Perspective on Satellite-Based Land Data Assimilation to Estimate Water Cycle Components in an Era of Advanced Data Availability and Model Sophistication

Gabriëlle J. M. De Lannoy[1*], Michel Bechtold[1], Clément Albergel[2], Luca Brocca[3], Jean-Christophe Calvet[4], Alberto Carrassi[5,6], Wade T. Crow[7], Patricia de Rosnay[8], Michael Durand[9], Barton Forman[10], Gernot Geppert[11], Manuela Girotto[12], Harrie-Jan Hendricks Franssen[13], Tobias Jonas[14], Sujay Kumar[15], Hans Lievens[1,16], Yang Lu[17,18], Christian Massari[3], Valentijn R. N. Pauwels[19], Rolf H. Reichle[20], Susan Steele-Dunne[21]

[1]KU Leuven, Department of Earth and Environmental Sciences, B-3001 Heverlee, Belgium

[2]European Space Agency Climate Office, ECSAT, Harwell Campus, Oxfordshire, Didcot OX11 0FD, UK

[3]National Research Council, Research Institute for Geo-Hydrological Protection, 06128 Perugia, Italy

[4]CNRM, Université de Toulouse, Météo-France, CNRS, 31057, Toulouse, France

[5]University of Reading, Department of Meteorology and NCEO, UK

[6]University of Bologna, Department of Physics and Astronomy "Augusto Righi", Italy

[7]USDA-ARS Hydrology and Remote Sensing Laboratory, Beltsville, MD USA

[8]European Centre for Medium-Range Weather Forecasts, Shinfield Park, RG2 9AX, Reading, UK

[9]Ohio State University, Columbus, OH, USA

[10]University of Maryland, Department of Civil and Environmental Engineering, College Park, Maryland, USA

[11]Deutscher Wetterdienst, Data Assimilation and Predictability, Offenbach, Germany

[12]University of California, Berkeley, Environmental Science and Policy Management, Berkeley, California, USA

[13]Forschungszentrum Jülich GmbH, Agrosphere (IBG-3), Jülich, Germany

[14]WSL Institute for Snow and Avalanche Research SLF, Davos, Switzerland

[15]NASA Goddard Space Flight Center, Hydrological Sciences Laboratory, Greenbelt, MD, USA

[16]Ghent University, Department of Environment, B-9000 Ghent, Belgium

[17]School of Civil Engineering, Sun Yat-sen University, Guangzhou 510275, China

[18]Guangdong Engineering Technology Research Center of Water Security Regulation and Control for Southern China, Sun Yat-sen University, Guangzhou 510275, China

[19]Monash University, Department of Civil Engineering, Clayton, Victoria, Australia

[20]NASA Goddard Space Flight Center, Global Modeling and Assimilation Office, Greenbelt, MD, USA

[21]Delft University of Technology, Department of Geoscience and Remote Sensing, Stevinweg 1, 2628 CN, Delft, The Netherlands

*** Correspondence:**
Corresponding Author
gabrielle.delannoy@kuleuven.be

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Abstract

The beginning of the 21st century is marked by a rapid growth of land surface satellite data and model sophistication. This offers new opportunities to estimate multiple components of the water cycle via satellite-based land data assimilation (DA) across multiple scales. By resolving more processes in land surface models and by coupling the land, the atmosphere, and other Earth system compartments, the observed information can be propagated to constrain additional unobserved variables. Furthermore, access to more satellite observations enables the direct constraint of more and more components of the water cycle that are of interest to end users. However, the finer level of detail in models and data is also often accompanied by an increase in dimensions, with more state variables, parameters, or boundary conditions to estimate, and more observations to assimilate. This requires advanced DA methods and efficient solutions. One solution is to target specific observations for assimilation based on a sensitivity study or coupling strength analysis, because not all observations are equally effective in improving subsequent forecasts of hydrological variables, weather, agricultural production, or hazards through DA. This paper offers a perspective on current and future land DA development, and suggestions to optimally exploit advances in observing and modeling systems.

1 Introduction

The distribution of water on Earth determines human livelihoods and is itself influenced by human activities. Estimating the water availability in various terrestrial compartments is essential for water resources management, agricultural monitoring, natural hazards and disaster risk assessment, biodiversity and planet health protection, numerical weather prediction (NWP), seasonal prediction, and climate change mitigation and adaptation. Currently, the most complete regional- to global-scale estimates of water-related variables are obtained by merging satellite data records into numerical models of Earth system processes through data assimilation (DA) (Asch et al., 2016). DA can combine the unprecedented amounts of satellite data with the steadily acquired process understanding of the past decades. Specifically, DA uses the satellite observations to correct errors in model simulations, including errors in unobserved variables. Thereby, DA adds value to the observations by inferring unobserved information, filling gaps and/or enhancing the spatial resolution of satellite data. In the geosciences, DA mostly refers to state estimation theory, but it more generally covers any technique that uses data to estimate the most accurate possible system state (Carrassi et al., 2018) and associated fluxes. Therefore, DA also encompasses model parameter optimization and the correction of boundary conditions, including meteorological forcings.

Land DA developments have been reviewed earlier (Reichle, 2008, Lahoz and De Lannoy, 2014, De Lannoy et al., 2016, Jin et al., 2018, Huang et al., 2019, Xia et al., 2019, Girotto et al., 2020, Durand et al., 2021, Baatz et al., 2021). In parallel to our paper, Kumar et al. (2022, in review) review and identify current community-agreed gaps and priorities for the future of state estimation via land DA. In this paper, we reflect on advances in observing, modeling and DA techniques, the associated opportunities and complexities of future land DA systems, and solutions to keep land DA efficient and effective, in the presence of rapid data growth and model sophistication in the first half of the 21st century. First, we summarize the state of the art of land DA for the estimation of water cycle variables (**Section 2**). Next, we offer a perspective on current observing, modeling and DA systems (**Section 3**) and on the future goals of land DA (**Section 4**). The focus will be on soil moisture, snow and vegetation estimation and how to extend the impact of satellite-based land DA to improved dynamic estimates of the atmosphere, vegetation, hydrological and biogeochemical cycles, as well as of natural hazards.

