Hydrology and Earth System Sciences Discussions



1 On the use of GRACE intersatellite tracking data for improved estimation

2 of soil moisture and groundwater in Australia

3 Natthachet Tangdamrongsub¹, Shin-Chan Han¹, Mark Decker²

4 ¹ School of Engineering, University of Newcastle, Callaghan, New South Wales, Australia

5 ² ARC Centre of Excellence for Climate System Science, University of New South Wales,

- 6 Sydney, New South Wales, Australia
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8 Abstract

9 An accurate estimation of soil moisture and groundwater is essential for monitoring the 10 availability of water supply in domestic and agricultural sectors. In order to improve the water storage estimates, previous studies assimilated terrestrial water storage variation 11 (ΔTWS) derived from Gravity Recovery and Climate Experiment (GRACE) into land surface 12 models. However, the GRACE-derived ΔTWS was generally computed from the high level 13 14 products (e.g., land grid). The gridded data products are subjected to several drawbacks such 15 as signal attenuation and/or distortion caused by ad hoc posteriori filters, and a lack of error covariance information. The consequence is undesired alteration of ΔTWS data and its 16 17 statistical property. To exploit the GRACE information rigorously and negate these 18 limitations, this study uses the fundamental GRACE satellite tracking Level 1B (L1B) data, 19 not the post-processed ΔTWS grid data. The approach combines the GRACE's least-squares 20 normal equation (full error variance-covariance information) of L1B data with the results 21 from the Community Atmosphere Land Exchange (CABLE) model to improve soil moisture 22 and groundwater estimates. This study demonstrates, for the first time, an importance of 23 using the raw GRACE data. The GRACE-combine (GC) approach is developed for optimal 24 least-squares combination maximizing the strength of the model and observations while 25 suppressing the weaknesses. The approach is applied to estimate the soil moisture and 26 groundwater over 10 Australian river basins and the results are validated against the satellite 27 soil moisture observation and the in-situ groundwater data. We demonstrate the GC approach 28 delivers evident improvement of water storage estimates, consistently from all basins, 29 yielding better agreement at seasonal and inter-annual time scales. Significant improvement 30 is found in groundwater storage while marginal improvement is observed in surface soil 31 moisture estimates likely due to limitation of GRACE's temporal and spatial resolution.

32

33 1. Introduction

34 The changes of Terrestrial Water Storage (ΔTWS) derived from the Gravity Recovery And 35 Climate Experiment (GRACE) data products have been used in the last decade to study 36 global water resources, including groundwater depletion in India and Middle East (Rodell et 37 al., 2009; Voss et al., 2013), water storage accumulation in Canada (Lambert et al., 2013), 38 flood-influenced water storage fluctuation in Cambodia (Tangdamrongsub et al., 2016). The 39 gravity data obtained from GRACE satellites are commonly processed and released in three 40 different product levels (L) that increase in the amount of processing, L1B – satellite tracking 41 data (Wu et al., 2006), L2 – global gravitational Stokes coefficients (Bettadpur, 2012), and 42 L3 – global grids (Landerer and Swenson, 2012). The original (L1B) GRACE information is





inevitably altered or sheered due to data processing and successive post-processing filterings,
 because the error covariance information is not propagated through each post-processing step.

45 The GRACE-derived ΔTWS has been computed widely from the higher-level products (e.g.,

46 L2 and L3) on which various ad hoc post-processing filters were applied (e.g., Gaussian

47 smoothing filter (Jekeli, 1981), destripe filter (Swenson and Wahr, 2006)). ΔTWS obtained

48 from these filters lacks proper error covariance information and is attenuated and distorted.

To overcome the signal attenuation in GRACE high-level products, empirical approaches
 have been developed, including the application of scale factors computed from land surface

models (Landerer and Swenson, 2012) to the GRACE L3 products. GRACE uncertainty in

52 high level product is usually unknown or assumed. For example, Zaitchik et al. (2008)

53 derived empirically a global average uncertainty that is variable depending on choices of

54 post-processing filters (Sakumura et al., 2014). Furthermore, GRACE error and sensitivity is

dependent on latitudes due to the orbit convergence toward poles (Wahr et al., 2006) and any

56 post-processing filters will alter the GRACE data and their error information. Rigorous

57 statistical error information is of equal importance to derivation of ΔTWS for data

assimilation and model calibration (Tangdamrongsub et al., 2017). ΔTWS and its uncertainty estimates should be formulated directly from L1B data considering the complete statistical

estimates should be formulated directly from L1B data considering the complete statisticalinformation.

The GRACE information is not fully exploited in many studies. For example, groundwater 61 62 storage variation (ΔGWS) is often computed by subtracting the soil moisture variation (ΔSM) 63 component simulated by the land surface model from GRACE-derived ΔTWS data (Rodell et al., 2009, Famiglietti et al., 2011), assuming the model ΔSM is error-free. This may result in 64 the inaccurate ΔGWS and the associated error estimate as the uncertainties of GRACE and of 65 66 the land surface model outputs are neglected in the combination of two noisy data. In data 67 assimilation application, albeit its importance, the GRACE uncertainty is commonly derived 68 empirically not necessarily reflecting the true GRACE error characteristics (e.g., Zaitchik et 69 al., 2008; Tangdamrongsub et al., 2015; Tian et al., 2017). For example, Girotto et al. (2016) 70 used L3 product and showed that it was necessary to adjust GRACE observation and its 71 uncertainty in order to make their water storage estimates more accurate. Similarly, Tian et 72 al. (2017) reported the need of applying a scale factor to GRACE uncertainty (from mascon 73 product) in their GRACE assimilation process. It is apparent that the use of post-processed 74 GRACE products often requires data tuning, leading possibly to an integration of incorrect 75 gravity information into the data assimilation system. Some recent studies began to employ 76 the full variance-covariance information in the data assimilation scheme (Eicker et al., 2014, 77 Schumacher et al., 2016; Tangdamrongsub et al., 2017), however, the GRACE signal used 78 were still affected by the post-processing filters.

79 This study aims to use the GRACE information of ΔTWS measurement directly from the raw 80 L1B data. The approach optimally combines the GRACE's least-squares normal equations 81 with the model simulation results from the Community Atmosphere Land Exchange 82 (CABLE, Decker, 2015) to improve ΔSM and ΔGWS estimates. The proposed approach 83 presents three main advantages. Firstly, one can exploit the full GRACE signal and error 84 information by using the normal equation data sets. Secondly, the approach is developed for 85 optimal least-squares combination, which maximizes the model and observation strength 86 while simultaneously supressing their weaknesses. Finally, the method bypasses empirical, 87 multiple-step post-processing filters.





- 88 The main objective of this study is to present the GRACE-combined (GC) approach to
- 89 estimate improved ΔSM and ΔGWS at regional scales. We demonstrate our approach applied
- 90 to 10 Australian river basins (Fig. 1a). We validate the top layer of ΔSM estimates against the
- 91 satellite soil moisture observation (the Advanced Microwave Scanning Radiometer aboard
- 92 EOS (AMSR-E), Njoku et al., 2003) over all 10 basins and the ΔGWS estimates against the
- 93 in-situ groundwater data available over Queensland and Victoria (Fig. 1b, 1c).
- 94 This paper is outlined as follows: Firstly, the derivation of GC approach is presented in Sect.
- 95 2 while the description of GRACE data processing, including the use of GRACE normal
- 96 equation is given in Sect. 3. Secondly, the CABLE modelling is outlined in Sect. 4. This
- 97 includes the derivation of model uncertainty based on the quality of precipitation data and the
- 98 model parameter inputs. The processing of validation data is also described in Sect. 4.
- 99 Thirdly, Sect. 5 presents the result of ΔSM and ΔGWS estimates and comparison to in-situ
- 100 data. The long-term trends in the Australian mass variation over the last 13 years is also
- 101 investigated in this section. In Sect. 6, the purposed approach is discussed in terms of

102 effectiveness, and data assimilation implementation.

