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Imtiaz Dharssi, Peter Steinle and Brett Candy

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1. ABSTRACT

Several Meteorological service agencies have developed Extended Kalman Filter based land data assimilation systems that, in principle, can analyse any model land variable. Such systems can make use of a wide variety of observation types, such as screen level observations and satellite based estimates such as retrieved surface soil moisture and retrieved skin temperature. Indirect measurements can be used and information propagated from the surface into the deeper soil layers. A key component of the system is the calculation of the Jacobians of the observation operator which describe the link between the observations and the land surface model variables. The Jacobians are estimated using finite difference by performing short model forecasts with perturbed initial conditions. This report examines the Jacobians that link observations of screen level variables, satellite derived surface soil moisture and satellite derived skin temperature to model soil temperature and moisture.

For a well behaved system the calculated values of the Jacobians should be nearly independent of the magnitude and sign of the perturbations used. This is investigated by comparing Jacobians calculated using perturbations of opposite signs. Jacobians values that are significantly affected by the sign of perturbation used are assumed to contain a gross error. A simple quality control scheme is developed to detect such gross errors. Analysis is also performed of the sensitivity of the calculated Jacobians to the magnitude of the perturbations used.

The calculated Jacobians that link screen level variables to model soil moisture show that there is strong coupling between the screen level and the soil. The coupling between the topmost model level soil moisture and the screen level is found to be due to a number of processes including bare soil evaporation, soil thermal conductivity, soil thermal capacity as well as transpiration by plants. Therefore, there is significant coupling both during the day and at night. The sign of the Jacobians linking screen level temperature to topmost model level soil moisture are usually negative during the day and tends to be positive during the night. The coupling between the the screen level and soil moisture in the deeper model layers is primarily through transpiration by plants. Therefore the coupling is only significant during the day and the vertical variation of the coupling is found to be significantly affected by the vegetation root depths. The calculated Jacobians that link screen level temperature to model soil temperature are found to be largest for the topmost model soil layer and become very small for the lower soil layers. These Jacobians are largest during the night and generally positive in value.

It is found that the Jacobians that link observations of surface soil moisture to model soil moisture are strongly affected by the soil hydraulic conductivity. Generally, for the JULES land surface model, the coupling between the surface and root zone soil moisture is weak. Finally, the Jacobians linking observations of skin temperature to model soil temperature and moisture are calculated. These Jacobians are found to have a similar spatial pattern to the Jacobians for observations of screen level temperature.

2. INTRODUCTION

The land surface states such as soil moisture, temperature and snow play an important role in land-atmosphere coupling. The very high albedo of snow, as well as the water storage and insulation properties means that snow can have a significant impact on numerical weather prediction (NWP) and seasonal forecasting. Soil moisture and temperature have a significant impact on screen level temperature and humidity, low clouds and precipitation, by influencing the exchange of heat and moisture between the land surface and the atmosphere (see for example Walker and Rowntree 1977; Timbal et al. 2002; Dharssi et al. 2009). Soil moisture is important for the prediction of summer-time precipitation at mid-latitudes over land (Koster et al. 2000). In particular, soil moisture plays an important role in the development of convective storms (Findell and Eltahir 1997). The land surface is also very important for the seasonal prediction of extreme events such as heat waves and drought (Weisheimer et al. 2011).

Data assimilation (DA) is extremely important for NWP since errors in the model initial conditions can grow rapidly and seriously degrade forecasts. The initial land surface state can have a significant impact on forecasts of screen level temperature and humidity as well as forecasts of precipitation. Specifying the model initial soil moisture and temperature state is especially difficult since there are few near real-time ground based observations of soil moisture and temperature. Therefore, indirect observations are usually used by land surface DA schemes to initialise the model soil moisture and temperature (Dharssi et al. 2011; de Rosnay et al. 2012). In addition, model soil moisture is highly model specific. For example, Koster et al. (2009) show that direct transfer of soil moisture values from one land surface model to a different land surface model is inappropriate and likely to lead to problems. Consequently, any land surface DA scheme must be consistent with the land surface model used by the NWP system. Inconsistencies in the analysed land surface fields could introduce spurious, long lived shocks to the NWP system and degrade forecasts.

3. LAND SURFACE ANALYSIS

A number of new space-borne remote sensing systems have been developed that provide information on surface soil moisture and temperature. However, most NWP centres still only use screen level observations (of temperature and humidity) for the operational analysis of soil moisture and temperature, e.g. ECMWF (de Rosnay et al. 2012), Meteo-France (Giard and Bazile 2000) and the German Weather Service (Hess et al. 2008). The Met Office is the first, and thus far only, NWP centre to operationally use satellite derived measurements of surface soil moisture (Dharssi et al. 2011) together with screen level observations (Best and Maisey 2002) for the analysis of soil moisture. Dharssi et al. (2011) find that assimilation of remotely sensed surface soil wetness measurements improves the agreement of the soil moisture analyses with ground based soil moisture observations and improves forecasts of screen level temperature and humidity.

Several Met services, such as ECMWF (de Rosnay et al. 2012; Drusch et al. 2009) and Meteo France (Mahfouf et al. 2009; Draper et al. 2011) have developed new Extended Kalman Filter (EKF) based land DA systems. Such EKF land DA systems can make more statistically optimal use of a wide variety of observation types, such as screen level observations and satellite based estimates such as retrieved Surface Soil Moisture (SSM), retrieved skin temperature , Leaf Area Index (LAI) and Fraction of Photosynthetically Active Radiation (FPAR). Indirect measurements can be used and information propagated from the surface into the deeper soil layers. Such EKF land DA systems are much more flexible and, in principle, any model land variable can be analysed; such as soil moisture, soil temperature, snow amount and vegetation properties such as LAI. For example an EKF based land DA system may,

- Use satellite estimates of surface soil moisture to analyse surface and root-zone soil moisture
- Use satellite estimates of skin temperature to analyse soil temperature and moisture
- Use observations of screen level temperature and humidity to analyse soil

temperature and moisture

- Use satellite estimates of FPAR to analyse soil moisture.

The EKF land DA system at ECMWF is now used operationally for soil moisture analysis. de Rosnay et al. (2012) show that the EKF has a more positive impact on NWP performance than the previously used Optimal Interpolation (OI) soil moisture nudging scheme. The EKF is found to make larger soil moisture increments in the surface soil layer than the OI scheme and much smaller increments in the lower soil layers. de Rosnay et al. (2012) suggest that this is because the EKF takes into account model vegetation properties such as vegetation root depth and fraction of vegetation roots in each model soil layer. While the simpler OI scheme doesn't use such vegetation information and merely scales the soil moisture increments by the model soil layer thickness. Since the lower model soil layers are much thicker than the model surface layer, this leads to unrealistically large soil moisture increments in the lower model soil layers by the OI scheme. In addition, the OI scheme assumes that the coupling between soil moisture and the screen level is only due to transpiration by plants. The EKF is much more comprehensive since all the active model land surface parameterisations determine the strength of coupling between soil moisture and the screen level. de Rosnay et al. (2012) find that the EKF soil moisture analyses are in better agreement with ground based soil moisture observations. Albergel et al. (2012) has compared global soil moisture measurements from over 200 ground based stations with remotely sensed soil moisture from SMOS (Soil Moisture and Ocean Salinity, Kerr et al. 2001), ASCAT (Advanced Scatterometer, Bartalis et al. 2007) and ECMWF EKF based soil moisture analyses that assimilate screen level observations and ASCAT derived surface soil moisture [1]. The correlation between the ECMWF EKF based soil moisture analyses and ground based observations is significantly higher than the correlations between SMOS or ASCAT derived soil moisture and ground based observations. This convincingly demonstrates the effectiveness of assimilating screen level observations to analyse soil moisture. The EKF land DA system at Meteo France is currently used for research only and the OI soil moisture nudging scheme is still used operationally. The generally neutral impact of the Meteo France EKF may be because of the simple two-layer land surface model used.

[1] ECMWF only use screen level observations for their operational soil moisture analyses. However, for testing they also assimilated ASCAT derived surface soil moisture. So far, ECMWF have found little benefit from assimilating ASCAT data but work is on-going, in particular to improve the bias correction.

The physically based soil moisture nudging scheme (Best and Maisey 2002) used operationally at the Met Office and Australian Bureau of Meteorology (Bureau) does use vegetation information including root depth and layer fractions of roots to determine the vertical distribution of soil moisture increments. In addition this scheme has been extended to include the effect of bare soil evaporation as well as transpiration to determine the strength of coupling between the soil moisture and screen level. Therefore, the physically based soil moisture nudging scheme is superior to the OI soil moisture nudging scheme. However, an EKF land DA system is much more flexible and uses the available information in a more statistically optimal manner and therefore the Bureau in collaboration with the Met Office are also developing an EKF land DA system (Candy et al. 2012).

3.1 The Extended Kalman Filter

The DA problem is kept manageable by assuming that the model land columns are independent of each other (a 1-dimensional approach). This assumption is also made by most land surface models, including JULES (Best et al. 2011). The standard EKF land DA analysis equations for each land column are given by

$$\mathbf{x}^{\mathbf{a}}(t_i) = \mathbf{x}^{\mathbf{b}}(t_i) + \mathbf{K}_i \left[\mathbf{o}(t_i) - h_i(\mathbf{x}^{\mathbf{b}})\right] \tag{1}$$

$$\mathbf{K}_i = \mathbf{B}\mathbf{H}_i^T \left(\mathbf{H}_i\mathbf{B}\mathbf{H}_i^T + \mathbf{R}\right)^{-1} \quad . \tag{2}$$

$\mathbf{x}(t_i)$ represents the state vector of a land column at time t_i with superscripts a and b standing for analysis and background. $\mathbf{o}(t_i)$ is the observation vector. $\mathbf{K}_i$ is the Kalman gain matrix at time t_i. $\mathbf{B}$ is the background error covariance matrix. $\mathbf{R}$ is the observation error covariance matrix. Both the $\mathbf{B}$ and $\mathbf{R}$ matrices are assumed to be diagonal and static in time. Normally, a Kalman filter updates $\mathbf{B}$ every cycle. However, this is difficult with the EKF since knowledge of the model error statistics is required. Several studies with EKF land DA systems have found no benefit from updating $\mathbf{B}$ (Sabater et al. 2007; Draper et al. 2009). The ECMWF EKF land DA system doesn't update $\mathbf{B}$ and most studies using the Meteo France EKF land DA system also don't update $\mathbf{B}$.

$\mathbf{H}_i$ is the Jacobian (linearisation) of the non-linear observation operator h_i and is defined using $h_i(\mathbf{x} + \boldsymbol{\Delta}) \simeq h_i(\mathbf{x}) + \mathbf{H}_i\boldsymbol{\Delta}$, where $\boldsymbol{\Delta}$ is a small perturbation to the model state $\mathbf{x}$. The elements of $\mathbf{H}_i$ are estimated using finite difference by individually perturbing each component of $\mathbf{x}$ by a a small scalar amount δ_j. A given element of $\mathbf{H}_i$ is calculated using

$$H_{kj} = \frac{y_k(\mathbf{x} + \delta_j) - y_k(\mathbf{x})}{\delta_j}. \tag{3}$$

$y_k(\mathbf{x} + \delta_j)$ is a short model forecast of observation type k (e.g. screen level temperature) starting from perturbed initial conditions $\mathbf{x}+\delta_j$. The number of perturbed forecasts required increases with the number of model variables to be analyses and the number of soil layers. For example, to analyse skin temperature and soil moisture and temperature on four soil levels would require ten perturbed forecasts, including the control $y(\mathbf{x})$. The length of a perturbed forecast is typically a few hours long but can be as short as one time-step, depending on the observation types assimilated.

The major computational cost of the EKF land DA system is the cost of running the perturbed forecasts. ECMWF use the fully coupled land/atmosphere model for the perturbed forecasts. Meteo France use an off-line land surface model (uncoupled to the atmosphere model) for the perturbed forecasts. Consequently the Meteo France EKF land DA system is computationally several orders of magnitude cheaper. The Bureau EKF land DA system also uses an off-line land surface model for the perturbation forecasts. Balsamo et al. (2007) and Mahfouf et al. (2009) have shown that the off line land surface model can be used to reliably calculate $\mathbf{H}_i$. The atmospheric forcing data for the off-line land surface model (precipitation, surface LW and SW radiation, air temperature and humidity, wind speed and surface pressure) are obtained from short range forecasts of the atmospheric model. Atmospheric forcing of air temperature and humidity are applied at a height of 20 m (which is above the screen level). This allows the EKF land DA system to also assimilate observations of screen level temperature and humidity (see Fig. 1 of Mahfouf et al. (2009) for a fuller explanation).

