Advances in model physics and their relevance to satellite data assimilation

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ABSTRACT

This paper provides an overview of ongoing activities where the use of model physics has allowed an increased usage of satellite observations in data assimilation systems and how it has also provided guidance on how to improve some aspects of physical parameterization schemes. First I present activities related to the assimilation of satellite radiances in cloudy areas. Then I focus on the assimilation of satellite radiances within land surface models. I finish by giving a list of future challenges in this area of research.

1 Introduction

Before the use of satellite radiances in variational data assimilation schemes, physical parameterizations were not part of analysis systems for Numerical Weather Prediction (NWP). Indeed the analysis was mostly static (three dimensional spatial schemes at a given time) and concerning large-scale atmospheric variables such as wind, temperature and surface pressure. Initialisation procedures highlighted the importance of providing dynamical balanced fields at synoptic scales, but were mostly based on adiabatic equations. The first signs that physical processes could play a significant role in data assimilation were identified through the "spin-up" problem[1] resulting from the analysis of the water vapour field. This problem is more acute in tropical regions for the following reasons: the lack of geostrophic balance, the importance of diabatic heating on the dynamical circulation, and the existence of a rather sparse network of conventional observations. Krishnamurti et al. (1988) proposed a "physical initialization" technique using satellite data in order to constrain the model diabatic heating rates with consistent dynamics. They proposed the inversion of a simple Kuo-type convection scheme, where the humidity correction Δq over an atmospheric column can be expressed as a function of a precipitation difference ΔRR between an observation "proxy" (e.g. derived from infra-red cloud top temperatures) and the model counterpart. Through a Newtonian relaxation of the dynamical fields towards analyses they were able to achieve consistent changes of the wind divergence with the humidity corrections. This led to reduced model spin-up and improved short-range tropical forecasts as shown in Figure 1. The next section will show that 4D-Var data assimilation is a better and more natural framework to address the physical initialisation problem.

2 4D-Var assimilation and model physics

When writing the cost function of the 4D-Var problem (with the classical notations proposed by Ide et al., 1997), one can ask the question: where does the model physics take place?

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[1] The spin-up corresponds to an imbalance of the water budget in the model at the beginning of the forecast, with either an excess in surface precipitation or surface evaporation.

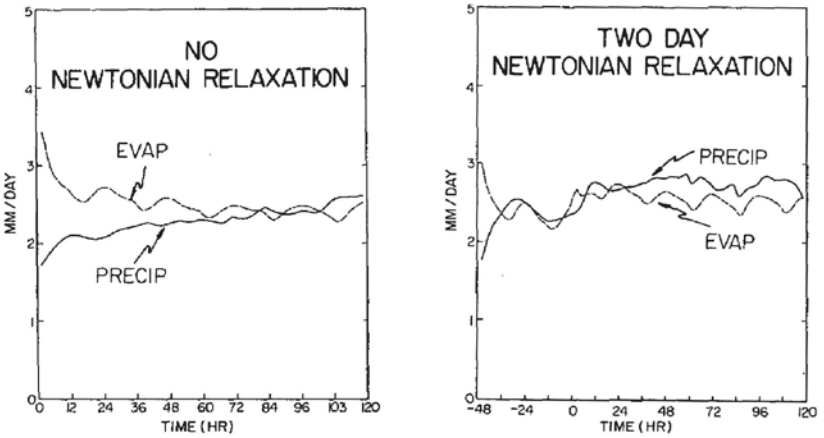

Figure 1: Illustration of the spin-up problem (imbalance of the water budget at the beginning of a numerical weather forecast) and of the use of "physical initialisation" to reduce it (NEWTONIAN RELAXATION) (taken from Krishnamurti et al., 1988).

$$J(\mathbf{x}_0) = \tfrac{1}{2}\, (\mathbf{x}_0 - \mathbf{x}_\mathrm{b})^\mathrm{T}\mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_\mathrm{b}) + \tfrac{1}{2}\, (H(\mathbf{x}_t) - \mathbf{y}_\mathrm{o})^\mathrm{T}\mathbf{R}^{-1}(H(\mathbf{x}_\mathrm{t}) - \mathbf{y}_\mathrm{o})$$

The model physics is present in the forward integrations with the non-linear NWP model M from which the background state $\mathbf{x}_\mathrm{b}$ is obtained (short-range forecast). The **B**matrix is also obtained from an ensemble of short-range forecasts using M. In the observation term, the non-linear model M is used to compute the model state $\mathbf{x}_t$ at the observation time t from the model state at the beginning of the assimilation window $\mathbf{x}_0$: $\mathbf{x}_t = M(\mathbf{x}_0)$. The model physics can also be part of the observation operator H (e.g. a boundary layer scheme to compute low level parameters such as $RH_{2\mathrm{m}}$ or $V_{10\mathrm{m}}$).