103

104 2. A method of combining GRACE L1B data with land surface model outputs

105 The statistical information of ΔTWS computed from a model can be written as:

106
$$\widetilde{h} = h + \epsilon; \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{C}), \tag{1}$$

- 107 where **h** is the "truth" (unknown) model state vector while \tilde{h} is the calculated state vector
- characterized with the model error ϵ . The model error is assumed to have zero mean and covariance **C**.
- 110 The term **h** is used to represent a vector including global ΔTWS grid, and terms with a
- subscript R (e.g., h_R , C_R) is used to represent only a regional set of ΔTWS (for example, in
- 112 Australia). As such, the observation equation over a region can be rewritten as:

113
$$\widetilde{h}_R = h_R + \epsilon; \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{C}_R).$$
(2)

- 114 As soil moisture and groundwater are the major components of ΔTWS in Australia (surface 115 water storage being insignificant), the vector h_R can be defined as:
- 116 $\boldsymbol{h}_{\boldsymbol{R}} = \boldsymbol{[}\Delta \boldsymbol{S}\boldsymbol{M}_{top} \quad \Delta \boldsymbol{S}\boldsymbol{M}_{rz} \quad \Delta \boldsymbol{G}\boldsymbol{W}\boldsymbol{S}\boldsymbol{]}^{T}, \tag{3}$
- 117 where ΔSM_{top} , ΔSM_{rz} , ΔGWS represent the vectors of top (surface) soil moisture, root zone 118 soil moisture, and groundwater storage variations, respectively.
- 119 A linearized GRACE satellite-tracking observation equation is formulated as:

120
$$y = \mathbf{A}x + e; e \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}), \tag{4}$$

121 where y is the observation vector containing the L1B inter-satellite ranging data, **A** is the

122 design (partial derivative) matrix relating the data and the Earth gravity field variations, \boldsymbol{x}

123 contains the Stokes coefficients of time-varying geopotential fields (e.g., Wahr et al., 1998),

124 and e is the L1B data noise, which has zero mean and covariance Σ . Eq. (4) can be modified

125 explicitly in terms of soil moisture and groundwater storage variations as:





126	$y = AS\overline{Y}Hh + e; e \sim \mathcal{N}(0, \Sigma),$	(5)
127	where S contains a factor used to convert ΔTWS to geopotential coefficient	nts considering the
128	load Love numbers (e.g., Wahr et al., 1998), $\overline{\mathbf{Y}}$ converts the gridded data i	nto the
129	corresponding spherical harmonic coefficients, and H is the operational m	atrix converting
130	$\Delta SM_{top}, \Delta SM_{rz}$, and ΔGWS to ΔTWS . This model is based on the assume	ption that the
131	GRACE orbital perturbation is a result of ΔTWS variation on the surface,	which is very
132	particular in Australia. For convenience, the term $\mathbf{Y} = \mathbf{S}\overline{\mathbf{Y}}$ is used in the fu	rther derivation. If

- 133 M is the number of model grid cells, N_{max} is the maximum degree of the geopotential
- 134 coefficients, and $L=(N_{max}+1)^2-4$ is the number of geopotential coefficients, the dimension of
- 135 **Y**, **H**, and **h** are $L \times M$, $M \times 3M$, and $3M \times 1$, respectively.
- 136 A least-squares solution of Eq. (5) is given as:

$$(\mathbf{H}^T \mathbf{Y}^T \mathbf{A}^T \mathbf{\Sigma}^{-1} \mathbf{A} \mathbf{Y} \mathbf{H}) \hat{\mathbf{h}} = \mathbf{H}^T \mathbf{Y}^T \mathbf{A}^T \mathbf{\Sigma}^{-1} \mathbf{y}.$$
 (6)

138 It can be simplified as:

137

139

$$\mathbf{H}^T \mathbf{Y}^T \mathbf{N} \ \mathbf{Y} \mathbf{H} \ \hat{\boldsymbol{h}} = \mathbf{H}^T \mathbf{Y}^T \boldsymbol{c}, \tag{7}$$

140 where $\mathbf{N} = \mathbf{A}^T \Sigma^{-1} \mathbf{A}$ and $\mathbf{c} = \mathbf{A}^T \Sigma^{-1} \mathbf{y}$. (The rationales of introducing **N** and **c** are explained

141 in the following section). Note that, the above derivations (Eq. (5) - Eq.(7)) are defined with

142 the global grid of h. For a regional application, Eq. (7) can be modified as:

143
$$\begin{bmatrix} \mathbf{H}_{R}^{T} \mathbf{Y}_{R}^{T} \mid \mathbf{H}_{o}^{T} \mathbf{Y}_{o}^{T} \end{bmatrix} \mathbf{N} \begin{bmatrix} \mathbf{Y}_{R} \mathbf{H}_{R} \\ \mathbf{Y}_{o} \mathbf{H}_{o} \end{bmatrix} \begin{bmatrix} \widehat{\boldsymbol{h}}_{R} \\ \widehat{\boldsymbol{h}}_{o} \end{bmatrix} = \begin{bmatrix} \mathbf{H}_{R}^{T} \mathbf{Y}_{R}^{T} \mid \mathbf{H}_{o}^{T} \mathbf{Y}_{o}^{T} \end{bmatrix} \boldsymbol{c}, \qquad (8)$$

where the subscript *R* indicates the grid ΔTWS only in a region of interest, and *o* for the rest of the globe. If the number of the model grid cells associated with *R* is *J* and that of the

146 outside cells is M-J. As such, the dimensions of \mathbf{Y}_R , \mathbf{H}_R , $\hat{\mathbf{h}}_R$, \mathbf{Y}_o , \mathbf{H}_o , $\hat{\mathbf{h}}_o$ are $L \times J$, $J \times 3J$, $3J \times 1$,

147 $L \times (M-J), (M-J) \times 3(M-J), 3(M-J) \times 1$, respectively. The dimension of N and c remain

unchanged, since they are essentially from the normal equations of the original GRACE L1Bdata (to be discussed in the following section).

From Eq. (8), the normal equations associated with ΔTWS in the region of interest can then be written as

152
$$\mathbf{H}_{R}^{T} \mathbf{Y}_{R}^{T} \mathbf{N} \mathbf{Y}_{R} \mathbf{H}_{R} \hat{\boldsymbol{h}}_{R} = \mathbf{H}_{R}^{T} \mathbf{Y}_{R}^{T} \boldsymbol{c} - \mathbf{H}_{R}^{T} \mathbf{Y}_{R}^{T} \mathbf{N} \mathbf{Y}_{o} \mathbf{H}_{o} \hat{\boldsymbol{h}}_{o}$$
(9)

153 or

154
$$\mathbf{N}_R \hat{\mathbf{h}}_R = \mathbf{c}_R \tag{10}$$

155 where $\mathbf{N}_R = \mathbf{H}_R^T \mathbf{Y}_R^T \mathbf{N} \mathbf{Y}_R \mathbf{H}_R$ and $\mathbf{c}_R = \mathbf{H}_R^T \mathbf{Y}_R^T \mathbf{c} - \mathbf{H}_R^T \mathbf{Y}_R^T \mathbf{N} \mathbf{Y}_o \mathbf{H}_o \hat{\mathbf{h}}_o$. As seen, Eq. (9) is the 156 regional representation of Eq. (7) where only the grid cells inside the study region are used, 157 while the contribution from the grid cells outside the region needs to be removed or 158 corrected. Combining the normal equation of Eq. (2) and Eq. (10), the optimal combined

159 solution of \hat{h}_R can be resolved as follows:

160
$$\widehat{h}_R = \left(\mathbf{C}_R^{-1} + \mathbf{N}_R\right)^{-1} \left(\mathbf{C}_R^{-1} \widetilde{h}_R + \mathbf{c}_R\right)$$
(11)





- 161 The computation of model covariance matrix C_R will be discussed in Sect. 4.2. The posteriori
- 162 covariance of \hat{h}_R can be estimated as follows:

163
$$\widehat{\boldsymbol{\Sigma}} = (\boldsymbol{C}_R^{-1} + \boldsymbol{N}_R)^{-1}, \qquad (12)$$

164 and the uncertainty estimate of \hat{h}_R is simply calculated as:

$$\sigma_{\hat{h}} = \sqrt{diag(\hat{\Sigma})},\tag{13}$$

166 where diag or represents the diagonal element of the given matrix.

