)
$$

572 with  $SM_{1 \text{ km}}^{\text{wef corr.}}$  being the WEF-corrected disaggregated soil moisture. Mathematically speaking, one should replace  $\texttt{SM}_{\texttt{SMOS}}$  with  $\sum \texttt{MEAN\_WEF} \cdot \texttt{SM}_{1 \text{ km}} / \sum \texttt{MEAN\_WEF}$ in (3) and (15) and run an iteration loop until convergence

of  $SM_{1 \text{ km}}^{\text{wef corr.}}$  values. However, the impact of the WEF on 576 disaggregated soil moisture is expected to be low so that the 577 simple correction in (18) is considered to be sufficient for the 578 purpose of the study. 579

*6) Disaggregation Output:* The downscaling relationship in 580 (3) is applied to each input data set, and the disaggregated soil 581 moisture data ensemble is averaged on each 1-km resolution 582 pixel within the study area. Averaging is a way to reduce 583 random uncertainties in the disaggregation output. In [17], [27], 584 disaggregated soil moisture was averaged in space (aggregated) 585 at the expense of downscaling resolution. Herein, temporal 586 averaging [30] is preferred to keep an optimal downscaling 587 resolution. Note that a condition to average disaggregated soil 588 moisture in time is the availability of thermal infrared data 589 at high temporal frequency. Another significant advantage of 590 applying DisPATCh to an input ensemble is to provide an 591 estimate of the uncertainty in 1-km resolution disaggregated 592 soil moisture, e.g., by computing the standard deviation within 593 the output ensemble. 594

IV. APPLICATION 595

To test DisPATCh under various surface and atmospheric 596 conditions, the algorithm is run during AACES-1 and AACES- 597 2 in different modes, by including (or not) a correction for 598 vegetation and atmospheric effects. In each case, disaggregated 599 SMOS soil moisture and HDAS measurements are compared 600 at 1-km resolution for all date-farm units with overlapping 601 HDAS/SMOS/MODIS data. 602

*A. Null Hypothesis* 603

In this study, the null hypothesis is defined as the application 604 of DisPATCh with parameter **SM <sup>p</sup>** set to zero in (8). Hence, 605 the downscaling relationship in (3) becomes 606

$$
SM_{1 \text{ km}} = SM_{SMOS} \tag{19}
$$

Il moisture, and an inflexion applying DisPATCh to an input ensemble is to provide an<br>it in some inconsistencies, estimate of the uncertainty in 1-km resolution disaggregated<br>that 1) potential exaporation soil moisture, e meaning that no 1-km information is used. Defining a null 607 hypothesis is useful to test whether DisPATCh is able to re- 608 produce the subpixel variability within the  $\sim 10 \text{ km}^2 \text{ sam}$  609 pling farms with better skill than simply assuming a uniform 610 moisture condition. Statistical results in terms of root mean 611 square difference, mean difference, correlation coefficient, and 612 slope of the linear regression between the SMOS soil moisture 613 disaggregated with (19) and *in situ* measurements are listed in 614 Table III. One observes that the root mean square difference 615 is generally explained by a (negative) bias in SMOS data and 616 that none of the correlations evaluated at 1-km resolution for 617 each farm separately is statistically significant (all calculated p- 618 values are larger than 0.10). Thus, the rationale for developing 619 DisPATCh is to improve the correlation at fine scale between 620 SMOS and ground soil moisture and to reduce the bias in 621 disaggregated SMOS data in the specific case where the bias 622 in SMOS data at the farm scale is due to the heterogeneity of 623 soil moisture within the SMOS pixel. 624

### TABLE III DisPATCh Is Run With No 1-km Information (**SM<sub>p</sub>Set to Zero) and Statistical Results Are Listed in Terms of Root Mean Square** DIFFERENCE (RMSD), MEAN DIFFERENCE (BIAS), CORRELATION COEFFICIENT (R), AND SLOPE OF THE LINEAR REGRESSION BETWEEN 1-km RESOLUTION DISAGGREGATED SMOS SOIL MOISTURE AND 1-km AGGREGATED IN SITU MEASUREMENTS. THE MEAN AND STANDARD DEVIATION OF GROUND MEASUREMENTS ( $\langle \rm SM_{HDAS} \rangle$ and  $\sigma_{HDAS}$ ), the Number of Considered 1-km PIXELS, AND STATISTICAL SIGNIFICANCE (P-VALUE) ARE ALSO LISTED FOR EACH DATE-FARM UNIT



### 625 *B. Visual Assessment of Disaggregation Images*

 As an example, DisPATCh is applied on DoY 49 over a 120 km by 80 km subarea including the farms F16, F17, F18, F19, and F20. The images of 1-km resolution disaggregated SMOS soil moisture are presented in Fig. 6. DisPATCh is run with **SM <sup>p</sup>** set to zero (null hypothesis) and in four distinct modes corresponding to the combinations of the "LST" (the official MODIS land surface temperature product is used) and "RAD" [the land surface temperature is derived from MODIS radiances using (14)] modes and the "Zone A+B+C" (the vegetation- transpiration dominated 1-km pixels are discarded) and "Zone A only" (only the soil evaporation-dominated 1-km pixels are selected) modes.

 In Fig. 6, the SMOS DGG nodes where level-2 soil moisture is successfully retrieved are overlaid on the image correspond- ing to the null hypothesis (resampled SMOS data with no 1-km information) for 6 am and 6 pm overpass times separately. The gaps in SMOS data in the lower middle part of the images are due to topography flagging over the Australian Alps. In the version-4 SMOS level-2 processor, soil moisture is not retrieved at the DGG nodes where the topography effects on simulated brightness temperatures exceed a certain threshold, so as to prevent large errors in soil moisture values. The appar- ent resolution of the null hypothesis image is 20 km because it is generated from the composition of four 40-km resolution resampled SMOS snapshot images, whose resampling grids are separated by 20 km (the SMOS level-2 data resampling strategy 651 was described in Section II-B.).

Note that the disaggregation products in the Zone A+B+C 653 mode cover an area larger than the area sampled by SMOS 654 data, because the SMOS resolution (about 40 km) is larger 655 than the SMOS product sampling length (about 15 km), but 656 does not provide disaggregated values at a distance larger than 657 20 km from the successful retrieval nodes. Concerning the Zone 658 A only mode, disaggregation products do not cover an area 659 larger than the SMOS sampling area because the Australian 660 Alps are surrounded by forests where the fraction of bare soil is 661 less than elsewhere in the area, and which correspond to Zone 662 B or C in the hourglass in Fig. 3. 663

When looking at the images obtained in the Zone A+B+C 664 mode in Fig. 6, one observes that the spatial structures of 665 1-km disaggregated SMOS soil moisture encompass, but does 666 not seem to be correlated with, the SMOS data sampling 667 length. However, a "boxy artifact" is still apparent at 20-km 668 resolution, which is the separation length of the SMOS data 669 resampling grids as explained in Section II-B. The notion of 670 "boxy artifact" was introduced by [39] to analyze the quality of 671 a disaggregation approach. The less apparent the low-resolution 672 boxes, the better the disaggregation skill of the algorithm to 673 spatially connect high-resolution disaggregated values between 674 neighboring low-resolution pixels, and thus to derive a realistic 675 high-resolution soil moisture field. When comparing the images 676 obtained in the Zone A+B+C mode with those obtained in the 677 LST

 $SM<sub>1 km</sub>$ 

 $\sigma_{SM, 1 km}$ 

 $\frac{SM_{1km}}{2}$ 

 $E17$ 



**O**SM, 1 km

Fig. 6. Images of disaggregation results over a 120 km by 80 km subarea on DoY 49. The disaggregated soil moisture (SM<sub>1 km</sub>) and its estimated uncertainty  $(\sigma_{\text{SM},1 \text{ km}})$  are compared in the LST and RAD modes and in the Zone A+B+C and Zone A only modes. Sampling farms are overlaid on all images. SMOS DGG nodes are overlaid on the image corresponding to the null hypothesis (no 1-km resolution information) presented at top.

 Zone A only mode, one observes that the 20-km resolution boxy artifact is less apparent in the Zone A only mode, consistent with the better sensitivity of MODIS-derived SEE with soil- dominated pixels (Zone A) than with mixed-surface (Zone B and C) pixels. In Fig. 6, the images obtained in the LST and RAD mode highlight different spatial structures. In general, there are less data gaps in the RAD than in the LST mode. However, ground validation data are required to assess their relative quality/accuracy.

687 As an assessment of the uncertainty in composited soil mois-688 ture disaggregation, the standard deviation within the disaggre-689 gation output ensemble is also reported for each disaggregation product in Fig. 6. The same observations can be made as with 690 the soil moisture images: spatial structures are more visible, and 691 the boxy artifact is less apparent in the RAD than in the LST 692 mode. In general, the estimated uncertainty in disaggregated 693 products is larger in the RAD than in the LST mode, regardless 694 of the Zone (A+B+C or A only) mode. 695

### *C. SMOS Weighting Function* 696

To evaluate the impact of the SMOS instrument weighting 697 function on disaggregation results, DisPATCh is run with (and 698 without) the WEF correction in (18). The expected effect of the 699



Fig. 7. Uncorrected versus WEF-corrected SMOS soil moisture for the entire data set.

 WEF is a bias at 40 km resolution on disaggregated soil mois- ture. Fig. 7 plots the uncorrected against WEF-corrected SMOS soil moisture for the entire data set including both AACES-1 and AACES-2 experiments. The WEF correction has very little impact on disaggregated soil moisture with a maximum difference between uncorrected and WEF-corrected SMOS soil 706 moisture of 0.02  $\text{m}^3/\text{m}^3$ , a mean difference of approximately 707 zero, and a standard deviation of 0.003  $\text{m}^3/\text{m}^3$ . Although the difference is small with this data set, WEF-corrected products are expected to be more realistic. Therefore, the correction in (18) is used in all the DisPATCh runs that follow.

### 711 *D. Quantitative Comparison With In Situ Measurements*

 Fig. 8 presents the scatterplots of 1-km resolution disaggre- gated SMOS soil moisture versus 1-km resolution aggregated *in situ* measurements for the ten date-farm units during AACES-1. On each graph are plotted the soil moisture dis- aggregated in the Zone A+B+C mode (empty squares) and the soil moisture disaggregated in the Zone A only mode (black squares). At the beginning of AACES-1, conditions are very dry so that SMOS retrievals are close to zero and the 720 variability of *in situ* measurements is low (about  $0.02 \text{ m}^3/\text{m}^3$ ). In such conditions, no useful information is expected from the application of DisPATCh, and the statistical results in terms of spatial correlation are not meaningful for DoY 28/F05, DoY 30/F07 and DoY 30/F08. While wetter conditions occur after DoY 30, cloud cover prevents DisPATCh to be run (MODIS data are unavailable) until DoY 46. On DoY 46, the average and standard deviation of *in situ* soil moisture measurements is 728 0.32 m<sup>3</sup>/m<sup>3</sup> and 0.06 m<sup>3</sup>/m<sup>3</sup>, respectively. The spatial variabil- ity of 1-km soil moisture is nicely captured by DisPATCh no- tably in the RAD mode. On DoY 49, the disaggregated SMOS soil moisture is still correlated with the *in situ* measurements made in three farms (F17, F18, and F20). On the last ground sampling day, disaggregation results are significantly correlated with *in situ* measurements in F19, but not in F20. The poor results obtained with DoY 51/F20 is probably due to the time gap (3 days) between ground sampling date (DoY 51) and MODIS overpass day (DoY 54).