As a consequence, the model physics is present in the gradient of the cost-function, required to solve the variational problem:

$$J(\mathbf{x}_0) = \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_\mathrm{b}) + \mathbf{M}^\mathrm{T}\mathbf{H}^\mathrm{T}\mathbf{R}^{-1}(\mathrm{H}(\mathbf{x}_t) - \mathbf{y}_\mathrm{o})$$

From the above formulation, the linearized physics should also appear in the adjoint operators $\mathbf{M}^\mathrm{T}$ and $\mathbf{H}^\mathrm{T}$. However it is not always the case. In practice, the linearization of physical parameterizations raises issues due to the presence of thresholds and non-linearities. There is a need for simplifications and regularizations to improve the validity of the tangent-linear approximation (e.g. Mahfouf, 1999). In a recent review, Janisková and Lopez (2012) provide a description of the ECMWF comprehensive package of linearized physics. When dealing with an incremental 4D-Var formulation with low resolution inner loops, an almost adiabatic version of the linearized NWP model can be sufficient (surface friction is nevertheless required to prevent spurious perturbations). When considering adjoint sensitivity studies, and examining forecast error reductions to observations sensitive to humidity, the use of linearized moist physics can be important for a fair interpretation of the relative importance of different observing systems (Janisková and Cardinali, 2014; personal communication). Finally, the linearized model physics is essential for the variational assimilation of observations sensitive to condensed water such as rainfall, cloudy satellite radiances, radar reflectivities, or lidar backscatter coefficients.

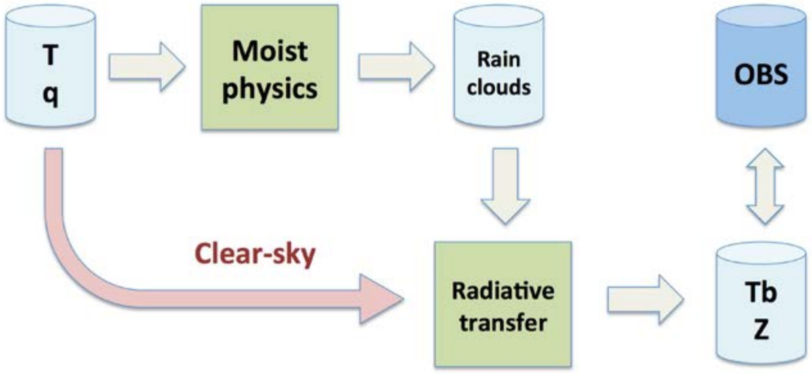

Figure 2: Schematic diagram showing how moist physics can be part of an observation operator to assimilation cloudy/rainy radiances (Tb) or radar reflectivities (Z).

From a satellite perspective, the 4D-Var assimilation systems have allowed to extract efficiently the information content from raw clear sky radiances over oceans. More recently, developments on an improved characterisation of surface temperature and/or surface emissivity have allowed 4D-Var systems to assimilate clear sky radiances over land and sea-ice (e.g. Karbou et al., 2005, 2010, 2014). Regarding infra-red cloudy radiances, a number of diagnostic techniques such as “CO2-slicing” or “1D-Var” provide information on cloud top pressure and effective cloud cover in order to assimilate clear sky radiances above clouds (e.g. Pangaud et al., 2009). In the microwave, the assimilation of cloudy/rainy radiances at low frequencies (below 50 GHz) has been successful at ECMWF (so-called “all sky radiances”) for a number of years thanks to the Janisková-Lopez package of moist linearized physics (Geer et al., 2010). The following areas remain challenging but the use of model physics could help:

- Cloudy satellite radiances (high frequency microwave and infra-red)
- Coupled assimilations with surfaces
- Satellite radiances in extreme atmospheric conditions (snow, cold surfaces)
- Measurements from active sensors

3 Assimilation of remote sensing observations in clouds

3.1 Diagnostic moist physics

When considering a package of diagnostic moist physics, the assimilation framework designed for clear sky variables can be kept unchanged. Indeed, as shown in Figure 2, the moist physics can be considered as part of the observation operator that converts temperature and humidity profiles (T, q) into hydrometeor profiles (cloud condensates, precipitation, cloud cover) before entering a radiative transfer scheme to compute brightness temperatures (T_b) or radar reflectivities (Z). A requirement is to have linearized versions of the moist physics in order to solve efficiently the variational problem. The papers from Geer (2014, this volume) and Janisková (2014, this volume) illustrate the assimilation of rainy microwave radiances and cloud radar/lidar measurements respectively.