167

165

168 3. GRACE data

169 **3.1 GRACE least-squares normal equations**

170 In this study, the least-squares normal equations are obtained from the ITSG-Grace2016 171 products (Mayer-Gürr et al, 2016; https://www.tugraz.at/institute/ifg/downloads/gravity-field-172 models/itsg-grace2016) between January 2003 and March 2016. All L1B data including KBR 173 inter-satellite tracking data, attitude, accelerometer, GPS based kinematic orbit data and 174 AOD1B corrections are reduced in terms of the normal equations. These data products are 175 usually used to compute the Earth's geopotential field to the maximum harmonic degree and 176 order of 90, or at a spatial resolution of ~220 km. The products contain the information of the 177 normal matrix **N** and the vector \boldsymbol{c} (as shown in Eq. (7)) as well as the a-priori time-varying 178 gravity field coefficients predicted with the GOCO05s solution (Mayer-Gürr et al., 2015). 179 Note that the solution of the ITSG-Grace2016 normal equation is the anomalous geopotential 180 coefficient vector (Δx), which is referenced to the a-priori time-varying gravity field (x_0), 181 through:

$$\mathbf{N}\,\Delta \mathbf{x} = \mathbf{d} \tag{14}$$

183 where d and x_0 are given. To obtain a complete gravity field variation between the study

184 period (x term in Eq. (4)), the a-priori time-varying gravity field, x_0 is firstly restored to

185 Eq. (14), and the mean gravity field (\bar{x}_0) computed from all x_0 between January 2003 and 186 March 2016 is then removed as follows:

187
$$\mathbf{N}\left(\Delta x + x_0 - \overline{x}_0\right) = d + N(x_0 - \overline{x}_0) \tag{15}$$

188 **N**
$$x = d + N(x_0 - \overline{x}_0)$$
 (16)

189 Therefore, in Sect. 2 (e.g., Eq. (7) – (11)), the matrix **N** remains unchanged while the vector c190 can be simply replaced by $c = d + N(x_0 - \overline{x}_0)$.

191

182

192 **3.2 GRACE-derived** ΔTWS products

193 Two monthly GRACE-derived ΔTWS products are also used, the CNES/GRGS Release 3

- 194 (RL3) (GRGS for short, Lemoine et al., 2015) and the JPL RL05M mascon-CRI version 2
- 195 product (mascon for short, Watkins et al., 2015; Wiese et al., 2016). The GRGS solution
- 196 provides ΔTWS at 1°×1° globally, derived from the Earth's geopotential coefficients up to the
- 197 maximum degree and order 80, and no filter nor scale factor is applied (L2 data product).





- 198 Mascon provides ΔTWS at equal-area 3° spherical cap grid globally. In contrast to the GRGS 199 solution, the mascon uses a gain factor derived from the land surface model (LSM) to restore
- 200 mitigated signals and reduce leakage errors (L3 data products) (Watkins et al., 2015; Wiese et
- al., 2016). Additionally, mascon provides the ΔTWS uncertainty together with the solution.
- 202 The uncertainty is computed based on several geophysical models (see Watkins et al. (2015)
- and Wiese et al. (2016) for more details). The uncertainty information is not available in theGRGS product.
- 205 The ΔTWS products are obtained between January 2003 and March 2016. The GRGS
- solution is retrieved from http://grgs.obs-mip.fr/grace/variable-models-grace-lageos/grace-
- 207 solutions-release-03 while the mascon is from http://grace.jpl.nasa.gov/data/get-
- 208 data/jpl_global_mascons. After retrieval, the long-term mean value between January 2003
- and March 2016 is computed and subtracted from the monthly products. To be consistent
- 210 with CABLE grid spacing (see Sect. 4), the spatial resolution of two datasets are resampled to
- 211 $0.5^{\circ} \times 0.5^{\circ}$ using the nearest grid values.
- 212 In this study, these two independent GRACE solutions are used for two main reasons:
- 213 1. To obtain the ΔTWS values outside Australia. As shown in Eq. (9), the \hat{h}_o vector 214 needs to be known, which can be from the GRACE-derived ΔTWS solution. We use 215 the GRGS solutions as the GRGS solution provides ΔTWS at a spatial resolution 216 comparable to the normal equation data.
- 217 2. To compare with the ΔTWS estimates from our approaches. Both GRGS and mascon 218 solutions are used to compare and validate our ΔTWS estimates.
- 219

220 4. Hydrology model and validation data

221 4.1 Model setup

222 The extensive description of the CABLE model is given in Decker (2015) and Ukkola et al. 223 (2016). This section describes the model setup and specific changes applied for this study. 224 CABLE can be used to estimate soil moisture and groundwater in terms of volumetric water 225 content every 3 hours at a 0.5°×0.5° spatial resolution. The soil moisture and groundwater storage can be simply computed by multiplying the estimates with thicknesses of various 226 227 layers. For soil moisture, the thickness of 6 soil layers is 0.022, 0.058, 0.154, 0.409, 1.085, 228 and 2.872 m, from top to bottom, respectively. The thickness of the groundwater layer is 229 modelled to be 20 m uniformly. Recalling Eq. (3), ΔSM_{top} is defined as the soil moisture storage variation at the top 0.022 m thick layer, while ΔSM_{rz} is the variation accumulated 230 231 over the second to the bottom soil layers (depth between 0.022 cm and 4.6 m).

232 CABLE is initially forced with the data from the Global Soil Wetness Project Phase 3

233 (GSWP3) (Dirmeyer et al., 2011; http://hydro.iis.u-tokyo.ac.jp/GSWP3), which is currently

available until December 2010. We replace GSWP3 forcing data with GLDAS data (Rodell

et al., 2004) to compute the water storage changes to 2016. The forcing data used in CABLE

are precipitation, air temperature, snowfall rate, wind speed, humidity, surface pressure, and

- short-wave and long-wave downward radiations. To investigate the impact of different
- 238 forcing data, the offline sensitivity study is conducted by comparing the water storage
- 239 estimates computed using:





240 1. All 8 forcing data components of GSWP3,

241 2. GSWP3 data with replacing one component obtained from GLDAS forcing data.

242 It is found that the water storage estimate is most sensitive to the replacement of precipitation 243 data, as expected, and relatively less sensitive to the change of other forcing components. We 244 use the GLDAS forcing data in this study and also further test 7 different precipitation data 245 products (see more details in Sect. 4.2). The forcing data are up/down sampled to a $0.5^{\circ} \times 0.5^{\circ}$

- spatial grid to reconcile with the CABLE spatial resolution.
- 247

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248 4.2 Model uncertainty

In this study, the CABLE uncertainty is derived from 210 ensemble estimates associated with 249 250 different forcing data and model parameters. The 7 different precipitation products (see Table 251 1) are used to run the model independently. Most products are available to present day while 252 GSWP3, Princeton, and MERRA are only available until December 2010, December 2012, 253 and February 2016, respectively. For each precipitation forcing, 30 ensembles are generated 254 by perturbing the model parameters within +/-10% of the nominal values. The perturbed size 255 of 10% is similar to Dumedah and Walker (2014). Based on the CABLE structure, the ΔSM 256 and ΔGWS estimates are most sensitive to the model parameters listed in Table 2. For 257 example, the fractions of clay, sand, and silt ($f_{clay}, f_{sand}, f_{silt}$) are used to compute soil 258 parameters including field capacity, hydraulic conductivity, and soil saturation which mainly 259 affect soil moisture storage. Similarly, the drainage parameters (e.g., q_{sub} , f_p) control the 260 amount of subsurface runoff, which has a direct impact on root zone soil moisture and 261 groundwater storages.