2 State of the Art

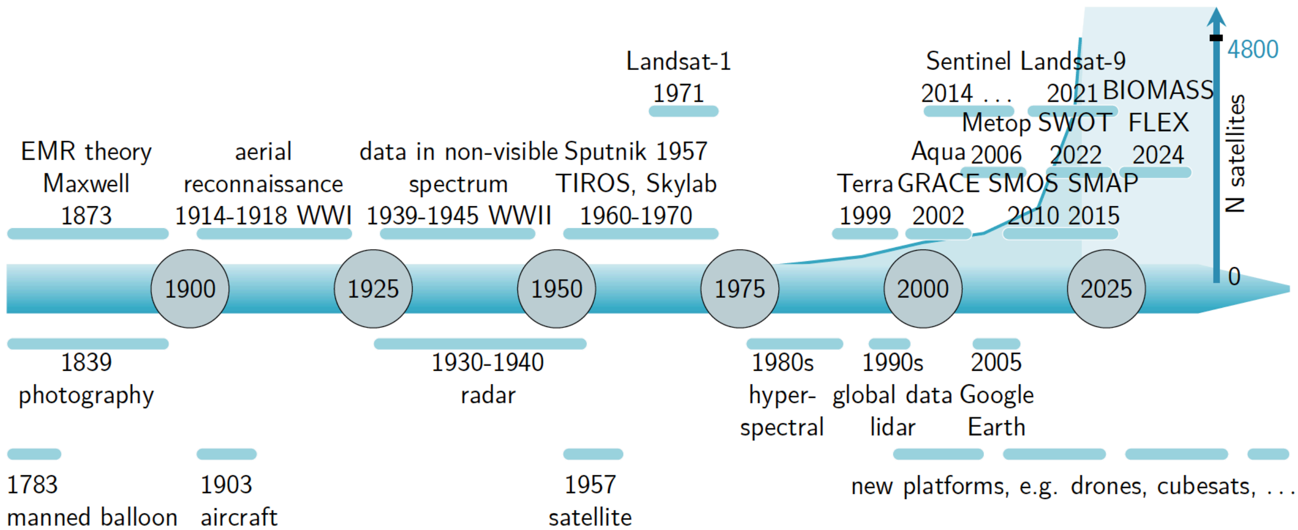

Figure 1. The 21st century within the history of remote sensing, which started with the understanding of electromagnetic radiation (EMR). Select satellite missions used for land DA are marked and discussed in the text.

The beginning of the 21st century has seen a sustained increase in remotely sensed data of the Earth system. **Figure 1** shows the exponential growth in satellite missions, with about 4,800 active satellite platforms orbiting our Earth in 2021 (https://www.statista.com/statistics/897719/number-of-active-satellites-by-year/), but only 20-25% collect Earth observations, and fewer than 1% are regularly used for land DA. Gravity measurements from the Gravity Recovery and Climate Experiment (GRACE) and GRACE Follow-On missions directly sense changes in total water storage but at a very coarse scale. Optical sensors (onboard the Terra, Landsat, and Sentinel-2 missions, among others) measure fine-scale water content proxies, e.g., snow cover extent, open water extent, vegetation, and soil color or temperature. Microwave sensors (onboard the Soil Moisture Ocean Salinity -SMOS-, Soil Moisture Active Passive -SMAP- and Sentinel-1 missions, the Advanced Microwave Scanning Radiometer onboard Aqua, and the Advanced SCATterometer -ASCAT- onboard Metop, among many more) are used to retrieve water amounts in the soil, vegetation and snow. The passive radiometer sensors collect brightness temperature data at a coarse resolution (~40 km), whereas active synthetic aperture radar (SAR) instruments can collect backscatter data at finer resolutions (< 1 km). Microwave sensors exploit the fact that the presence of water directly affects the dielectric properties of the soil, vegetation and snow, and it strongly influences the emission and scattering of microwave radiation (Ulaby et al., 2014). Insight into how radiation interacts with water in different land compartments is summarized in radiative transfer models, which can be used in two ways: (i) to invert the observed radiance into geophysical "retrieval" products (e.g., soil moisture, vegetation or snow water content), or (ii) as so-called observation operators to map simulated land surface variables to satellite-observed signals (e.g., brightness temperature or backscatter).

Many land DA systems have used microwave observations to estimate surface and deeper soil moisture (de Rosnay et al., 2014, De Lannoy et al., 2016, Reichle et al., 2019), and related variables such as discharge (Lievens et al., 2015, De Santis et al., 2021), turbulent fluxes (Lu et al., 2020), and even groundwater in peatlands (Bechtold et al., 2020). With the activation of dynamic vegetation models, the assimilation of optical vegetation indices (e.g., leaf area index) and microwave vegetation optical depth (Fairbairn et al., 2017, Kumar et al., 2020, Mucia et al., 2022) has gained interest, including to improve evapotranspiration (ET) and runoff. DA of thermal satellite data has also been popular for ET and soil moisture estimation (Crow et al., 2008), but studies on the intersection between the water and energy cycle will not be further discussed, to keep the focus on water cycle variables. At the finer scale, optical and radar satellite data have been assimilated in crop models to update canopy or soil state variables and ultimately estimate transpiration, agricultural biomass and yield (Jin et al., 2018, Lu et al., 2022). Under frozen conditions, the assimilation of optical snow cover fraction or microwave-based snow depth has been explored (Helmert et al., 2018, Girotto et al., 2021).