738 Statistical results in terms of root mean square difference, 739 mean difference, correlation coefficient, and slope of the linear regression between the SMOS soil moisture disaggregated in 740 the Zone A+B+C mode and aggregated *in situ* measurements 741 are listed in Table IV. Statistical significance (p-value) is also 742 reported for each date-farm unit to select statistically significant 743 (p-value < 0.10) results. Although the disaggregation of SMOS 744 data on extensively dry DoY 30 does not provide any additional 745 information (soil is uniformly dry), the observed correlation 746 between disaggregated (LST mode) and *in situ* soil moisture 747 is statistically significant, and the correlation coefficient value 748 is negative  $(-0.70 \text{ and } -0.95 \text{ at } F07 \text{ and } F08$ , respectively). 749 One plausible explanation is the opposite effect of soil temper- 750 ature on HDAS soil moisture measurements and on MODIS- 751 derived soil evaporative efficiency: a slight undercorrection of 752 the temperature-corrected hydraprobe measurements at high 753 temperature [18] results in a slight increase of soil moisture 754 estimate with soil temperature, while an increase of soil temper- 755 ature makes soil evaporative efficiency decrease. Nevertheless, 756 the possible impact of soil temperature on HDAS measurements 757 is very low with a slope of the linear regression between 758 disaggregated SMOS and *in situ* soil moisture calculated as 759 −0.08 and −0.03 for F07 and F08, respectively. When selecting <sup>760</sup> statistically significant results (p-value  $< 0.10$ ) and discarding 761 data for DoY 30, the mean correlation coefficient and slope in 762 RAD mode are 0.75 and 0.58, respectively.  $763$ 

on on disaggregated soil mois-<br>
estimate with solic respective, whis an interest or solic experiment of several solic experiment of solic server and the set including buth AACES-1 is very low with a slope of the linear re Fig. 9 presents the scatterplots of 1-km resolution disaggre- 764 gated SMOS soil moisture versus 1-km resolution aggregated *in* 765 *situ* measurements for the five date-farm units during AACES- 766 2. On each graph are plotted the soil moisture disaggregated in 767 the Zone A+B+C mode (empty squares) and the soil moisture 768 disaggregated in the Zone A only mode (black squares). The 769 surface conditions of AACES-2 were relatively wet with a mean 770 soil moisture value estimated as  $0.29 \text{ m}^3/\text{m}^3$ . The disaggre- 771 gated SMOS soil moisture does not correlate well with *in situ* 772 measurements with a p-value larger than 0.10 for all sampling 773 days, except for DoY 256/F07 in LST mode (see Table IV). The 774 negative correlation coefficient  $(-0.73)$  obtained on DoY 256 is 775 discussed when comparing the Zone A+B+C and Zone A only 776 modes in Section IV-F. In general, statistical results in Table IV 777 indicate that DisPATCh does not succeed in representing the 778 variability of soil moisture at 1-km resolution during AACES- 779 2. In fact, DisPATCh is based on the tight coupling that occurs 780 between soil moisture and evaporation under high evaporative 781 demand conditions [40]. This coupling seems to be weak in 782 September over the study area so that the disaggregation results 783 at 1-km resolution are not reliable. 784

For DoY 264/F13, however, an interesting feature is ob- 785 served on the graph corresponding to the RAD and Zone A 786 only modes. When removing the (three) black squares with 787 the largest errorbars, the correlation coefficient and the slope 788 of the linear regression between disaggregated and *in situ* 789 observations becomes 0.9 and 0.7, respectively. This suggests 790 that: 1) the standard deviation within the disaggregation output 791 ensemble can be a good estimate of the uncertainty in the 792 composited disaggregation product; and 2) the applicability of 793 DisPATCh is greatly dependent on the quality of MODIS land 794 surface temperature. Note that in this study, a choice was made 795 to maximize the number of data points used in the comparison 796 with *in situ* measurements. Consequently, all the cloud-free 797



Fig. 8. Scatterplots of 1-km resolution disaggregated SMOS soil moisture versus 1-km resolution aggregated *in situ* measurements for each of the ten date-farm data sets during AACES-1. The filled circles correspond to disaggregation with no 1-km information, empty squares to Zone A+B+C mode and black squares to Zone A only mode. For the Zone A only mode, the uncertainty in disaggregated soil moisture is represented by vertical errorbars.

 MODIS land surface temperature data were used regardless of the MODIS land surface temperature quality index. Further research should be conducted to assess whether selecting the MODIS pixel with the best MODIS land surface temperature quality index would improve the disaggregation results. This would be possible using the AACES airborne data, which cover a much larger area than *in situ* measurements.

### 805 *E. Atmospheric Corrections*

 The impact of atmospheric corrections on DisPATCh output is analyzed by comparing the disaggregation results obtained in the LST and RAD mode. Quantitative comparison between LST and RAD modes is provided in Table IV in terms of root mean square difference, mean difference, correlation coeffi- cient, and slope of the linear regression between disaggregated SMOS soil moisture and aggregated *in situ* measurements. Correlation coefficient and slope values are reported only if the p-value (statistical significance) is lower than 0.10. It is apparent that statistical results are better in the RAD than in the LST mode. When including all dates, the mean bias is 816 decreased from  $-0.05 \text{ m}^3/\text{m}^3$  in LST mode to  $-0.03 \text{ m}^3/\text{m}^3$  817 in RAD mode during AACES-1. When selecting statistically 818 significant results (p-value  $<$  0.10) and discarding data for 819 DoY 30, the mean correlation coefficient and slope is 0.75 and 820 0.58 in RAD mode, and 0.65 and 1.5 in LST mode, respectively. 821 Note that the improvement is very significant for DoY 46/F16 822 with a correlation coefficient and slope increasing from about 823 zero to 0.7 and 0.8, respectively. 824

The fact that the results obtained in RAD mode are superior 825 to those obtained in LST mode indicates that the atmospheric 826 corrections of the official MODIS land surface temperature 827 add significant uncertainties in the disaggregation products. 828 One rationale may be that the information used in atmospheric 829 corrections (notably air temperature and water vapor profile 830 data) are subjected to large uncertainties at 5-km resolution. 831 As DisPATCh is based on the spatial variations of MODIS 832 temperature relative to the 40 km scale mean, the atmospheric 833 corrections on the land surface temperature data are not nec- 834 essary at 5 km (as it is done in the MODIS temperature 835

### TABLE IV

DISPATCH Is Run in the Zone A+B+C Mode and Statistical Results Are Listed in Terms of Root Mean Square Difference (RMSD), MEAN DIFFERENCE (BIAS), CORRELATION COEFFICIENT (R), AND SLOPE OF THE LINEAR REGRESSION BETWEEN 1-km RESOLUTION DISAGGREGATED SMOS SOIL MOISTURE AND 1-km AGGREGATED IN SITU MEASUREMENTS. THE RESULTS OBTAINED USING THE RADIANCE-DERIVED LAND SURFACE TEMPERATURE DATA (RAD MODE) AND USING THE OFFICIAL MODIS LAND SURFACE TEMPERATURE DATA (LST MODE IN PARENTHESIS) ARE COMPARED. THE MEAN AND STANDARD DEVIATION OF GROUND MEASUREMENTS ((SM<sub>HDAS</sub>) AND σ<sub>HDAS</sub>), THE NUMBER OF CONSIDERED 1-km PIXELS AND STATISTICAL SIGNIFICANCE ( P-VALUE) ARE ALSO LISTED FOR EACH DATE-FARM UNIT



days DoY 28-30.

836 algorithm). An atmospheric correction at 40-km resolution is 837 sufficient and provides even better disaggregation results that 838 applying an atmospheric correction at 5-km resolution.

### 839 *F. Vegetation Cover*

 The impact of vegetation cover on DisPATCh output during AACES-1 is analyzed by comparing the disaggregation results obtained in the Zone A+B+C and Zone A only mode. Quan- titative comparison between Zone A+B+C and Zone A only modes is provided in Tables IV and V in terms of root mean square difference, mean difference, correlation coefficient, and slope of the linear regression between disaggregated SMOS soil moisture and aggregated *in situ* measurements. It is apparent that statistical results are generally better in the Zone A only than in the Zone A+B+C mode for both LST and RAD modes. In the RAD mode for instance, the mean correlation coefficient is increased from 0.75 in the Zone A+B+C mode (Table IV) to 0.89 in the Zone A only mode (Table V). Also the mean slope is closer to 1 as it switches from 0.58 in the Zone A+B+C mode (Table IV) to 0.91 in the Zone A only mode (Table V). Con- sequently, results are consistent with the hourglass approach in Fig. 3 that predicts a lower sensitivity of MODIS-derived soil temperature to soil moisture in Zone B and C, Zone A having the highest potential for estimating soil moisture variability 858 from MODIS temperature. 859

On DoY 256, the negative correlation appearing in Zone 860 A+B+C mode (Table IV) is not significant in Zone A only mode 861 (Table V), suggesting that the contradictory result obtained on 862 DoY 256 is probably an artifact due to the small sample size. 863

Note that one drawback of the Zone A only mode is the larger 864 amount of data gaps in the soil moisture images. Therefore, 865 the use of both modes is a compromise between application 866 coverage and accuracy in the disaggregation output. 867

### *G. Distinguishing Between SMOS and DisPATCh Errors* 868

By solving the extent mismatch between 40-km resolution 869 remote sensing observation and localized *in situ* measurements, 870 DisPATCh could be used as a tool to help improve the validation 871 strategies of SMOS data in low-vegetated semi-arid regions. It 872 also would reduce the coverage requirements identified by [41] 873 for airborne validation campaigns. However, such a validation 874 approach requires separating the different error sources that 875 may be attributed to SMOS soil moisture and to DisPATCh. 876 One solution is to estimate the errors attributed to DisPATCh 877 and then deduce the errors attributed to SMOS soil moisture. To 878 estimate the errors that are associated with the disaggregation 879



Fig. 9. Scatterplots of 1-km resolution disaggregated SMOS soil moisture versus 1-km resolution aggregated *in situ* measurements for each of the five datefarm data sets during AACES-2. The filled circles correspond to disaggregation with no 1-km information, empty squares to Zone A+B+C mode and black squares to Zone A only mode. For the Zone A only mode, the uncertainty in disaggregated soil moisture is represented by vertical errorbars.

 methodology, it is suggested to analyze the spatial correla- tion between 1-km disaggregated SMOS soil moisture and *in situ* measurements. If the correlation is significant, then the disaggregation product is likely to be sufficiently accurate for validating SMOS data.

 Note that the errors in DisPATCh are in part coupled with the errors in SMOS soil moisture, particularly because SMOS is an input to DisPATCh. However, any uncertainties in SMOS soil moisture should not impact the disaggregation results at a distance shorter than the SMOS data sampling length (15 km). This is the reason why such a validation strategy should be conducted with ground measurements made within a distance radius of 15 km.

In this study case, five date-farm units including DoY 893 46/F15, DoY 46/F16, DoY 49/F17, DoY 49/F18, and DoY 894 49/F20 indicate a significant correlation between disaggregated 895 SMOS soil moisture and *in situ* measurements. For these units, 896 the root mean square error in disaggregated SMOS soil mois- 897 ture is mainly explained by a bias in disaggregated soil moisture 898 (see Table IV). However, no conclusion can be drawn from 899 these data because: 1) the bias is sometimes positive (DoY 900 46/F15, DoY 49/F20), and sometimes negative (DoY 46/F16, 901 DoY 49/F17, DoY 49/F18); and 2) the comparison is made only 902 once for each farm, which does not allow analyzing the tempo- 903 ral behavior. Such a validation approach could be undertaken 904 in the near future using the OzNet (http://www.oznet.org.au/, 905 [42]) soil moisture monitoring network, providing continuous 906 measurements at 68 sites within the Murrumbidgee catchment 907 area. 908

### *H. Subpixel Variability and Assimilation Perspectives* 909

**EXERCT:**<br>
1. Subpixel Variability and Assimilation Perspectives<br>
2.2<br>
1. Subpixel Variability and Assimilation Perspectives<br>
2.2<br>
2.2<br>
2.3<br>
1. Subpixel Computed as the standard uncertainty in disaggregated<br>
1. Subpixel C DisPATCh is successively run in LST or RAD mode and in 910 Zone A+B+C or Zone A only mode during AACES-1. Fig. 10 911 plots for each case the estimated uncertainty in disaggregated 912 soil moisture (computed as the standard deviation of the disag- 913 gregation output ensemble) against the subpixel variability of 914 1-km resolution *in situ* measurements (computed as the stan- 915 dard deviation of the *in situ* measurements made within 916 1-km pixels). The data corresponding to DoY 51 are plotted 917 separately because of the time gap between HDAS/SMOS 918 (DoY 51) and MODIS (DoY 54) collection time. It is interest- 919 ing to observe that the estimated uncertainty in disaggregated 920 soil moisture is closely related to the observed subpixel vari- 921 ability of *in situ* measurements. Hence,  $\sigma_{\rm SM,1 \ km}$  could be used 922 as a proxy for representing the soil moisture variability at scales 923 finer than 1-km resolution. Concerning the data on DoY 51, the 924 linear regression is clearly off the 1:1 line. This is consistent 925 with a decrease of the spatial variability in soil moisture during 926 a dry down period [43]. In particular, the spatial variability 927 in soil moisture is expected to be lower on DoY 54 than on 928  $DoY 51.$  929

The correlation between the estimated uncertainty in disag- 930 gregated soil moisture and the subpixel soil moisture variability 931 makes an additional link between DisPATCh output and assim- 932 ilation schemes into hydrological models. A number of optimal 933 assimilation methodologies have been developed to combine 934 model predictions with remote sensing observations. However, 935 any so-called optimal assimilation technique stops being opti- 936 mal if the uncertainty in remotely sensed data is unknown or 937 estimated with a large uncertainty. In the perspective of assim- 938 ilating disaggregated SMOS data into land surface models, one 939 should keep in mind that the error information on observable 940 variables is as crucial as the observations themselves, e.g., [44]. 941

### V. SUMMARY AND CONCLUSION 942

DisPATCh is an algorithm dedicated to the disaggregation of 943 soil moisture observations using high-resolution soil tempera- 944 ture data. It converts soil temperature fields into soil moisture 945 fields given a semi-empirical soil evaporative efficiency model 946