From ensemble generations, total K = 210 sets of the ensemble water storage estimates (h_e) are obtained:

$$\mathcal{H}_{R} = [h_{e}|_{k=1} \quad h_{e}|_{k=2} \quad h_{e}|_{k=3} \quad \dots \quad h_{e}|_{k=K}]$$
(17)

and the mean value of \mathcal{H}_R is computed as follows:

$$\widetilde{\boldsymbol{h}}_{\boldsymbol{R}} = \frac{1}{\kappa} \sum_{k=1}^{K} \boldsymbol{h}_{\boldsymbol{e}} |_{\boldsymbol{k}}$$
(18)

267 Note that due to the absence of GSWP3, Princeton, and MERRA data, the number of 268 ensembles reduce to K = 180 after December 2010, K = 150 after December 2012, and K =269 120 after February 2016, respectively. The mean value is removed from each ensemble 270 member, $\mathcal{H}_{R}' = \mathcal{H}_{R} - \tilde{h}_{R}$, and the error covariance matrix of the model is empirically 271 computed as:

$$\mathbf{C}_{R} = \mathcal{H}_{R}' (\mathcal{H}_{R}')^{T} / (K - \mathbf{1})$$
(19)

273 The \tilde{h}_R (Eq. (18)) and C_R (Eq. (19)) terms can be directly used in Eq. (11).

Note that the sampling error caused by finite sample size might lead to spurious correlations in the model covariance matrix (Hamill et al., 2001). The effect can be reduced by applying an exponential decay with a particular spatial correlation length to C_R . In this study, the correlation length is determined based on the empirical covariance of model estimated ΔTWS . The covariance function of ΔTWS is firstly assumed isotropic, and it is computed

empirically based on the method given in Tscherning and Rapp (1974). The distance where





the maximum value of the variance decreases to half is defined as the correlation length. The obtained values vary month-to-month, and the mean value of 250 km is used in this study.

282 It is emphasized that the model omission error caused by imperfect modelling of hydrological

283 process within the LSM is not taken into account in the above description. We assume for

such model error by increasing 20% of the model covariance. (i.e., multiplying C_R by 1.2).

286 4.3 Validation data

287 4.3.1 Satellite soil moisture observation

288 The satellite observed surface soil moisture data is obtained from the Advanced Microwave 289 Scanning Radiometer-Earth Observing System (AMSR-E) cooperating the Land Parameter 290 Retrieval Model (Njoku et al., 2003). The observation is used to validate our estimates of top 291 soil moisture changes (ΔSM_{top}). The AMSR-E product provides volumetric water content in 292 the top layer derived from a passive microwave data (from NASA EOS Aqua satellite) and 293 forward radiative transfer model. In this study, the level 3 product, available daily between 294 June 2002 and June 2011 at $0.25^{\circ} \times 0.25^{\circ}$ spatial resolution is used (Owe et al., 2008). The 295 measurements from ascending and descending overpasses are averaged for each frequency 296 band (C and X). Then, the monthly mean value is computed by averaging the daily data 297 within a month. To obtain the variation of the surface soil moisture, the long-term mean 298 between June 2002 and June 2011 is removed from the monthly data. Regarding the different 299 depth measured in CABLE and AMSR-E, the CDF-matching technique (Reichle and Koster, 300 2004) is used to reduce the bias between the top soil moisture model and the observation. 301 Since there is no satellite observed or ground measured root zone soil moisture data for 302 meaningful comparison with our results, particularly at continental scale. Validation of 303 ΔSM_{rz} at regional and continental scales is currently unachievable due to a complete lack of observations at this spatial scale. 304

305

306 4.3.2 In-situ groundwater

The in-situ groundwater level from bore measurements are obtained from 2 different ground observation networks (see Fig. 1). The data in Queensland are obtained from Department of Natural Resources and Mines (DNRM) while the data in Victoria is from Department of

310 Environment and Primary Industries (DWPI). More than 10,000 measurements are available

311 from each network, but the data gap and outliers are present. Therefore, the bore

312 measurement is firstly filtered by removing the sites that present no data or data gap longer

than 30 months during the study period.

To obtain the monthly mean value, the hourly or daily data are averaged in a particular

315 month. The outliers are detected and fixed using the Hampel filter (Pearson, 2005) where the

316 remaining data gaps are filled using the cubic spline interpolation. To obtain the groundwater

level variation, the long-term mean groundwater level computed between the study period is

318 removed from the monthly values. The groundwater level variation (ΔL) is then converted to

319 ΔGWS using $\Delta GWS = S_y \cdot \Delta L$, where S_y is specific yield. Based on Chen et al. (2016), $S_y =$

320 0.1 is used for the Victoria network. Specific yields of Queensland's network have been

found ranging from 0.045 (Rassam et al., 2013) to 0.06 (Welsh 2008), and an averaged $S_y =$





322 0.05 is used in this study. Finally, the mean value computed from all data (in each network) is

- 323 used to represent the in-situ data of the network.
- 324

325 **5. Results**

326 5.1 Model-only performance

- 327 We study the model ΔTWS changes under different meteorological forcing and land
- parameterization. Total 210 estimates of monthly TWS (sum of SM_{top} , SM_{rz} , and GWS) are
- 329 obtained between January 2003 and March 2016 from the ensemble run based on 7 different
- 330 precipitation inputs. Then, the averaged values of the *TWS* estimates are computed from the
- 331 30 precipitation-associated ensemble members. This results in 7 sets of monthly mean *TWS*
- estimates from 7 different precipitation data. For each set, the monthly ΔTWS is computed by
- removing the long-term mean computed between January 2003 and March 2016.
- The precipitation-based ΔTWS are then compared with the GRACE-mascon solution (see
- 335 Sect. 3.2) over 10 different Australian basins. The comparison is carried out between January
- 336 2003 and March 2016. Due to the availability of the data, the periods used are shorter in cases
- 337 of GSWP3, Princeton, and MERRA precipitation (see Table 1). The metric used to evaluate a
- 338 goodness of fit between CABLE run and GRACE mascon estimates is the Nash-Sutcliff (NS)
- coefficient (see Eq. (A1)) (Fig. 2).
- 340 Figure 2 demonstrates CABLE ΔTWS varies noticeably by precipitation as well as locations.
- 341 The area-weighted average values (see Eq. (A2)) computed from Princeton, GSWP3, and
- 342 TRMM yields the model ΔTWS reasonably agreeing with GRACE by giving the NS
- 343 coefficient greater than 0.45, while MERRA, PERSIANN, and GLDAS show NS = \sim 0.3. The
- less agreement is mainly due to the quality of rainfall estimates over Australia. The NS of
- 345 ECMWF is around 0.4.
- 346 All model ensembles are consistent with the GRACE data over Timor Sea and inner parts of
- Australia (e.g., LKE, MRD, NWP) where the NS value can reach as high as 0.9 (see e.g.,
- 348 TRMM over TIM). On the contrary, the less agreement is found mostly over the coastal
- 349 basins. Very small or even negative NS values indicate the misfit between CABLE and
- 350 GRACE mascon solutions, and they are observed over Indian Ocean (see GLDAS), North
- 351 East Coast (see GSWP3, PERSIANN, TRMM), South East Coast (see MERRA, TRMM),
- 352 South West Coast (see GSWP3, GLDAS, MERRA), and South West Plateau (see MERRA).
- 353 By averaging all ΔTWS estimates from 7 different precipitation, the mean-ensemble estimate
- 354 (MN) delivers the best agreement with GRACE as seen by the highest average NS value (MN
- of AVG = 0.55) among all ensembles. Particularly, NS values are greater than 0.4 in all
- 356 basins and no negative NS values are presented in MN. In average, it can be clearly seen that
- 357 using the mean value (MN) is a viable option to increase the overall performance of the
- ΔTWS estimates. Therefore, only CABLE MN result will be used in further analyses. The
- 359 comparison with the GRGS GRACE solution was also evaluated (not shown here) and the
- overall results are similar to Fig. 2.
- 361 **5.2 Impact of GRACE on storage estimates**
- 362 **5.2.1 Contribution of GRACE**





- 363 This section investigates the impact of the GC approach on the estimates of various water
- 364 storage components. The ΔTWS estimate obtained from the GC approach is demonstrated in
- 365 Sect. 5.1, by comparing with the independent GRACE mascon solution. Figure 2 shows the
- 366 GC result yields the highest NS values in all basins, outperforming all other CABLE runs. In 367 average (AVG), the NS value increases by ~35% (0.55 to 0.74) from the MN case. The
- similar behaviour is also seen when compared with the GRGS GRACE solution (not shown);
- 369 the average NS value increases from 0.50 to 0.74. This is not surprising as the GC approach
- 370 uses the fundamental GRACE tracking data as GRACE mascon and GRGS solutions do.
- 371 Improvement of NS coefficient indicates merely the successfulness of integrating GRACE
- 372 data and the model estimates.