In practice, land DA systems are developed by merging the theoretical insights in DA, which provide a portfolio of algorithms, with the operational and physical constraints of land surface observations and modeling. An overview of regional and global land DA systems is given by Xia et al. (2019). The observations consist either of satellite retrieval products (soil moisture: Dharssi et al., 2011, Liu et al., 2011, Rodriguez-Fernandez et al., 2019; vegetation: Albergel et al., 2017, Kumar et al., 2020; snow: De Lannoy et al., 2010) or direct satellite signals (related to soil moisture: De Lannoy and Reichle, 2016, Lievens et al., 2017, Muñoz-Sabater et al., 2019, Reichle et al., 2019; snow: Larue et al., 2018, Xue et al., 2018), and most land DA systems consider far fewer observations than state variables (this characterizes DA in the geosciences at large). For example, one surface soil moisture retrieval every few days can update soil moisture in multiple soil layers and possibly vegetation, or one weekly snow cover fraction observation can update the water amount in different snow layers, while the model state evolves at sub-hourly time steps. Furthermore, most land DA systems are one-dimensional, i.e., they update each soil-vegetation-snow column (grid cell) independently and the analysis update is strictly limited to the observed columns. This formulation does not exploit the capability of many DA approaches to propagate information across the model domain from observed to unobserved areas. If communication among different columns is made possible via the physics-based model or via spatial error correlations, thus making the DA system spatially distributed, then state variables in neighboring (observed or unobserved) columns within the influence radius of a given observation are analyzed together (Reichle and Koster, 2003, De Lannoy et al., 2010, Magnusson et al., 2014, Reichle et al., 2019).

The above studies all aim at state estimation via particle or Kalman filtering variants (other DA methods such as variational DA or direct insertion have also been used) to correct the land surface state for short-term and interannual errors in the meteorological forcings (in offline systems, i.e., not coupled to an atmospheric model) or other unmodeled temporary deviations in some water compartments. In this process, only a few DA systems effectively assign the DA corrections to the source of errors, such as for example snowfall or precipitation input to obtain good snow depth or total water storage estimates (Winstral et al., 2019, Girotto et al., 2021). Most DA systems do not conserve mass, unless the water budget is explicitly constrained (Pan et al., 2012).

To correct land surface estimates for longer-term or systematic deviations, and to minimize water budget imbalances, satellite data can be used more effectively for parameter estimation. These parameters can be part of the prognostic model (Han et al., 2014, Kolassa et al., 2020), the diagnostic radiative transfer model (De Lannoy et al., 2013, Rains et al., 2022), or represent a bias factor for meteorological input (Wrzesien et al., 2022). Long-term model calibration could be seen as a form of long-term DA or history matching. Alternatively, DA for sequential parameter updating (with or without simultaneous state updating) allows to account for time-varying parameters (Montzka et al., 2011, Magnusson et al., 2016).

3 Perspective on Current Observing, Modeling and DA Systems

3.1 Observations

The spaceborne observations of many water cycle variables have been improving in radiometric, spatial, and temporal resolution, but dedicated missions are not yet available for all parts of the water budget. Soil moisture is now routinely measured at a coarse resolution by dedicated L-band satellite missions (SMOS, SMAP, Kerr et al., 2010, Entekhabi et al., 2014), and can also be inferred from shorter wavelength C-band sensors onboard meteorological satellite missions (ASCAT, Figa-Saldana et al., 2002). Finer-scale estimates can be obtained from current C-band SAR or optical sensors, and the upcoming NASA-ISRO L-band SAR (NISAR, Rosen and Kumar, 2021) and ESA High Priority Candidate Mission Radar Observation System for Europe in L-band (ROSE-L, Pierdicca et al., 2019) are expected to improve fine-scale soil moisture estimates.

There is currently no mission devoted to SWE, but various passive microwave sensors have been combined to produce coarse-scale SWE products (Luojus et al., 2021). The complexity of snow itself and its presence in complex terrain require more insight on how different types of radiation interact with snow to support the development of a dedicated mission (e.g. Ku and X-band) for fine-scale SWE observation. Multi-frequency missions such as the planned Copernicus Imager Microwave Radiometer (CIMR) will become relevant for SWE remote sensing in the future. Meanwhile, existing sensors have been used in an opportunistic way (e.g., snow depth from Sentinel-1 radar, Lievens et al., 2022), and upcoming missions such as NISAR and ROSE-L will further help to estimate high resolution SWE.

The water stored in vegetation is also not yet fully observed from space. Several optical vegetation indices (e.g., leaf area index) approximate the vegetation health and transpiration (Bannari et al., 2009). More recently, the microwave-based vegetation optical depth (VOD) products have shown promise to represent biomass, vegetation structure and water (Steele-Dunne, 2017, Wigneron et al., 2021, Chaubell et al., 2020). The upcoming BIOMASS Earth Explorer mission (Quegan et al., 2019) promises to explore long wavelength (P-band) measurements to estimate the total biomass in whole forest layers. Recent studies also aim at the estimation of plant transpiration from novel solar induced fluorescence (SIF) retrievals (Maes et al., 2020). The upcoming FLEX Earth Explorer mission (Drusch et al., 2017) will collect SIF data to serve agricultural purposes. Ultimately, advancing VOD and SIF-based retrievals and gaining insights in how vegetation affects microwave radiation or fluorescence will lead to better estimates of the water, carbon and energy cycle when combined with dynamic vegetation and crop yield modeling.