3.2 The Land Surface Model

The ACCESS (Australian Community Climate and Earth-System Simulator) system is used at the Bureau for NWP. MOSES2 (Essery et al. 2001) or JULES are used to represent the land surface processes in the NWP versions of ACCESS . JULES is scientifically very similar to MOSES2. However, the JULES code is much more flexible than MOSES2; incorporating advanced Fortran 90 features such as the use of Modules and in particular JULES can be run off-line.

Therefore, the Bureau EKF land DA system, in development, uses JULES. The soil is discretised into four layers of 0.1, 0.25, 0.65 and 2 m thickness (from top to bottom). The vertical discretisation for the soil hydrology is the same as that for the thermodynamics, i.e. the positions of the soil moisture levels coincides with the soil temperature levels. The soil hydrology is based on a finite difference form of the Richards equation and Darcy's law. The van Genuchten (1980) equations are used to describe the relationship of soil hydraulic conductivity and soil suction to the unfrozen volumetric soil moisture. The van Genuchten soil parameters depend on the soil texture (size distribution of the soil particles and the soil organic carbon content). A new high resolution soil textures map is used that merges data from three separate sources; Harmonised World Soil Database (HWSD, FAO et al. 2008), State Soil Geographic Database (United States region, Miller and White 1998) and point observations of soil sand, silt and clay fractions. Currently, there is no vertical variation of soil texture.

The soil thermodynamics is represented by diffusive heat exchanges between the soil layers and by heat advection between the soil layers by the fluxes of moisture. The freezing and melting of soil water are also represented and the associated latent heat is included in the thermodynamic calculations.

The land surface model uses 5 vegetation tiles (broadleaf trees, needleleaf trees, C3 (temperate) grass, C4 (tropical) grass and shrubs) and 4 non-vegetation tiles (urban, inland open water, bare soil and land ice). Transpiration by plants extracts soil water directly from the soil layers via the plant roots while bare soil evaporation extracts soil water from the top soil layer only. The ability of plants to access water from each soil layer is determined by the root density distribution and soil moisture availability. The broadleaf trees are assumed to have a root depth of $d_r = 3\ m$, needleleaf trees have $d_r = 1\ m$, grasses and shrubs have $d_r = 0.5\ m$ and the total depth of the model soil $z_t = 3\ m$.

The bulk stomatal resistance in the absence of soil moisture stress is calculated by a photosynthesis model (Mercado et al. 2007) and depends on incident radiation, vegetation type, surface air temperature and humidity deficit. The bulk stomatal resistance includes a dependency on the soil moisture content via a soil moisture availability factor. To reduce computational costs, the parameter values from the tiles within a land column can be aggregated so that a single energy balance equation is solved per land column.

4. EXPERIMENTS AND RESULTS

In order to avoid compensating effects through temporal averaging, results are presented for one time period only; the off-line perturbed forecasts are started from initial conditions valid at 3Z 16/01/2011. The length of the perturbed forecasts is three hours. Perturbed forecasts with shorter (longer) lengths of one (five) hour(s) have also been tried. The Jacobians for the screen level observations appear not to be significantly affected by the forecast length. However, the Jacobians for the surface soil moisture observations are significantly affected by the forecast length. A simple Quality Control (QC) is applied to the computed Jacobians shown in the following figures and the simple QC scheme is described in section 4.1.2 . Jacobian elements are calculated for the region 48S to 45N; 125W to 178E (a global investigation would require greater computational effort and thus slow progress). Figure 1 shows the model initial conditions for snow amount and level 1 soil temperature. During January much of the northern hemisphere land is covered by snow.

4.1 The Jacobians of the Observation Operator for the Screen Level Observations

Screen level observations of temperature and humidity can be assimilated to analyse soil moisture and temperature when there is strong coupling between the screen level and the soil. The Jacobians of screen level temperature with respect to soil moisture ($\Delta T_{2m}/\Delta\theta_l \equiv H_{T_{2m},\theta_l}$), in the four model soil layers, are shown in Fig. 2. For soil layers two to four, the coupling between screen level temperature and soil moisture is primarily through transpiration by vegetation. Consequently the coupling occurs during daylight. Negative Jacobians values means that an increase in soil moisture leads to a cooling of the screen level. For the surface soil layer, the picture is more complicated as there is strong coupling both during the day and at night. The Jacobians have a positive value in some places and a negative value in others and this is investigated in the next section.

The Jacobians of screen level specific humidity with respect to soil moisture ($\Delta q_{2m}/\Delta\theta_l$) are shown in Fig. 3. The spatial pattern shown in Fig. 3 is similar to Fig. 2. However, for screen level specific humidity, the Jacobian values are primarily positive meaning that an increase in soil moisture leads to an increase in screen level humidity.

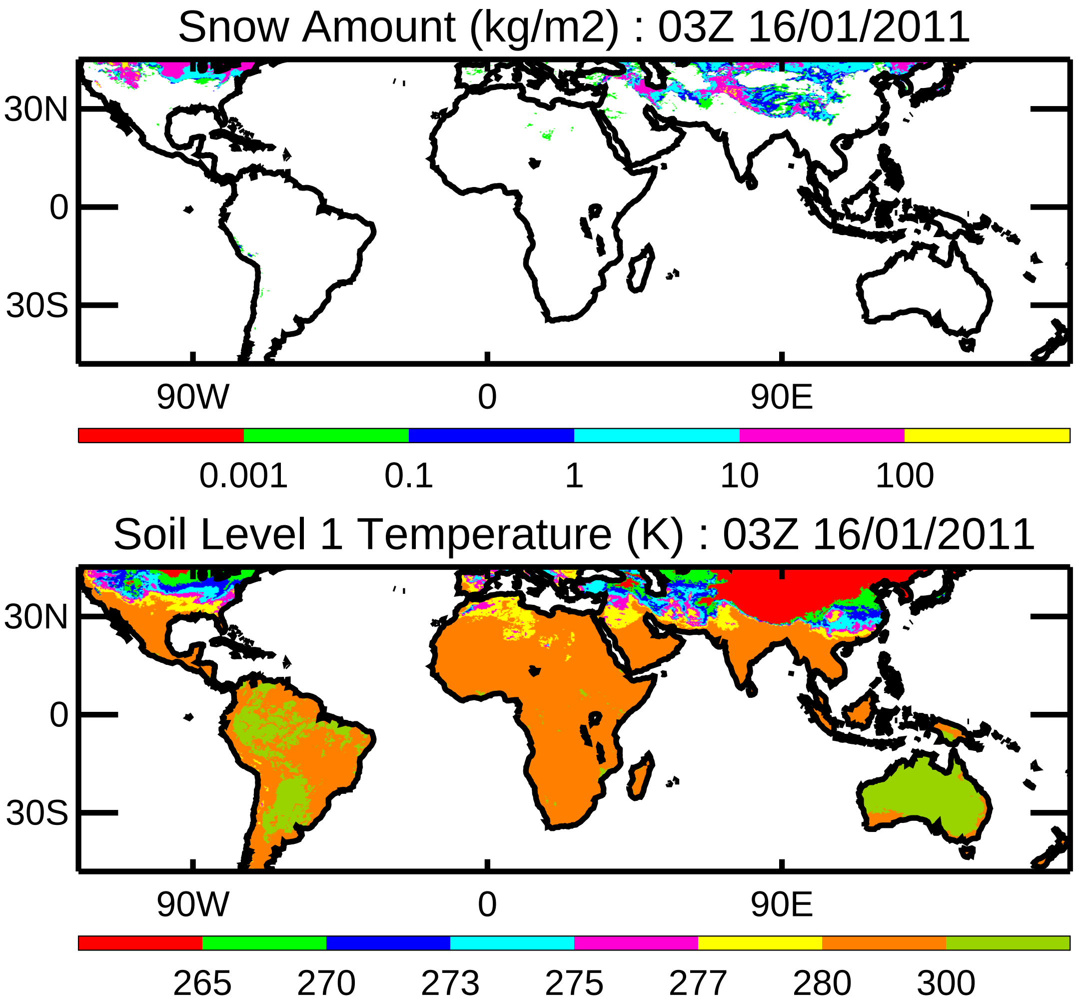

Fig. 1 Initial conditions for model snow amount (top panel) and level 1 soil temperature (lower panel) at 3Z 16/01/2011.

The Jacobians of screen level temperature with respect to soil temperature ($\Delta T_{2m}/\Delta T_l$) are shown in Fig. 4. The Jacobians are largest for soil level 1 and become very small for soil levels 3 and 4. The Jacobians are largest during the night and generally positive in value. This is consistent with the experience of ECMWF who find that their soil temperature nudging scheme is more effective during the night and winter when screen level errors are less likely to be related to soil moisture (Mahfouf et al. 2000).

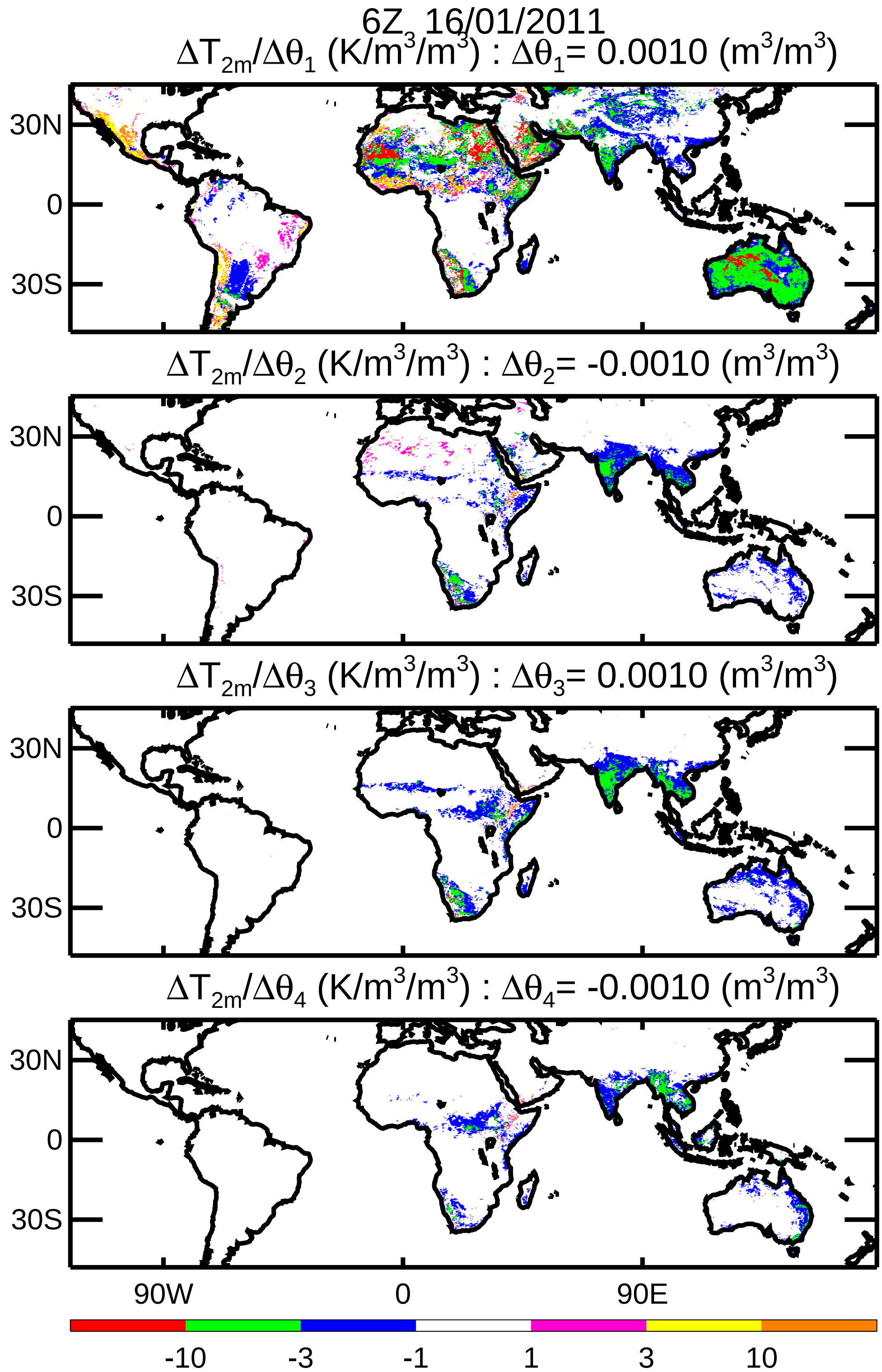

Fig. 2 The computed Jacobians of screen level temperature with respect to volumetric soil moisture in the four model soil layers. The Jacobians are valid at 6Z 16/01/2011 and are calculated using three hour long perturbed forecasts with initial soil moisture perturbations of magnitude $|\Delta\theta_l| = 10^{-3}\ m^3/m^3$. The sign of $\Delta\theta_l$ can be positive or negative and for illustration is alternated between soil layers.