### TABLE V

DISPATCH Is Run in the Zone A Only Mode, and Statistical Results Are Listed in Terms of Root Mean Square Difference (RMSD), MEAN DIFFERENCE (BIAS), CORRELATION COEFFICIENT (R), AND SLOPE OF THE LINEAR REGRESSION BETWEEN 1-km RESOLUTION DISAGGREGATED SMOS SOIL MOISTURE AND 1-km AGGREGATED IN SITU MEASUREMENTS. THE RESULTS OBTAINED USING THE RADIANCE-DERIVED LAND SURFACE TEMPERATURE DATA (RAD MODE) AND USING THE OFFICIAL MODIS LAND SURFACE TEMPERATURE DATA (LST MODE IN PARENTHESIS) ARE COMPARED. THE MEAN AND STANDARD DEVIATION OF GROUND MEASUREMENTS ((SM<sub>HDAS</sub>) AND <sub>HDAS</sub>), THE NUMBER OF CONSIDERED 1-km Pixels and Statistical Significance (p-Value) Are Also Listed for Each Date-Farm Unit



DoY 28-30.

 and a first-order Taylor series expansion around the field-mean soil moisture. In this study, the disaggregation approach is ap- plied to 40-km resolution version-4 SMOS level-2 soil moisture using 1-km resolution MODIS data. The objective is to test DisPATCh under different surface and atmospheric conditions using the very intensive ground measurements collected in southeastern Australia during the 2010 summer and winter AACES campaigns. Those measurements are aggregated at the downscaling resolution (1 km) and subsequently compared to the disaggregated SMOS soil moisture. Over the study area, climatic (evaporative demand), meteorologic (presence of clouds), and vegetation (cover and water status) conditions are strong constraints on disaggregation results. The quality of disaggregation products varies greatly according to season: while the correlation coefficient between disaggregated and *in situ* soil moisture is 0.7 during the summer AACES, it is about zero during the winter AACES, consistent with a weaker coupling between evaporation and surface moisture in temperate than in semi-arid climate. Moreover, vegetation cover prevents the soil temperature to be retrieved from thermal infrared data and the vegetation water stress may increase the remotely sensed land surface temperature independent of near- surface soil moisture. By separating the 1-km pixels where MODIS temperature is mainly controlled by soil evaporation,

from those where MODIS temperature is controlled by both 971 soil evaporation and vegetation transpiration, the correlation 972 coefficient between disaggregated and *in situ* soil moisture is 973 increased from 0.70 to 0.85 during the summer AACES cam- 974 paign. Also, cloud cover totally obscures the surface during rain 975 events, and on clear sky days, the water vapor in the atmosphere  $976$ significantly affects the quality of land surface temperature 977 data. It is found that the 5-km resolution atmospheric correction 978 of the official MODIS temperature data has significant impact 979 on DisPATCh output. An alternative atmospheric correction at 980 40-km resolution increases the correlation coefficient between 981 disaggregated and *in situ* soil moisture from 0.72 to 0.82 during 982 the summer AACES. 983

The above limitations must be kept in mind when using 984 DisPATCh as a tool for validating SMOS soil moisture. Over 985 semi-arid areas, disaggregation can solve the extent mismatch 986 between the 40-km resolution SMOS data and localized *in situ* 987 measurements. However, the validation of SMOS using Dis- 988 PATCh requires separation of the errors associated with SMOS 989 data and the errors associated with DisPATCh. As SMOS data 990 are an input to DisPATCh, the errors in DisPATCh are also 991 linked to the uncertainty in SMOS soil moisture. Nevertheless, 992 one way to identify the error sources specifically attributed 993 to DisPATCh is to analyze the spatial correlation between 994



Fig. 10. Estimated uncertainty in disaggregated soil moisture ( $\sigma_{SM}$ , 1 km) versus subpixel variability of 1 km resolution *in situ* measurements for DisPATCh run in LST or RAD mode and Zone A+B+C or Zone A only mode.

 disaggregated SMOS data and the *in situ* measurements made at a distance larger than the downscaling resolution (1 km with MODIS data) and smaller than the SMOS data sampling length 998 (15 km).

999 Based on the results obtained using the AACES *in situ* 1000 measurements, several improvements of DisPATCh can be 1001 suggested:

- 1002 Use of the MODIS land surface temperature quality index 1003 to select the SMOS pixels with the highest MODIS data 1004 quality.
- 1005 Correcting the MODIS land surface temperature for to-1006 pography and illumination effects [45]. Within a 40-km 1007 SMOS resolution pixel, the elevation range may be very 1008 significant and thus induce a variability in land sur-1009 face temperature that is not attributed to surface soil 1010 moisture.
- 1011 Use of ancillary air temperature data to constrain the 1012 estimation of end-members. The unstressed vegetation 1013 temperature  $T_{v,min}$  could be set to the air temperature 1014 instead of the minimum MODIS land surface temperature. 1015 This would make the estimation of  $T_{v,min}$  less dependent 1016 on the representativeness of the surface conditions met 1017 within the SMOS pixel [24].
- 1018 Accounting for the dependency of soil evaporative effi-1019 ciency to potential evaporation, by replacing the model in 1020 [26] with the model in [38].
- 1021 Estimating an optimal downscaling resolution for each 1022 season: as the sensitivity of soil evaporative efficiency to 1023 soil moisture is lower in the winter months than in the sum-1024 mer months, aggregating DisPATCh output may improve 1025 the quality of disaggregation products at the expense of 1026 spatial resolution [17].

A robust disaggregation methodology of SMOS soil moisture 1027 at 1-km resolution, which would provide both disaggregated 1028 soil moisture and its uncertainty at 1-km resolution is a crucial 1029 step toward the application of SMOS data to hydrological 1030 studies. 1031

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**Olivier Merlin**, photograph and biography not available at the time of 1207 publication. 1208

**Christoph Rüdiger**, photograph and biography not available at the time of 1209 publication. 1210 1211 **Ahmad Al Bitar**, photograph and biography not available at the time of 1212 publication.

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**Jeffrey P. Walker**, photograph and biography not available at the time of 1215 publication. 1216 publication.

**Yann H. Kerr**, photograph and biography not available at the time of 1217 publication.

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# Disaggregation of SMOS Soil Moisture in Southeastern Australia 123 DISaggiegation of Sivios Son Iviolistule<br>23 Olivier Merlin, Christoph Rüdiger, Ahmad Al Bitar, Philippe Richaume, Jeffrey P. Walker, and Yann H. Kerr

 *Abstract***—Disaggregation based on Physical And Theoretical scale Change (DisPATCh) is an algorithm dedicated to the dis- aggregation of soil moisture observations using high-resolution soil temperature data. DisPATCh converts soil temperature fields into soil moisture fields given a semi-empirical soil evaporative efficiency model and a first-order Taylor series expansion around the field-mean soil moisture. In this study, the disaggregation approach is applied to soil moisture and ocean salinity (SMOS) data over the 500 km by 100 km AACES (Australian Airborne Calibration/validation Experiments for SMOS) area. The 40-km resolution SMOS surface soil moisture pixels are disaggregated at 1-km resolution using the soil skin temperature derived from moderate resolution imaging spectroradiometer (MODIS) data, and subsequently compared with the AACES intensive ground measurements aggregated at 1-km resolution. The objective is to test DisPATCh under various surface and atmospheric conditions. It is found that the accuracy of disaggregation products varies greatly according to season: while the correlation coefficient be- tween disaggregated and** *in situ* **soil moisture is about 0.7 during the summer AACES, it is approximately zero during the winter AACES, consistent with a weaker coupling between evaporation and surface soil moisture in temperate than in semi-arid climate. Moreover, during the summer AACES, the correlation coefficient between disaggregated and** *in situ* **soil moisture is increased from 0.70 to 0.85, by separating the 1-km pixels where MODIS temper- ature is mainly controlled by soil evaporation, from those where MODIS temperature is controlled by both soil evaporation and vegetation transpiration. It is also found that the 5-km resolution atmospheric correction of the official MODIS temperature data has a significant impact on DisPATCh output. An alternative at- mospheric correction at 40-km resolution increases the correlation coefficient between disaggregated and** *in situ* **soil moisture from 0.72 to 0.82 during the summer AACES. Results indicate that**

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O. Merlin is with the Centre d'Etudes Spatiales de la Biosphère (CESBIO), 31401 Toulouse, France (e-mail: olivier.merlin@cesbio.cnes.fr).

C. Rüdiger (e-mail: chris.rudiger@monash.edu).

A. Al Bitar (e-mail: ahmad.albitar@cesbio.cnes.fr).

P. Richaume (e-mail: philippe.richaume@cesbio.cnes.fr).

J. P. Walker (e-mail: jeff.walker@monash.edu).

Y. H. Kerr (e-mail: yann.kerr@cesbio.cnes.fr).

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**DisPATCh has a strong potential in low-vegetated semi-arid areas** 37 **where it can be used as a tool to evaluate SMOS data (by reducing** 38 **the mismatch in spatial extent between SMOS observations and** 39 **localized** *in situ* **measurements), and as a further step, to derive** 40 **a 1-km resolution soil moisture product adapted for large-scale** 41 **hydrological studies.** 42

*Index Terms***—AACES, calibration/validation, disaggregation,** 43 **Disaggregation based on Physical And Theoretical scale Change** 44 **(DisPATCh), field campaign, moderate resolution imaging spectro-** 45 **radiometer (MODIS), soil moisture and ocean salinity (SMOS).** 46

### I. INTRODUCTION 47

**EVALUATION** Disappergation hasted non-linearized And Theoretical scale Change and occur and Theoretical scale Change (Change And Theoretical scale Change Matter priority (MOIS) and Theoretical scale Change (Change Theore **P** ASSIVE MICROWAVE remote sensing has the capability 48 to provide key elements of the terrestrial hydrological 49 cycle such as surface soil moisture [1], [2] and overland pre- 50 cipitation [3], [4]. Nevertheless, due to the large discrepancy 51 between the observation scale (several tens of km) and the scale 52 of physical interactions with the land surface (one wavelength 53 or several cm), the radiative transfer models applied to passive 54 microwave remote sensing data are only semiphysically based. 55 Consequently, the retrieval process of land surface parameters 56 from microwave brightness temperatures requires ancillary data 57 for calibration and validation purposes [5]. It also requires a 58 strategy to use such ancillary data since ground-based sampling 59 is often made over a small area/point, which constrasts with 60 the large integrated extent of spaceborne passive microwave 61 observations.

The soil moisture and ocean salinity (SMOS), [6]) satellite 63 was launched on November 2, 2009. Over land, the SMOS 64 mission aims at providing  $\sim$ 5 cm surface soil moisture data 65 at a spatial resolution better than 50 km and a repeat cycle of 66 less than 3 days. The payload is a 2-D interferometer equipped 67 with 69 individual L-band antennas regularly spaced along Y- 68 shaped arms. This new concept allows observing all pixels in 69 the 1000 km wide field of view at a range of incidence angles. 70 It also allows reconstructing brightness temperatures on a fixed 71 sampling grid [7]. 22

Since the SMOS launch, various field experiments (the 73 HOBE site in Denmark [8], the Mali site in Western Africa 74 [9], the SMOSMANIA site in Southwestern France [10] just 75 to name a few) have been undertaken to validate SMOS recon- 76 structed brightness temperatures and soil moisture retrievals. 77 The AACES (Australian Airborne Calibration/validation 78 Experiment for SMOS, [11]) is one of the most compre- 79 hensive campaigns worldwide dedicated to SMOS calibra- 80 tion/validation. A series of two experiments were undertaken 81 in 2010, AACES-1 in January-February (Austral summer) and 82

 AACES-2 in September (Austral winter). The data collected in AACES include 1-km resolution airborne L-band brightness temperature mapped over a 500 km by 100 km area, 20 days of very intensive ground measurements and 20 5 km by 2 km ground sampling areas.

 Even though the AACES ground measurements are very extensive, it is not feasible to cover the whole extent of a SMOS pixel by ground sampling alone. This is the reason why most validation strategies of spaceborne passive microwave data using *in situ* measurements have been based on the as- sumption that local observations are representative of a much larger spatial extent (i.e., the size of a microwave pixel). In the heterogeneous case where this assumption does not hold, up- scaling approaches [12], [13] have been developed to relate the available ground observations to satellite scale soil moisture. Such approaches are very useful over sites which have been monitored for a long time and where extensive measurements have been made over a range of spatial scales. However, aggre- gation rules are difficult to build over sites which have been set up recently, or where no extensive field campaigns have been undertaken.

 This study develops a methodology to facilitate the cali- bration and validation of SMOS data using localized ground measurements, such as those collected during AACES. The methodology combines upscaling (aggregation) and downscal- ing (disaggregation) approaches to make remote sensing and *in situ* observations match at an intermediate spatial resolution of 1 km. The key step in the procedure is a disaggregation algorithm of passive microwave soil moisture using kilometric optical data [14]–[16]. Disaggregating SMOS soil moisture can solve the disparity of spatial scales between satellite and *in situ* observations. However, the validation of spaceborne data by means of a disaggregation approach requires the uncertainties and potential error sources in downscaled data to be assessed. Generally speaking, disaggregation is a compromise between downscaling resolution and accuracy. The higher downscaling resolution, the more disaggregated values are spatially repre- sentative of ground observations, but typically have a lower accuracy and vice versa [17]. In this context, a disaggrega- tion algorithm named Disaggregation based on Physical And Theoretical scale Change (DisPATCh) is applied to 40-km resolution SMOS soil moisture over the AACES area using 1- km resolution Moderate resolution Imaging Spectroradiometer (MODIS) data. The objective is to test DisPATCh under various surface and atmospheric conditions. Specifically, the impact of climatic (evaporative demand), meteorologic (presence of clouds), and vegetation (cover and water status) conditions on 1-km resolution disaggregated soil moisture is evaluated both qualitatively by visual assessment of disaggregation images and quantitatively by comparing DisPATCh output with AACES intensive ground measurements.