Figure 3 shows the GC results of ΔTWS as well as ΔSM_{top} , ΔSM_{rz} , and ΔGWS in different basins. The monthly time-series and the de-seasonalized time-series are shown. In general,

375 GRACE tends to increase ΔTWS when the model ΔTWS (MN) is predicted to be

underestimated (see e.g., LKE, MRD, NWP, SWP, TIM between 2011 and 2012) and by

377 decrease ΔTWS when determined to be overestimated (see all basins between 2008 and

378 2010). A clear example is seen over Gulf of Carpentaria (Fig. 3d), where CABLE

overestimates ΔTWS and produces phase delay between 2008 and 2010. The over estimated

- amplitude and phase delay seen in CABLE ΔGWS during this above period (Fig. 3c) is
- 381 caused by an overestimation of soil and groundwater storage. The positively biased soil and
- 382 groundwater storage causes a phase delay by increasing the amount of time required for the
- subsurface drainage (baseflow) to reduce to soil and groundwater stores. The overestimation
- 384 of water storage is the result of overestimated precipitation or underestimated

evapotranspiration. The amplitude and phase of the water storage estimate are adjustedtoward GRACE observation in the GC approach.

- The impact of GRACE varies across the individual storage as well as across the geographical location (climate regime). In general, the major contributors to ΔTWS are ΔSM_{rz} and ΔGWS .
- 389 Due to a small store size (only ~2 cm thick), ΔSM_{top} contributes only ~2 % to ΔTWS . As
- 390 such, ΔSM_{rz} , and ΔGWS have greater variations, which commonly lead to greater uncertainty
- 391 compared to ΔSM_{top} , and therefore, the stores anticipate greater shares from the GRACE
- 392 update. This behaviour is seen over all basins where the differences between CABLE-

```
393 simulated and GC \Delta SM_{rz}, and \Delta GWS estimates are greater (compared to \Delta SM_{top}).
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394 Furthermore, the impact of GRACE on ΔSM_{rz} , and ΔGWS is different across the continent. 395 For example, over central and southern Australia (see e.g., LKE, MRD, NWP, SWP), the dry 396 climate is responsible for a small amount of groundwater recharge and most of the infiltration 397 is stored in soil compartments. In this climate condition, ΔSM_{rz} amplitude is significantly 398 larger than ΔGWS and it plays a greater role in ΔTWS , and consequently, the GRACE 399 contribution is mostly seen in ΔSM_{rz} component. Different behaviour is seen over the northern Australia (GOC, NEC, TIM) where ΔGWS amplitude are greater (~40 % of ΔTWS) 400 401 compared to other basins (only ~17 % of ΔTWS). This is due to the sufficient amount of 402 rainfall over the wet climate region, replenishing groundwater recharges and resulting in 403 greater variability in ΔGWS . Therefore, compared to the dry climate basin, the GRACE 404 contributes to ΔGWS over these basins by the larger amount. 405

406 5.2.2 Impact on long-term trend estimates





- 407 The spatial patterns of the long-term trends of water storage changes over January 2003 and
- 408 March 2016 are analysed before and after applying the GC approach (Fig. 5). For
- 409 comparison, the long-term trends of ΔTWS derived from the mascon and GRGS solutions are
- also shown (Fig. 5a, 5b). From Fig. 5d, GRACE effectively changes the long-term trend
- 411 estimates in most basins in a way the spatial pattern of the ΔTWS trend of the GC solution
- 412 consistent to the mascon and GRGS solutions, while satisfying the model processes and
- 413 keeping the spatial resolution. The trend of ΔSM_{top} is insignificant (Fig. 5e) and the GC
- 414 approach does not change (Fig. 5f). The largest adjustment is seen in ΔSM_{rz} and ΔGWS
- 415 components, to be consistent with the GRACE data in most basins (Fig. 5h, 5j).
- 416 GRACE shows significant changes in the ΔTWS trend estimates particularly over the
- 417 northern and western parts of the continent. The model estimates around the Gulf of

418 Carpentaria basin show a strong negative trend that is inconsistent from the GRACE data. It

- 419 is found that underestimated precipitation after 2012 is likely the cause of such an
- 420 incompatible negative trend (see Fig. 3d). Applying the GC approach clearly improves the
- trend (Fig. 5c vs. 5d). The other example is seen over the western part of the continent (see
- 422 rectangular area in Fig. 5c, 5d) where the averaged long-term trend of ΔTWS was predicted
- to be -0.4 cm/year but changed to be -1.2 cm/year (see also Sect. 5.4) by the GC approach.
- The precipitation over the western Australia is understood to be overestimated after 2012,
- 425 evidently seen by that the model ΔTWS is always greater than the GC solution (see e.g., Fig.
- 3h, 4d, 4p). The GC approach reveals that the water loss over the western Australia is at least
 twice greater than what has predicted by the CABLE model.
- In addition, the shortage of water storage in the south-eastern part of the continent from the millennium drought (McGrath et al., 2012) has been recovered (seen as a positive water storage trend in Fig. 5) after the rainfall between 2009 and 2012, while the western part is still drying out (seen as negative trends). The trend estimates in terms of mass change is discussed in more detail in Sect. 5.4.
- 433

434 5.2.3 Reduction of uncertainty

- 435 Influenced by climate pattern, the uncertainty of water storage estimates significantly varies 436 across Australia. The uncertainty of the model estimate is computed from the variability 437 induced by different precipitation and model parameters while the uncertainty of GC solution 438 is computed using Eq. (13). As expected, larger uncertainties are observed in ΔSM_{rz} and 439 ΔGWS than in ΔSM_{top} (an order of magnitude smaller) since ΔSM_{top} is smaller than others 440 (Fig. 6). Over the wet basins, larger amplitude of the water storage leads to larger uncertainty, 441 seen over Gulf of Carpentaria, North East Coast, South East Coast, and Timor Sea where the 442 CABLE-simulated ΔTWS uncertainty is approximately 28 % larger than other basins. The 443 smaller uncertainty is found over the dry regions (e.g., LKE, SWP). In most basins, the 444 uncertainty of ΔSM_{rz} is larger than the ΔGWS , except the wet basins (e.g., GOC, NEC, TIM) 445 where the greater groundwater recharge leads to a larger uncertainty of ΔGWS .
- 446 Figure 6 demonstrates how much the formal error of each of storage components is reduced
- 447 by the GC approach. Overall, the estimated CABLE uncertainties averaged over all basins
- 448 (AVG) are 0.2, 4.0, 4.0, and 5.7 cm for ΔSM_{top} , ΔSM_{rz} , ΔGWS , and ΔTWS , respectively.





449 With the GC approach, the uncertainties of ΔSM_{top} , ΔSM_{rz} , ΔGWS , and ΔTWS decrease by 450 approximately 26%, 35%, 39%, and 37%, respectively.

451 It is worth mentioning that the model uncertainty is mainly influenced by the meteorological 452 forcing data. The uncertainty of precipitation derived from 7 different precipitation products 453 is shown in Fig. 6e. The spatial pattern of the precipitation uncertainty is correlated with the 454 uncertainty of water storage estimates. The larger water storage uncertainty is deduced from the larger precipitation uncertainty. The quality of precipitation forcing data is found to be an 455 456 important factor to determine the accuracy of water storage computation.

457

458 5.3 Comparison with independent data

459 5.3.1 Soil moisture