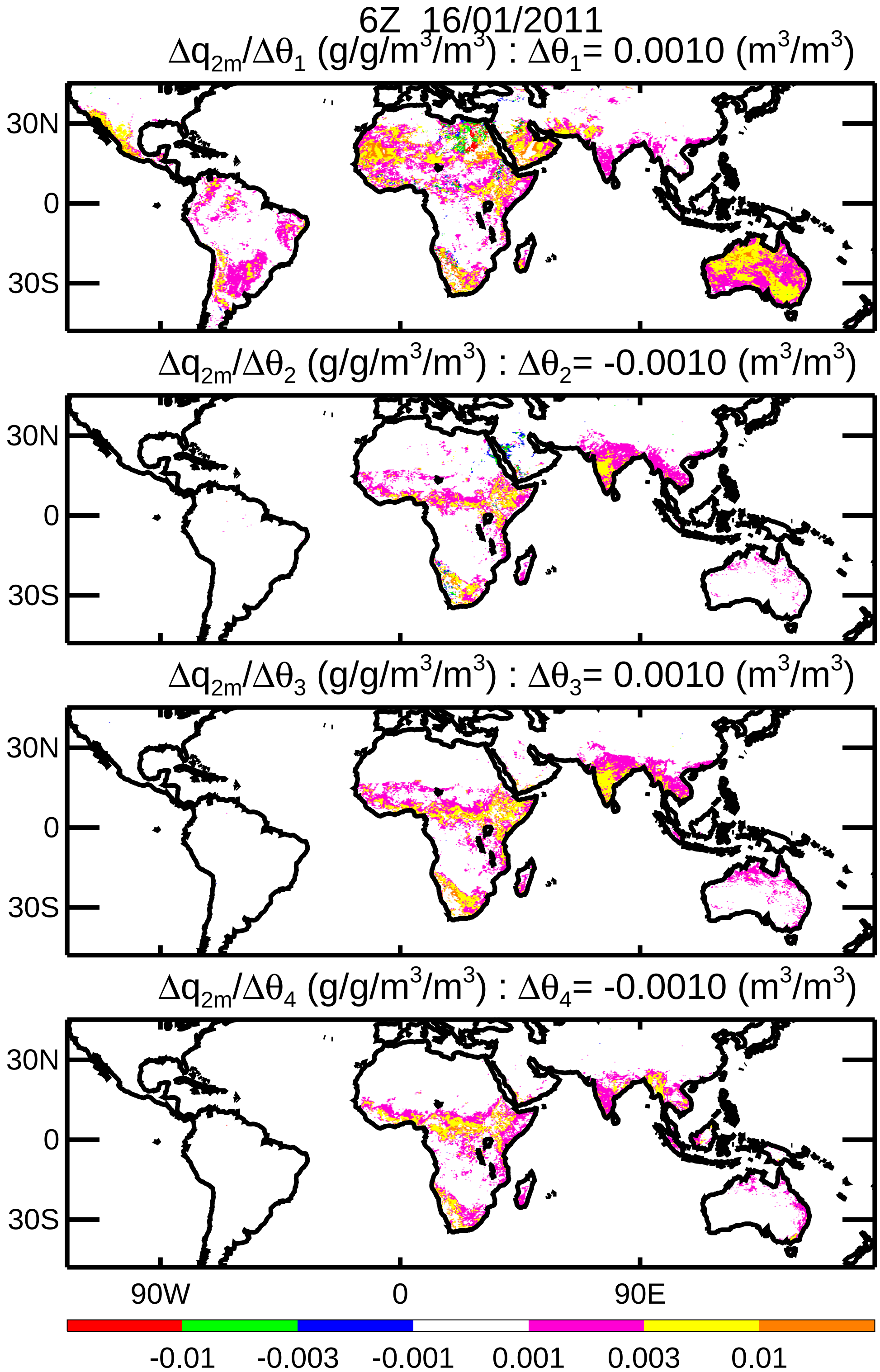

Fig. 3 The computed Jacobians of screen level specific humidity with respect to volumetric soil moisture in the four model soil layers. The Jacobians are valid at 6Z 16/01/2011 and are calculated using three hour long perturbed forecasts with soil moisture perturbations of magnitude $10^{-3}\ m^3/m^3$.

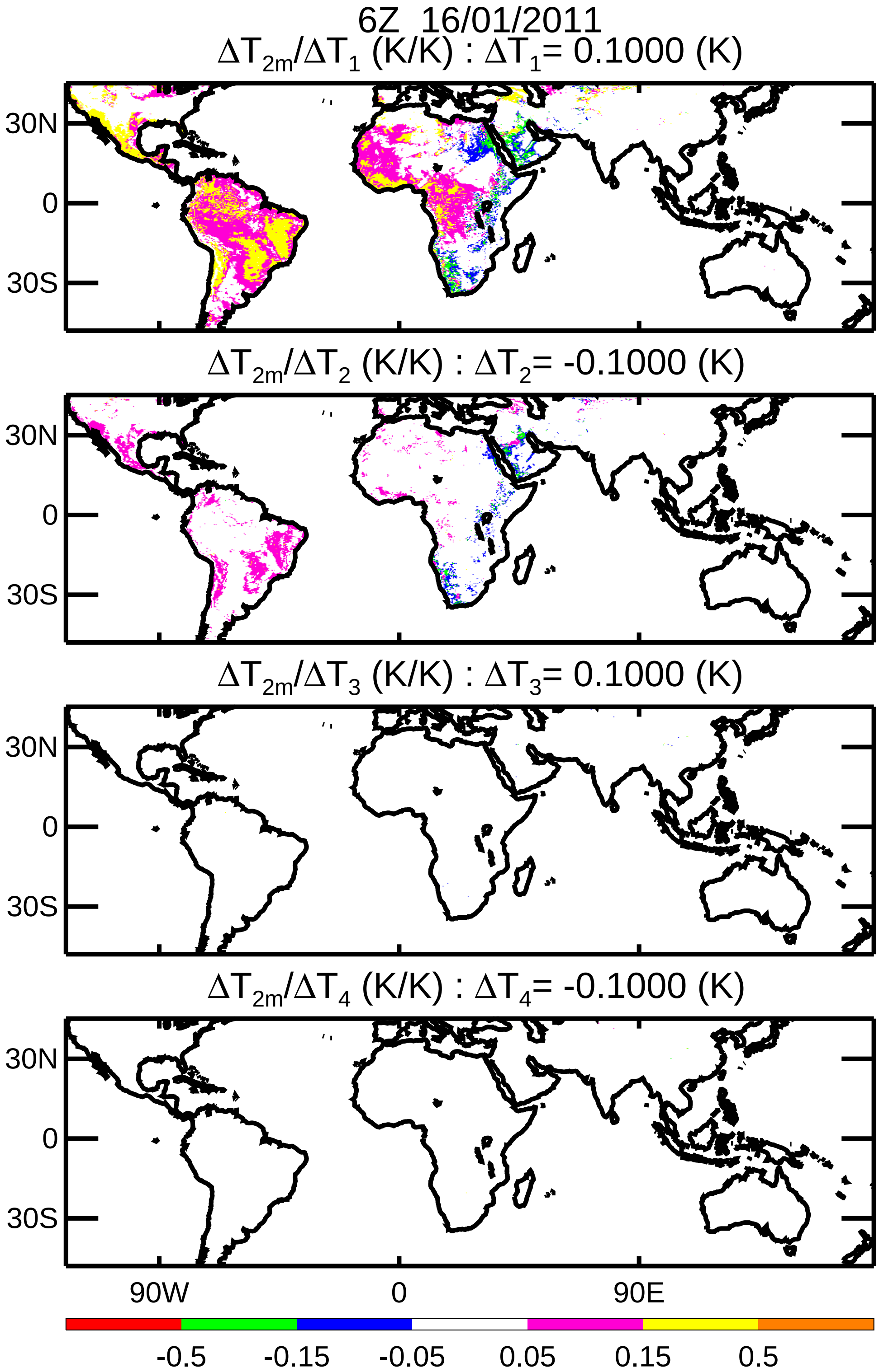

Fig. 4 The computed Jacobians of screen level temperature with respect to soil temperature in the four model soil layers. The Jacobians are valid at 6Z 16/01/2011 and are calculated using three hour long perturbed forecasts with soil temperature perturbations of magnitude 10^{-1} K.

4.1.1 Effect of Land Surface Parameterisations

To investigate the impact of the land surface model parameterisations on the calculation of the Jacobians, experiments are performed where the parameterisations are modified or switched off. Figure 5 shows the Jacobians of screen level temperature with respect to the soil moisture in the topmost model soil layer ($\Delta T_{2m}/\Delta\theta_1$) when bare soil evaporation is switched off. Comparing Fig. 5 with the top panel of Fig. 2 shows that bare soil evaporation can produce strong coupling between screen level temperature and surface soil moisture, both during the day and night. Switching off bare soil evaporation reduces the magnitude of $\Delta T_{2m}/\Delta\theta_1$ in the interior of Australia, the Sahara and parts of south America. In some night time regions, switching off bare soil evaporation causes $\Delta T_{2m}/\Delta\theta_1$ to swap sign and have positive instead of negative values. With bare soil evaporation switched off, $\Delta T_{2m}/\Delta\theta_1$ is predominantly negative in the daytime region and predominantly positive in the night time region.

Both the soil thermal conductivity and soil heat capacity are strongly affected by soil moisture. Therefore, these two processes may be responsible for the positive values of $\Delta T_{2m}/\Delta\theta_1$ in night-time regions, observed in Fig. 5. The JULES soil thermal conductivity (λ_s) is calculated using (Peters-Lidard et al. 1998; Dharssi et al. 2009)

$$\lambda_s = (\lambda_{sat} - \lambda_{dry})K_e + \lambda_{dry} \tag{4}$$

where λ_{sat} is the soil thermal conductivity when the soil is saturated and λ_{dry} is the soil thermal conductivity when the soil is dry. λ_{sat} and λ_{dry} are both dependent on soil texture. For the model medium soil texture, $\lambda_{sat} = 1.6\ Wm^{-1}K^{-1}$ and $\lambda_{dry} = 0.2\ Wm^{-1}K^{-1}$. The Kersten number ($K_e$) is given by

$$K_e = \begin{cases} \log_{10}\dfrac{\theta}{\theta_s} + 1.0 & \dfrac{\theta}{\theta_s} \geq 0.1 \\ \\ 0 & \text{otherwise} \end{cases} \quad . \tag{5}$$

For investigation, the parameterisation of soil thermal conductivity is modified so that it becomes independent of soil moisture,

$$\lambda_s^{modified} = (\lambda_{sat} + \lambda_{dry})/2 \quad . \tag{6}$$

Figure 6 shows the Jacobians $\Delta T_{2m}/\Delta\theta_1$ when the parameterisation of soil ther-

