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SPECIALTY SECTION

This article was submitted to
Water and Hydrocomplexity,
a section of the journal
Frontiers in Water

RECEIVED 20 May 2022

ACCEPTED 21 July 2022

PUBLISHED 11 August 2022

CITATION

Camporese M and Giroto M (2022)
Recent advances and opportunities in
data assimilation for physics-based
hydrological modeling.
Front. Water 4:948832.
doi: 10.3389/frwa.2022.948832

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Recent advances and opportunities in data assimilation for physics-based hydrological modeling

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Data assimilation applications in integrated surface-subsurface hydrological models (ISSHMs) are generally limited to scales ranging from the hillslope to local or meso-scale catchments. This is because ISSHMs resolve hydrological processes in detail and in a physics-based fashion and therefore typically require intensive computational efforts and rely on ground-based observations with a small spatial support. At the other end of the spectrum, there is a vast body of literature on remote sensing data assimilation for land surface models (LSMs) at the continental or even global scale. In LSMs, some hydrological processes are usually represented with a coarse resolution and in empirical ways, especially groundwater lateral flows, which may be very important and yet often neglected. Starting from the review of some recent progress in data assimilation for physics-based hydrological models at multiple scales, we stress the need to find a common ground between ISSHMs and LSMs and suggest possible ways forward to advance the use of data assimilation in integrated hydrological models.

KEYWORDS

integrated surface-subsurface hydrological models, land surface models, remote sensing, data assimilation, groundwater, soil moisture

Introduction

Physics-based hydrological modeling

Physics-based hydrological models are important in earth and environmental sciences thanks to their inherent capability of being applicable to the widest possible range of scales and environmental conditions (Fatichi et al., 2016). These models are increasingly being used to predict future water resources quantity and quality in response to climate and land use change, to monitor and assess hydroclimatic hazards (such as floods and droughts), and in general to understand the intertwined dynamics between the hydrological, atmospheric, and carbon cycles. They are playing an ever-increasing role, also thanks to their capabilities of considering multiple compartments of the terrestrial water cycle (Clark et al., 2015). Depending on the scale of interest, we refer here to two different categories of physics-based hydrological models: local to meso-scale integrated

surface-subsurface hydrological models (ISSHMs) and continental to global-scale land surface and hydrological models (LSMs/GHMs).

Integrated surface-subsurface hydrological models (Furman, 2008; Maxwell et al., 2014; Paniconi and Putti, 2015; Kollet et al., 2018) typically resolve the Richardson-Richards equation (or some approximation of it) in the subsurface, coupled with some form of the shallow water equation for surface flow. Although their spatial resolution varies widely (from a few meter to several hundred meters), due to their high computational requirements and need for detailed parameterization, ISSHMs are usually applied to relatively small spatial domains (i.e., from hillslope to regional or meso-scale catchments), with a handful of notable recent exceptions at the continental scale (Keune et al., 2016, 2018; Maxwell and Condon, 2016; Kollet et al., 2018; Condon and Maxwell, 2019; Condon et al., 2020a,b).

Global hydrological and land surface models (LSM/GHM), on the other hand, were first developed in the context of earth system modeling to resolve energy and mass balance processes at the interface between the land surface and the atmosphere. Their spatial resolution typically ranges from 10 to 50 km, which are often inadequate to fully capture the fine-scale variability of surface and subsurface hydrological processes. As an example, they typically lack the representation of processes in highly heterogeneous areas such as mountains and coasts, which are also amongst the most vulnerable regions to hydro-climatic hazards (Balica et al., 2012; Elalem and Pal, 2015).

Regardless of the scale of interest, both ISSHMs and LSM/GHMs rely on accurate representation of the hydrological physical processes as well as input meteorological forcing data (e.g., precipitation, air temperature, wind speed, etc.), and parameters (e.g., land cover, soil type, soil properties, etc.), all of which can be difficult to obtain and can lead to large uncertainties in modeled hydrological states and fluxes (Collier et al., 2018), especially when generalizing a model to larger spatial domain. These uncertainties (and errors) inherently affect all estimates of hydrological states (e.g., water table or soil moisture) obtained through modeling. However, they can be quantified and limited through data assimilation approaches.