3.2 Prognostic moist physics

With increased spatial resolutions, the description of clouds is becoming more explicit in NWP models. Convective scale models (around 1km grid mesh) can resolve vertical motions in clouds with prognostic variables describing the evolution of condensed hydrometeors (dynamical transport and microphysical conversions between species). It means that the simulation of cloudy radiances can be more realistic since more direct information is available on condensed hydrometeors. In most parameterized convection schemes cloud variables are rather poorly described (see for example Mahfouf (2005) or Mahfouf and Bilodeau (2009)) but new promising approaches are being developed (Piriou et al., 2007). On the other hand, the complexity of cloud schemes can be such that the number of new variables to initialise increases a lot, with additional non-linearities, thresholds and tunable parameters. In theory, new prognostic variables imply an extension of the control vector and also a dedicated estimation of the corresponding **B**-matrix (e.g. Michel et al., 2011).

Martinet et al. (2013) have perfomed a number of preliminary activities towards the assimilation of cloudy IASI radiances, by examining situations where a 1D-Var assimilation can be performed (overcast and homogeneous scenes both in the model and in the observations) that led to unbiased and Gaussian errors statistics. On the small number of pixels satisfying the above criteria, a 1D-Var scheme is able to reduce significantly background errors for ice opaque clouds and to a lesser extent low level liquid clouds. A dedicated **B**-matrix for the Météo-France convective scale model AROME has been derived. Despite promising results, this preliminary study cannot be easily extended to the 3D-Var framework of AROME.

A more suitable framework could be ensemble data assimilation systems as illustrated by Chambon et al. (2013) with the mesoscale model WRF and the Maximum Likelihood Ensemble Filter. Satellite microwave radiances over land (SSMI/S, AMSR-E and MHS) have been used to initialise the hydrometeors from WRF. The **B**-matrix for the hydrometeors is computed from the ensemble leading to flow dependent statistics. They have shown that it does not alleviate completely issues associated with discontinuities in cloud physics: the generation of model precipitation where observed is more difficult than the suppression of model precipitation where is has not been observed, since in the first case background error statistics for hydrometeors remain rather low. In order to account for errors in cloud location and radiative transfer modelling a specific bias correction scheme has been defined based on a “symmetric scattering index” over land.

Prognostic cloud schemes have to define microphysical properties of condensates (density, shape, size distribution) for the conversions between species and their transport. Radiative transfer schemes have also to make similar assumptions in order to compute the radiative properties of particles within an atmospheric volume. These assumptions are not necessarily consistent since these modules, which are coupled through data assimilation systems, are developed independently. For example, when considering the assimilation of microwave radiances for frequencies above 50 GHz, scattering effects by solid particles within clouds (snow, ice, graupel, hail) have to be considered since they contribute to a strong reduction of brightness temperatures measured by spaceborne instruments. Common assumptions are to assume that ice particles are solid spheres and snow particles are soft spheres (mixture of air and ice), since the Mie theory provides analytical scattering properties for these simple shapes. The Marshall-Palmer Particle Size Distribution (PSD) is often chosen since it leads to simple analytical expressions of the various moments. Recently, Geer and Boardo (2014) have relaxed these assumptions that are made in the RTTOV-SCATT radiative transfer model (Bauer et al., 2006). They have used scattering properties obtained by Liu (2008) from the Discrete Dipole Approximation (DDA) method for a number of solid particles of various shapes. They have also relaxed the Marshall Palmer distribution by using the "normalized" PSD formulations from Field et al. (2007) with mass-diameter formulations (giving combined information on density and shape) from Kulie et al. (2010). They have considered the data assimilation framework of the ECMWF global system that allows a systematic comparison between observed and simulated brightness temperatures over a large sample of cloudy systems (Figure 3). By defining a number of criteriaon the innovation departures, they found an optimal particle shape (sector snowflakes) that improves the simulation of brightness temperatures over the whole microwave spectrum of existing instruments. As mentioned above, these changes were done independently from the description of microphysical processes representing clouds in the ECMWF NWP model. The level of complexity of microphysical schemes for the assimilation ofobservations sensitive to hydrometeors (e.g. radar reflectivity, liquid water content, total number concentration) has been recently challenged by Laroche et al. (2005) who pointed out, in an idealized framework, that three moment schemes might be required for such purpose and that second moment schemes could have a behaviour less desirable than simple one moment schemes.