460 The ΔSM_{top} estimates are compared with the AMSR-E derived soil moisture. The processing 461 of AMSR-E data is described in Sect 4.3.1. The performance is assessed using Nash-Sutcliff coefficients, given in Table 3. In general, CABLE (MN) shows a good performance in the top 462 soil moisture simulation showing NS value of >0.4 for most of the basins. The top soil 463 464 moisture estimate shows slightly better agreement with the C-band measurement of the 465 AMSR-E product. This is likely caused by the greater emitting depth of the C-band measurement (~1 cm), which is closer to the depth of the top soil layer (~2 cm) used in this 466 467 study (Njoku et al., 2003).

The GC approach leads to a small bit of improvement of the top soil estimate consistently 468 469 from C- and X-band measurements and from all basins. No degradation of the NS value is 470 observed in the GC solutions. The largest improvement is seen over LKE and NEC, where 471 NS increases by 10 - 15%. For other regions, the change in the NS coefficient may be

- 472 incremental.
- 473

474 5.3.2 Groundwater

475 The ΔGWS estimates from the model and the GC method are compared with the in situ data 476 obtained from 2 different ground networks in Queensland and Vitoria. For each network, all 477 ΔGWS data inside the groundwater network boundary (see polygons in Fig. 1) are used to 478 compute the average ΔGWS time series. From the comparison given in Fig. 7, it is found that 479 the GC solutions of ΔGWS follows the overall inter-annual pattern of CABLE but with a 480 considerably larger amplitude. This results in a better agreement with the in situ ΔGWS data 481 seen from both networks. The NS coefficient of ΔGWS between the estimates and the in situ 482 data are given in Table 4. The CABLE ΔGWS performs significantly better in Queensland 483 (NS = ~0.5) than Victoria (NS = ~0.3). Significant improvement is found from the GC 484 solutions in both networks, where the NS value increases from 0.5 to 0.6 (\sim 22 %) in 485 Queensland and from 0.3 to 0.6 (~85 %) in Victoria. Even greater improvement is seen when the inter-annual patterns are compared. The NS value increase from 0.5 to 0.7 (~ 32 %), and 486 487 0.4 to 0.8 (~93 %) in Queensland and Victoria, respectively. 488 The comparison of the long-term trend of ΔGWS is also evaluated. The estimated trends in

489 Queensland and Victoria are given in Table 4. Beneficially from the GC approach, the ΔGWS

490 trend is improved by approximately 20 % (from 0.4 to 0.6, compared to 1.6 cm/year) in





- 491 Queensland. Increasing of ΔGWS is mainly influenced by the large amount of rainfall during
- 492 the 2009 2012 La Niña episodes (see Fig. 7a). In Victoria, significant improvement of
- 493 ΔGWS trend by about 76 % (from 0.1 to -0.2, compared to -0.3 cm/year) is observed.
- 494 Similar improvement of long-term trend estimates is seen in de-seasonalized time series
- 495 (improves by ~15 % in Queensland and by ~74 % in Victoria). Decreasing of ΔGWS in
- 496 Victoria is mainly due to the highly-demanded groundwater consumption by agriculture and
- domestic activities (van Dijk et al., 2007; Chen et al., 2016). As the groundwater
- 498 consumption is not parameterized in CABLE, the decreasing of ΔGWS estimate cannot
- 499 properly captured in the model simulation. Applying GC approach effectively reduces the
- 500 model deficiency and improves the quality of the groundwater estimations.
- 501

502 **5.4 Assessment of mass variation in the past 13 years**

503 Australia experiences significant climate variability; for example the millennium drought starting from late '90 (Van Dijk et al., 2013) and extremely wet condition during several La 504 505 Niña episodes (Trenberth 2012; Han 2017). These periods are referred as "Big Dry" and "Big 506 Wet" (Ummenhofer et al., 2009; Xie et al., 2016). To understand the total water storage 507 (mass) variation influenced by these two distinct climate variabilities, the water storage 508 change obtained from the GC approach during Big Dry and Big Wet is separately 509 investigated over 10 basins. The time window between January 2003 and December 2009 is defined as the Big Dry period while between January 2010 and December 2012 is defined as 510 511 the Big Wet period following Xie et al. (2016). In each period, the long-term trends of GC 512 estimates of ΔTWS , ΔSM_{top} , ΔSM_{rz} , and ΔGWS are firstly calculated. Then, the total water 513 storage variation (in meter) is simply obtained by multiplying the long-term trend (in m/year) 514 with the number of years in the specific period, 7 years for Big Dry and 3 years for Big Wet. 515 To obtain the mass variation, the water storage variation is multiplied by the area of the basin and the density of water (1000 kg/m³). The estimated mass variations during Big Dry and Big 516 Wet are displayed in Fig. 8. The long-term mass variation of the entire period (January 2003 517 518 - March 2016) is also shown.

519 During Big Dry (2003 – 2009), a significant loss of total storage (40 – 60 Gton over 7 years) 520 is observed over LKE, MRD, NWP, and SWP basins. The largest groundwater loss of >20 521 Gton is found from LKE and MRD. No significant change is observed over the tropical 522 climate regions (e.g., GOC, NEC). The mass loss mostly occurs in the root zone and 523 groundwater compartments where the sum of ΔSM_{rz} and ΔGWS explains more than 90% of 524 the ΔTWS value. The mass loss is also observed in ΔSM_{top} but >10 times smaller than 525 ΔSM_{rz} and ΔGWS .

- 526 During Big Wet (2010 2012), the basins like LKE, MRD and TIM exhibit the significant 527 total storage gain of >100 Gton. The gain is particularly larger in ΔSM_{rz} over the basins that
- total storage gain of >100 Gton. The gain is particularly larger in ΔSM_{rz} over the basins that experienced the significant loss during Big Dry. For example, over LKE and MRD, the gain
- 529 of ΔSM_{rz} is approximately 2 3 times greater than ΔGWS . It implies that most of the
- 530 infiltration (from the 2009 2012 La Niña rainfall) is stored as soil moisture through the long
- 531 drought period, and that the groundwater recharge is secondary to the ΔSM_{rz} increase.
- 532 The opposite behaviour is observed over the basins (such as NEC and GOC) that experienced 533 mass gain during Big Dry. The water storage gain is greater in ΔGWS compared to ΔSM_{rz} . In





- 534 NEC, ΔGWS gain is ~8 times larger than ΔSM_{rz} during Big Wet. The soil compartment may
- 535 be saturated during Big Dry and additional infiltration from the Big Wet precipitation leads to
- 536 an increased groundwater recharge. The ΔSM_{rz} loss observed over GOC is simply caused by
- 537 the timing selection of Big Wet period, which ends earlier (~ 2011) in GOC than in other
- basins. The ΔSM_{rz} gain becomes ~26 Gton if the Big Wet period is defined as 2008 2011.
- 539 During the post-Big Wet period (2012 and afterwards), the decreasing trend of water storage
- 540 is observed from all basins (see Fig. 3, 4). This is mainly caused by the decrease in
- precipitation after 2012 and by gradual water loss through evapotranspiration (Fasullo et al.,2013).