Spaceborne observation of water fluxes such as total ET and discharge remains a challenge. Intermittent satellite-based discharge estimates can be derived from optical and altimeter data (Abdella et al., 2021, Tarpanelli et al., 2021). The Surface Water and Ocean Topography (SWOT) mission will soon enable frequent spaceborne observations of river stage for large rivers to allow inference of discharge (Biancamaria et al., 2016; Frasson et al., 2021). Currently, no mission is specifically dedicated to ET measurements (Fisher et al., 2017), and ET is most typically inferred from satellite-observed surface or skin temperature (related to sensible heat) as the residual of a simple energy balance model (Anderson et al., 2021), or indirectly obtained via soil moisture and VOD DA in a land surface model (Martens et al., 2017). Most high-resolution ET methods based on optical sensors suffer from low coverage (clear-sky conditions, low revisit times) and from large discrepancies among the various products. The ECOsystem Spaceborne Thermal Radiometer Experiment on Space Station (ECOSTRESS, Fisher et al., 2020) mission helped evaluating the use of thermal infrared observations at fine spatial and temporal resolutions to define future ET mission requirements. The future Land Surface Temperature Monitoring (LSTM, or Sentinel-8) and Thermal infraRed Imaging Satellite for High-Resolution Natural resource Assessment (TRISHNA, Roujean et al., 2021) missions promise to advance ET measurements in the coming decade. The quantification of other water fluxes, such as irrigation fluxes, from satellite observations is still in its infancy (Kumar et al., 2015, Massari et al., 2021, Dari et al., 2022).

Most DA systems use satellite observations that are directly related to land surface state variables (e.g., soil moisture, temperature, vegetation, snow) to improve subsequent state and flux forecasts. Conversely, the *assimilation of satellite-based flux observations* (e.g., ET, runoff, irrigation) is relatively less explored and limited to regional applications (Hartanto et al., 2017, Gavahi et al., 2020), because only a few global flux products are available (mainly ET) and they heavily depend on model background which might be inconsistent with the assimilation model. Furthermore, the diagnostic flux DA requires a careful design to link flux observations to prognostic state or parameter updates that are memorized in the system for improved forecasts. The latter can be achieved e.g., via selecting particles with a self-consistent combination of parameter, state and flux values in particle filters or via an adequate observation operator in Kalman filter-based techniques (Pauwels et al., 2006).

New sensor technologies have not only helped to observe more variables, but also increased the resolution of data. For example, SAR data can regularly monitor soil moisture and surface water at km-scale resolution, albeit with more noise, longer revisit times or smaller coverage than coarser-scale data. Even if some (mainly commercial) sensors are indeed able to measure with high levels of detail, observations with meter-scale resolution are unlikely to make it into equally fine-scale land DA systems for global applications any time soon (**Section 4.2**).

The level of satellite observation processing desirable for land DA is the subject of a debate that should strengthen the collaboration between geophysical retrieval and DA communities in the future. Land DA uses satellite observations either in the form of gridded radiances collected by the sensor or as the associated geophysical retrievals. Just like retrieval DA, radiance DA has been used to update the land surface state (examples below) and parameters in the land surface or radiative transfer model (Han et al., 2014). Radiance DA requires a forward model to relate the land surface state (soil moisture, temperature, snow, vegetation water content) and parameters (clay fraction, vegetation scattering albedo) to the satellite radiance signals as part of the observation operator (Reichle et al., 2014). The observation operator can also deal with the difference in spatial support of the observations and simulations in a multiscale DA system, e.g., to downscale coarse-scale observations to a finer resolution. Some studies report little DA skill difference between radiance and geophysical retrieval assimilation (De Lannoy and Reichle, 2016, Aires et al., 2021), and other studies show that radiance DA can circumvent biases associated with retrievals. For example, for deep mountain snow, SWE retrievals can be significantly biased (e.g. Wrzesien et al., 2017), but microwave radiance DA allowed both Li et al. (2017) and Kim et al. (2019) to achieve unbiased SWE estimates. Furthermore, DA of radiances facilitates the simultaneous updating of multiple state variables (e.g., soil moisture, temperature and vegetation) more elegantly than DA of the various associated individual retrieval products with cross-correlated errors. Radiance DA is also physically more self-consistent than retrieval DA, because retrievals are constrained by background information that may deviate from that of the model. E.g., soil moisture retrieval may use temperature information, and soil or vegetation parameters from data sources that are different from those of the model. The physical consistency makes radiance DA particularly attractive for coupled land-atmosphere DA (de Rosnay et al., 2022).

Finally, the observation error characterization is more traceable for radiance DA. In the realm of DA algorithms, the use of (nonlinear) observation operators enables solving DA as a nonlinear optimization problem, without (or with limited) relying on linearity assumptions. In short, *satellite observations should be provided along with good observation operators that can support land DA*.

The spatio-temporal characterization of the observation error (that is, retrieval or instrument error, plus representativeness error) is a key element to successful DA systems. New sensor developments would thus ideally be preceded by a synthetic *observing system simulation experiment* (Crow et al., 2005) to quantify the tolerable levels of uncertainty for efficient DA. Furthermore, observations and model estimates typically have distinct biases, which are ideally resolved, explained, or removed prior to state updating (see **Section 3.3** and **4.1**). *This requires that satellite missions span enough years to quantify climatological biases in observation space*, and this has so far limited the use of short-lived exploratory missions onboard new platforms (e.g., drones, cubesats) in DA systems.