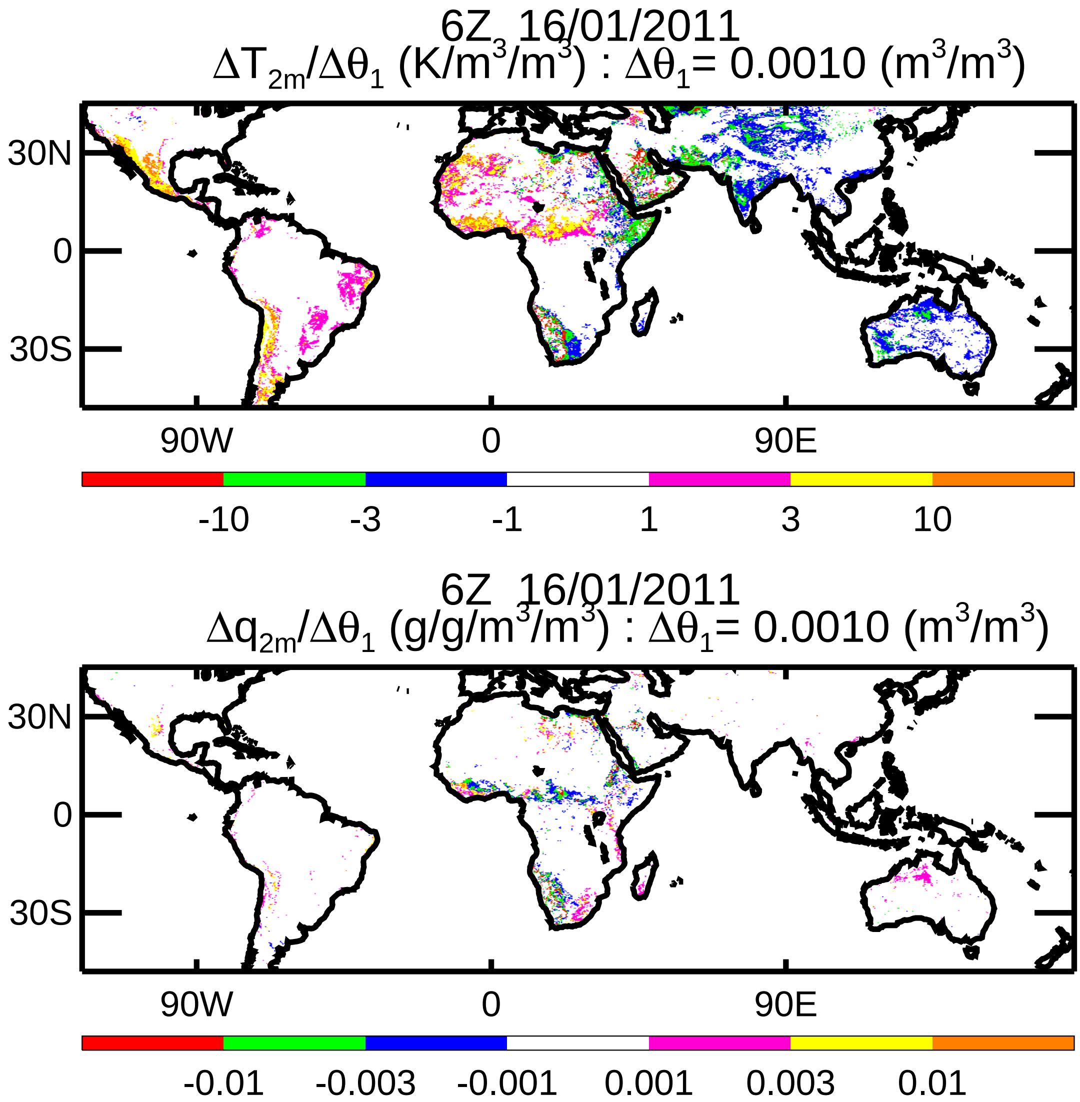

Fig. 5 The computed Jacobians of screen level temperature (top panel) and specific humidity (lower panel) with respect to volumetric soil moisture in the topmost model soil layer when bare soil evaporation is switched off. The Jacobians are valid at 6Z 16/01/2011 and are calculated using three hour long perturbed forecasts with soil moisture perturbations of magnitude 10^{-3} m^3/m^3. This figure can be compared with the top panels of Figs. 2 and 3.

mal conductivity is modified and bare soil evaporation is switched off. Comparing Figs. 5 and 6 shows that modifying the parameterisation of soil thermal conductivity significantly reduces the coupling between screen level temperature and topmost level soil moisture in many regions, both during the day and night. However, some night-time regions with positive values of $\Delta T_{2m}/\Delta\theta_1$ still persist. This suggests that other processes, such as the relation between soil heat capacity and soil moisture, are also important.

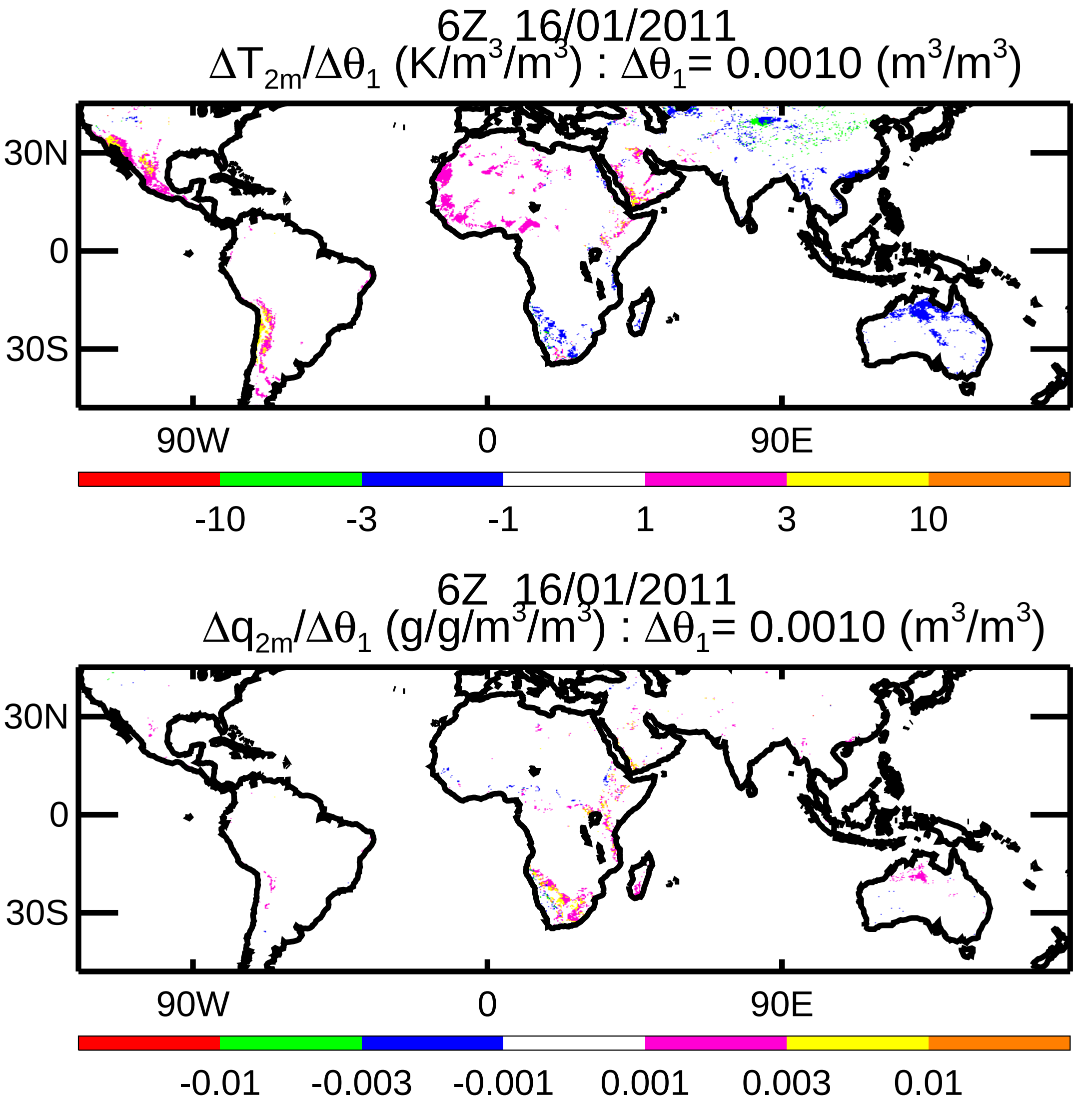

Fig. 6 The computed Jacobians of screen level temperature (top panel) and specific humidity (lower panel) with respect to volumetric soil moisture in the topmost model soil layer when bare soil evaporation is switched off and the parameterisation of soil thermal conductivity is modified so that it it independent of soil moisture. The Jacobians are valid at 6Z 16/01/2011 and are calculated using three hour long perturbed forecasts with soil moisture perturbations of magnitude 10^{-3} m^3/m^3. This figure can be compared with Fig. 5 and the top panels of Figs. 2 and 3.

The preceding analysis shows that there is strong coupling between soil moisture and screen level temperature and humidity. The coupling between the topmost model level soil moisture and the screen level is due to a number of processes including bare soil evaporation, soil thermal conductivity, soil thermal capacity as well as transpiration by plants. Although transpiration by plants only occurs during the day, the other processes can also occur at night. Therefore, there is significant coupling both during the day and at night and the sign of the Jacobians of $\Delta T_{2m}/\Delta\theta_1$ can be positive or negative. $\Delta T_{2m}/\Delta\theta_1$ is usually negative during the day and tends to be positive during the night.

The coupling between the soil moisture in the deeper model layers and the screen level is primarily through transpiration by plants. Therefore the coupling is only significant during the day. The vertical variation of the coupling is significantly affected by the vegetation root depths. Figure 7 shows the computed Jacobians $\Delta T_{2m}/\Delta\theta_l$ when the vegetation root depths are doubled. Increasing the vegetation root depth causes stronger coupling with the deeper soil layers, i.e. increases the magnitude of $\Delta T_{2m}/\Delta\theta_4$ and reduces the magnitude of $\Delta T_{2m}/\Delta\theta_2$. This is because a doubling of vegetation root depth causes the fraction of roots in soil layer four to increase and the fraction of roots in soil layer two to decrease.

4.1.2 Linearity and Quality Control

For a well behaved system the calculated values of the Jacobian elements H_{kj} should be nearly independent of the magnitude and sign of the perturbations δ_j. This is investigated by comparing Jacobian elements calculated using perturbations of opposite signs. H^+ (H^-) represents Jacobians calculated using a positive (negative) perturbation. A high correlation between H^+ and H^- indicates linearity while a low correlation indicates problems.

For the computed Jacobian elements $\Delta T_{2m}/\Delta\theta_1$ the correlation between H^+ and H^- is only 0.44 when using perturbation values of $|\Delta\theta_1| = 10^{-3}\ m^3/m^3$. Using alternative perturbation values of $|\Delta\theta_1| = 10^{-4}$ or $10^{-2}\ m^3/m^3$ doesn't show improvement. The low correlation is caused by a small proportion of grid points where H^+ differs significantly from H^- (grid points contain gross errors). Grid points containing gross errors are identified using the following heuristic criteria

$$\text{Gross Error where } |H^+ - H^-|/(0.1\epsilon_{kj} + |H^+| + |H^-|) > 0.5\ , \qquad (7)$$

where $\epsilon_{kj} = \sigma_{o,k}/\sigma_{b,j}$ and $\sigma_{o,k}$ ($\sigma_{b,j}$) is the expected error in observed (model) estimates of variable k (j). Assuming $\sigma_{o,T2m} = 2\ K$ and $\sigma_{b,\theta 1} = 0.04\ m^3/m^3$ gives $\epsilon_{kj} = 50\ K/m^3/m^3$ for $\Delta T_{2m}/\Delta\theta_1$. Grid points containing gross errors predominantly occur in arid regions ($\theta_1 < 0.1\ m^3/m^3$) during night-time; such as the Sahara at 3Z (see Fig. 8). Such grid points also show large values for $|H^+|+|H^-|$ (see Fig. 9).