Data assimilation

Data Assimilation (DA) refers to a suite of statistical techniques that incorporate observation data into mathematical models, with the goal of optimizing estimates of the system state (and possibly parameters). The results of a DA framework should be a statistically optimal estimate, superior to that from either the model or observations alone (Evensen et al., 2022). DA was pioneered by meteorologists and has been used to improve operational weather forecasts for decades. The first application of data assimilation in ISSHMs dates to the early

2000s (Paniconi et al., 2003). Since then, much progress has been made, also thanks to the widespread diffusion of ensemble-based assimilation methods such as the ensemble Kalman filter and its variants (Evensen, 2003). Data assimilation for LSM/GHMs has a similar history, with significant advancements over the past decade for estimating hydrological land surface variables (Reichle et al., 2002; de Rosnay et al., 2014).

In general, LSM/GHM DA previous developments involve univariate data assimilation, i.e., assimilation of one observation to adjust model states (e.g., soil moisture) or parameters such as precipitation scaling factors (e.g., Liu and Margulis, 2019; Girotto et al., 2021), albedo (Navari et al., 2018), and vegetation properties (Smith et al., 2020). More recently, the scientific community started to target multi-observational approaches. The simultaneous assimilation of multiple observation data strongly improves model predictions compared with single observation and/or state estimation alone (e.g., Girotto et al., 2019; Kumar et al., 2019; Khaki et al., 2020). Data assimilation applications in ISSHMs typically involve the assimilation of multiple measurements in both the surface (soil moisture, streamflow) and subsurface compartments (pressure head, water table depth) with or without the update of model parameters (e.g., Camporese et al., 2009a,b; Pasetto et al., 2012; Rasmussen et al., 2015, 2016; Zhang et al., 2015, 2016; Ridler et al., 2018; Gebler et al., 2019; He et al., 2019).

While promising in overcoming models and observations uncertainties, current literature in data assimilation for physically based hydrological studies agree that: (i) it is very challenging to improve model estimates in one compartment assimilating measurements from another (Camporese et al., 2009b; Zhang et al., 2016; Botto et al., 2018); (ii) the joint update of system states and model parameters usually leads to better results (Botto et al., 2018; Gebler et al., 2019); (iii) data assimilation applications in integrated surface-subsurface hydrological models are generally limited to scales that go from the hillslope (Botto et al., 2018; Gebler et al., 2019) to local-scale (He et al., 2019) or meso-scale catchments (Rasmussen et al., 2016; Ridler et al., 2018), mainly due to computational constraints; (iv) the robustness of the assimilation application depends upon the accurate characterization of the combined modeling and observation uncertainties, a task that can be particularly challenging especially for large spatial domains (Kumar et al., 2017).

Statement of the problem: The scale gap

From the analysis of recent literature in hydrological data assimilation, a distinct scale gap emerges. Ground observations can have a high time resolution but are typically characterized by a very small spatial support, making them ideal for assimilation in local catchment-scale or hillslope models, where the size of the computational cell/element can be of the same order

of magnitude of the measurement volume. However, they are expensive with respect to the (limited) spatial coverage they offer. At the other end of the spectrum, satellite-based observations are under continuous development to reduce their uncertainties and provide additional information, thanks to their large spatial coverage; for this reason, they are commonly assimilated in LSMs/GHMs. However, their use with ISSHMs have been hindered by their typically coarse resolution, which is not consistent with scale requirements of ISSHMs (Samaniego et al., 2010; Or et al., 2015; Or, 2020). In addition, hyper-resolution modeling at continental to global scales with ISSHMs still requires prohibitive computational efforts for them to be used in ensemble-based data assimilation frameworks. The main goal of this mini-review is to discuss possible new directions for hydrological modeling, observations, and DA methodologies, which could lead to advances in data assimilation for larger spatial domains or to unlock the potential of remote sensing data for assimilation in physics-based hydrological models.