3.2 Models

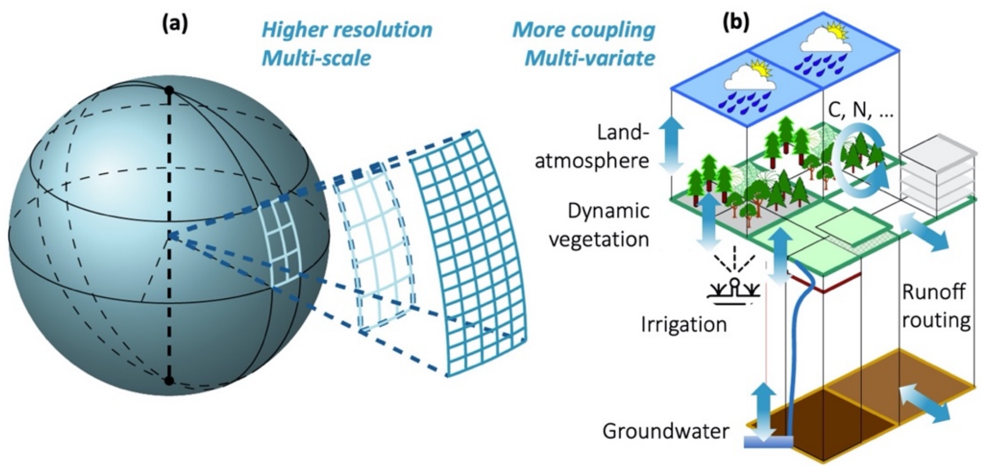

Figure 2. Land surface model sophistication increased in the 21st century towards (a) higher resolutions, by resolving multi-scale hydrological processes and improving model parameterizations, and (b) coupling of more processes, by replacing simplistic parameterizations and including more interactions between variables in multiple compartments.

The beauty of nature is that it is intelligible and can be captured in general physical laws, despite its complexity in the details. This knowledge is indispensable to add value to observations, and to inter- and extrapolate them to unobserved variables. In the last decades, a slow but steady increase in sophistication of large-scale land surface modeling and DA systems has been achieved (Fisher and Koven, 2020) by (i) improving model parameterizations (Balsamo et al., 2009) and resolving multiscale processes (**Figure 2a**), (ii) improving prognostic representations of hydrological processes, such as e.g., lateral subsurface flows in aquifers (Shrestha et al., 2014), snow processes (Bartelt and Lehning, 2002, Deschamps-Berger et al., 2022), peatland-specific processes (Bechtold et al., 2020), (iii) improving prognostic representations of vegetation (Clark et al., 2011), biogeochemical cycles including the nitrogen cycle (Oleson et al., 2013) and phosphorus cycle (Goll et al., 2017), (iv) activating anthropogenic processes, such as irrigation (Lawston et al., 2017), or by (v) land-atmosphere coupling (**Figure 2b**).

By shifting from parameterized to physically resolved modeling (e.g., static parameterized to prognostic dynamic vegetation) and by coupling more processes, the DA impact of a single observation *can reach more unobserved, but model-resolved, compartments*. For example, snow depth DA can improve discharge and low-level atmospheric estimates (Griessinger et al., 2019, Lahmers et al., 2022, Rudisill et al., 2021), and backscatter DA can update dynamic vegetation and soil moisture, to eventually update irrigation (Modanesi et al., 2022). Efforts are ongoing to advance land DA in coupled land-atmosphere models (de Rosnay et al., 2014, Boussetta et al., 2015, Carrera et al., 2019, Reichle et al., 2021b) to make good on the promise to improve NWP and subseasonal to seasonal predictions (Kumar et al., 2022). As a matter of fact, the use of physics-based models has also been pivotal to the success of atmospheric DA in NWP to propagate information to unobserved areas (Kalnay, 2002). At the same time, several studies with current state-of-the-art land surface models also reported limited success (Crow et al., 2020, Hung et al., 2022) in propagating information from one compartment to another, which suggests that the modeling (parameterization) of the coupling and fluxes between land compartments as well as DA strategies need further research.

Surprisingly few new prognostic physics-based models (or model components) have been developed in response to the growing number of satellite data. This might be because we have reached the maximal desired structural complexity for large-scale applications, or because the coarse resolution of many satellite data integrates too much spatial variability, complicating a clean local physical interpretation of processes. As both model simulations and satellite observations become available at higher resolutions and for longer time spans, more spatial and temporal scales get resolved (**Figure 2a**). This might possibly deepen our process understanding, limit parameterizations and ultimately help hyper-resolution modeling (Wood et al., 2011) and DA.

Alternative ways of model development are emerging, which in fact have the potential to use the growing amount of (possibly coarse-scale) data and artificial intelligence rather than our human intelligence to build a model. Specifically, *machine learning* (ML) holds promise (Nearing et al., 2020) to develop models for multiple variables directly from multiple types of observations. E.g., ML can be used to diagnose how satellite-observed signals can be related to a set of land surface variables via complex interactions. Especially for microwave-based observation operators (Xue et al., 2018, Shan et al., 2022), ML might currently be more efficient than trying to fully understand and parameterize all radiation interactions. It is however unclear if ML is capable of entirely replacing prognostic land surface models in Earth system models, given that ML is not well-suited for nonstationary systems (e.g., under climate change), or to support the inference of unobserved land variables, because ML typically employs supervised learning that requires the existence of observations prior to training. More pragmatically and potentially more successfully, ML might complement physically based descriptions in a hybrid fashion (Reichstein et al., 2019). Note that in this subsection, ML is presented as a tool for model development. **Section 3.3** discusses how ML can be used for DA.

Ideally, models offer a framework to propagate observations to unobserved variables, but models are imperfect, and their uncertainties originate from errors in the numerical schemes, unresolved scales, parameters, initial conditions, meteorological input (in offline systems) or missing processes. Via DA, the model state, parameters or forcing inputs will be updated to correct the model trajectory. If parameterizations are replaced with physically resolved process descriptions and the associated parameters would become physically measurable, then the need to update parameters should reduce in favor of more state updating. Similarly, when offline forcing inputs are replaced with coupled land-atmosphere modeling and constrained by atmospheric observations, then the need to update meteorological input in land surface models should reduce in favor of more state updating.