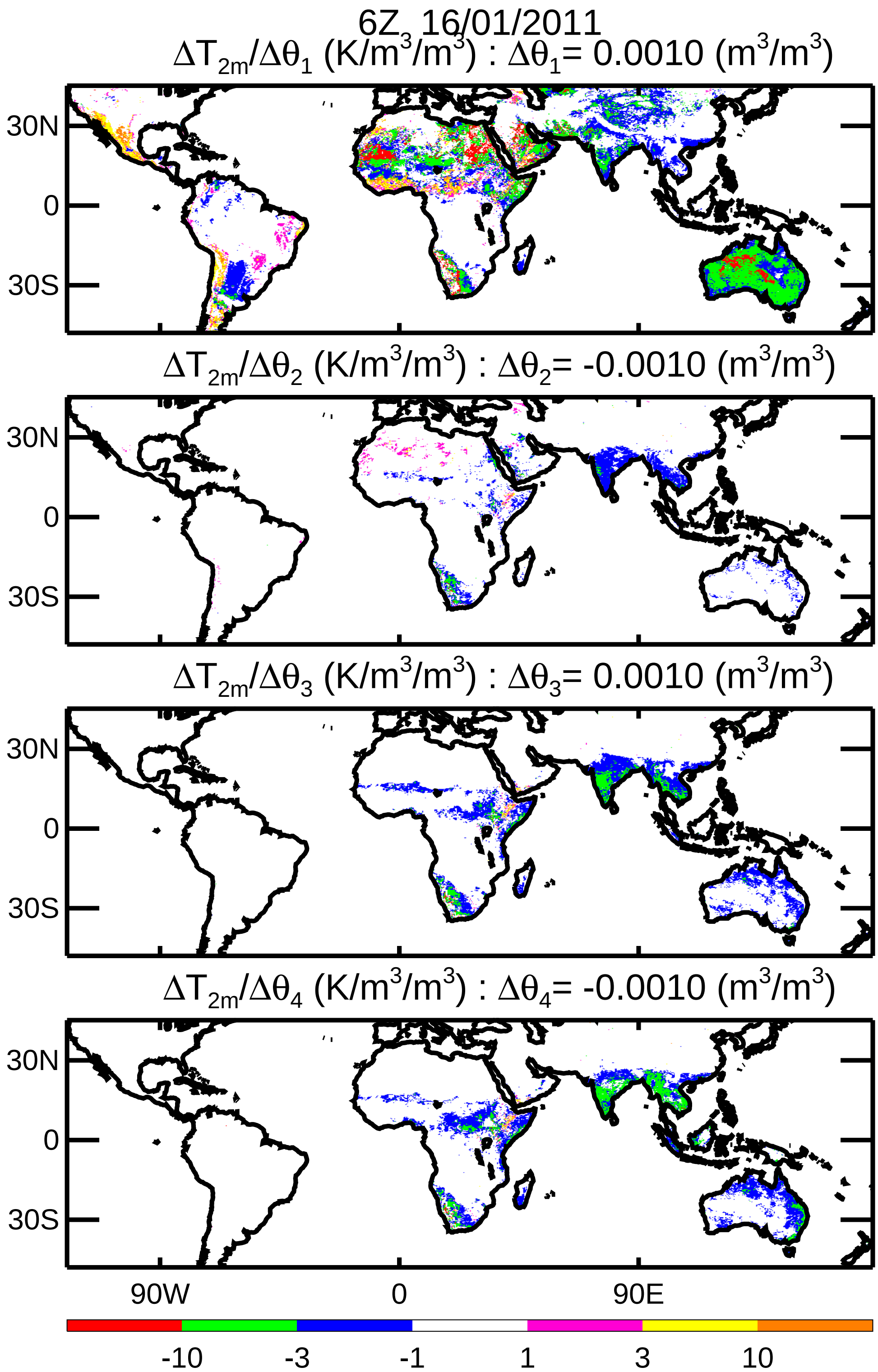

Fig. 7 The computed Jacobians of screen level temperature with respect to volumetric soil moisture in the four model soil layers when the vegetation root depths are doubled. The Jacobians are valid at 6Z 16/01/2011 and are calculated using three hour long perturbed forecasts with soil moisture perturbations of magnitude $10^{-3}\ m^3/m^3$. This figure can be compared with Fig. 2 which shows the computed Jacobians for the default vegetation root depths.

Table 1 Correlation between H^+ and H^- with and without the application of the simple QC scheme. H^+ (H^-) represents Jacobian elements $\Delta T_{2m}/\Delta\theta_1$ calculated using a positive (negative) level 1 soil moisture perturbation ($\Delta\theta_1$) and three hour long perturbation forecasts. The columns labelled *Gross Error* show the proportion of grid points that are identified by Eq. 7 to contain gross error. The numbers in brackets are for Jacobian elements calculated using one hour long perturbation forecasts.

$\lvert\Delta\theta_1\rvert$	no QC		after simple QC	
(m^3/m^3)	Correlation	Gross Error	Correlation	Gross Error
10^{-4}	0.19 (-0.09)	0.2% (0.1%)	0.99 (0.99)	0.1% (0.0%)
10^{-3}	0.44 (0.43)	0.4% (0.3%)	0.98 (0.97)	0.2% (0.2%)
10^{-2}	0.60 (0.60)	2.7% (2.5%)	0.79 (0.72)	1.8% (2.1%)

For illustration, this report assume that $\sigma_{o,T2m} = 2\ K$, $\sigma_{o,q2m} = 2 \times 10^{-3}\ g/g$, $\sigma_{o,\theta 1} = 0.04\ m^3/m^3$ $\sigma_{o,T*} = 5\ K$, $\sigma_{b,\theta} = 0.04\ m^3/m^3$ and $\sigma_{b,T} = 2\ K$. However, these values are likely to be revised before operational implementation.

The computed Jacobian elements $\Delta T_{2m}/\Delta T_1$ (relating screen level temperature to model level 1 soil temperature) also show some grid points with gross errors. This time the gross errors predominantly occur near the snow line where the model level 1 soil temperature is in the range $265\ K < T_1 < 280\ K$ (see Figs. 10 and 11).

A simple Quality Control (QC) scheme is implemented that rejects Jacobian elements where $|H_{kj}| > \epsilon_{kj}/2$ and where $265\ K < T_1 < 280\ K$. The advantage of this simple QC scheme is that it is computationally cheap since it doesn't require knowledge of both H^+ and H^-. After the application of the simple QC scheme the correlation between H^+ and H^- increases to values close to 1. The simple QC scheme detects about half the grid points with gross errors. Table 1 shows the correlation between H^+ and H^- for $\Delta T_{2m}/\Delta\theta_1$ both with and without the application of the simple QC scheme.

4.1.3 Sensitivity to Magnitude of Perturbations

Figure 12 shows the sensitivity of the calculated Jacobians for screen level temperature to the magnitude of the volumetric soil moisture perturbations, for the Australia region. The results indicates that the system is well behaved for perturbation values in the range of 10^{-4} to $10^{-2}\ m^3/m^3$, a perturbation value of $10^{-3}\ m^3/m^3$ is found to be close to optimal. A similar analysis using the calcu-

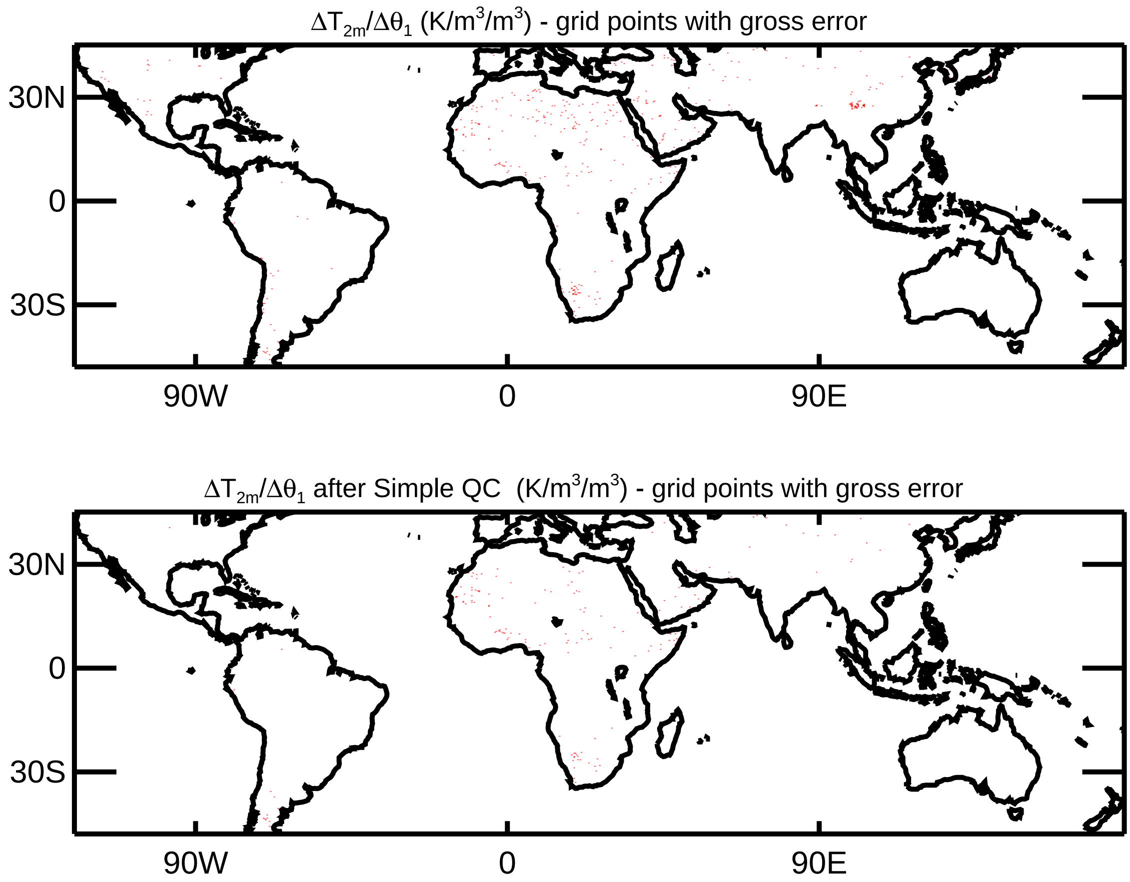

Fig. 8 Location of grid points where the Jacobian elements $\Delta T_{2m}/\Delta\theta_1$ contain a gross error. The Jacobian elements are calculated using finite difference and level 1 soil moisture perturbation values of $|\Delta\theta_1| = 10^{-3}\ m^3/m^3$. Gross errors are identified using Eq. 7, the upper (lower) panel shows results without (with) the application of the simple QC scheme.

lated Jacobians for screen level specific humidity also shows that a soil moisture perturbation value of $10^{-3}\ m^3/m^3$ is close to optimal (results not shown). The Jacobians for screen level specific humidity are less sensitive to the magnitude of the soil moisture perturbation. For skin and soil temperature, results indicate that the system is well behaved for perturbation values in the range of 10^{-2} to $1\ K$, a perturbation value of $10^{-1}\ K$ is found to be close to optimal. ECMWF use a volumetric soil moisture perturbation value of $10^{-2}\ m^3/m^3$ while Meteo France use perturbation values less than $10^{-4}\ m^3/m^3$. Meteo France use perturbation values of about $3 \times 10^{-3}\ K$ for temperature while ECMWF don't use their EKF to analyse skin or soil temperature.

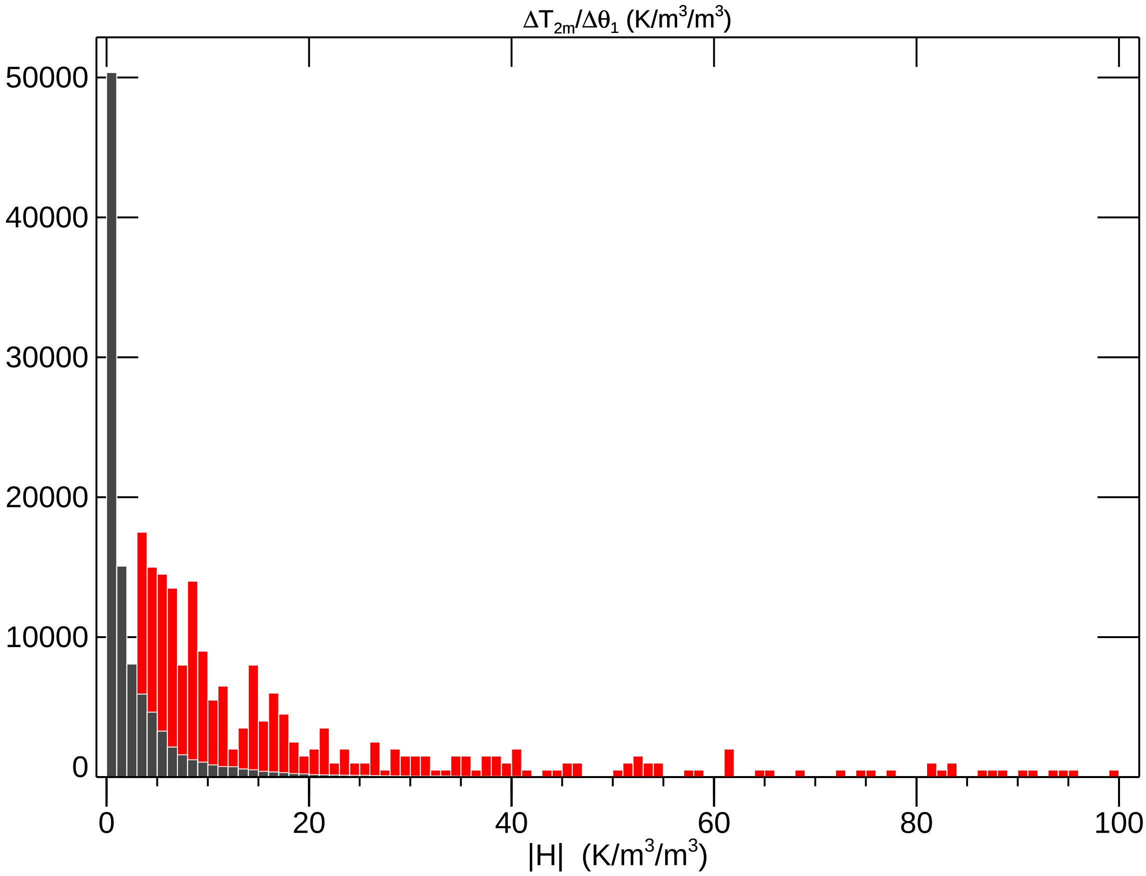

Fig. 9 Histogram distributions of $(|H^+| + |H^-|)/2$ for the Jacobian elements $\Delta T_{2m}/\Delta\theta_1$. H^+ (H^-) represents Jacobian elements calculated using a positive (negative) level 1 soil moisture perturbation of $|\Delta\theta_1| = 10^{-3}\ m^3/m^3$. The distribution for grid points that do not contain a gross error, according to Eq. 7, is shown in black. The distribution for grid points that do contain a gross error is shown in red, this distribution has been scaled by a factor of 500.