Bridging the gaps between spatial scales

In the following, we discuss recent developments, outstanding challenges, and possible research directions in physics-based hydrological modeling (Section Recent advances and outstanding challenges in physically based hydrological modeling), relevant observations (Section Recent advances and outstanding challenges in observation data), and assimilation systems (Section Data assimilation for non-gaussian systems).

Recent advances and outstanding challenges in physically based hydrological modeling

In many cases, the breadth of differences in the data generated from *in-situ* and remote sensing observations raises significant questions on how to best use these data in modeling development and testing. Land surface and groundwater have intertwined processes, yet their scientific modeling fields are still disconnected.

Over the past decade, the LSM/GHM modeling community has been embracing hyper-resolution (~1-km or finer) integrated surface-subsurface hydrological modeling (Wood et al., 2011; Bierkens et al., 2015; Condon et al., 2021), therefore providing the opportunity for the two modeling categories (ISSHMs and LSM/GHMs) to start meeting in the middle while resolving regional to continental scale surface-subsurface hydrological processes. Moving LSM/GHMs to higher resolutions and/or ISSHMs to larger scales is posing huge challenges, mainly represented by uncertainties due to the lack

of fine scale model processes and parameters knowledge (Beven and Cloke, 2012). Some of these challenges are listed as follows.

First, while meso-scale natural processes, such as precipitation-induced runoff or evaporation, are included in most LSM/GHMs, more local anthropogenic processes, such as irrigation, are rarely modeled, especially in LSMs (Bierkens et al., 2015). Human driven processes can directly control the groundwater (GW) table, for instance, by lowering the GW table through pumping and by increasing recharge *via* flood irrigation. To date, representing human-induced impacts in continental to global scale hydrological models remains a major challenge, mostly due to the lack of accurate global irrigation information (Wada et al., 2017).

Second, despite advancements in land surface model complexity, most LSM/GHMs route moisture in the vertical dimension only, and allow no lateral communication between vertical soil columns, i.e., they do not represent GW dynamics. Such an assumption implies that controls of GW on land-surface interactions, and consequently hydro-climatic hazards, may be overlooked (Keune et al., 2016; Maxwell and Condon, 2016). Subsurface flow can also be crucial for a series of applications including (and not limited to) drought monitoring, flood predictions, and water resources management. Only recently, the land surface community started to recognize that lateral groundwater flow significantly interacts with surface processes such as vegetation dynamics (Gochis et al., 2018; Zeng et al., 2018; Forrester and Maxwell, 2020; Rummeler et al., 2022), hydro-climatic hazards (Felsberg et al., 2021), and atmospheric forecasting (Getirana et al., 2020) and consequently to put efforts in representing this process (e.g., Batelis et al., 2020).

Third, although the number of high-resolution datasets such as topography, land use, geology, and soil properties are increasing, these data are also the products of remote sensing, land surface models, statistical downscaling techniques, or combinations thereof and thus affected by inaccuracies and uncertainties.

Finally, executing physically based models at high spatial resolution, while resolving surface and subsurface water dynamics in a coupled way and over large regions is computationally demanding, both in terms of CPU time and storage requirements (Kollet et al., 2010; Maxwell, 2013).

These challenges suggest the need to develop new modeling approaches at continental and global scales that can properly simulate hydrological processes (especially lateral subsurface flows) at resolutions compatible with remote sensing data (i.e., resolutions used in the LSM/GHM community). To this end, machine learning and deep learning techniques are recently being explored to emulate complex subsurface physical processes (Radmanesh et al., 2020; Tran et al., 2021) and also to link modeled estimates with indirect measurements of the state variables (e.g., to link moisture states to radiances observations, Section Earth observations).