543 The overall water storage change in the last 13 years demonstrates that the severe water loss 544 from most basins during Big Dry (the millennium drought) is balanced with the gain during 545 Big Wet (the La Niña). The negative ΔTWS estimated during Big Dry becomes positive in LKE, MRD, and SEC and less negative in TIM, and the greatest gain is observed from NEC 546 547 by ~50 Gton during 13 year-period (see Fig. 8c). However, the water mass loss is still 548 detected over the western basins (e.g., IND, NWP, SWP, SWC), and their magnitudes are 549 even larger than the mass loss during Big Dry. For example, the greatest ΔTWS loss of ~79 550 Gton is observed over NWP, which is ~25 Gton greater than the loss during Big Dry (see Fig. 551 8a and 8c). The basin is less affected by the La Niña, and the rainfall during Big Wet is 552 clearly inadequate to support the water storage recovery in the basin. Rainfall deficiency also 553 reduces the groundwater recharge, resulting in even more decreasing of ΔGWS , compared to 554 the Millennium Drought period (see Fig. 8j and 8l). The continual decrease in water storage 555 over western basins is likely caused by the interaction of complex climate patterns like El 556 Niño Southern Oscillation, Indian Ocean Dipole, and Southern Annular Mode cycles 557 (Australian Bureau of Meteorology, 2012; Xie et al., 2016).

558

567

559 **6. Further development of GC approach**

560 6.1 Comparison of GC approach with alternatives

561 The simplest approach to estimate ΔGWS is to subtract the model soil moisture component 562 from GRACE ΔTWS data, without considering uncertainty in the model output, as used in 563 Rodell et al. (2009) and Famiglietti et al. (2011). This method is called Approach 1 (App 1). 564 In Approach 2 (App 2) as in Tangdamrongsub et al. (2017), by accounting for the uncertainty 565 of model outputs and GRACE data, the water storage states are updated through a Kalman 566 filter:

$$\widehat{\boldsymbol{h}}_{R} = \widetilde{\boldsymbol{h}}_{R} + \boldsymbol{H}\boldsymbol{C}_{R}^{T}(\boldsymbol{H}\boldsymbol{R}\boldsymbol{H}^{T} + \boldsymbol{C}_{R})^{-1}(\boldsymbol{b} - \boldsymbol{H}\widetilde{\boldsymbol{h}}_{R})$$
(20)

568 where \tilde{h}_R , H, C_R are described in Sect. 2, *b* is an observation vector containing GRACE-569 derived ΔTWS , and **R** is an error variance-covariance matrix of the observation. The 570 GRACE-derived ΔTWS and its error information is obtained from the mascon solution. The 571 matrix **R** is a (diagonal) error variance matrix since no covariance information is given in the 572 mascon product.

573 The ΔGWS estimates from App1, App2 and GC in Queensland and Victoria are shown in

Fig. 9. It is clearly seen that ΔGWS from App1 are overestimated while the one from App2

575 fits the ground data significantly better. This behaviour was also seen in Tangdamrongsub et





576 al. (2017) that the water storage estimates tend to be overestimated when error components 577 such as spatial correlation error were neglected as in App1. ΔGWS from App2 shows clear 578 improvements in terms of NS coefficients in both networks. Considering the de-seasonalized 579 ΔGWS estimates, in Queensland, the trend increases from 0.39 \pm 0.03 to 0.42 \pm 0.03 cm/year 580 (improves by 1.5%), and the NS value increases from 0.46 to 0.53. In Victoria, the trend 581 decreases from 0.73 ± 0.10 to 0.46 ± 0.05 cm/year (improves by 27%), and the NS value 582 increases from -0.89 to 0.30. Although App2 is not yet as good as the GC solution based on 583 the most comprehensive error propagation, this simple test demonstrates an important of 584 considering the uncertainty. The reason of App2 being less accurate than GC is likely due to 585 too simplified error information implemented in App2.

586

597

587 6.2 GC data assimilation approach

588 We so far discussed the GC approach to update the water storage estimates independently 589 every month. The approach can be easily expanded to sequentially update the model initial 590 states whenever the GRACE observation is available (for example, every day) as in data 591 assimilation (DA) like ensemble Kalman filter (Evensen, 2003) and particle filter (Weerts 592 and El Serafy, 2006). We briefly describe a way of modifying the GC approach suitable for 593 DA. The ensemble of simulated monthly water storage estimates is predicted based on the set 594 of ensemble forcing data and model parameters. This is simply running CABLE for K 595 (number of ensemble) times. When GRACE observation is available, the updated state is 596 computed:

$$\widehat{h}_{Re} = (C_R + N_R)^{-1} (C_R \widetilde{h}_{Re} + c_{Re})$$
(21)

598 where the subscript *e* represents the ensemble or perturbed version of the original vector or matrix (see e.g., Eq. (11)). The dimension of \hat{h}_{Re} , \tilde{h}_{Re} , c_{Re} is $3J \times K$. The estimated \hat{h}_{Re} can 599 600 be directly used as in the initial state for the next time step for CABLE run (Eicker et al., 601 2014; Tangdamrongsub et al., 2015; Tian et al., 2017), or used in the repeated run to avoid 602 any spurious jump of the water storage estimates between the each step (Forman et al., 2012; 603 Tangdamrongsub et al., 2017). This sequential update process can be carried out as long as 604 desired. The feasibility of GRACE DA has been demonstrated with "devised" uncertainty (covariance) information. As a future work, we will develop new DA approach on the basis 605 of full error information of GRACE data by using the least-squares normal equation and thus 606 607 carrying the error information from the fundamental (satellite tracking) data level. 608

609 7. Conclusion

610 This study presents an approach of combining the raw GRACE observation with model

simulation to improve water storage estimates over Australia. Distinct from other methods,

612 we exploit the fundamental GRACE satellite tracking data and the full data error variance-

613 covariance information to avoid alteration of signal and measurement error information

614 present in higher level data products.

615 We compare groundwater storage estimates from GC approach and two other approaches,

616 subject to inclusion of GRACE uncertainty in ΔGWS calculation. Validating three results of

617 ΔGWS against the in situ groundwater data, we find that the GC approach delivers the most





- 618 accurate groundwater estimate, followed by the approach based on incomplete information of
- 619 GRACE's data error. The poorest estimate of groundwater storage is seen when the GRACE
- 620 uncertainty is completely ignored. This confirms the critical value of using the complete
- 621 GRACE signal and error information at the raw data level.
- The analysis of water storage change between 2003 and 2016 reveals that half of the
- 623 continent (5 out of 10 basins) is still not fully recovered from the Millennium Drought. The
- TWS decrease in Western Australia has been most characteristic and the GC approach finds
- 625 that the water loss mainly occur in groundwater layer. Rainfall inadequacy is attributed to the
- 626 continual dry condition, leading to a greater decreasing of groundwater recharge and storage 627 over Western Australia.
- 628 The land surface model we used is deficient in anthropogenic groundwater consumption. The
- model calibration will never help and the groundwater consumption must be brought in by
- 630 external sources. On the contrary, the statistical approach like our GC approach may be
- 631 useful to fill in the missing component and lead to a more comprehensive water storage
- 632 inventory.
- 633 However, it is difficult to constrain different water storage components by only using total
- storage observation like GRACE. In addition, it is challenging to improve surface soil
- 635 moisture varying rapidly in time, using a monthly mean GRACE observation. Tian et al.
- 636 (2017) utilized the satellite soil moisture observation from the Soil Moisture and Ocean
- 637 Salinity (SMOS, Kerr et al., 2001) in addition to GRACE data for their data assimilation and