 The AACES, SMOS, and MODIS data used in this study are first described. Next, the disaggregation methodology is presented followed by a step-by-step description of the Dis- PATCh algorithm. Results of the comparison between disag- gregated SMOS soil moisture and *in situ* measurements are then reported. To test DisPATCh under various surface and atmospheric conditions, the algorithm is run during AACES-1

and AACES-2 in different modes, by including (or not) a 141 correction for vegetation and atmospheric effects. Finally, some 142 perspectives in the use of DisPATCh for validating SMOS data 143 using ground-based sampling are given. 144

### II. DATA COLLECTION AND PREPROCESSING 145

The AACES experiments were planned to provide ground 146 and airborne soil moisture data over an area of approximately 147 500 km by 100 km during the two main seasons in the 148 Murrumbidgee river catchment, in southeastern Australia. The 149 first AACES campaign (AACES-1) was undertaken in summer 150 2010 from January 18 to February 21, and the second campaign 151 (AACES-2) was undertaken in the following Austral winter 152 from September 11 to September 24 [11]. Fig. 1 presents the 153 study area including the 20 5 km by 2 km ground sampling 154 focus areas. The background image is the MODIS 250-m res- 155 olution 16-day normalized difference vegetation index (NDVI) 156 product of February 2, 2010. The climate of the Murrumbidgee 157 catchment area ranges from semi-arid in the west to alpine in 158 the east, with a strong rainfall and potential evapotranspiration 159 gradient in the west-east direction. Land use is extensive graz- 160 ing in the west, cropping in the center, and mostly grazing/forest 161 in the east (refer to [11] for a detailed account of AACES). 162

*A. HDAS* 163

If over sites when they been studied that increases the C attention and the search that increases the MODIS 250-m respective measurements focus areas. The background image is the MODIS 250-m respective measurements focus During both AACES-1 and AACES-2, a spatially enabled 164 platform (Hydraprobe Data Acquisition System, HDAS) was 165 used to collect extensive measurements of near-surface soil 166 moisture. HDAS is a handheld system combining a soil dielec- 167 tric sensor (Hydraprobe) and a pocket PC with GPS receiver, 168 allowing for direct storage of location and measurement within 169 the GIS software. HDAS measurements were calibrated using 170 the approach presented in [18] with a root mean square error 171 of point estimate of about  $0.03 \text{ m}^3/\text{m}^3$ . The sampling coverage 172 was two 5 km by 2 km farms per day during AACES-1 and one 173 5 km by 2 km farm per day during AACES-2. Within each farm, 174 a total of six adjacent 5 km long transects separated by 330 m 175 were walked to cover each area of  $10 \text{ km}^2$ , and three separate 176 HDAS measurements were made along transects every 50 m. 177

In this study, HDAS soil moisture data are aggregated at 178 1-km resolution by averaging all measurements made within 179 each pixel of the MODIS resolution grid. Out of concern for 180 spatial representativeness of *in situ* observations, only the 1-km 181 pixels whose ground sampling covers more than two third of 182 its surface area are kept for comparison with disaggregation 183 results. The 1-km average of HDAS measurements is denoted 184  $\langle SM_{\rm HDAS} \rangle$  and the standard deviation of *in situ* measurements 185 (denoted  $\sigma_{\text{HDAS}}$ ) computed to estimate the subpixel variability 186 at 1-km resolution. 187

*B. SMOS* 188

The version-4 SMOS level-2 soil moisture product is used. 189 This product (released on March 24, 2011) was produced from 190 the reprocessed level 1C data, and the version-4 level-2 soil 191 moisture algorithm. SMOS has a 6 am (ascending) and 6 pm 192



Fig. 1. Overview of the study area. During AACES, ten 100 km by 50 km patches were overflown by an airborne L-band radiometer. Within each patch, two 5 km by 2 km subareas were sampled to collect spatial soil moisture measurements. In this study, DisPATCh is run over a 640 by 240 km area including the whole AACES area, and disaggregation results are evaluated over the ground sampling areas.

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The samp (descending) equator crossing time. The sampling grid of the SMOS level-2 soil moisture product is called DGG or discrete global grid [19], [20] and has a node separation of about 15 km. The DGG provides a discretization that is higher than the SMOS natural pixel size, which is 40 km on average, ranging from 30 km at boresight to 90 km at high incidence angles. In this study, the disaggregation procedure takes advan- tage of the oversampling of SMOS data to potentially reduce (and provide an estimate of) random errors in disaggregated SMOS data. Instead of using a single snapshot SMOS im- age, DisPATCh uses four (overlapping) independent snapshots, which are generated by: 1) sliding a 40-km resolution grid; and 2) extracting the DGG nodes approximately centered on each 40 km pixel. The extraction of SMOS DGG nodes is presented in [21]. The DGG node(s) that fall(s) near the center of the 208 40-km resolution pixels with a  $+/-10$ -km tolerance are se- lected. If more than one DGG is selected, the associated soil moisture values are averaged to produce a single value for each 40-km resolution pixel. The 40-km resolution grid that fits the study area corresponds to what is termed here Resampling 1. Similarly, Resampling 2, 3, and 4 are performed by sliding the 214 40-km resolution grid to coordinates  $(+20 \text{ km}, 0), (0, -20 \text{ km}),$  and ( +20 km, −20 km), respectively. The four 40-km resolu- tion SMOS data sets are then used independently as input to DisPATCh.

### 218 *C. MODIS*

219 The MODIS data used in this paper are composed of:

220 • Version-5 MODIS/Terra land surface temperature and

221 emissivity daily level-3 global 1-km grid product 222 (MOD11A1) and version-5 MODIS/Aqua land surface

temperature and emissivity daily level-3 global 1-km grid 223 product (MYD11A1). The land surface temperature data 224 set is the main component of DisPATCh. It is used to 225 estimate 1-km resolution soil evaporative efficiency at 226 10 am (Terra data) and 1 pm (Aqua data) [22]. 227

- Version-5 MODIS/Terra vegetation indices 16-day level-3 228 global 1-km grid product (MOD13A2). The NDVI data set 229 is used in DisPATCh to estimate the fractional vegetation 230 cover at 1-km resolution [23].
- Version-5 MODIS/Terra+Aqua albedo 16-day level-3 232 global 1-km grid product (MCD43B3). The surface albedo 233 data set is used in DisPATCh to estimate the vegetation 234 temperature at maximum water stress from the space land 235 surface temperature albedo [24]. The MCD43B3 product 236 provides 1-km data describing both directional hemispher- 237 ical reflectance (black-sky albedo) at local solar noon 238 and bihemispherical reflectance (white-sky albedo). In this 239 study, surface albedo refers to the MODIS shortwave white 240 sky albedo. 241
- MODIS/Terra level-1B calibrated radiances swath 1-km 242 grid product (MOD021KM) and MODIS/Aqua level- 243 1B calibrated radiances swath 1-km grid product 244 (MYD021KM). The radiance data set is used to derive 245 a land surface temperature data set that differs from the 246 official MOD11A1 and MYD11A1 products with respect 247 to atmospheric correction. 248

Products MOD11A1, MYD11A1, MOD13A2, and 249 MCD43B3 were downloaded through the NASA Warehouse 250 Inventory Search Tool (WIST http://wist.echo.nasa.gov/) and 251 products MOD021KM and MYD021KM were downloaded 252 through the NASA Level 1 and Atmosphere Archive and Dis- 253 tribution System (LAADS http://ladsweb.nascom.nasa.gov). 254

TABLE I SCALE AND OFFSET VALUES USED TO CONVERT TERRA (AND AQUA ) MODIS RADIANCE DATA TO PHYSICAL RADIANCE VALUES OVER THE AACES AREA

Thermal band	Scale (W m <sup><math>-2</math></sup> sr <sup><math>-1</math></sup> )	Offset $(-)$
	$8.4002 \cdot 10^{-4}$ $(6.5081 \cdot 10^{-4})$   1577 (2036)	
	$7.2970 \cdot 10^{-4}$ (5.7100 $\cdot 10^{-4}$ ) 1658 (2119)	

255 All products were projected in UTM 55 South with a sampling 256 interval of 1000 m using the MODIS reprojection tool.

257 The level-1B calibrated radiance data ( $R_{31}$  and  $R_{32}$  for bands 258 31 and 32, respectively) were converted from digital number 259 (DN) to radiance in W m<sup>-2</sup> sr<sup>-1</sup> using the radiance scales and 260 offsets provided with each MODIS granule as listed in Table I

$$
R_{\lambda} = \text{Scale}_{\lambda} \times (\text{DN}_{\lambda} - \text{Offset}_{\lambda}) \tag{1}
$$

261 The radiance values were then converted to brightness temper-262 ature in K using the inverse of the Planck function [25]

$$
Tb_{\lambda} = \frac{c_2}{\lambda \ln\left(1 + \frac{c_1}{R_{\lambda}\lambda^5}\right)}\tag{2}
$$

263 with  $c_1 = 1.19107 \times 10^8$   $\mu$ m<sup>5</sup> W m<sup>-2</sup> sr<sup>-1</sup> and  $c_2 =$ 264  $1.43883 \times 10^4 \mu$ m K, for center wavelength of the given band 265 (11.0186  $\mu$ m and 12.0325  $\mu$ m for 31 and 32 band, respectively).

### 266 *D. Overlapping HDAS, SMOS, and MODIS Data and* 267 *Generating an Input Data Set*

 As indicated in Table II, HDAS soil moisture, SMOS soil moisture, and cloud-free MODIS land surface temperature data have overlapped on five days during AACES-1 (on January 28 and 30 and February 15, 18, and 20) and on five days during AACES-2 (on September 11, 13, 21, 22, and 24). On each sampling day, two farms were sampled during AACES-1 (except on February 18 when three farms were sampled), and one farm was sampled during AACES-2, so that disaggregation results can be evaluated for ten date-farm units during AACES-1 and five date-farm units during AACES-2.

 DisPATCh is applied to an input ensemble composed of the different combinations of available SMOS (ascending orbit at 6 am and/or descending orbit at 6 pm) and MODIS (onboard Terra platform at 10 am and/or Aqua platform at 1 pm) data. To increase the quantity of input data sets, the MODIS data col- lected on the day before and the day after the SMOS overpass date are also included. For SMOS data on day of year (DoY) 51, the clear sky MODIS data collected on DoY 54 are used. Note that one implicitly assumes that no rainfall occurs between MODIS and SMOS overpasses, and that the spatial variability captured by MODIS is relatively similar to the actual variabil- ity of surface soil moisture at the time of SMOS overpass. Moreover, the SMOS data oversampling is used to generate four (overlapping) 40-km resolution SMOS grids on which DisPATCh is run independently, thus increasing the number of downscaled data that could be used in the validation. It is reminded that the spacing (about 15 km) between neighboring SMOS DGG nodes is smaller than the SMOS resolution (about

40 km). By combining the four SMOS grids, the two potential 296 SMOS data sets (two orbits in one day) and the six potential 297 MODIS data sets (three days including two overpasses each), 298 the maximum number of input data sets is 48. The generation 299 of input data sets is shown in Fig. 2 and the number of daily 300 input data sets is indicated for each date-farm unit in Table II. 301

### III. DISAGGGREGATION ALGORITHM 302

DisPATCh converts 1-km resolution MODIS-derived soil 303 temperature fields into 1-km resolution surface soil moisture 304 fields given a semi-empirical soil evaporative efficiency model 305 [26] and a first-order Taylor series expansion around the 306 40-km resolution SMOS observation. DisPATCh is an im- 307 proved version of the algorithms in [16] and [27], and mainly 308 differs with regard to the representation of the vegetation water 309 status. In previous versions [16], [27], the soil temperature was 310 derived from MODIS land surface temperature by assuming 311 that vegetation was unstressed so that vegetation temperature 312 was uniformly set to the minimum surface temperature ob- 313 served within the SMOS pixel. In this study, the approach in 314 [28] is implemented to take into account vegetation water status 315 in the estimation of soil temperature. 316

### *A. Disaggregation Methodology* 317

DN<sub>A</sub> - Offsets, (1) differs with regard to the representation of the vegatition water<br>states. In previous versions [16], [27], the soil temperature with<br>certain and states. In previous versions [16], [27], the soil tempe The disaggregation procedure decouples the soil evaporation 318 from the 0–5 cm soil layer and the vegetation transpiration 319 from the root-zone soil layer by separating MODIS surface 320 temperature into its soil and vegetation components as in the 321 triangle or trapezoidal method [28], [29]. MODIS-derived soil 322 temperature is then used to estimate soil evaporative efficiency, 323 which is known to be relatively constant during the day on clear 324 sky conditions. MODIS-derived soil evaporative efficiency is 325 finally used as a proxy for surface (0–5 cm) soil moisture 326 variability within the SMOS pixel. The link between surface 327 soil moisture and soil evaporative efficiency at different scales 328 is ensured by a downscaling relationship and a soil evapo- 329 rative efficiency model, as described below in more detail. 330 The originality of DisPATCh relies on a dynamical land cover 331 classification (based on the hourglass approach in [28]) that 332 takes into account the subpixel variability of the sensitivity of 333 soil evaporative efficiency to surface soil moisture. 334