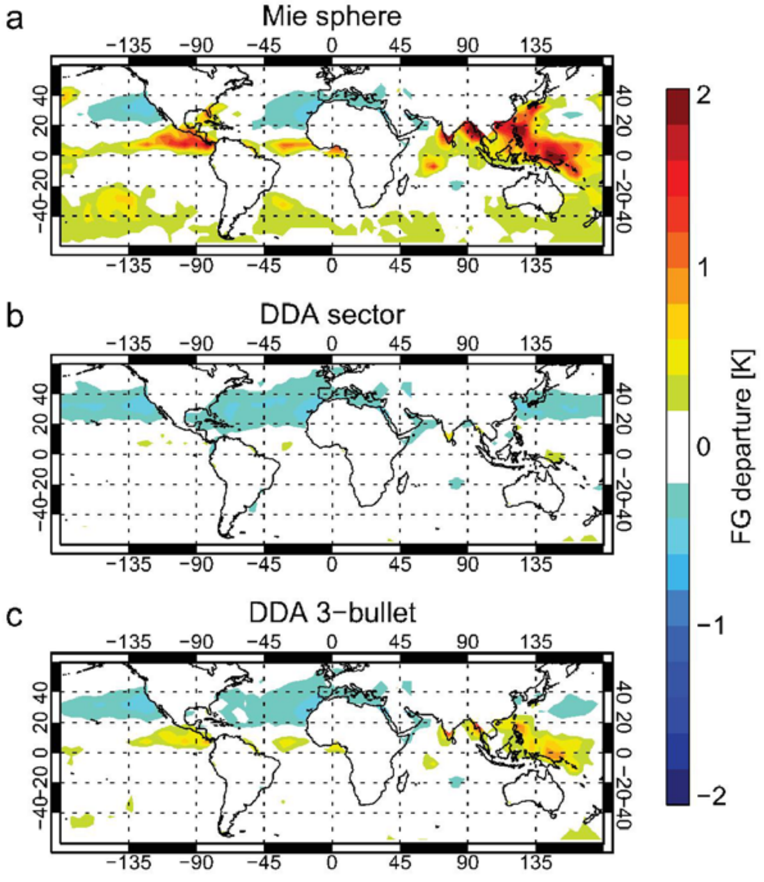

Figure 3: Mean background departures in the 52.8 GHz channel on SSMI/S for three choices of snow optical properties (June 2012): (a) Spheres with Mie theory, (b) Sector snowflake with DDA, (c) 3-bullet rosette with DDA. Model simulations are short range forecasts from the ECMWF model coupled to the RTTOV-SCATT radiative transfer scheme (taken from Geer and Boardo, 2014).

4 Assimilation of remote sensing observations for the surface

During the last decade, there have been a number of satellite missions providing useful information on continental surfaces in particular on superficial soil moisture (ASCAT[2], SMOS[3], SMAP[4]). The availability of these new satellite data have led to a number of improvements regarding the description of land surfaces compatible with NWP modelling and also with observation operators for the simulation of satellite products. For example, the fact that satellite pixels have a footprint between 20 and 40 km that encompasses many surface types, requires horizontal heterogeneities to be accounted for in the forward modelling. At low microwave frequencies the emission of a vegetated surface is very different from that of an open water surface (lake) or of a snow covered area. Indeed, instruments like SMOS, dedicated to probe water in the soil, are also sensitive to liquid water present in other media (vegetation, lakes, oceans, snow), as it can be clearly seen in the ECMWF monthly monitoring presented in Figure 4.

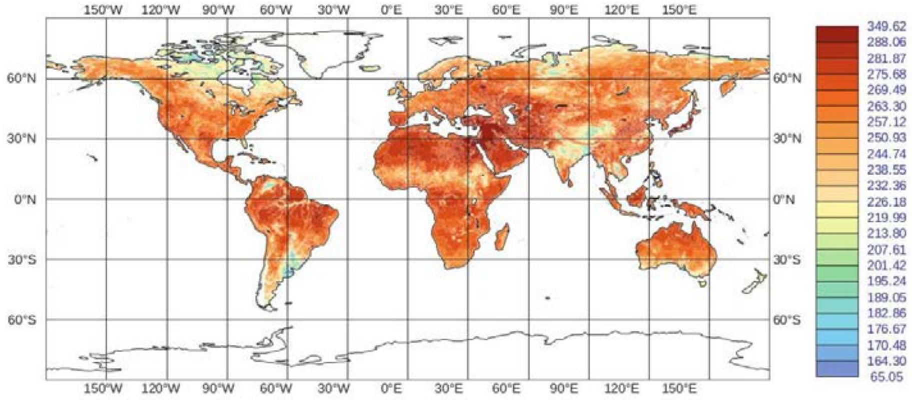

Figure 4: Monthly mean (16/08/2014 to 13/07/2014) of observed SMOS T_b in XX polarisation at 40^o angle (taken from the ECMWF operational monitoring).