4.2 The Jacobians of the Observation Operator for the Assimilation of Surface Soil Moisture Measurements

Several new space-borne remote sensing systems, operating at microwave frequencies, have been developed that provide a more direct retrieval (than using screen level observations) of surface soil moisture, e.g. SMOS, ASCAT and AMSR-2 (Advanced Microwave Scanning Radiometer-2, Oki et al. 2010). These systems provide global data coverage and the horizontal resolution is similar to global NWP models. At microwave frequencies the dielectric constant of liquid water ($\simeq$ 70) is much higher than that of the soil mineral particles ($<$ 5) or ice. An increase in soil moisture leads to an increase in the dielectric constant of the soil which leads to a decrease in soil emissivity and an increase in soil reflectivity.

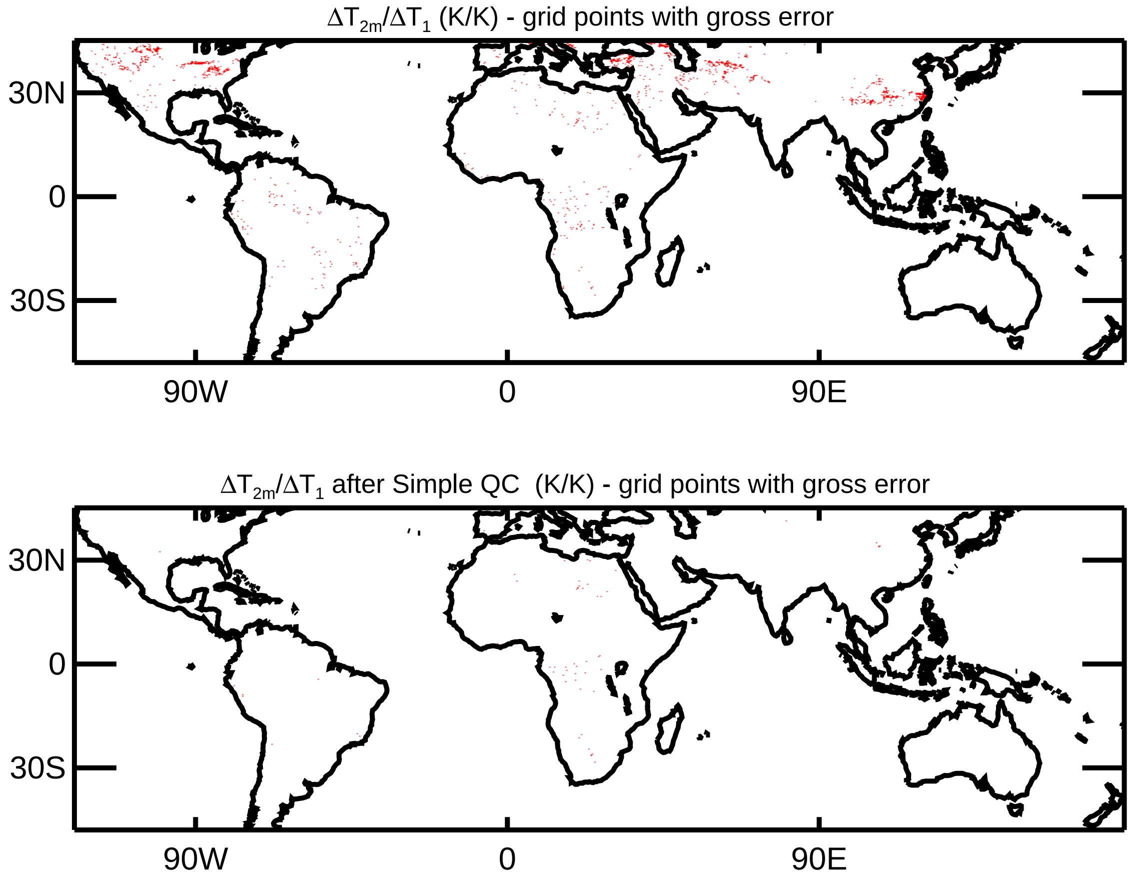

Fig. 10 Location of grid points where the Jacobian elements $\Delta T_{2m}/\Delta T_1$ contain a gross error. The Jacobian elements are calculated using finite difference and level 1 soil temperature perturbation values of $|\Delta T_1| = 10^{-1}\ K$. Gross errors are identified using Eq. 7, the upper (lower) panel shows results without (with) the application of the simple QC scheme.

Therefore, satellite based measurements of microwave brightness temperature (passive system) or backscatter (active system) can be used to derive estimates of surface soil moisture (SSM) using a retrieval algorithm.

Measurements of SSM can be assimilated to update both the model surface and root zone soil moisture by using the Jacobians $\Delta\theta_1/\Delta\theta_l \equiv H_{\theta_1,\theta_l}$ that are computed using Equation 3. The computed Jacobians are shown in Fig. 13. The results show that generally, for JULES, the coupling between the surface and root zone soil moisture is weak. $\Delta\theta_1/\Delta\theta_3$ and $\Delta\theta_1/\Delta\theta_4$ are close to zero. $\Delta\theta_1/\Delta\theta_2$ is non-zero in regions where the soil is close to saturation and consequently the hydraulic conductivity is high. $\Delta\theta_1/\Delta\theta_1 \equiv H_{\theta_1,\theta_1}$ is close to unity in most regions, the exceptions are where the soil moisture is close to saturation and Jacobian values as low as 0.5 can occur. Increasing the length of the perturbation forecasts does significantly increase the coupling between the surface and root zone soil mois-

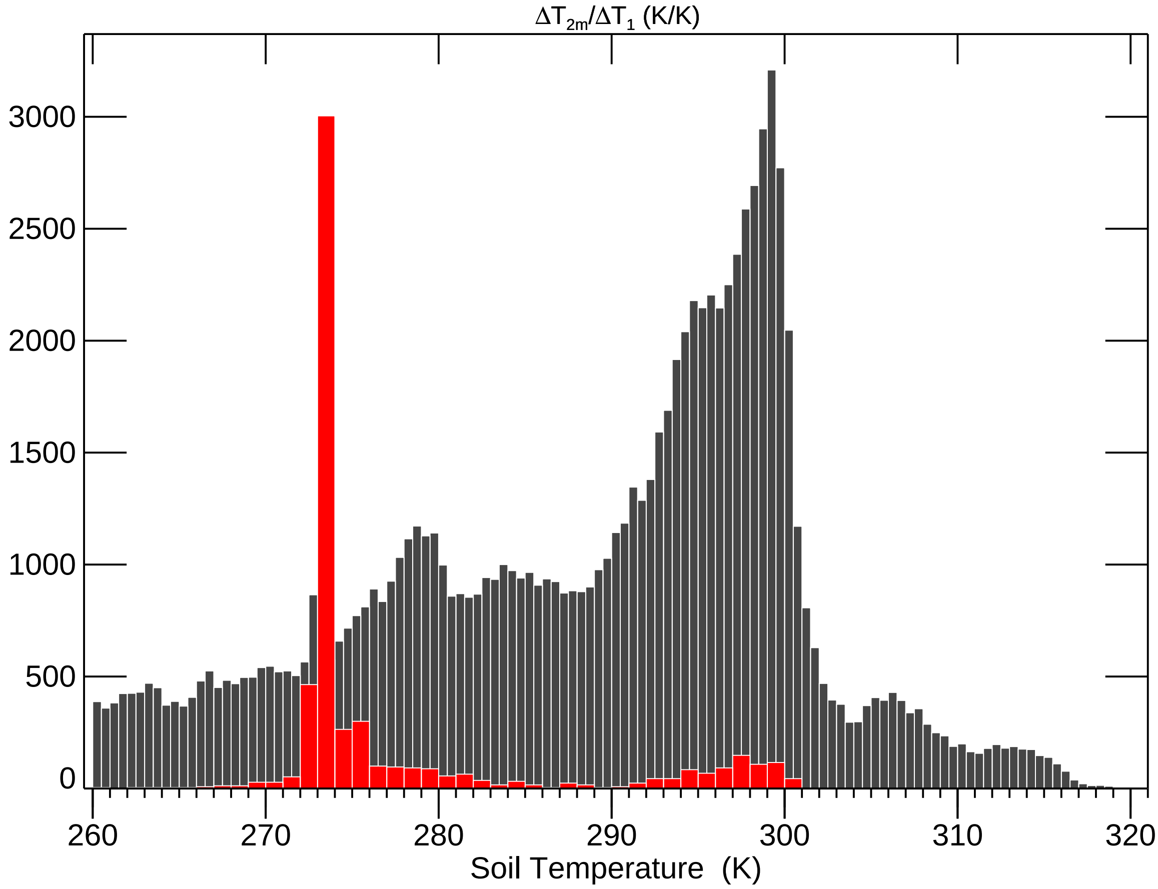

Fig. 11 Histogram distribution, shown in black, of level 1 soil temperature for the Jacobian elements of $\Delta T_{2m}/\Delta T_1$ that do not contain a gross error according to Eq. 7. The level 1 soil temperature distribution for grid points that do contain a gross error is shown in red, this distribution has been scaled by a factor of 4. The Jacobian elements are calculated using finite difference and level 1 soil temperature perturbations of $|\Delta T_1| = 10^{-1}\ K$.

ture. Draper (2011) has also used the JULES land surface model to calculate the Jacobians for measurements of SSM over the Australia region and found similar results.

The van Genuchten (1980) equations describe the model relationship between the soil hydraulic conductivity (K_{VG}) and the unfrozen volumetric soil moisture θ^u.

$$K_{VG} = K_s S_e^L \left[1 - (1 - S_e^{1/m})^m\right]^2, \tag{8}$$

where the soil wetness $S_e = (\theta^u - \theta_r)/(\theta_s - \theta_r)$, $L = 0.5$ and $m = 1 - 1/n$. θ_s, θ_r, K_s , α and n are the van Genuchten soil parameters and depend on the soil texture (size distribution of the soil particles and the soil organic carbon content). Equa-