*1) Downscaling Relationship:* The downscaling relation- 335 ship can be written as 336

$$
SM_{1 \text{ km}} = SM_{SMOS} + \frac{\partial SM_{mod}}{\partial SEE} \times (SE_{MODIS,1 \text{ km}} - \langle SEE_{MODIS,1 \text{ km}} \rangle_{40 \text{ km}})
$$
(3)

with **SM<sub>SMOS</sub>** being the SMOS soil moisture (for clarity, 337 the variables defined at SMOS scale are written in bold), 338  $SEE_{\text{MODIS}}$  the MODIS-derived soil evaporative efficiency (ra- 339) tio of actual to potential evaporation),  $\langle$ SEE<sub>MODIS</sub> $\rangle$ <sub>40 km</sub> its 340 average within a SMOS pixel and ∂**SMmod**/∂**SEE** the partial 341 derivative evaluated at SMOS scale of soil moisture with re- 342 spect to soil evaporative efficiency. Note that the linearity of (3) 343 implies that a possible bias in SMOS data would produce the 344

### TABLE II

LIST OF OVERLAPPING HDAS, SMOS, AND MODIS (MOD11A1 AND MYD11A1) DATA DURING AACES-1 AND AACES-2. ONLY THE SMOS DATA COLLECTED ON THE SAME DAY AS GROUND SAMPLING HAVE BEEN CONSIDERED. THE MODIS DATA CONSIDERED AS INPUT TO DISPATCH HAVE BEEN COLLECTED WITHIN PLUS OR MINUS ONE DAY EITHER SIDE THE GROUND SAMPLING (AND SMOS OVERPASS) DATE. ON EACH SAMPLING DATE, THE RESULTANT NUMBER OF INPUT DATA SETS TO DISPATCH IS ALSO INDICATED





Fig. 2. Schematic diagram presenting the combination of SMOS and MODIS to generate an ensemble of input data to DisPATCh. The output data are composite d at 1-km resolution by computing the average  $(SM_{1 \text{ km}})$  and standard deviation  $(\sigma_{SM,1 \text{ km}})$  of disaggregated SMOS soil moisture.

 same bias in disaggregated data [30]. Consequently, although the possible presence of a bias in SMOS data limits the accuracy in the disaggregated soil moisture, it is not a limiting factor to the applicability of DisPATCh. MODIS derived soil evaporative efficiency is expressed as a linear function of soil temperature

$$
SEE_{\text{MODIS},1 \text{ km}} = \frac{\mathbf{T}_{\mathbf{s},\mathbf{max}} - T_{\mathbf{s},1 \text{ km}}}{\mathbf{T}_{\mathbf{s},\mathbf{max}} - \mathbf{T}_{\mathbf{s},\mathbf{min}}} \tag{4}
$$

350 with  $T<sub>s</sub>$  being the MODIS-derived soil skin temperature,  $T_{s, max}$  the soil skin temperature at  $SEE = 0$  and  $T_{s, min}$ 352 the soil skin temperature at  $SEE = 1$ . The linearity of the relationship between soil evaporative efficiency and surface soil temperature was verified using the physically based dual source energy budget model in [31] using a synthetic data set composed of a range of surface soil moisture values and differ- ent atmospheric conditions (results not shown). End-members **T s** ,**min** and **T s** ,**max** are estimated from the polygons obtained

by plotting MODIS surface temperature against MODIS NDVI 359 and MODIS albedo as in [24]. Derivation of soil temperature is 360 based on a linear decomposition of the surface temperature into 361 its soil and vegetation components as a good approximation of 362 the relationship with fourth power for temperatures [32], [33] 363 and consistent with the triangle method. MODIS-derived soil 364 skin temperature is expressed as  $365$ 

$$
T_{\rm s,1\ km} = \frac{T_{\rm MODIS} - f_{\rm v,1\ km} T_{\rm v,1\ km}}{1 - f_{\rm v,1\ km}}
$$
(5)

with  $T<sub>MODIS</sub>$  being the 1-km resolution MODIS land sur-366 face temperature,  $f_v$  the MODIS-derived fractional vegetation 367 cover, and  $T_v$  the vegetation temperature. In this study, vegeta- 368 tion temperature is estimated using the approach proposed by 369 [28]. In (5), fractional vegetation cover is written as  $370$ 

$$
f_{\rm v,1\ km} = \frac{\rm NDVI_{MODIS} - NDVI_{s}}{\rm NDVI_{v} - NDVI_{s}} \tag{6}
$$

 with NDVI<sub>MODIS</sub> being the 1-km resolution MODIS NDVI, **NDVI <sup>s</sup>** the NDVI corresponding to bare soil, and **NDVI <sup>v</sup>** the NDVI corresponding to full-cover vegetation. Minimum and maximum NDVI values are set to 0.15 and 0.90, respectively. In [16], the accuracy and robustness of the disaggregation methodology were tested using three different formulations of soil evaporative efficiency [26], [34], [35]. Results based on the NAFE'06 data set [36], which was collected over a 60 km by 40 km area in the AACES area, indicated that the model in [26] was better adapted for conditions where soil properties are unknown at high resolution. Consequently, the partial derivative in (3) is computed using the soil evaporative efficiency model 383 in [26]

$$
SEE_{\text{mod}} = \frac{1}{2} - \frac{1}{2}\cos(\pi \cdot SM / SM_{\text{p}})
$$
 (7)

 with **SM <sup>p</sup>** being a soil parameter (in soil moisture unit). In [26], **SM <sup>p</sup>** was set to the soil moisture at field capacity. In DisPATCh, **SM <sup>p</sup>** is retrieved at 40-km resolution from SMOS and aggregated MODIS data [16]. By inverting (7), one obtains

$$
SM_{\text{mod}} = \frac{SM_{\text{p}}}{\pi} \cos^{-1}(1 - 2 \text{SEE})
$$
 (8)

 *2) Vegetation Temperature:* Vegetation temperature in (5) is estimated at 1-km resolution with the "hourglass" approach in [28]. By plotting the diagonals in the quadrilateral in Fig. 3, four areas are distinguished in the space defined by surface temperature and fractional vegetation cover. In zone A, land surface temperature is mainly controlled by soil evaporation leading to optimal sensitivity to surface soil moisture. In zone D, land surface temperature is mainly controlled by vegetation transpiration with no sensitivity to surface soil moisture. In zones B and C, land surface temperature is controlled by both soil evaporation and vegetation transpiration with intermediate (average) sensitivity to surface soil moisture. Based on this un- derstanding, vegetation temperature is estimated in a different manner in each zone.

402 For a given data point located in Zone A, vegetation temper-403 ature is

$$
T_{\mathbf{v},1 \text{ km}} = (\mathbf{T}_{\mathbf{v},\mathbf{min}} + \mathbf{T}_{\mathbf{v},\mathbf{max}})/2
$$
 (9)

404 with  $T_{v,min}$  and  $T_{v,max}$  being the vegetation temperature 405 at minimum and maximum water stress, respectively. End-406 members  $T_{v,min}$  and  $T_{v,max}$  are estimated from the poly-407 gons obtained by plotting MODIS surface temperature against 408 MODIS NDVI and MODIS albedo as in [24].

409 For a given data point located in Zone B, vegetation temper-410 ature is

$$
T_{\mathbf{v},1 \text{ km}} = (T_{\mathbf{v},\text{min},1 \text{ km}} + \mathbf{T}_{\mathbf{v},\text{max}})/2 \tag{10}
$$

411 with  $T_{\rm v,min,1\ km}$  being the vegetation temperature associated 412 with  $\text{SEE} = 0$  ( $T_s = \mathbf{T}_{s,\text{max}}$ ).

413 For a given data point located in Zone C, vegetation temper-414 ature is

$$
T_{\rm v,1\ km} = (\mathbf{T}_{\mathbf{v},\mathbf{min}} + T_{\rm v,max,1\ km})/2 \tag{11}
$$



Fig. 3. Polygon defined in the land surface temperature-fractional vegetation cover space contains four distinct zones A, B, C, and D. In Zone A (soildominated area), the estimated vegetation temperature is constant leading to optimal sensitivity of estimated soil temperature to surface soil moisture. In Zone D, the estimated soil temperature is constant with no sensitivity to surface soil moisture. In Zone B and C (mixed surface), surface temperature is both controlled by soil evaporation and vegetation transpiration with intermediate (average) sensitivity of estimated soil temperature to surface soil moisture. DisPATCh can be run in the Zone A+B+C mode or in the Zone A only mode.



Fig. 4. Temperature end-members  $T_{s,min}$ ,  $T_{s,max}$ ,  $T_{v,min}$ , and  $T_{v,max}$  are estimated from the surface temperature-fractional vegetation cover space and the surface temperature-surface albedo space within two given SMOS pixels. In (b), the pixel corresponding to the largest MODIS albedo has a fractional vegetation cover larger than 0.5, so that  $T_{v, max}$  is set to its surface temperature. In (d), the pixel corresponding to the largest MODIS albedo has a fractional vegetation cover lower than 0.5, so that  $T_{\mathbf{v},\mathbf{max}}$  is set to  $T_{\mathbf{v},\mathbf{min}}$ .

415 with  $T_{v, \text{max}, 1 \text{ km}}$  being the vegetation temperature associated 416 with  $\text{SEE} = 1$  ( $T_s = T_{s,\text{min}}$ ).

417 For a given data point located in Zone D, vegetation temper-418 ature is

$$
T_{\rm v,1\ km} = (T_{\rm v,min,1\ km} + T_{\rm s,max,1\ km})/2 \tag{12}
$$

 *3) End-Members:* End-members **T s** ,**min** , **T s** ,**max** , **T v** ,**min** and **T v** ,**max** are estimated by combining the spatial information provided by the surface temperature-fractional vegetation cover space and the surface temperature-albedo space plotted using MODIS data collected in a 40-km resolution SMOS pixel. An illustration is provided in Fig. 4 for two given SMOS pixels.

- 425 • **T v** ,**min**: the vegetation temperature at minimum vegeta-426 tion water stress is set to the minimum MODIS surface 427 temperature in the SMOS pixel [see Fig. 4(a) and (c)].
- 428 • **T v** ,**max**: the vegetation temperature at maximum vegeta-429 tion water stress is set to the MODIS surface temperature 430 of the pixel with the maximum value of MODIS albedo in 431 the SMOS pixel [see Fig. 4(b)]. If the fractional vegetation 432 cover of that pixel is lower than 0.5 [see Fig. 4(d)], the veg-433 etation temperature at maximum vegetation water stress 434 is alternatively set to **T v** ,**min**, meaning that vegetation is 435 unstressed within the SMOS pixel. The condition based 436 on fractional vegetation cover is lower than 0.5 aims to 437 increase the robustness of the determination approach of

**T v** ,**max**, particularly in the SMOS pixels where all surface 438 conditions are not met. 439

- $T_{\rm s,min}$ : the soil temperature at SEE = 1 is extrapolated 440 along the wet soil edge at  $f_v = 0$ . The wet soil edge 441 is defined as the line passing through  $(1, \mathbf{T}_{\mathbf{v},\mathbf{min}})$  and 442 through the data point such that all the data points with 443  $f_{\rm v}$  < 0.5 are located above the wet soil edge [see Fig. 4(a) 444 and (c)].  $445$
- $\mathbf{T}_{\mathbf{s},\mathbf{max}}$ : the soil temperature at SEE = 0 is extrapolated 446 along the dry soil edge at  $f_v = 0$ . The dry soil edge 447 is defined as the line passing through  $(1, T_{\mathbf{v},\mathbf{max}})$  and 448 through the data point such that all the data points with 449  $f_{\rm v}$  < 0.5 are located below the dry soil edge [see Fig. 4(a) 450 and (c)].  $451$

### *B. Atmospheric Correction* 452

In MOD11A1 and MYD11A1 products, the land surface 453 temperature is derived from MODIS thermal radiances using 454 the split window algorithm [37] 455

$$
T_{\text{MODIS}} = C + \left(A_1 + A_2 \frac{1 - \epsilon}{\epsilon} + A_3 \frac{\Delta \epsilon}{\epsilon^2}\right) \frac{Tb_{31} + Tb_{32}}{2} + \left(B_1 + B_2 \frac{1 - \epsilon}{\epsilon} + B_3 \frac{\Delta \epsilon}{\epsilon^2}\right) \frac{Tb_{31} - Tb_{32}}{2} \tag{13}
$$

456 with  $T b_{31}$  and  $T b_{32}$  being the brightness temperatures mea-457 sured in the MODIS bands 31 and 32, respectively,  $\epsilon_{31}$  and  $\epsilon_{32}$  the surface emissivities estimated in the respective bands, and  $A_1$ ,  $A_2$ ,  $A_3$ ,  $B_1$ ,  $B_2$ ,  $B_3$ , and C regression coefficients. These coefficients are available during algorithm execution via a look up table stratified by subranges of near surface air temperature and total column water vapor. These input field are obtained at a 5-km resolution from the MODIS07\_L2 product.