An improved description of inland water surfaces has been proposed by Balsamo et al. (2012) using the prognostic lake scheme FLake. These requirements, in terms of data assimilation, also mean that high resolution physiographic databases (regularly updated) are needed to describe accurately sub-grid surface heterogeneities in land surface schemes developed for NWP models. Another important constraint on land surface schemes with this new type of observation, comes from the fact that remote-sensing instruments probe at most the first 5 cm of soil. Indeed, the water contained in the top soil layer is not the main driver of surface evapotranspiration that is of primary interest in NWP models. What dominates the strength of water losses in the atmosphere or in rivers is the water content over a deeper layer (few meters): the root-zone.

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[2] ASCAT: Advanced Scatterometer on board METOP satellites that measures the backscattered radiation from the surface in C-band.

[3] SMOS: Soil Moisture Ocean Salinity is an ESA mission with a L-band radiometer having a synthetic aperture antenna launched in 2009.

[4] SMAP: Soil Moisture Active Passive is a NASA mission having a L-band radiometer with a real aperture and a L-band radar to be launched in 2015.

The usefulness of these satellite data relies on the capacity of land surface schemes to transfer background departures located in the superficial soil layer into relevant increments in the root-zone layer. This transfer of information is schematically presented in Figure 5 for the simulation of SMOS brightness temperatures using the community microwave radiative transfer model CMEM[5].Most of Land Data Assimilation Systems (LDAS) use either an Extended Kalman Filter (EKF) approach (ECMWF, Météo-France, Met Office) or an Ensemble Kalman Filter (EnKF) approach (Environment Canada, NASA, USDA) in order to perform the inversion presented in Figure 5.

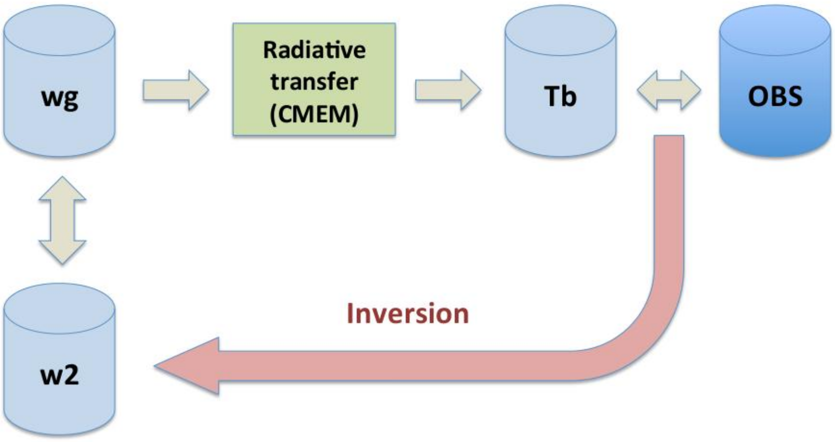

Figure 5: Schematic description of a Land Data Assimilation System for the assimilation of L-band Tb (brighntess temperatures). The superficial soil moisture w_g is used in the observation operator CMEM whereas the analysis provides correction for the soil moisture in the root-zone w_2, through an inversion process.

The link between the superficial and deep soil moisture reservoirs can be easily understood with the simple two layer version of the ISBA scheme (Noilhan and Mahfouf, 1996) based on the force-restore method. The two prognostic equations are written as:

$$\frac{\partial w_g}{\partial t} = \frac{C_1}{\rho_w d_1}\left[P_g - E_g(T_s)\right] - \frac{C_2}{\tau}\left(w_g - w_{g2}\right) \qquad d_1 = 1 \text{ cm}$$

$$\frac{\partial w_2}{\partial t} = \frac{1}{\rho_w d_2}\left[P_g - E_g - E_{tr}(T_s)\right] - D \qquad d_2 \approx 2 \text{ m}$$

with τ=1 day, d_1=1 cm, d_2 (between 1 and 2 m), C_1 and C_2 are time constant scaling parameters function of soil texture and soil moisture. The various fluxes (precipitation P_g, bare soil evaporation E_g, vegetation transpiration E_{tr} and gravitational drainage D) are schematically displayed in Figure 6.

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[5] CMEM: Community Microwave Emission Model.