- showed a clear improvement in the top soil moisture estimate. The GC approach with
- 639 complementary observations at higher temporal resolution should be considered particularly
- 640 to enhance the surface soil moisture computation.
- 641 Finally, the GC approach can be simply extended for GRACE data assimilation. Assimilating
- the raw GRACE data into land surface models like CABLE enables the model state and
- 643 parameter to be adjusted with the realistic error information, allowing reliable storage
- 644 computation. The GC data assimilation will be developed in our future study.
- 645

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- 650 least-squares normal equations.
- 651





652 Appendix: Nash-Sutcliff coefficient and area-weighted average

653 Nash-Sutcliff coefficient (NS) is computed as follows:

$$NS = \mathbf{1} - \frac{\sum_{i=1}^{N} (\mathbf{y}_i - \hat{\mathbf{x}}_i)^2}{\sum_{i=1}^{N} (\mathbf{y}_i - \bar{\mathbf{y}})^2}$$
(A1)

- where y is an observation vector, \overline{y} is the mean of the observation, \hat{x} is a vector containing
- the simulated result, i is the index of observation, and N is the number of observation.
- 657 Area-weighted average (\overline{Z}) is compute as follows:

$$\bar{Z} = \frac{\sum_{j=1}^{M} w_j \bar{z}_j}{\sum_{j=1}^{M} w_j}$$
(A2)

659 where w is the area size, \bar{z} is the mean value inside the considered area, j is the area index,

660 and M is the number of considered area.

661





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- 852





- 853 **Table 1.** Precipitation data from 7 different products used in this study, the Global Soil
- 854 Wetness Project Phase 3 (GSWP3), the Global Land Data Assimilation System (GLDAS),
- the Tropical Rainfall Measuring Mission (TRMM), the Modern-Era Retrospective Analysis
- 856for Research and Applications (MERRA), the European Centre for Medium-Range Weather
- 857 Forecasts (ECMWF), the Princeton's Global Meteorological Forcing Dataset (Princeton), and
- the Precipitation Estimation from Remotely Sensed Information using Artificial Neural
- 859 Networks (PERSIANN). The temporal resolution of all products are 3 hours. Most products
- are available to present while GSWP3, MERRA, and Princeton terminate earlier.

Product	Availability	Spatial	References
		resolution	
GSWP3	1901/01 -	$0.5^{\circ} \times 0.5^{\circ}$	Dirmeyer et al. (2006)
	2010/12		-
GLDAS	2000/03 -	0.25°×0.25°	Rodell et al. (2004)
(NOAH025SUBP 3H)	present		
TRMM (3B42)	1998/01 -	0.25°×0.25°	Huffman et al. (2007)
	present		
MERRA	1980/01 -	$0.5^{\circ} \times 0.67^{\circ}$	Rienecker et al. (2011)
(MSTMNXMLD.5.2.0)	2016/02		
ECMWF (ERA-Interim)	1979/01 -	$0.75^{\circ} \times 0.75^{\circ}$	Dee et al. (2011)
	present		
Princeton (V2 0.5°)	1987/01 –	$0.5^{\circ} \times 0.5^{\circ}$	Sheffield et al. (2005)
	2012/12		
PERSIANN (3 hr)	2002/03 -	0.25°×0.25°	Sorooshian et al. (2000)
	present		

861

862

863 Table 2. Model parameters that are sensitive to SM and GWS estimates. The following

parameters were perturbed using the additive noise with the boundary conditions given in the
last column. The further parameter description can be found in Decker (2015) and Ukkola et
al. (2016).

Parameter	Name	Spatial	Perturbed
		variability	range
$f_{\text{clay}}, f_{\text{sand}}, f_{\text{silt}}$	Fraction of clay, sand, and silt	Yes	0 – 1
$f_{\rm sat}$	Fraction of grid cell that is saturated	No	810 - 990
$q_{ m sub}$	Maximum rate of subsurface drainage	No	0.009 - 0.01
	assuming a fully saturated soil column		
fp	Tuneable parameter controlling drainage speed	No	1.9 - 2.2





- 869 **Table 3**. NS coefficients between top soil moisture estimates and the satellite soil moisture
- observations from AMSR-E products over 10 different Australian basins. The area-weighted
- average value (AVG) is also shown.

	C-band		X-band	
	CABLE	GC	CABLE	GC
GOC	0.67	0.68	0.58	0.60
IND	0.53	0.54	0.41	0.41
LKE	0.48	0.53	0.36	0.42
MRD	0.77	0.80	0.75	0.78
NEC	0.34	0.39	0.14	0.19
NWP	0.33	0.36	0.38	0.42
SEC	0.68	0.68	0.69	0.71
SWC	0.85	0.85	0.89	0.89
SWP	0.55	0.56	0.46	0.48
TIM	0.44	0.45	0.16	0.16
AVG	0.53	0.56	0.47	0.50

872

873

- **Table 4**. NS coefficient and long-term trend of ΔGWS estimated from the model-only and
- 875 GC solutions in Queensland and Victoria groundwater network. The long-term trend of the
- 876 in-situ data is also shown.

	Queensland		Victoria			
	In-situ	CABLE	GC	In-situ	CABLE	GC
Original time-series						
NS [-]	-	0.49	0.60	-	0.34	0.63
Trend	1.60 ± 0.05	0.39 ± 0.02	0.63 ± 0.05	$-0.27 \pm$	0.10 ± 002	-0.18 ± 0.03
[cm/year]				0.05		
De-seasonalized time-series						
NS [-]	-	0.50	0.66	-	0.43	0.83
Trend	1.60 ± 0.05	0.39 ± 0.02	0.57 ± 0.04	$-0.25 \pm$	0.10 ± 0.02	-0.16 ± 0.03
[cm/year]				0.05		







878

879 Figure 1. (a) Geographical location of 10 Australian river basins. Red and blue polygons

880 indicate the boundaries of groundwater networks in Queensland (b) and Victoria (c),

881 respectively. Triangles (in b and c) represent the selected bore locations used in this study.







Figure 2. NS coefficients between the model and GRACE-mascon ΔTWS over 10 Australian basins (in ordinate). The NS values were computed based on CABLE ΔTWS computed with 7 different precipitation data (in abscissa), GSWP3 (GS), GLDAS (GL), ECMWF (EC), MERRA (MR), PERSIANN (PR), TRMM (TR). The NS value of the mean ΔTWS estimates (the average of 7 variants) is also shown (MN). The area-weighted average NS value over all basins is also shown (AVG). The NS value of ΔTWS from the GRACE-combined (GC) approach is shown in the last column. The full name of the basins can be found in Fig. 1.







892

Figure 3. The monthly time series of ΔSM_{top} , ΔSM_{rz} , ΔGWS , and ΔTWS estimated from model (blue) and GC (red) solutions over Gulf of Carpentaria (GOC), Indian Ocean (IND),

895 Lake Eyre (LKE), Murray-Darling (MRD), and North East Coast (NEC). The de-

seasonalized time series is also shown.







898

899 Figure 4. Similar to Fig. 3, but estimated over North West Plateau (NWP), South East Coast

900 (SEC), South West Coast (SWC), South West Plateau (SWP), and Timor Sea (TIM).







Figure 5. Long-term trends of ΔTWS (c, d), ΔSM_{top} (e, f), ΔSM_{rz} (g, h), and ΔGWS (i, j) estimated from the model-only (left) and the GC solutions (right). Results of GRACE ΔTWS independently from mascon (a) and GRGS solution (b) are also shown. The eastern part of North West Plateau basin is shown as a rectangle polygon in (c) and (d).







908

909 **Figure 6.** Uncertainties of ΔSM_{top} , ΔSM_{rz} , ΔGWS , and ΔTWS estimated from the model

910 (blue) and the GC solutions (red) in 10 different Australian basins. The uncertainty of the

911 precipitation is shown in (e). The area-weighted average value (AVG) is also shown.







913

Figure 7. The monthly time series of ΔGWS estimated from the model, GC solutions, and measured from the in situ groundwater network in Queensland (a) and Victoria (b). Deseasonalized time series are shown in thick lines.







919 **Figure 8.** Mass changes (Gton, Giga tonne) of ΔTWS , ΔSM_{top} , ΔSM_{rz} , and ΔGWS estimated 920 from GC solutions over 10 Australian basins in 3 different periods, Big Dry (January 2003 – 921 December 2009), Big Wet (January 2010 – December 2012), and entire period (January 2003 922 – March 2016).

923







Figure 9. Δ*GWS* estimated from Approach 1 (App1) and Approach 2 (App2) in Queensland
(a) and Victoria (b). The in-situ groundwater network data and the GC solutions are also
shown. De-seasonalized time series are shown in thick lines.