 Given that regression coefficients in (13) are provided at 5-km resolution, the atmospheric corrections on the MODIS land surface temperature product are actually made at 5-km resolution. To test whether atmospheric corrections on MODIS temperature have an impact on disaggregation results, a differ- ent procedure is proposed to obtain another temperature data set whose atmospheric corrections are operated at the scale of a SMOS pixel, i.e., at 40-km resolution (instead of 5-km resolution for the official MODIS temperature product). The approach is to normalize the mean MODIS radiance-derived brightness temperature at the SMOS resolution. Normalization is done by adjusting the minimum and maximum mean MODIS brightness temperature to the minimum and maximum value of the official MODIS land surface temperature product within the SMOS pixel, respectively. The new temperature noted  $T_{\text{MODIS}}^{\text{unif. corr.}}$  (uniform atmospheric corrections) is written

$$
T_{\text{MODIS}}^{\text{unif. corr.}} = T_{\text{MODIS,min}} + (T_{\text{MODIS,max}} - T_{\text{MODIS,min}})
$$

$$
\times \frac{Tb_{31} + Tb_{32} - \text{Min}(Tb_{31} + Tb_{32})}{\text{Max}(Tb_{31} + Tb_{32}) - \text{Min}(Tb_{31} + Tb_{32})} \quad (14)
$$

 with T**MODIS** ,**min** and T**MODIS** ,**max** being the minimum and maximum MODIS land surface temperature within the SMOS pixel, and **Min**() and **Max**() the function that returns the mini- mum and maximum value within the SMOS pixel, respectively. Note that the underlying assumptions of (14) are:

- 485 near surface air temperature and column water vapor vary
- 486 at scales larger than 40 km (size of a SMOS pixel).
- 487 surface emissivity is close to 1.

### 488 *C. Algorithm*

 The steps used in applying DisPATCh include: 1) select- ing the SMOS pixels with at least 90% (clear sky) MODIS- retrieved land surface temperature coverage; 2) computing soil evaporative efficiency over nominal MODIS pixels with (4); 3) estimating soil evaporative efficiency over non-nominal MODIS pixels; 4) retrieving parameter **SM <sup>p</sup>**; 5) applying the downscaling relationship of (3); 6) correcting disaggregated soil moisture by the SMOS pixel weighting function; and 7) compositing on a daily basis the disaggregation output en- semble [21]. The input and output data and their link within DisPATCh are summarized in Fig. 5.

 *1) Selecting Clear Sky SMOS Pixels:* A threshold of 90% cloud-free MODIS coverage is used to select the SMOS pix- els to be disaggregated. In the official MODIS land surface temperature product (MOD11A1 for Terra and MYD11A1 for Aqua), the data affected by the presence of clouds are already masked. Hence, selection of the 90% clear sky SMOS pixels is



Fig. 5. Schematic diagram presenting the input and output data of DisPATCh.

directly based on the MODIS land surface temperature product 506 masking. 507

It resolution (instead of  $\theta$ -final control instead of the same of the same of the same of the correction and maximum mean MODIS and maximum means and maximum means and maximum means are corrections) is written<br>  $\lim_{n \to \$ *2) Non-Nominal Pixels:* Nominal MODIS pixels are de- 508 fined as the 1-km resolution pixels that do not include open 509 water and where land surface temperature is actually retrieved. 510 Open water pixels are flagged in the algorithm when MODIS 511 NDVI retrievals yield negative values. The soil evaporative 512 efficiency of open water pixels is set to 1. The emerged pixels 513 where land surface temperature is not retrieved (due to the 514 presence of some clouds within the SMOS pixel) are processed 515 as pixels with mean surface conditions. In practice, the soil 516 evaporative efficiency of cloudy pixels (which represent less 517 than 10% of the surface area within the SMOS pixel) is set to 518 the mean soil evaporative efficiency calculated over the clear 519 sky MODIS pixels. Allocating a soil evaporative efficiency 520 value to non-nominal pixels allows DisPATCh to be run over a 521 wider range of SMOS pixels, including those partially covered 522 by clouds. However, non-nominal 1-km resolution pixels are 523 flagged and discarded from the disaggregation output ensemble. 524

> *3) Forested Areas:* In this study, DisPATCh is applied to all 525 the SMOS pixels where the soil moisture retrieval is successful, 526 even those including forest class, as long as the 1 km MODIS 527 pixels are in Zone A, B or C (see Fig. 3). This choice is 528 relevant here because the AACES extensive data were almost 529 exclusively collected in agricultural areas (cropping/grazing), 530 so forests for this study are not an issue. In the case of a 531 mixed SMOS pixel including a significant fraction of forest, 532 DisPATCh should be applied to the surface area of the dominant 533

534 class, thus excluding the surface area of the minority land cover 535 classes.

536 *4) Calibration:* The soil moisture parameter **SM <sup>p</sup>** used to 537 compute ∂**SMmod**/∂**SEE** in (3) is estimated by inverting the 538 SEE model in (7) at SMOS resolution

$$
SM_{p} = \frac{\pi \cdot SM_{SMOS}}{\cos^{-1} \left(1 - 2\langle SEE_{MODIS,1 \text{ km}}\rangle_{40 \text{ km}}\right)} \tag{15}
$$

 A value of **SM <sup>p</sup>** is obtained for each SMOS pixel and each input data set. Note that the main assumption limiting validity of the calibration approach is the soil evaporative efficiency model [26] itself. The soil evaporative efficiency model in [26] was chosen for its simplicity (one parameter) and its ability to represent the general behavior of soil evaporative efficiency over the full range of soil moisture: particularly the null deriva- tive at zero and at maximum soil moisture, and an inflexion point in between [38]. However, it has some inconsistencies. In particular, [38] have indicated that 1) potential evaporation is physically reached at soil saturation and not at field capac- ity; therefore the model in [26] should be (strictly speaking) parameterized by the soil moisture at saturation and not by the soil moisture at field capacity, and 2) soil evaporative efficiency varies with potential evaporation, meaning that the soil moisture parameter (set to the soil moisture at field capacity in [26]) should theoretically vary in time with atmospheric evaporative demand. Consequently, the **SM <sup>p</sup>** retrieved from SMOS and MODIS data using the model in [26] is definitely not the soil moisture at field capacity as in [26], although it could be in part related to it. In this study, **SM <sup>p</sup>** is therefore considered to be a fitting parameter self-estimated by DisPATCh.

 *5) Weighting Function:* A SMOS pixel WEighting Function (WEF) is used to take into account the impact of soil mois- ture distribution on the SMOS scale soil moisture as seen by SMOS radiometer. A centrosymmetric analytical approxima-tion MEAN\_WEF is provided in [19], [20]

$$
MEAN\_WEF(\rho) = C_{\text{MWEF2}} + WEF_A \left( \frac{\rho}{C_{\text{MWEF1}}} \cdot \frac{\pi}{C_{\text{WEF1}}} \right)
$$
\n(16)

566 with  $\rho$  being the distance from the SMOS pixel center, and 567  $C_{\text{MWEF1}} = 40 \text{ km}, C_{\text{MWEF2}} = 0.027, C_{\text{WEF1}} = 73.30 \text{ and}$ 

$$
WEF_A(\rho') = \frac{\left[\operatorname{sinc}(C_{WEF1} \cdot \rho')\right]^{C_{WEF2}}}{1 + C_{WEF3} \cdot \rho'^{C_{WEF4}}} \tag{17}
$$

568 with  $\rho'$  being the distance in the director cosines coordinates, 569 sinc $(x) = \sin(x)/x$ , and  $C_{\text{WEF2}} = 1.4936$ ,  $C_{\text{WEF3}} = 524.5$ 570 and  $C_{\text{WEF4}} = 2.103$ .

571 A correction is applied to disaggregated soil moisture in (3)

$$
SM_{1 \text{ km}}^{\text{wef corr.}} = SM_{1 \text{ km}} + \frac{\sum \text{MEAN\_WEF}(\rho) \cdot SM_{1 \text{ km}}(\rho)}{\sum \text{MEAN\_WEF}(\rho)} - SM_{\text{SMOS}} \quad (18)
$$

572 with  $SM_{1 \text{ km}}^{\text{wef corr.}}$  being the WEF-corrected disaggregated soil moisture. Mathematically speaking, one should replace  $\texttt{SM}_{\texttt{SMOS}}$  with  $\sum \texttt{MEAN\_WEF} \cdot \texttt{SM}_{1 \text{ km}} / \sum \texttt{MEAN\_WEF}$ in (3) and (15) and run an iteration loop until convergence

of  $SM_{1 \text{ km}}^{\text{wef corr.}}$  values. However, the impact of the WEF on 576 disaggregated soil moisture is expected to be low so that the 577 simple correction in (18) is considered to be sufficient for the 578 purpose of the study. 579

*6) Disaggregation Output:* The downscaling relationship in 580 (3) is applied to each input data set, and the disaggregated soil 581 moisture data ensemble is averaged on each 1-km resolution 582 pixel within the study area. Averaging is a way to reduce 583 random uncertainties in the disaggregation output. In [17], [27], 584 disaggregated soil moisture was averaged in space (aggregated) 585 at the expense of downscaling resolution. Herein, temporal 586 averaging [30] is preferred to keep an optimal downscaling 587 resolution. Note that a condition to average disaggregated soil 588 moisture in time is the availability of thermal infrared data 589 at high temporal frequency. Another significant advantage of 590 applying DisPATCh to an input ensemble is to provide an 591 estimate of the uncertainty in 1-km resolution disaggregated 592 soil moisture, e.g., by computing the standard deviation within 593 the output ensemble. 594

IV. APPLICATION 595

To test DisPATCh under various surface and atmospheric 596 conditions, the algorithm is run during AACES-1 and AACES- 597 2 in different modes, by including (or not) a correction for 598 vegetation and atmospheric effects. In each case, disaggregated 599 SMOS soil moisture and HDAS measurements are compared 600 at 1-km resolution for all date-farm units with overlapping 601 HDAS/SMOS/MODIS data. 602

*A. Null Hypothesis* 603

In this study, the null hypothesis is defined as the application 604 of DisPATCh with parameter **SM <sup>p</sup>** set to zero in (8). Hence, 605 the downscaling relationship in (3) becomes 606

$$
SM_{1 \text{ km}} = SM_{SMOS} \tag{19}
$$

Il moisture, and an inflexion applying DisPATCh to an input ensemble is to provide an<br>it in some inconsistencies, estimate of the uncertainty in 1-km resolution disaggregated<br>that 1) potential exaporation soil moisture, e meaning that no 1-km information is used. Defining a null 607 hypothesis is useful to test whether DisPATCh is able to re- 608 produce the subpixel variability within the  $\sim 10 \text{ km}^2 \text{ sam}$  609 pling farms with better skill than simply assuming a uniform 610 moisture condition. Statistical results in terms of root mean 611 square difference, mean difference, correlation coefficient, and 612 slope of the linear regression between the SMOS soil moisture 613 disaggregated with (19) and *in situ* measurements are listed in 614 Table III. One observes that the root mean square difference 615 is generally explained by a (negative) bias in SMOS data and 616 that none of the correlations evaluated at 1-km resolution for 617 each farm separately is statistically significant (all calculated p- 618 values are larger than 0.10). Thus, the rationale for developing 619 DisPATCh is to improve the correlation at fine scale between 620 SMOS and ground soil moisture and to reduce the bias in 621 disaggregated SMOS data in the specific case where the bias 622 in SMOS data at the farm scale is due to the heterogeneity of 623 soil moisture within the SMOS pixel. 624

### TABLE III DisPATCh Is Run With No 1-km Information (**SM<sub>p</sub>Set to Zero) and Statistical Results Are Listed in Terms of Root Mean Square** DIFFERENCE (RMSD), MEAN DIFFERENCE (BIAS), CORRELATION COEFFICIENT (R), AND SLOPE OF THE LINEAR REGRESSION BETWEEN 1-km RESOLUTION DISAGGREGATED SMOS SOIL MOISTURE AND 1-km AGGREGATED IN SITU MEASUREMENTS. THE MEAN AND STANDARD DEVIATION OF GROUND MEASUREMENTS ( $\langle \rm SM_{HDAS} \rangle$ and  $\sigma_{HDAS}$ ), the Number of Considered 1-km PIXELS, AND STATISTICAL SIGNIFICANCE (P-VALUE) ARE ALSO LISTED FOR EACH DATE-FARM UNIT



### 625 *B. Visual Assessment of Disaggregation Images*

 As an example, DisPATCh is applied on DoY 49 over a 120 km by 80 km subarea including the farms F16, F17, F18, F19, and F20. The images of 1-km resolution disaggregated SMOS soil moisture are presented in Fig. 6. DisPATCh is run with **SM <sup>p</sup>** set to zero (null hypothesis) and in four distinct modes corresponding to the combinations of the "LST" (the official MODIS land surface temperature product is used) and "RAD" [the land surface temperature is derived from MODIS radiances using (14)] modes and the "Zone A+B+C" (the vegetation- transpiration dominated 1-km pixels are discarded) and "Zone A only" (only the soil evaporation-dominated 1-km pixels are selected) modes.