Recent advances and outstanding challenges in observation data

Earth observations

Earth observation data (aka satellite or remote sensing) is essential to monitor hydrologic variables such as soil moisture and groundwater table because it provides a bird's-eye view of the Earth's dynamics. In the last several decades, the number of spaceborne sensors has rapidly increased. These observing systems can detect subsurface hydrologic states such as the soil moisture at various spatial and temporal resolutions (e.g., from ~ 1 to 40 km resolutions, Entekhabi et al., 2010; Fang et al., 2021). Despite this apparent wealth of new data, there are lingering methodological challenges to translate these types of observations into water table depth. In fact, the basic remote sensing principle involves the direct interaction between an incident radiation (e.g., natural solar radiation or active radiation sent from a sensor) and the targets of interest. Groundwater is a hidden resource and therefore cannot be directly observed and measured from space. Ground-based water table depth monitoring and reporting are scarce and variable across the globe, and frequently limited to developed regions. For this reason, little is still known about the global patterns of the water table depth and its interactions with the land, urban and natural ecosystems, hindering our capabilities to fully exploit the potential of water table information in data assimilation for global-scale integrated hydrological modeling.

Possible ways forward are offered by the fact that groundwater can be indirectly observed through other quantities, for example evaporation fluxes (Miralles et al., 2011) and total terrestrial water storage (TWS) (Famiglietti and Rodell, 2013).

Water table dynamics are linked to the atmosphere through evapotranspiration and recharge. From a water budget perspective, the accurate account of water losses *via* evapotranspiration and runoff should lead to improved estimates of recharge fluxes, and thus water table depth. Recent studies have shown that assimilation of remotely sensed evapotranspiration estimates can inform the groundwater table dynamics (Gelsinari et al., 2020).

Since 2002, TWS estimates have been derived from the Gravity Recovery and Climate Experiment (GRACE) and its follow-on mission (GRACE-FO). These missions provide valuable information on groundwater conditions beyond what can be seen at the surface (Li et al., 2012; Scanlon et al., 2018) because it measures the water storage changes in the entire terrestrial water storage (i.e., including snow, vegetation biomass, surface soil moisture, root-zone soil moisture, and GW). However, limitations still exist for using GRACE data in operational groundwater dynamics monitoring. The major limitations are related to (i) the data delivery latency; (ii) the relatively coarse spatial and temporal resolutions of GRACE observations; and (iii) the fact that TWS is an

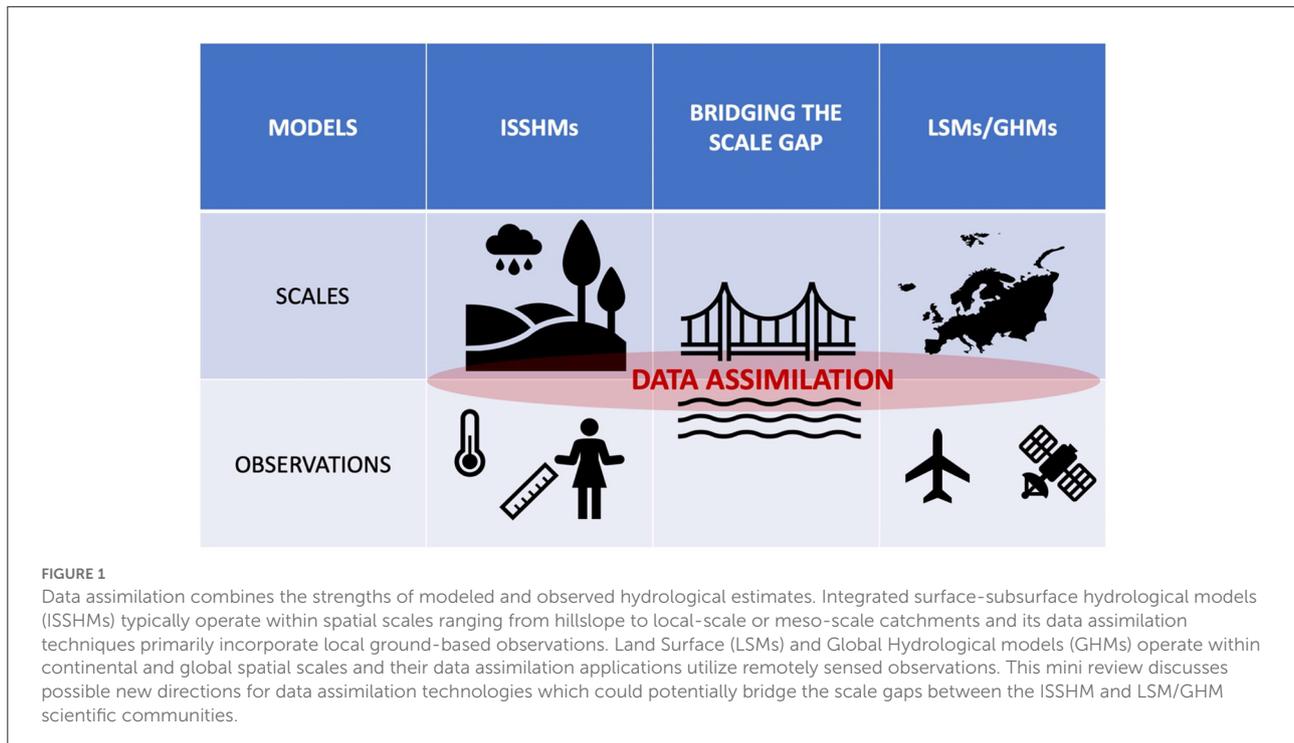
aggregated observation of multiple water storage components. The assimilation of GRACE data in an LSM allows us to downscale the TWS observations spatially and temporally into its various water storage components such as surface and root zone soil moisture and groundwater table (Giroto et al., 2016; Kumar et al., 2016).