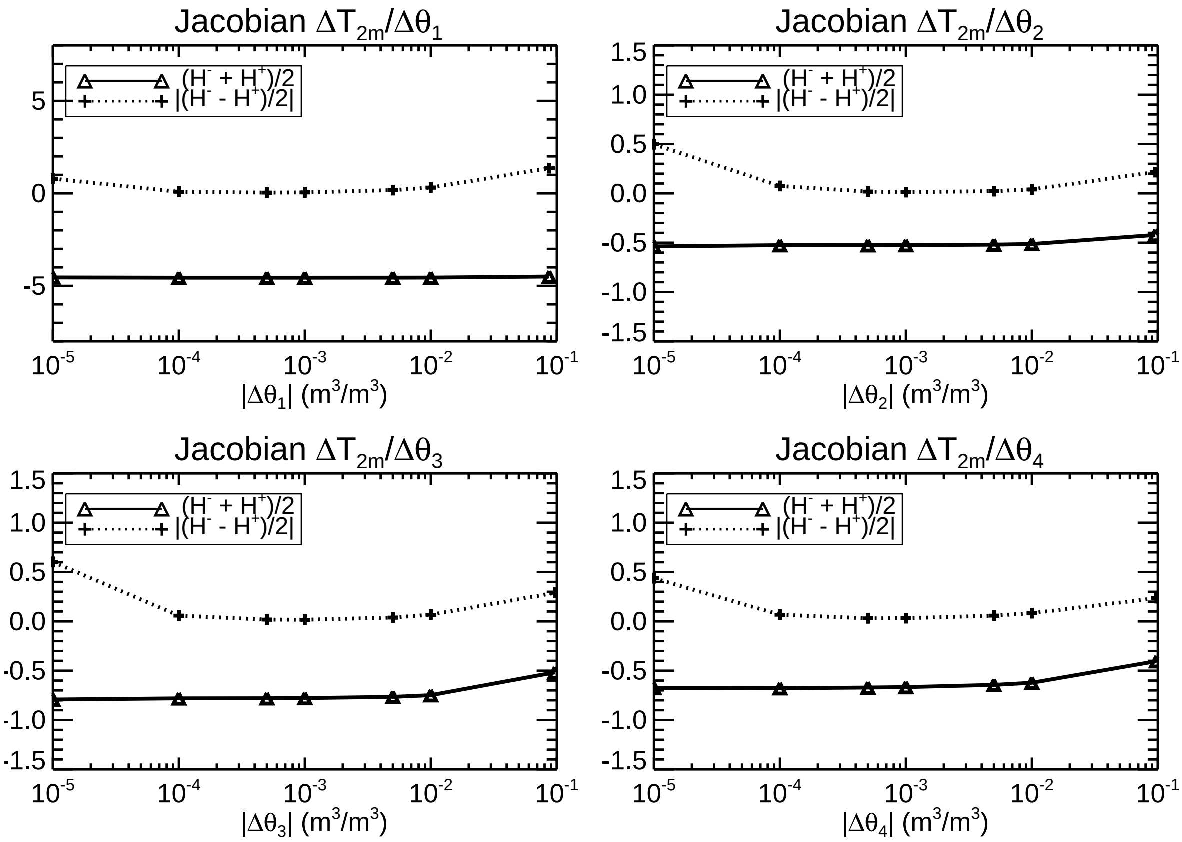

Fig. 12 The sensitivity of the calculated Jacobians for screen level temperature to the magnitude of the volumetric soil moisture perturbations $|\Delta\theta_l|$ in soil layer l. H^- represents Jacobian values calculated using a negative perturbation while H^+ represents Jacobian values calculated using a positive perturbation. For a well behaved EKF system $|H^- - H^+|$ should be close to zero. The dotted line shows $|H^- - H^+|/2$ averaged over the Australia region while the solid line shows $(H^- + H^+)/2$ averaged over Australia. The results indicates that the system is well behaved for $|\Delta\theta_l|$ values in the range of 10^{-4} to 10^{-2} m^3/m^3.

tion 8 shows that the hydraulic conductivity is very sensitive to changes in soil moisture. Small changes in soil moisture can lead to order of magnitude changes in soil hydraulic conductivity. For example, when $S_e = 1$, $K_{VG} = K_s$ while when $S_e = 0.9$ and $n = 1.18$, $K_{VG} = K_s \times 10^{-2}$. In addition, K_s is strongly affected by soil texture. For coarse textured soils the model assumes $K_s = 1.95 \times 10^{-2}\ mm/s$ while for medium textured soils $K_s = 2.8 \times 10^{-3}\ mm/s$. Consequently, uncertainty in soil texture can also lead to order of magnitude uncertainty in soil hydraulic conductivity. Figure 14 shows the computed Jacobians $\Delta\theta_1/\Delta\theta_2$ when the soil hydraulic conductivity is increased by a factor of ten. The coupling between the SSM and the root zone has increased significantly.

Using four different land surface models with different coupling strengths and syn-

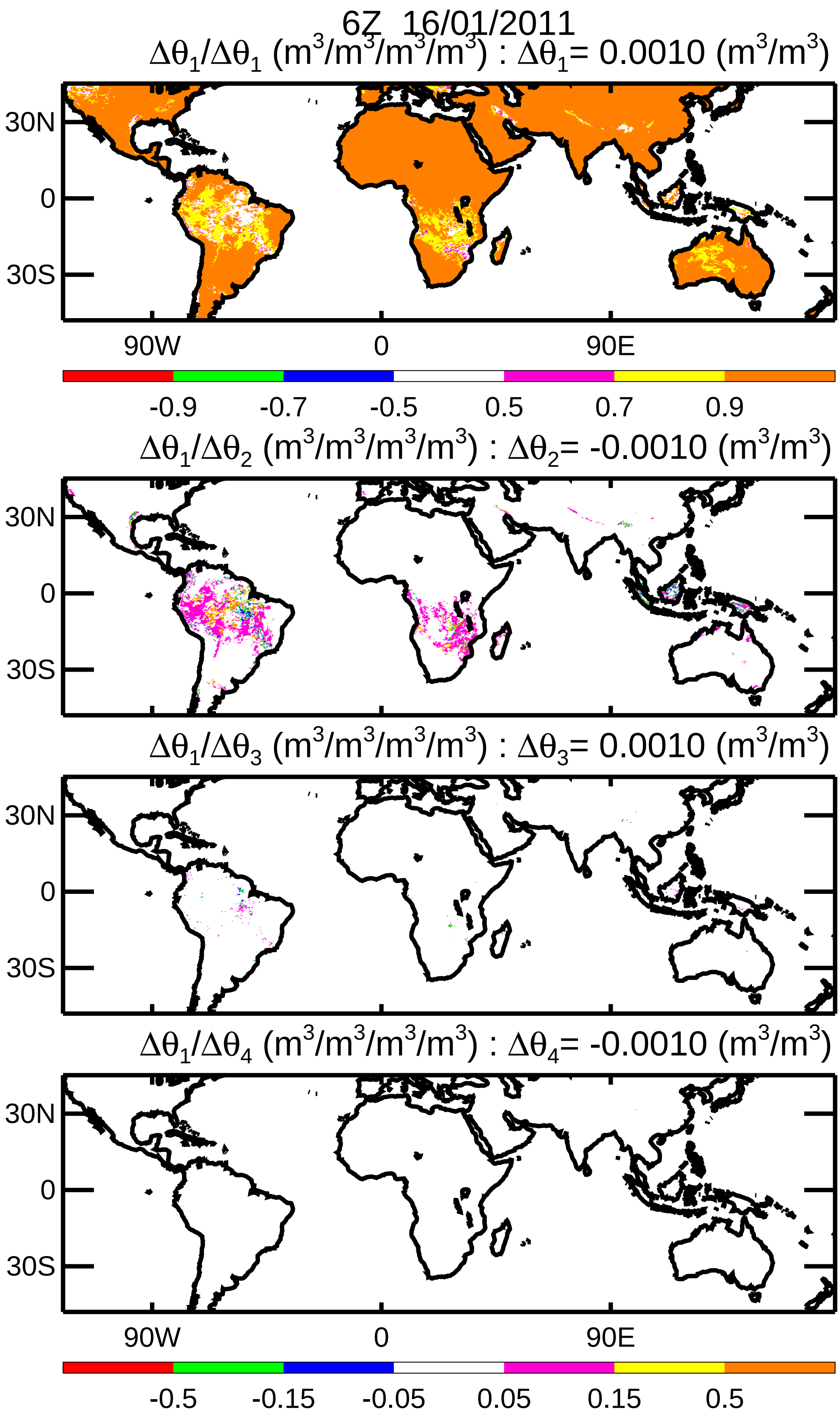

Fig. 13 The computed Jacobians of surface volumetric soil moisture with respect to volumetric soil moisture in the four model soil layers. The Jacobians are valid at 6Z 16/01/2011 and are calculated using three hour long perturbed forecasts with soil moisture perturbations of magnitude $10^{-3}\ m^3/m^3$.

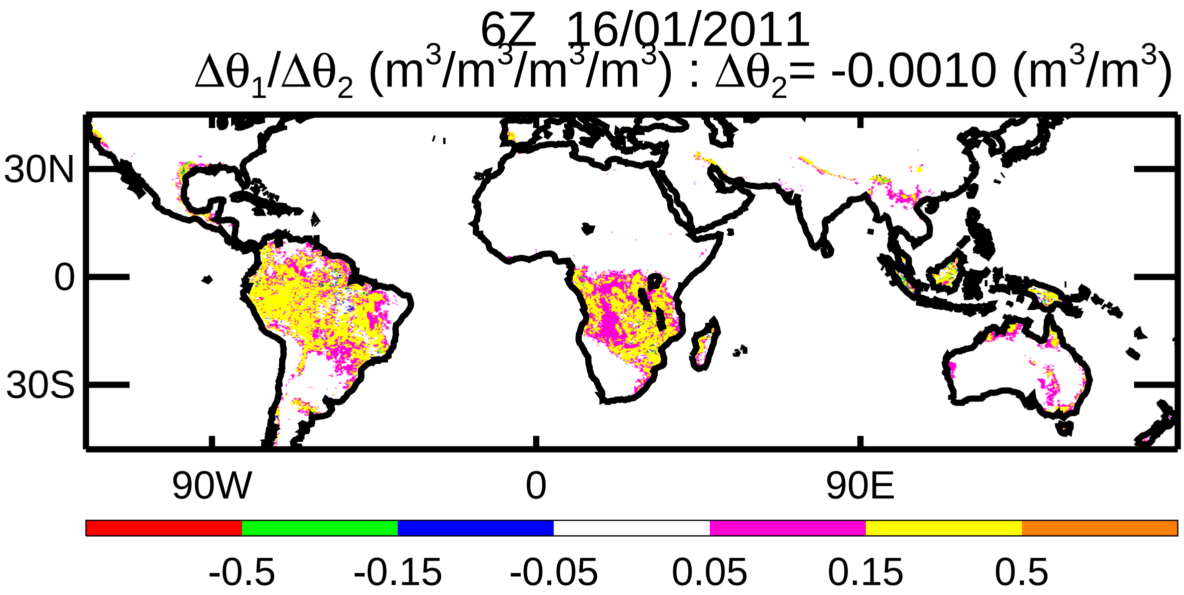

Fig. 14 The computed Jacobians of surface volumetric soil moisture with respect to volumetric soil moisture in the second model soil layer when the soil hydraulic conductivity is increases by a factor of ten. The Jacobians are valid at 6Z 16/01/2011 and are calculated using three hour long perturbed forecasts with soil moisture perturbations of magnitude $10^{-3}\ m^3/m^3$. This figure can be compared with the second panel of Fig. 13.

thetic observations of SSM, Kumar et al. (2009) find that the potential of SSM assimilation to improve root zone soil moisture is higher when the coupling between the SSM and root zone soil moisture is stronger. Given that the true strength of coupling between the SSM and root zone soil moisture is unknown, the non-identical twin, assimilation experiments of Kumar et al. (2009) suggest that it is better to over-estimate rather than under-estimate the coupling between the SSM and root zone soil moisture. Therefore, artificially increasing the model soil hydraulic conductivity by a factor of ten may be an effective technique to improve the assimilation of satellite derived SSM. However, careful and comprehensive testing will be required to fully validate all the consequences of such an approach.

4.3 The Jacobians of the Observation Operator for Surface Skin Temperature

Best and Maisey (2002) show that in unstable conditions, to a good approximation

$$\Delta T_* = \Delta T_{2m} / \left(1 - \mu\, r_{a,2m}/r_a\right) \quad . \tag{9}$$

Where r_a ($r_{a,2m}$) is the aerodynamic resistance between the surface and first model level (screen level) and $\mu \simeq 0.9$. Therefore, it is expected that the computed Jacobians between surface skin temperature and soil moisture ($\Delta T_*/\Delta\theta_l$) should show a similar spatial pattern to the Jacobians between screen level temperature and soil moisture ($\Delta T_{2m}/\Delta\theta_l$) but have a larger magnitude (since the denominator in Eq 9 is less than 1). Figure 15 shows the computed Jacobians $\Delta T_*/\Delta\theta_l$ and that there is significant coupling between surface skin temperature and soil moisture. Therefore, in principle, it will be possible to assimilate satellite measurements of T_* to analyse soil moisture. However, for a variety of reasons, model and satellite derived surface skin temperature exhibit very different climatologies and consequently bias correction will be required. As expected, comparing Figs. 15 and 2 shows that, the spatial variation of $\Delta T_*/\Delta\theta_l$ is very similar to $\Delta T_{2m}/\Delta\theta_l$ and the magnitudes are much larger. Figure 16 shows the computed Jacobians $\Delta T_*/\Delta T_l$ and that there is significant coupling between surface skin temperature and model level 1 soil temperature. There are also strong similarities between $\Delta T_*/\Delta T_l$ and $\Delta T_{2m}/\Delta T_l$. Ghent et al. (2010) have assimilated measurements of surface skin temperature for the Africa region using the JULES land surface model and found improvements to model surface fluxes and soil moisture.