 In Fig. 6, the SMOS DGG nodes where level-2 soil moisture is successfully retrieved are overlaid on the image correspond- ing to the null hypothesis (resampled SMOS data with no 1-km information) for 6 am and 6 pm overpass times separately. The gaps in SMOS data in the lower middle part of the images are due to topography flagging over the Australian Alps. In the version-4 SMOS level-2 processor, soil moisture is not retrieved at the DGG nodes where the topography effects on simulated brightness temperatures exceed a certain threshold, so as to prevent large errors in soil moisture values. The appar- ent resolution of the null hypothesis image is 20 km because it is generated from the composition of four 40-km resolution resampled SMOS snapshot images, whose resampling grids are separated by 20 km (the SMOS level-2 data resampling strategy 651 was described in Section II-B.).

Note that the disaggregation products in the Zone A+B+C 653 mode cover an area larger than the area sampled by SMOS 654 data, because the SMOS resolution (about 40 km) is larger 655 than the SMOS product sampling length (about 15 km), but 656 does not provide disaggregated values at a distance larger than 657 20 km from the successful retrieval nodes. Concerning the Zone 658 A only mode, disaggregation products do not cover an area 659 larger than the SMOS sampling area because the Australian 660 Alps are surrounded by forests where the fraction of bare soil is 661 less than elsewhere in the area, and which correspond to Zone 662 B or C in the hourglass in Fig. 3. 663

When looking at the images obtained in the Zone A+B+C 664 mode in Fig. 6, one observes that the spatial structures of 665 1-km disaggregated SMOS soil moisture encompass, but does 666 not seem to be correlated with, the SMOS data sampling 667 length. However, a "boxy artifact" is still apparent at 20-km 668 resolution, which is the separation length of the SMOS data 669 resampling grids as explained in Section II-B. The notion of 670 "boxy artifact" was introduced by [39] to analyze the quality of 671 a disaggregation approach. The less apparent the low-resolution 672 boxes, the better the disaggregation skill of the algorithm to 673 spatially connect high-resolution disaggregated values between 674 neighboring low-resolution pixels, and thus to derive a realistic 675 high-resolution soil moisture field. When comparing the images 676 obtained in the Zone A+B+C mode with those obtained in the 677



Fig. 6. Images of disaggregation results over a 120 km by 80 km subarea on DoY 49. The disaggregated soil moisture (SM<sub>1 km</sub>) and its estimated uncertainty  $(\sigma_{\text{SM},1 \text{ km}})$  are compared in the LST and RAD modes and in the Zone A+B+C and Zone A only modes. Sampling farms are overlaid on all images. SMOS DGG nodes are overlaid on the image corresponding to the null hypothesis (no 1-km resolution information) presented at top.

 Zone A only mode, one observes that the 20-km resolution boxy artifact is less apparent in the Zone A only mode, consistent with the better sensitivity of MODIS-derived SEE with soil- dominated pixels (Zone A) than with mixed-surface (Zone B and C) pixels. In Fig. 6, the images obtained in the LST and RAD mode highlight different spatial structures. In general, there are less data gaps in the RAD than in the LST mode. However, ground validation data are required to assess their relative quality/accuracy.

687 As an assessment of the uncertainty in composited soil mois-688 ture disaggregation, the standard deviation within the disaggre-689 gation output ensemble is also reported for each disaggregation product in Fig. 6. The same observations can be made as with 690 the soil moisture images: spatial structures are more visible, and 691 the boxy artifact is less apparent in the RAD than in the LST 692 mode. In general, the estimated uncertainty in disaggregated 693 products is larger in the RAD than in the LST mode, regardless 694 of the Zone (A+B+C or A only) mode. 695

### *C. SMOS Weighting Function* 696

To evaluate the impact of the SMOS instrument weighting 697 function on disaggregation results, DisPATCh is run with (and 698 without) the WEF correction in (18). The expected effect of the 699



Fig. 7. Uncorrected versus WEF-corrected SMOS soil moisture for the entire data set.

 WEF is a bias at 40 km resolution on disaggregated soil mois- ture. Fig. 7 plots the uncorrected against WEF-corrected SMOS soil moisture for the entire data set including both AACES-1 and AACES-2 experiments. The WEF correction has very little impact on disaggregated soil moisture with a maximum difference between uncorrected and WEF-corrected SMOS soil 706 moisture of 0.02  $\text{m}^3/\text{m}^3$ , a mean difference of approximately 707 zero, and a standard deviation of 0.003  $\text{m}^3/\text{m}^3$ . Although the difference is small with this data set, WEF-corrected products are expected to be more realistic. Therefore, the correction in (18) is used in all the DisPATCh runs that follow.

### 711 *D. Quantitative Comparison With In Situ Measurements*

 Fig. 8 presents the scatterplots of 1-km resolution disaggre- gated SMOS soil moisture versus 1-km resolution aggregated *in situ* measurements for the ten date-farm units during AACES-1. On each graph are plotted the soil moisture dis- aggregated in the Zone A+B+C mode (empty squares) and the soil moisture disaggregated in the Zone A only mode (black squares). At the beginning of AACES-1, conditions are very dry so that SMOS retrievals are close to zero and the 720 variability of *in situ* measurements is low (about  $0.02 \text{ m}^3/\text{m}^3$ ). In such conditions, no useful information is expected from the application of DisPATCh, and the statistical results in terms of spatial correlation are not meaningful for DoY 28/F05, DoY 30/F07 and DoY 30/F08. While wetter conditions occur after DoY 30, cloud cover prevents DisPATCh to be run (MODIS data are unavailable) until DoY 46. On DoY 46, the average and standard deviation of *in situ* soil moisture measurements is 728 0.32 m<sup>3</sup>/m<sup>3</sup> and 0.06 m<sup>3</sup>/m<sup>3</sup>, respectively. The spatial variabil- ity of 1-km soil moisture is nicely captured by DisPATCh no- tably in the RAD mode. On DoY 49, the disaggregated SMOS soil moisture is still correlated with the *in situ* measurements made in three farms (F17, F18, and F20). On the last ground sampling day, disaggregation results are significantly correlated with *in situ* measurements in F19, but not in F20. The poor results obtained with DoY 51/F20 is probably due to the time gap (3 days) between ground sampling date (DoY 51) and MODIS overpass day (DoY 54).

738 Statistical results in terms of root mean square difference, 739 mean difference, correlation coefficient, and slope of the linear regression between the SMOS soil moisture disaggregated in 740 the Zone A+B+C mode and aggregated *in situ* measurements 741 are listed in Table IV. Statistical significance (p-value) is also 742 reported for each date-farm unit to select statistically significant 743 (p-value < 0.10) results. Although the disaggregation of SMOS 744 data on extensively dry DoY 30 does not provide any additional 745 information (soil is uniformly dry), the observed correlation 746 between disaggregated (LST mode) and *in situ* soil moisture 747 is statistically significant, and the correlation coefficient value 748 is negative  $(-0.70 \text{ and } -0.95 \text{ at } F07 \text{ and } F08$ , respectively). 749 One plausible explanation is the opposite effect of soil temper- 750 ature on HDAS soil moisture measurements and on MODIS- 751 derived soil evaporative efficiency: a slight undercorrection of 752 the temperature-corrected hydraprobe measurements at high 753 temperature [18] results in a slight increase of soil moisture 754 estimate with soil temperature, while an increase of soil temper- 755 ature makes soil evaporative efficiency decrease. Nevertheless, 756 the possible impact of soil temperature on HDAS measurements 757 is very low with a slope of the linear regression between 758 disaggregated SMOS and *in situ* soil moisture calculated as 759 −0.08 and −0.03 for F07 and F08, respectively. When selecting <sup>760</sup> statistically significant results (p-value  $< 0.10$ ) and discarding 761 data for DoY 30, the mean correlation coefficient and slope in 762 RAD mode are 0.75 and 0.58, respectively.  $763$ 

on on disaggregated soil mois-<br>
estimate with solic respective, whis an interest or solic experiment of several solic experiment of solic server and the set including buth AACES-1 is very low with a slope of the linear re Fig. 9 presents the scatterplots of 1-km resolution disaggre- 764 gated SMOS soil moisture versus 1-km resolution aggregated *in* 765 *situ* measurements for the five date-farm units during AACES- 766 2. On each graph are plotted the soil moisture disaggregated in 767 the Zone A+B+C mode (empty squares) and the soil moisture 768 disaggregated in the Zone A only mode (black squares). The 769 surface conditions of AACES-2 were relatively wet with a mean 770 soil moisture value estimated as  $0.29 \text{ m}^3/\text{m}^3$ . The disaggre- 771 gated SMOS soil moisture does not correlate well with *in situ* 772 measurements with a p-value larger than 0.10 for all sampling 773 days, except for DoY 256/F07 in LST mode (see Table IV). The 774 negative correlation coefficient  $(-0.73)$  obtained on DoY 256 is 775 discussed when comparing the Zone A+B+C and Zone A only 776 modes in Section IV-F. In general, statistical results in Table IV 777 indicate that DisPATCh does not succeed in representing the 778 variability of soil moisture at 1-km resolution during AACES- 779 2. In fact, DisPATCh is based on the tight coupling that occurs 780 between soil moisture and evaporation under high evaporative 781 demand conditions [40]. This coupling seems to be weak in 782 September over the study area so that the disaggregation results 783 at 1-km resolution are not reliable. 784

For DoY 264/F13, however, an interesting feature is ob- 785 served on the graph corresponding to the RAD and Zone A 786 only modes. When removing the (three) black squares with 787 the largest errorbars, the correlation coefficient and the slope 788 of the linear regression between disaggregated and *in situ* 789 observations becomes 0.9 and 0.7, respectively. This suggests 790 that: 1) the standard deviation within the disaggregation output 791 ensemble can be a good estimate of the uncertainty in the 792 composited disaggregation product; and 2) the applicability of 793 DisPATCh is greatly dependent on the quality of MODIS land 794 surface temperature. Note that in this study, a choice was made 795 to maximize the number of data points used in the comparison 796 with *in situ* measurements. Consequently, all the cloud-free 797



Fig. 8. Scatterplots of 1-km resolution disaggregated SMOS soil moisture versus 1-km resolution aggregated *in situ* measurements for each of the ten date-farm data sets during AACES-1. The filled circles correspond to disaggregation with no 1-km information, empty squares to Zone A+B+C mode and black squares to Zone A only mode. For the Zone A only mode, the uncertainty in disaggregated soil moisture is represented by vertical errorbars.

 MODIS land surface temperature data were used regardless of the MODIS land surface temperature quality index. Further research should be conducted to assess whether selecting the MODIS pixel with the best MODIS land surface temperature quality index would improve the disaggregation results. This would be possible using the AACES airborne data, which cover a much larger area than *in situ* measurements.

### 805 *E. Atmospheric Corrections*

 The impact of atmospheric corrections on DisPATCh output is analyzed by comparing the disaggregation results obtained in the LST and RAD mode. Quantitative comparison between LST and RAD modes is provided in Table IV in terms of root mean square difference, mean difference, correlation coeffi- cient, and slope of the linear regression between disaggregated SMOS soil moisture and aggregated *in situ* measurements. Correlation coefficient and slope values are reported only if the p-value (statistical significance) is lower than 0.10. It is apparent that statistical results are better in the RAD than in the LST mode. When including all dates, the mean bias is 816 decreased from  $-0.05 \text{ m}^3/\text{m}^3$  in LST mode to  $-0.03 \text{ m}^3/\text{m}^3$  817 in RAD mode during AACES-1. When selecting statistically 818 significant results (p-value  $<$  0.10) and discarding data for 819 DoY 30, the mean correlation coefficient and slope is 0.75 and 820 0.58 in RAD mode, and 0.65 and 1.5 in LST mode, respectively. 821 Note that the improvement is very significant for DoY 46/F16 822 with a correlation coefficient and slope increasing from about 823 zero to 0.7 and 0.8, respectively. 824

The fact that the results obtained in RAD mode are superior 825 to those obtained in LST mode indicates that the atmospheric 826 corrections of the official MODIS land surface temperature 827 add significant uncertainties in the disaggregation products. 828 One rationale may be that the information used in atmospheric 829 corrections (notably air temperature and water vapor profile 830 data) are subjected to large uncertainties at 5-km resolution. 831 As DisPATCh is based on the spatial variations of MODIS 832 temperature relative to the 40 km scale mean, the atmospheric 833 corrections on the land surface temperature data are not nec- 834 essary at 5 km (as it is done in the MODIS temperature 835

### TABLE IV

DISPATCH Is Run in the Zone A+B+C Mode and Statistical Results Are Listed in Terms of Root Mean Square Difference (RMSD), MEAN DIFFERENCE (BIAS), CORRELATION COEFFICIENT (R), AND SLOPE OF THE LINEAR REGRESSION BETWEEN 1-km RESOLUTION DISAGGREGATED SMOS SOIL MOISTURE AND 1-km AGGREGATED IN SITU MEASUREMENTS. THE RESULTS OBTAINED USING THE RADIANCE-DERIVED LAND SURFACE TEMPERATURE DATA (RAD MODE) AND USING THE OFFICIAL MODIS LAND SURFACE TEMPERATURE DATA (LST MODE IN PARENTHESIS) ARE COMPARED. THE MEAN AND STANDARD DEVIATION OF GROUND MEASUREMENTS ((SM<sub>HDAS</sub>) AND σ<sub>HDAS</sub>), THE NUMBER OF CONSIDERED 1-km PIXELS AND STATISTICAL SIGNIFICANCE ( P-VALUE) ARE ALSO LISTED FOR EACH DATE-FARM UNIT



days DoY 28-30.