Another interesting opportunity is given by processes linking changes in GW level to deformation of the Earth's crust and thus vertical land motion (Erban et al., 2014; Darvishi et al., 2021). As opposed to tectonic and sediment compaction, the vertical land motion associated with surface water or groundwater table changes can be visible at sub-annual temporal scales. Some GW systems are more susceptible to compaction compared to others. In some cases, depletion and recharge of aquifers can cause vertical land motion with rates up to ~ 10 cm/year (Carlson et al., 2020). Elastic deformation typically results in small-magnitude recoverable displacements (on the mm to cm scale) of the land surface (Shirzaei et al., 2020). When the effective stress exceeds a stress threshold, the deformation is inelastic and results in permanent (irreversible) subsidence. Recent studies have quantified the elastic contributions to vertical land motion and related it to GW (Chaussard and Farr, 2019; Smith and Knight, 2019; Hsu et al., 2020; Lu et al., 2020; Ojha et al., 2020; Tangdamrongsub and Šprlák, 2021). Deriving accurate global soil compaction parameters and modules to be coupled to hydrological models can be complex, if not impossible. For data assimilation, this limitation can be addressed with the development of an artificial intelligence (i.e., neural network) forward model to link vertical deformation to changes in the variable of interest (i.e., groundwater table) (Smith and Majumdar, 2020; Naghibi et al., 2022).

In addition to improved estimates of the driving forces, as detailed above, an accurate, detailed and spatio-temporal assessment of groundwater fluxes requires also a reliable estimate of soil and aquifer parameters, to avoid errors in parameters leading to over- or underestimation of fluxes. Starting from prior parameter distributions that can be extracted from globally available datasets (e.g., Batjes, 1997; Hengl et al., 2017), data assimilation allows for their dynamic update, which can lead to improved model predictions (e.g., Hung et al., 2022).

Intermediate-Scale sensing technologies

One possible way forward to expand the capabilities of DA for integrated hydrological modeling is offered by novel sensing technologies at intermediate scales that go beyond the local support scale typical of ground observations. While traditional soil moisture, water table, and pressure head observations have a support volume of a few cubic centimeters or decimeters, fiber optics sensing (FOS), airborne electro-magnetic methods (AEMs), cosmic ray neutron sensing (CRNS), and unmanned aerial vehicles (UAVs) represent relatively cheap (compared to the possible extent of the surveys) options to collect



hydrologically relevant data at scales ranging from tens of meters to hundreds of kilometers.

Fiber optic sensing can be used to measure, among other variables, strain, displacement, pressure, and temperature with high spatial resolution for distances of several kilometers (Leone, 2022). Fiber optic distributed temperature sensing (FO-DTS), in particular, represents a promising technique to measure soil water at high spatial resolutions (<1 m), thanks to the relationship between soil thermal properties and soil moisture content (Sayde et al., 2010, 2014; Steele-Dunne et al., 2010; Striegl and Loheide, 2012; Dong et al., 2017; Vidana Gamage et al., 2018). However, to the best of our knowledge, FOS data have never been used for DA studies in integrated hydrological modeling and still represent an underexploited opportunity.