3.3 DA Methods

The choice of DA method for a given application is arguably often driven by the research group's repository of source code, and it is rarely optimal in a mathematical sense (Carrassi et al., 2018). However, the discontinuity (e.g., via activation thresholds) and non-differentiability of land surface processes (including prognostic soil-water-vegetation-snow and diagnostic radiation interactions) is a valid reason to *favor ensemble Kalman or particle-based techniques* (Evensen et al., 2022), instead of variational methods that require model adjoints, which are difficult to obtain and maintain. Furthermore, ensemble- and particle-based DA can diagnose flow-dependent forecast error estimates for nonlinear land surface models. Like in other areas of climate science, filters dominate operational land DA systems because they naturally support the sequential inclusion of satellite observations, provided they are available to describe an optimal current state for subsequent forecasts. For longer-term re-analysis solutions, or for slowly varying variables, smoothers (Dunne and Entekhabi, 2006, Margulis et al., 2015) gather observations over a sliding retrospective time window to obtain the best historical solution.

The key to any DA method is in the *treatment of the forecast and observation errors*. State estimation assumes random errors. In the ensemble Kalman filter (EnKF) or particle filter (PF), the distribution of the random forecast error accumulated between assimilation time steps is diagnosed from an ensemble of realizations, and ensemble generation is an art by itself (choice of perturbations, variable transformations to obtain Gaussianity, covariance inflation, localization; Carrassi et al., 2018). The observation errors are typically set to a constant standard deviation parameter that reflects the instrument or retrieval error, increased by the representativeness error that also includes observation operator error (Tijana et al., 2018). The forecast and observation error estimates are typically hyperparameters optimized by manual tuning of DA diagnostics (Reichle et al., 2017), because automated adaptive filtering (Crow and Reichle, 2008, De Lannoy et al., 2009) remains too inefficient. Most DA methods rely on the assumption of unbiased sources of information, and thus biases are typically removed prior to DA via, e.g., cumulative distribution function matching between the assimilated observations and the model simulations (Reichle and Koster, 2004, Kumar et al., 2012); consequently, DA analyses are consistent with the (potentially erroneous) model climatology. Ideally, biases are disentangled to estimate (De Lannoy et al., 2007, Pauwels et al., 2013) and possibly remove forecast or observation bias, or perhaps to identify the impact of water management or other human activity (e.g., unmodeled groundwater pumping and irrigation; Kumar et al., 2015, Girotto et al., 2017).

The nature of the errors associated with different land variables is very different. **Figure 3** illustrates how soil moisture has a more bounded error growth than snow or vegetation, and that a single DA update reduces the forecast error for a longer time in variables with longer error autocorrelation lengths. *More research is needed on how to best address these various types of errors for different variables via different DA methods and different bias treatments.* For example, state-only updating without observation bias correction was advantageous to correct the accumulated snow and the associated river discharge in Smyth et al. (2019) and Lahmers et al. (2022), but in other studies, snow observation bias correction (De Lannoy et al., 2012, Liu et al., 2013) or bias correction to snowfall (Magnusson et al., 2016) was preferred. Similarly, Albergel et al. (2017) and Kumar et al. (2020) used a bias-blind filter for vegetation updating, but omitting bias correction for vegetation observations can possibly cause undesirable sawtooth timeseries and inferior ET and runoff estimates when assimilating intermittent observations, when the model is pushed out of its statistical equilibrium. The need for observation bias correction might depend on the boundedness of variables and the coupling between variables in different models, i.e., whether there is strong circular coupling equilibrium (vegetation-transpiration-soil moisture-vegetation) or rather a dominant one-way coupling (snowpack-discharge).

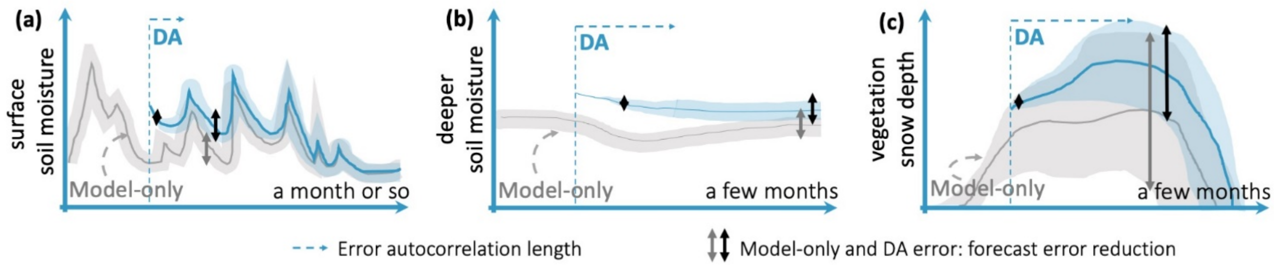

Figure 3. Different error characteristics of (a) surface soil moisture, (b) deeper soil moisture, and (c) vegetation or snow depth, for (gray) model-only and (blue) DA simulations. The semi-transparent plumes represent ensemble uncertainties.

Finally, most of the above considerations hold for DA in the traditional sense of merging physics-based model variables with satellite observations. New, data-driven methods such as ML offer an alternative to DA and can in some ways be similar to four-dimensional variational DA (by including the time dimension as in smoothers). Like DA (Geer et al., 2021), ML can be used to obtain better state estimates, bias estimates (Pan et al., 2021) or parameter estimates (Mudunuru et al., 2022). *Novel hybrid DA-ML methods* (Bonavita et al., 2020) are showing success in discovering and emulating unresolved-scale processes, whenever a chronic lack of data makes the task extremely difficult for pure ML. In the context of coupled atmosphere-ocean modeling, DA-ML has shown promising results (Brajard et al., 2021) and its future use in a land-atmosphere context could be attractive.