The simplicity of ISBA equations allows the estimate of the analytical Jacobians that relate sensitivity of the superficial soil moisture at a given time T to changes in deep soil moisture at the beginning of an assimilation window:

$$\frac{\partial w_g^T}{\partial w_2^0} = 1 - \exp\left(-\frac{C_2 T}{\tau}\right) < 1$$

This expression assumes that the surface forcing (precipitation minus evaporation: $P_g - E_g$) can be neglected (nighttime and dry periods). This Jacobian is lower than one and increases with the length of the assimilation window T (restore of the surface layer to the equilibrium value from the root-zone layer). When computing the Jacobians in finite differences as displayed in Figure 7 at 12 UTC and 24 UTC on 1 July 2006 (over Western Europe these are close to local times), it appears that the largest values (some of them being above one) are obtained during the day when the radiative forcing is large, in contradiction with the analytical expression and with the physical understanding on how information can be transferred from the superficial to the deep layer. This spurious behaviour can be explained by a weakness of the non-linear scheme that projects onto the linearized version.

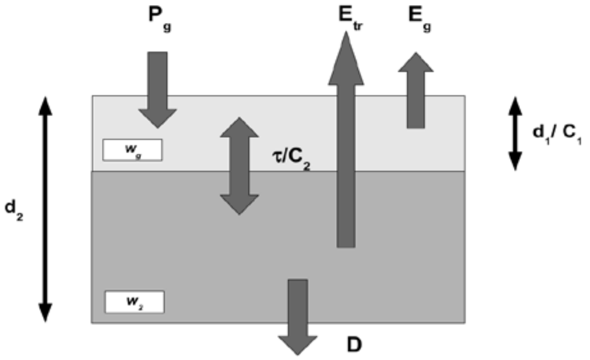

Figure 6: Schematic description of the two-layer land surface scheme ISBA.

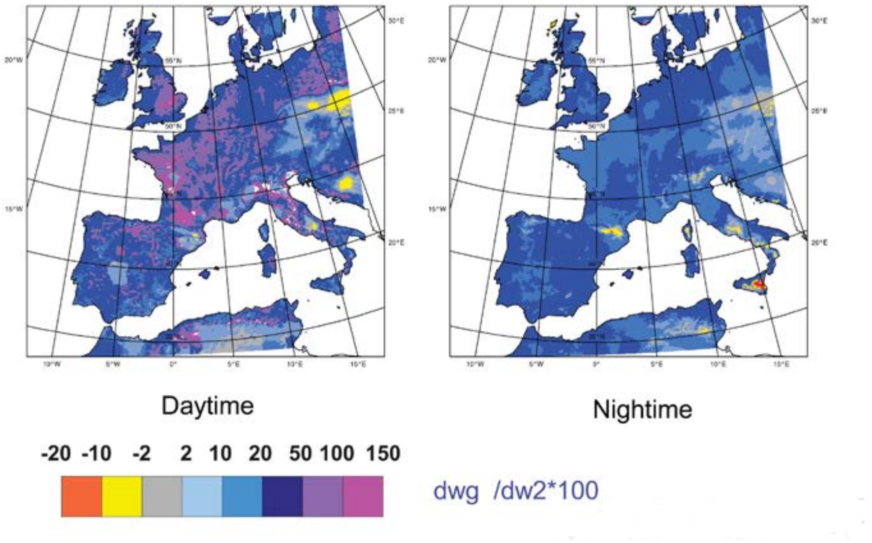

Figure 7: Jacobians of the ISBA scheme ∂w_g/∂$w_2$computed in finite differences for the 1 July 2006 at 12 UTC (left panel) and 00 UTC (right panel). The length of the assimilation window is T=24 hours.

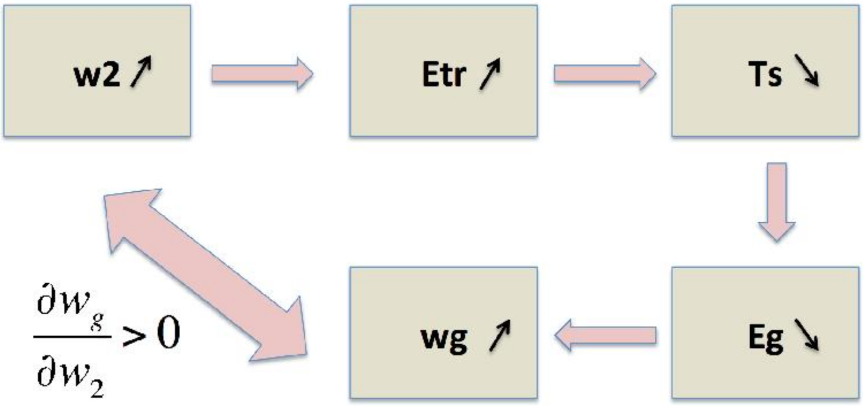

Figure 8: Explanation of spurious values of Jacobians $\partial w_g/\partial w_2$ *in the two-layer ISBA scheme, when the two layers are linked through the surface energy balance (one single surface temperature* T_s *for bare soil and vegetation).*