836 algorithm). An atmospheric correction at 40-km resolution is 837 sufficient and provides even better disaggregation results that 838 applying an atmospheric correction at 5-km resolution.

### 839 *F. Vegetation Cover*

 The impact of vegetation cover on DisPATCh output during AACES-1 is analyzed by comparing the disaggregation results obtained in the Zone A+B+C and Zone A only mode. Quan- titative comparison between Zone A+B+C and Zone A only modes is provided in Tables IV and V in terms of root mean square difference, mean difference, correlation coefficient, and slope of the linear regression between disaggregated SMOS soil moisture and aggregated *in situ* measurements. It is apparent that statistical results are generally better in the Zone A only than in the Zone A+B+C mode for both LST and RAD modes. In the RAD mode for instance, the mean correlation coefficient is increased from 0.75 in the Zone A+B+C mode (Table IV) to 0.89 in the Zone A only mode (Table V). Also the mean slope is closer to 1 as it switches from 0.58 in the Zone A+B+C mode (Table IV) to 0.91 in the Zone A only mode (Table V). Con- sequently, results are consistent with the hourglass approach in Fig. 3 that predicts a lower sensitivity of MODIS-derived soil temperature to soil moisture in Zone B and C, Zone A having the highest potential for estimating soil moisture variability 858 from MODIS temperature. 859

On DoY 256, the negative correlation appearing in Zone 860 A+B+C mode (Table IV) is not significant in Zone A only mode 861 (Table V), suggesting that the contradictory result obtained on 862 DoY 256 is probably an artifact due to the small sample size. 863

Note that one drawback of the Zone A only mode is the larger 864 amount of data gaps in the soil moisture images. Therefore, 865 the use of both modes is a compromise between application 866 coverage and accuracy in the disaggregation output. 867

### *G. Distinguishing Between SMOS and DisPATCh Errors* 868

By solving the extent mismatch between 40-km resolution 869 remote sensing observation and localized *in situ* measurements, 870 DisPATCh could be used as a tool to help improve the validation 871 strategies of SMOS data in low-vegetated semi-arid regions. It 872 also would reduce the coverage requirements identified by [41] 873 for airborne validation campaigns. However, such a validation 874 approach requires separating the different error sources that 875 may be attributed to SMOS soil moisture and to DisPATCh. 876 One solution is to estimate the errors attributed to DisPATCh 877 and then deduce the errors attributed to SMOS soil moisture. To 878 estimate the errors that are associated with the disaggregation 879



Fig. 9. Scatterplots of 1-km resolution disaggregated SMOS soil moisture versus 1-km resolution aggregated *in situ* measurements for each of the five datefarm data sets during AACES-2. The filled circles correspond to disaggregation with no 1-km information, empty squares to Zone A+B+C mode and black squares to Zone A only mode. For the Zone A only mode, the uncertainty in disaggregated soil moisture is represented by vertical errorbars.

 methodology, it is suggested to analyze the spatial correla- tion between 1-km disaggregated SMOS soil moisture and *in situ* measurements. If the correlation is significant, then the disaggregation product is likely to be sufficiently accurate for validating SMOS data.

 Note that the errors in DisPATCh are in part coupled with the errors in SMOS soil moisture, particularly because SMOS is an input to DisPATCh. However, any uncertainties in SMOS soil moisture should not impact the disaggregation results at a distance shorter than the SMOS data sampling length (15 km). This is the reason why such a validation strategy should be conducted with ground measurements made within a distance radius of 15 km.

In this study case, five date-farm units including DoY 893 46/F15, DoY 46/F16, DoY 49/F17, DoY 49/F18, and DoY 894 49/F20 indicate a significant correlation between disaggregated 895 SMOS soil moisture and *in situ* measurements. For these units, 896 the root mean square error in disaggregated SMOS soil mois- 897 ture is mainly explained by a bias in disaggregated soil moisture 898 (see Table IV). However, no conclusion can be drawn from 899 these data because: 1) the bias is sometimes positive (DoY 900 46/F15, DoY 49/F20), and sometimes negative (DoY 46/F16, 901 DoY 49/F17, DoY 49/F18); and 2) the comparison is made only 902 once for each farm, which does not allow analyzing the tempo- 903 ral behavior. Such a validation approach could be undertaken 904 in the near future using the OzNet (http://www.oznet.org.au/, 905 [42]) soil moisture monitoring network, providing continuous 906 measurements at 68 sites within the Murrumbidgee catchment 907 area. 908

### *H. Subpixel Variability and Assimilation Perspectives* 909

**EXERCT:**<br>
1. Subpixel Variability and Assimilation Perspectives<br>
2.2<br>
1. Subpixel Variability and Assimilation Perspectives<br>
2.2<br>
2.2<br>
2.3<br>
1. Subpixel Computed as the standard uncertainty in disaggregated<br>
1. Subpixel C DisPATCh is successively run in LST or RAD mode and in 910 Zone A+B+C or Zone A only mode during AACES-1. Fig. 10 911 plots for each case the estimated uncertainty in disaggregated 912 soil moisture (computed as the standard deviation of the disag- 913 gregation output ensemble) against the subpixel variability of 914 1-km resolution *in situ* measurements (computed as the stan- 915 dard deviation of the *in situ* measurements made within 916 1-km pixels). The data corresponding to DoY 51 are plotted 917 separately because of the time gap between HDAS/SMOS 918 (DoY 51) and MODIS (DoY 54) collection time. It is interest- 919 ing to observe that the estimated uncertainty in disaggregated 920 soil moisture is closely related to the observed subpixel vari- 921 ability of *in situ* measurements. Hence,  $\sigma_{\rm SM,1 \ km}$  could be used 922 as a proxy for representing the soil moisture variability at scales 923 finer than 1-km resolution. Concerning the data on DoY 51, the 924 linear regression is clearly off the 1:1 line. This is consistent 925 with a decrease of the spatial variability in soil moisture during 926 a dry down period [43]. In particular, the spatial variability 927 in soil moisture is expected to be lower on DoY 54 than on 928  $DoY 51.$  929

The correlation between the estimated uncertainty in disag- 930 gregated soil moisture and the subpixel soil moisture variability 931 makes an additional link between DisPATCh output and assim- 932 ilation schemes into hydrological models. A number of optimal 933 assimilation methodologies have been developed to combine 934 model predictions with remote sensing observations. However, 935 any so-called optimal assimilation technique stops being opti- 936 mal if the uncertainty in remotely sensed data is unknown or 937 estimated with a large uncertainty. In the perspective of assim- 938 ilating disaggregated SMOS data into land surface models, one 939 should keep in mind that the error information on observable 940 variables is as crucial as the observations themselves, e.g., [44]. 941

### V. SUMMARY AND CONCLUSION 942

DisPATCh is an algorithm dedicated to the disaggregation of 943 soil moisture observations using high-resolution soil tempera- 944 ture data. It converts soil temperature fields into soil moisture 945 fields given a semi-empirical soil evaporative efficiency model 946

### TABLE V

DISPATCH Is Run in the Zone A Only Mode, and Statistical Results Are Listed in Terms of Root Mean Square Difference (RMSD), MEAN DIFFERENCE (BIAS), CORRELATION COEFFICIENT (R), AND SLOPE OF THE LINEAR REGRESSION BETWEEN 1-km RESOLUTION DISAGGREGATED SMOS SOIL MOISTURE AND 1-km AGGREGATED IN SITU MEASUREMENTS. THE RESULTS OBTAINED USING THE RADIANCE-DERIVED LAND SURFACE TEMPERATURE DATA (RAD MODE) AND USING THE OFFICIAL MODIS LAND SURFACE TEMPERATURE DATA (LST MODE IN PARENTHESIS) ARE COMPARED. THE MEAN AND STANDARD DEVIATION OF GROUND MEASUREMENTS ((SM<sub>HDAS</sub>) AND <sub>HDAS</sub>), THE NUMBER OF CONSIDERED 1-km Pixels and Statistical Significance (p-Value) Are Also Listed for Each Date-Farm Unit



DoY 28-30.

 and a first-order Taylor series expansion around the field-mean soil moisture. In this study, the disaggregation approach is ap- plied to 40-km resolution version-4 SMOS level-2 soil moisture using 1-km resolution MODIS data. The objective is to test DisPATCh under different surface and atmospheric conditions using the very intensive ground measurements collected in southeastern Australia during the 2010 summer and winter AACES campaigns. Those measurements are aggregated at the downscaling resolution (1 km) and subsequently compared to the disaggregated SMOS soil moisture. Over the study area, climatic (evaporative demand), meteorologic (presence of clouds), and vegetation (cover and water status) conditions are strong constraints on disaggregation results. The quality of disaggregation products varies greatly according to season: while the correlation coefficient between disaggregated and *in situ* soil moisture is 0.7 during the summer AACES, it is about zero during the winter AACES, consistent with a weaker coupling between evaporation and surface moisture in temperate than in semi-arid climate. Moreover, vegetation cover prevents the soil temperature to be retrieved from thermal infrared data and the vegetation water stress may increase the remotely sensed land surface temperature independent of near- surface soil moisture. By separating the 1-km pixels where MODIS temperature is mainly controlled by soil evaporation,

from those where MODIS temperature is controlled by both 971 soil evaporation and vegetation transpiration, the correlation 972 coefficient between disaggregated and *in situ* soil moisture is 973 increased from 0.70 to 0.85 during the summer AACES cam- 974 paign. Also, cloud cover totally obscures the surface during rain 975 events, and on clear sky days, the water vapor in the atmosphere  $976$ significantly affects the quality of land surface temperature 977 data. It is found that the 5-km resolution atmospheric correction 978 of the official MODIS temperature data has significant impact 979 on DisPATCh output. An alternative atmospheric correction at 980 40-km resolution increases the correlation coefficient between 981 disaggregated and *in situ* soil moisture from 0.72 to 0.82 during 982 the summer AACES. 983

The above limitations must be kept in mind when using 984 DisPATCh as a tool for validating SMOS soil moisture. Over 985 semi-arid areas, disaggregation can solve the extent mismatch 986 between the 40-km resolution SMOS data and localized *in situ* 987 measurements. However, the validation of SMOS using Dis- 988 PATCh requires separation of the errors associated with SMOS 989 data and the errors associated with DisPATCh. As SMOS data 990 are an input to DisPATCh, the errors in DisPATCh are also 991 linked to the uncertainty in SMOS soil moisture. Nevertheless, 992 one way to identify the error sources specifically attributed 993 to DisPATCh is to analyze the spatial correlation between 994



Fig. 10. Estimated uncertainty in disaggregated soil moisture ( $\sigma_{SM}$ , 1 km) versus subpixel variability of 1 km resolution *in situ* measurements for DisPATCh run in LST or RAD mode and Zone A+B+C or Zone A only mode.

 disaggregated SMOS data and the *in situ* measurements made at a distance larger than the downscaling resolution (1 km with MODIS data) and smaller than the SMOS data sampling length 998 (15 km).

999 Based on the results obtained using the AACES *in situ* 1000 measurements, several improvements of DisPATCh can be 1001 suggested:

- 1002 Use of the MODIS land surface temperature quality index 1003 to select the SMOS pixels with the highest MODIS data 1004 quality.
- 1005 Correcting the MODIS land surface temperature for to-1006 pography and illumination effects [45]. Within a 40-km 1007 SMOS resolution pixel, the elevation range may be very 1008 significant and thus induce a variability in land sur-1009 face temperature that is not attributed to surface soil 1010 moisture.
- 1011 Use of ancillary air temperature data to constrain the 1012 estimation of end-members. The unstressed vegetation 1013 temperature  $T_{v,min}$  could be set to the air temperature 1014 instead of the minimum MODIS land surface temperature. 1015 This would make the estimation of  $T_{v,min}$  less dependent 1016 on the representativeness of the surface conditions met 1017 within the SMOS pixel [24].
- 1018 Accounting for the dependency of soil evaporative effi-1019 ciency to potential evaporation, by replacing the model in 1020 [26] with the model in [38].
- 1021 Estimating an optimal downscaling resolution for each 1022 season: as the sensitivity of soil evaporative efficiency to 1023 soil moisture is lower in the winter months than in the sum-1024 mer months, aggregating DisPATCh output may improve 1025 the quality of disaggregation products at the expense of 1026 spatial resolution [17].

A robust disaggregation methodology of SMOS soil moisture 1027 at 1-km resolution, which would provide both disaggregated 1028 soil moisture and its uncertainty at 1-km resolution is a crucial 1029 step toward the application of SMOS data to hydrological 1030 studies. 1031

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**Olivier Merlin**, photograph and biography not available at the time of 1207 publication. 1208

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