4 Perspective on Future DA Development

4.1 Land DA Goals of the Future: Priorities

From its origin in atmospheric and ocean sciences, DA for state updating provides the best-possible initial conditions for subsequent forecasts. Properly estimating the initial state is critically important in chaotic systems (Carrassi et al, 2022), where small errors can grow exponentially in time and where the characteristics of such growth are themselves unpredictable. By contrast, land systems are usually asymptotically stable. Therefore, initial errors are typically internalized in the state (memory) until the system reaches an equilibrium after some time. Nevertheless, in a coupled land-atmosphere system, a small land initialization error could result in exponential error growth in the atmosphere. Seemingly small improvements obtained via land DA are therefore critical for NWP and seasonal predictions, provided the coupling mechanisms for long-term predictability are well represented. In land-only applications, state updating is essential to reset cumulative vegetation or snow variables for seasonal-scale yield or discharge forecasts, or to adjust soil moisture or input forcings for more accurate short-term hazard predictions of landslides (Felsberg et al., 2021), fires (Jensen et al., 2018), floods (Massari et al., 2018), and droughts (Li et al., 2019).

However, DA is not equally effective in all circumstances. For example, soil moisture updating can generally improve streamflow predictions (Mahanama et al., 2012, Reichle et al., 2021a), but might not be effective to reduce errors in the fast runoff component which are dominated by rainfall errors (Mao et al., 2020). Similarly, the influence of soil moisture on ET depends on the seasons, the coupling strength between soil moisture and ET in different climate regimes (Dong et al., 2020) and the ability of the assimilation model to accurately capture that coupling (Crow et al., 2020). To use data and resources most efficiently in a century when ever more data are becoming available (**Section 4.2**), one should wonder which specific type of observations at what time and location has the largest impact on land DA analyses and beyond. A suggestion for future research is thus to explore *targeted land DA*. This requires that we first determine which type of observations are most useful to improve the forecast skill of particular land or atmosphere variables under the given circumstances, via sensitivity studies, forecast sensitivity-based observation impact studies, or coupling strength analyses. The land DA community can learn from the NWP community, which already has a strong grasp on how much various observations contribute to forecast skill (Eyre et al., 2021). Thereafter, we can efficiently assimilate those observations that likely have the most impact. The limitation is that satellite observations are collected in fixed orbits and not necessarily at the strategically most optimal location or time, so the main goal of targeting observations is a careful selection of the available observations.

Apart from state updating, satellite DA should be further explored for parameter estimation to (i) improve inherited static global soil and vegetation parameter databases that served older model generations, and to (ii) assign values to newly resolved parameters that will emerge from the sophistication of land surface models, e.g. to parameterize dynamic vegetation growth or water table dynamics. Parameter estimation is in principle possible using the same DA framework used for state estimation. Nevertheless, the success of parameter updating depends on the model sensitivity to that specific parameter and to its correlation with the observed quantities. The latter could be automatically estimated via the ensemble (for the EnKF) or the particles (for the PF), thus further promoting the use of this family of methods. Recently, hybrid EnKF-PF methods have been developed precisely to use the EnKF for the "more linear" state update and the PF for the "more nonlinear" parameter updates (van Leeuwen et al., 2019). Those methods could prove effective in land DA as well. Finally, parameter updating is particularly relevant for long-term applications, because DA frameworks for state-only updating rely on the assumption of the system being autonomous and stationary and are thus not theoretically suitable if a system is subject to climate change or human activities that cause changes in the system's equilibrium. This is a broader issue for DA and goes well beyond the realm of land DA. Usually, the assumption is that by sequentially updating the system state and parameters we drive the conditional posterior probability toward the new equilibrium, yet rigorous mathematical results along these lines are still missing.

DA can be used to correct the state, parameters or forcings for unmodeled or poorly modeled processes, such as e.g. human activities. For example, Saharan dust deposited on snow should result in a sudden update of the parameterized or simulated albedo to ensure correct snow melt estimates. A forest fire, deforestation, land use change, or crop rotation within or across years (Boas et al., 2021) all require updates of vegetation model parameters or states. Such events will be followed by a gradual adjustment to a new soil moisture equilibrium both in the model and reality, but the transition time might differ, because some (unobserved) model parameters that determine the transition time are not in line with reality. The same is true for land systems in the presence of climate change, which might necessitate gradually changing model parameters. How to *combine long-term updates for poorly modeled processes via parameter updating with short-term state updating* should be explored in the future.

DA diagnostics of observation-minus-forecast and analysis-minus-forecast residuals allow an evaluation of the optimality of the DA system (Desroziers, 2005, Reichle et al., 2017). These diagnostics could in the future also help to identify (and improve) times and locations of poorly modeled processes, or system transitions from steady state to a new equilibrium.

DA aims at blending multiple sources of information seamlessly. However, in one-dimensional DA systems, no horizontal information propagation is achieved, which can result in artificial spatial patterns (e.g., swath edges or cloud screening imprinted in the DA analysis). When the land DA is coupled to an atmospheric model, such spatial discontinuities could lead to undesirable triggering of turbulence (Alapaty et al., 1997). Furthermore, only a part of the model variables might be included in the DA state vector. E.g., only a few soil moisture layers might be updated out of all soil-vegetation variables, or only the land variables and no atmospheric variables might be updated in a coupled DA system. To *avoid unphysical discontinuities* at the border between domains (e.g., land vs. atmosphere, or observed vs. non-observed land) or at the interface between variables, *spatially distributed and multivariate DA methods* are recommended, where multiple state variables of the land surface and coupled processes are updated.