The fact of using a single energy balance for the bare soil and the vegetated parts of the surface (same surface temperature T_s) together with a strong non-linear behaviour of vegetation transpiration near the wilting point (w_{wilt})[6] induces an unphysical link between w_g and w_2. It is schematically presented in Figure 8. An increase in w_2 (near w_{wilt}) enhances (significantly) vegetation transpiration E_{tr} that cools the surface. A decrease in surface temperature T_s reduces bare soil evaporation E_g that in turns reduces the water losses of the superficial layer (e.g. therefore increases w_g). This positive Jacobian $\partial w_g/\partial w_2$ will induce significant changes in w_2 from w_g observations, during day time when evaporation is large and also when the soil is rather dry (non-linearities near w_{wilt}). A consequence is that, in a data assimilation system, satellite observations sensitive to w_g will appear more informative than they actually are. It is also important to notice, through studies described in Kumar et al. (2009) and in Parrens et al. (2014), that a two-layer scheme enhances deep layer corrections since the actual physical transfers (through vertical gradients of water potential) are neglected. With multi-layer soil schemes, Jacobians have strong seasonal variations with lower values in winter affecting a deep soil layer and higher values in summer over a much shallower layer (Parrens et al., 2014). The structure of bulk soil schemes prevents from describing such processes that are relevant for a realistic assimilation of superficial soil moisture information from remote-sensing.

Recently, Albergel et al. (2012) have revised the link between superficial soil moisture w_g and bare soil evaporation E_g in the ECMWF land surface scheme HTESSEL (Balsamo et al., 2009). Such revised formulation has been proposed through a systematic comparison between simulated and observed SMOS brightness temperatures over semi-arid regions. Simulated values were significantly lower than the observed ones, indicating too high values of superficial soil moisture contents. Indeed, in the original version of HTESSEL, E_g was set to zero when w_g reached the wilting point. Such critical soil moisture value is meaningful over vegetated areas but is not justified over bare soil surfaces (Mahfouf and Noilhan, 1991).

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[6] wilting point: rather dry soil moisture value below which the vegetation cannot extract water from the soil through its root system.

By setting $E_g = 0$ for a completely dry soil ($w_g = 0$), a better agreement was found with in-situ observations (Figure 9) and a large increase in SMOS brightness temperatures has been noticed over semi-arid regions of the globe (Figure 10). It is important to underline the fact that bare soil evaporation being negligible in both formulations, the response of the atmosphere is unchanged. Therefore, the use of remote-sensing observations for land data assimilation provides additional constraints on surface schemes as part of the observation operator in order to achieve a better consistency between the various components of the water and energy budgets (fluxes and storage values).

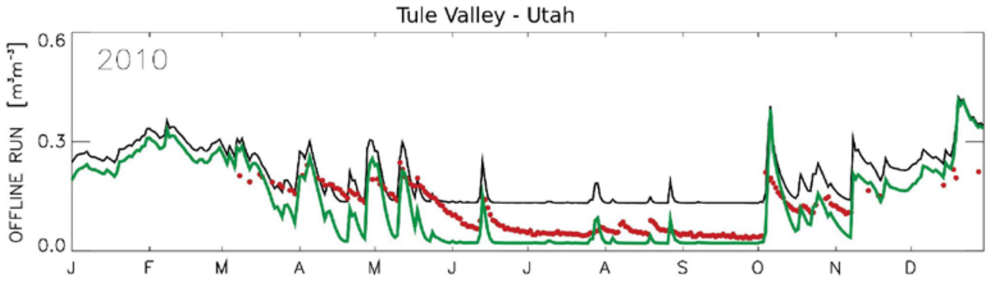

Figure 9: Illustration of volumetric soil moisture time-series for one site in Utah (Tule Valley) for 2010. The black line is for BEVAP OLD (control experiment without the new bare ground evaporation formulation: $E_g(w_g = w_{wilt}) = 0$), green line is for BEVAP NEW (test with new formulation: $E_g(w_g = 0) = 0$) and red dots are for in situ observations of soil moisture (taken from Albergel et al., 2012).