5. CONCLUSIONS AND FUTURE WORK

To take full advantage of the available global satellite measurements of the land surface as well as screen level observations an EKF based land surface data assimilation system is under development at the Bureau in collaboration with the Met Office. Such a system is flexible and can make more statistically optimal use of a wide variety of observation types. The most important aspect of the EKF land data assimilation system is the calculation of the Jacobians of the observation operator that describe the link between the observations and the land surface model variables. The Jacobians are computed using finite difference by perturbing each model variable to be analysed, in-turn, and performing short model forecasts. The number of perturbed forecasts required increases with the number of model variables to be analyses and the number of soil layers. Other works such as Mahfouf et al. (2009) and Drusch et al. (2009) have also looked at the calculation of the Jacobians. However, this work examines the Jacobians in much greater detail than before. In addition, this is the first work to use the JULES land surface model to compute the Jacobians for screen level observations and measurements of surface skin temperature.

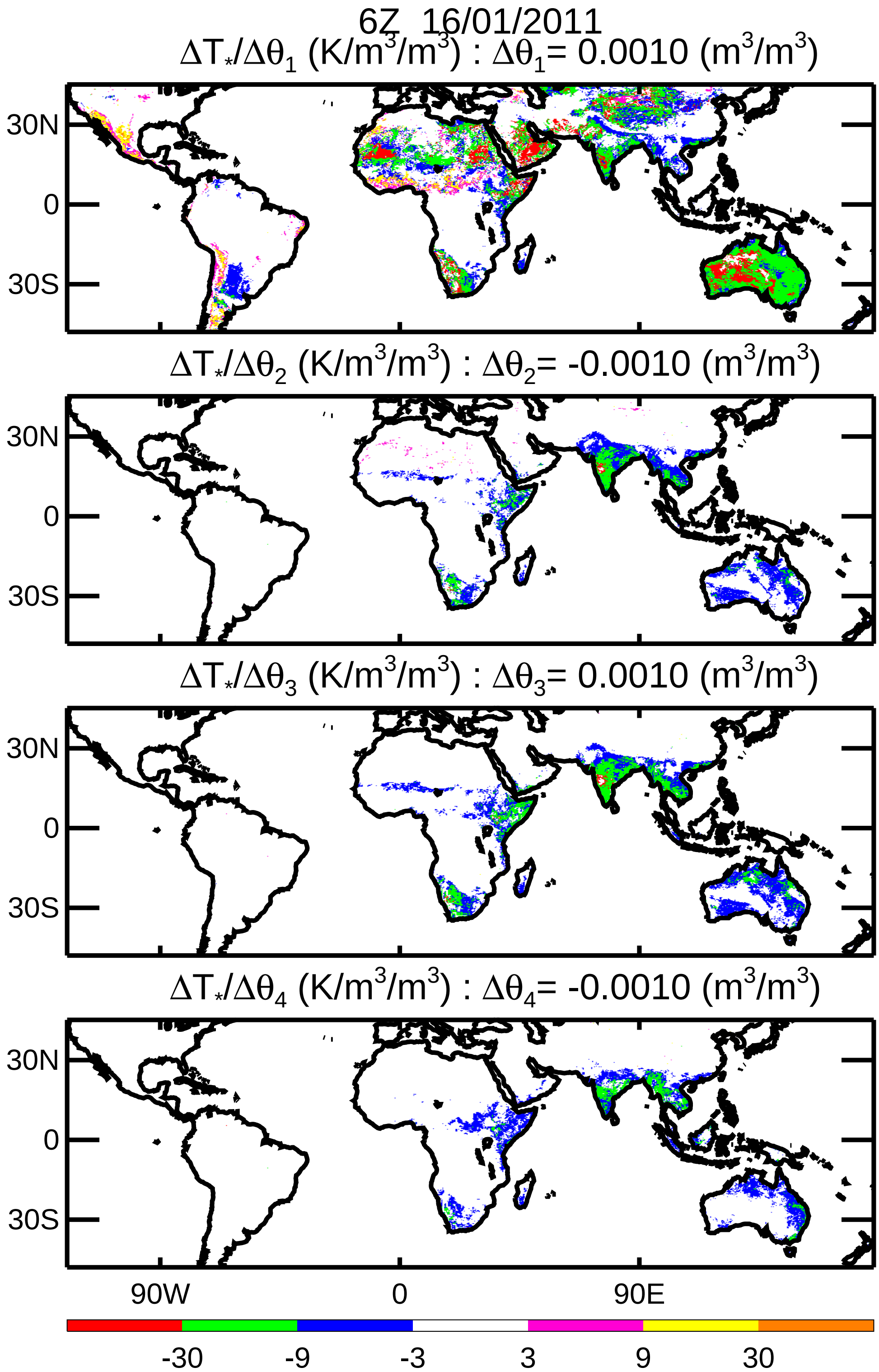

Fig. 15 The computed Jacobians of surface skin temperature with respect to volumetric soil moisture in the four model soil layers. The Jacobians are valid at 6Z 16/01/2011 and are calculated using three hour long perturbed forecasts with soil moisture perturbations of magnitude $10^{-3}\ m^3/m^3$. This figure can be compared with Fig. 2 but note the change in scale.

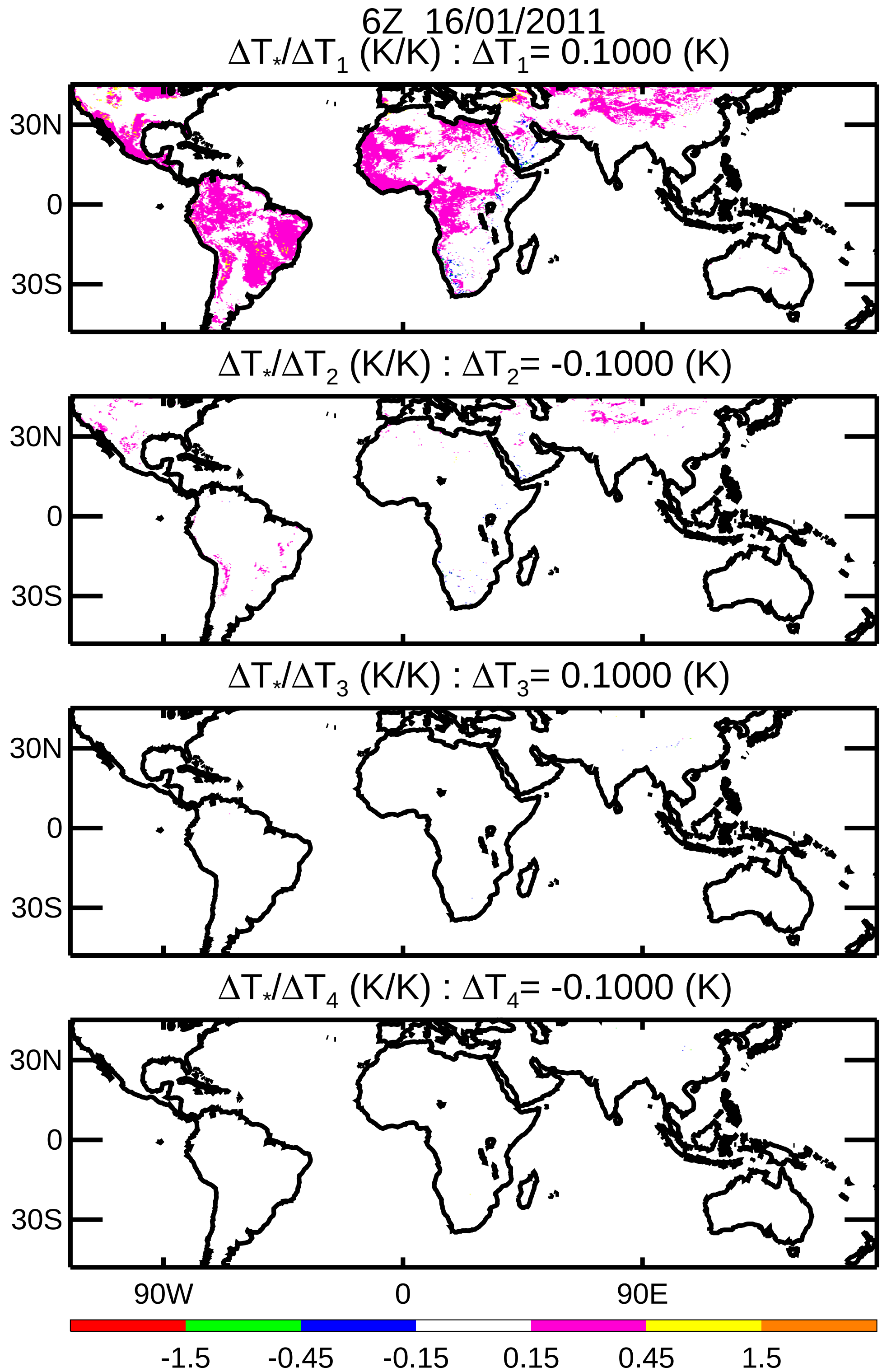

Fig. 16 The computed Jacobians of surface skin temperature with respect to soil temperature in the four model soil layers. The Jacobians are valid at 6Z 16/01/2011 and are calculated using three hour long perturbed forecasts with soil temperature perturbations of magnitude 10^{-1} K. This figure can be compared with Fig. 4 but note the change in scale.

Results show that quality control of the computed Jacobians is very important. Two quality control schemes are compared; a computationally expensive scheme that doubles the number of perturbed forecasts required and a simple quality control scheme that is computationally cheap. The use of the simple quality control scheme is found to give adequate results. Results also show that the computed Jacobians can be sensitive to the size of the perturbations used. Perturbations that are too small cause problems due to numerical rounding while perturbations that are too large cause problems due to non-linearities in the model. Experiments show that volumetric soil moisture perturbation values in the range of 10^{-4} to 10^{-2} m^3/m^3 give good results and a perturbation value of 10^{-3} m^3/m^3 is close to optimal. For skin and soil temperature perturbations, experiments indicate that a perturbation value of 10^{-1} K is close to optimal.

This is the first work to look at the effect of land surface parameterisations on the computed Jacobians. As expected, the parameterisation details have a significant impact. Experiments are performed where the parameterisations are modified or switched off. Results show that the coupling between the soil moisture in the topmost model layer and the screen level is due to a number of processes including bare soil evaporation, soil thermal conductivity, soil thermal capacity as well as transpiration by plants. The coupling between the soil moisture in the lower model layers and the screen level is due to transpiration by plants. This result is significant as it explains why the coupling with the soil moisture in the topmost model layer is much stronger than the coupling with the soil moisture in the lower model layers. Consequently, soil moisture increments in the topmost model layer will be larger than would be the case if the coupling were only due to transpiration. In addition, improving the analysis of topmost model layer soil moisture will have a significant impact on forecasts of screen level temperature and humidity.

The Jacobians linking observations of surface soil moisture with soil moisture in the lower model layers have been computed. Experiments show that artificially increasing the soil hydraulic conductivity by a factor of ten significantly increases the coupling between the surface and root zone soil moisture. Otherwise, for JULES, the coupling between the surface and root zone soil moisture is weak. Small uncertainty in soil moisture or soil texture can lead to order of magnitude uncertainty in soil hydraulic conductivity. In addition, Kumar et al. (2009) suggest that it is better to over-estimate rather than under-estimate the coupling between the surface and root zone soil moisture. Consequently, artificially increasing the model soil hydraulic conductivity by a factor of ten may be an effective technique to improve the assimilation of satellite derived surface soil moisture.

The Jacobians linking observations of skin temperature to model soil temperature and moisture have also been computed. These Jacobians have a similar spatial pattern to the Jacobians linking observations of screen level temperature to model soil temperature and moisture but are larger in magnitude. Consequently, assimilation of satellite derived skin temperature may also significantly improve the analysis of model soil temperature and moisture.

Further efforts are now required to determine the most optimal values of the spatially varying background (observation) error covariance matrices $\mathbf{B}$ ($\mathbf{R}$). In order to achieve operational implementation of the EKF land DA scheme, pre-operational trials will need to be performed to assess the impact on the analysis and forecast of soil moisture and atmospheric fields (Candy et al. 2012).This work is on-going.

It is well known that model soil moisture is model specific (Koster et al. 2009). Results indicate that the Jacobians are also model specific. Consequently, careful examination of the Jacobians might allow significant insight into the behaviour of land surface models. It would be a useful exercise to examine and compare the Jacobians computed using the CABLE land surface model (Kowalczyk et al. 2006). This would be a good starting point towards modifying the JULES based EKF land data assimilation scheme for CABLE. Development of a CABLE based land data assimilation scheme is a pre-requisite for using CABLE in the ACCESS NWP system. It is intended that CABLE will be integrated into the JULES framework (Law et al. 2012) and this will simplify the task of using CABLE for NWP.

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