As an extension of multivariate DA, the use of coupled DA is seen as another key area of desired DA development (de Rosnay et al., 2022). Strongly-coupled DA intends to inform one component of the climate system (e.g., the land) by using observations of the other (e.g., the atmosphere) and vice-versa (Penny and Hamill, 2017). This contrasts with the so called "weakly-coupled DA" in which the analysis update only affects the model compartment where data are collected, but then a coupled model is used in the forecast step. The model usually acts as a dynamical way of propagating information from the observed to the unobserved component, and weakly-coupled DA is usually developed first towards the ultimate goal of strongly-coupled DA. The spatio-temporal difference between processes in the coupled media (e.g., land-atmosphere) make it extremely difficult to construct a suitable error covariance across them (Tondeur et al., 2020). *The sophistication of DA techniques will need to grow with a stronger coupling* of the simulated water, energy and biogeochemical cycles (Baatz et al., 2021) in land surface, terrestrial ecosystem and atmospheric modeling and with the use of multivariate constraints across the various compartments of these coupled systems.

4.2 Increased Dimensions of Future Land DA: Challenges and Opportunities

Most visions for future land DA include multisensor DA (Durand et al., 2021), multivariate DA (Kumar et al., 2022), and multi-scale DA with a push towards finer resolutions. Our priorities above should be viewed against the backdrop of these foreseen developments, and here we highlight some associated opportunities. A multisensor approach is recommended to constrain more water cycle variables (Girotto et al., 2019) and obtain finer spatial and temporal resolutions, e.g., to benefit from the higher accuracy of coarse-scale observations and from the spatial detail in fine-scale observations (De Lannoy et al., 2012, Lievens et al., 2017). The use of multiple independent observations also has the *potential to mitigate equifinality problems, i.e., to identify the state variable, input or parameter correction, or combination thereof, that results in the most effective constraint (e.g., particle selection)*. As discussed above, multivariate DA is needed for physical consistency and to reach more unobserved variables in more sophisticated systems. Higher-resolution (km-scale) DA systems promise to better resolve local land details for improved NWP and land-atmosphere reanalysis products. Higher resolutions for coupled land surface-subsurface models also better represent runoff processes at the hillslope scale, and narrow valleys with underlying groundwater bodies, which affect the simulation of ET (Shrestha et al., 2018). Furthermore, high-resolution estimates are needed for agricultural applications and hazard estimation.

From the viewpoint of system theory, these desires for high-resolution multivariate and multisensor DA translate into *larger dimensions of state and observation error covariances, which necessitates practical and computationally affordable solutions*. Larger updated state vectors require larger ensemble sizes to mitigate the sampling error in the ensemble-based error covariances, or beg for alternative solutions to partition the state into less-dependent groups of correlated variables that can be updated sequentially (thus making the ensemble covariance essentially block-diagonal). Indeed, the latter grouping of state variables conceptually mimics the idea of localization to filter out spurious error correlations in spatially distributed DA systems, and is also the essence of weakly-coupled DA systems.

Assimilating more observations from multiple sensors, multiple products, or high-resolution datasets increases the dimensions of the observation error covariance matrix. Spatially neighboring observations, or joint soil moisture and vegetation retrievals from the same microwave sensor, cannot be assimilated independently due to associated error correlations. *Solutions can be found in directly assimilating radiances rather than multiple derived retrieval products, targeting only those observations that have most impact on the forecast* (**Section 4.1**), *and thinning the observations* (Waller et al., 2018). A second problem with assimilating multiple observations is that they each might have their own bias, represent something different than the model variables, and/or might cause contradicting updates (Girotto et al., 2019). Appropriate uncertainty estimates and bias removal partly solve this problem, and allow DA to update the temporal variability, while preserving the model's climatological water distribution as a strong constraint (Pan et al., 2012). *Ideally, when observation biases get resolved and we find adequate ways to relate modeled and observed land estimates in absolute terms, then the multitude of observations should be used to also correct the modeled terrestrial water partitioning, and thereby create the correct climatological land conditions to support the correct coupling regimes.*

Finally, using models, observations and DA at ever finer resolutions inevitably requires advanced computational infrastructure, more background information, e.g., on land surface processes, soil and land use parameters, high-resolution meteorological information (for off-line land simulations), and a DA method that can address the problem complexity (Carrassi et al., 2018). Furthermore, fine-scale estimates are by their nature more uncertain than the aggregated counterparts. In the future, we will have to balance the advantages of resolving more detail against the curse of dimensionality.

5 Conclusion

Satellite-based land DA is an interdisciplinary field of research that yields the most complete and consistent estimates of terrestrial water cycle variables. The growing amount of satellite data and the sophistication of modeling systems in the 21st century require efficient land DA systems to fuse observations and models into meaningful information for end users. Land DA can convert the intermittent swaths of satellite signals into temporally and spatially complete, gridded fields of soil moisture, snow or vegetation estimates and related variables, including land surface fluxes such as ET and runoff. By coupling the land with atmosphere or groundwater processes, and by resolving vegetation or snow parameterization schemes with physics-based processes, observations have the potential to update more unobserved variables, and to have an impact beyond the land surface. This is especially the case for NWP, crop monitoring, hazard (landslides, fires, floods, droughts) assessment, and carbon management.

Large, dynamical modeling systems that include more resolved or coupled processes, require sophisticated DA techniques (perhaps supplemented with ML) to optimally distribute the observed information into improved estimates of the multivariate state, parameters, or boundary conditions. The exponential growth of satellite data will support improved constraints of the advanced modeling frameworks, but the growing dimensions in land DA will also necessitate the development of efficient DA algorithms. It will thus become increasingly important to select the most suitable levels of observation processing and the most impactful observations for assimilation, because not all observations are equally efficient all the time in DA systems. We can curb the growth of state and observation dimensions in the DA problem by considering targeted DA, rather than a mass integration of all data.

6 Conflict of Interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

7 Author Contributions

GDL developed the paper structure and wrote the initial draft, all co-authors contributed to the shaping of the paper contents and to the writing and editing of the paper.

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