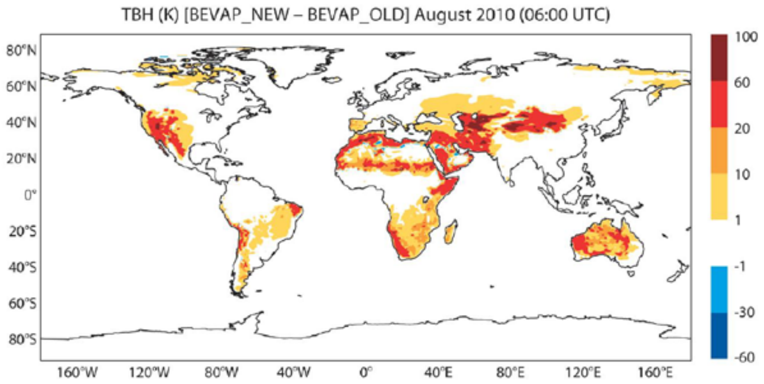

Figure 10: Map of differences between SMOS Tb (horizontal polarisation, 40^o incidence angle in K) simulated using ECMWF model fields from BEVAP NEW ($E_g(0) = 0$) and BEVAP OLD ($E_g(w_{wilt}) = 0$) for August 2010 (06:00 UTC) (taken from Albergel et al., 2012).

5 Conclusions and perspectives

During the last ten years there has been significant progress in the assimilation of satellite data in synergy with an increased usage of model physics:

- More realistic microphysical processes in cloud and precipitation schemes have allowed the assimilation of cloudy and rainy radiances (and radar reflectivities) instead of surface precipitation.
- Improved surface modelling is paving the way towards the assimilation of satellite data from dedicated missions (SMOS, SMAP): lake modelling, multi-layer soil schemes, improved description of land evaporation, multiple energy balance (mosaic approach).

The example of ECMWF regarding the synergy between land surface modelling and land data assimilation developments is quite remarkable with that respect. The level of complexity in the description of the surface physics has been made consistent with observations to be assimilated whereas comparisons of model outputs in observation space have proven to be a useful diagnosis of systematic errors that led to improved physics and observation operator descriptions.

There is a strong interest in prognostic microphysical schemes in NWP models to provide an improved coupling with observation operators (T_b and Z) (e.g. two-moment schemes with explicit condensation from aerosol nuclei, three-moment schemes for radar reflectivity assimilation). Ensemble assimilation techniques offer a natural extension of the control vector to hydrometeors with associated B matrix (Lorenc, 2014; this volume). However, non-linearities and thresholds present in the model physics will remain but they will be more difficult to identify and cure. Indeed, there is an interest in evaluating model physics (as part of the observation operator) in terms of Jacobians, in order to identify spurious behaviours (Chevallier and Mahfouf, 2001; Fillion and Mahfouf, 2003, Duerinckx et al., 2014). Jacobians can also be compared with more complex (reference) schemes (Garand et al., 2001). The current increased usage of satellite radiances over land, allows surface retrievals (of either surface temperature or surface emissivity) but they remain “sink variables” (e.g. Guedj et al., 2011). This would require a coupling between land and atmospheric assimilation systems (but not necessarily in a synchronous manner). This statement is also valid for other surfaces (e.g. ocean state, snow, sea ice). Developments of dynamical vegetation schemes with improved radiative transfer in the canopy will allow the assimilation of quantities such as FAPAR[7], LAI[8], and BRDF[9]. The future satellite missions with new instruments will put requirements on additional information from the model physics: the polarized multi-angular instrument 3MI on EPS-SG (solar spectrum, aerosols), the sub-millimeter radiometer ICI on EPS-SG (cloud ice description), the wide swath altimeter SWOT (continental hydrology).

High resolution NWP models (sub-kilometric scale) will require new detailed surface physiography data bases (PROBA-V, COPERNICUS Sentinel program), the inclusion of 3D effects (surface, clouds), and they raise the upscaling issues to satellite footprint in the observation operator (Duffourg et al., 2010). Additional spectral bands might be required to solve surface energy balance in order to simulate the spectral signature from various surface properties such as vegetation and snow. An important issue concerns the microphysical consistency across the electromagnetic spectrum (between solar, infra-red and microwave) where a synergy between active and passive instruments could help. This consistency should extend to microphysical schemes developed for NWP models. Finally, open questions concern the handling of model errors in data assimilation systems, closely linked to weaknesses in the description of physical processes through parameterization schemes, and that need to be prescribed (random part) in or removed (systematic part) from ensemble systems.

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[7] FAPAR: Fraction of Observed Photosynthetically Active Radiation.

[8] LAI: Leaf Area Index.

[9] BRDF: Bidirectional Reflectance Distribution Function.

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