Much progress has been made in the past decade to assimilate hydrogeophysical observations in hydrological models. In particular, Electrical Resistivity (ER) data, thanks to their sensitivity to soil moisture and salinity, have demonstrated their usefulness in parameterizing subsurface systems (e.g., Camporese et al., 2015; Crestani et al., 2015; Manoli et al., 2015; Tso et al., 2020). However, all these studies have focused on local-scale systems, while hydrogeophysics now offers the opportunity to survey large extensions of land with AEM methods. They potentially allows for the estimation of key groundwater parameters, such as hydraulic conductivity, with remotely sensed geophysical data collected over thousands of square kilometers, while still being able to capture heterogeneities at scales of interest for physics-based hydrological models ($\sim 10^1$ m) (e.g., Christensen et al., 2017; Knight et al., 2018;

Vittecoq et al., 2019). So far, AEM surveys have been typically conducted to get a static picture of the subsurface structure and parameters. However, if repeated over time (despite their costs), these surveys might provide valuable datasets to be used in data assimilation studies for integrated hydrological modeling, such as variations of groundwater levels over large areas, which could complement information provided by GRACE.

Cosmic ray neutron probes are used in several fields of hydrology as they offer the possibility of estimating average snow water equivalent (Schattan et al., 2017) and soil moisture over areas of 130–240 m of radius and to depths of ~ 15 –80 cm, depending on the soil moisture itself (Köhli et al., 2015). Using an Ensemble Adjustment Kalman Filter, Patil et al. (2021) assimilated neutron counts for a 655 km² catchment into the Noah-MP land surface model, showing that incorporating information from CRNS can improve parameter and soil moisture estimates and paving the way for future applications also in ISSHMs.

The increasing use of UAVs in all science disciplines, whereby multiple types of sensors can be easily deployed over relatively large areas, also provides us with plenty of opportunities to assimilate high-resolution data at intermediate scales. Assimilation of UAV-collected data is becoming common in weather modeling (Sun et al., 2020; Jensen et al., 2021) and crop modeling (Yu et al., 2019; Peng et al., 2021). However, incorporation of UAV data in physics-based hydrological modeling is still largely unexplored. Tang et al. (2018) used river bathymetry data collected through UAV surveys, in conjunction with measurements of hydraulic head assimilated

via EnKF, to improve model predictions and parameters with HydroGeoSphere (Brunner and Simmons, 2012), an ISSHM, for a river catchment in Switzerland. Given the capabilities of UAV-mounted sensors to measure a wide range of hydrological (e.g., soil moisture) and vegetation (e.g., leaf area index) variables, we see much room for DA studies in physics-based hydrological modeling in the next few years.

Data assimilation for non-gaussian systems

A common approach in data assimilation is the ensemble Kalman filter (EnKF; Evensen, 2003) that dynamically and sequentially updates model error covariance information by producing an ensemble of model predictions, which are individual model realizations perturbed by the assumed model error (Reichle et al., 2002). EnKF systems have been targeted by both ISSHMs (e.g., Camporese et al., 2009b; Pasetto et al., 2012) and LSM/GHMs (de Rosnay et al., 2014; Kumar et al., 2016; Giroto et al., 2019). Some common challenges include the need of spatially localizing EnKF covariances to remove spurious correlations, and most importantly its assumption of multi-gaussianity, which must be met for both system states and observations. If this assumption is not satisfied, the EnKF only gives sub-optimal results or, in the worst cases, fails to give an adequate representation of the variables of interest. Other, arguably more sophisticated methods, include particle filter (PF) techniques (e.g., Crisan, 2001) or combinations of EnKF and PF (e.g., Stordal et al., 2011). Like the EnKF, the PF is a sequential Monte Carlo approach, but it does not depend on the assumption of Gaussian distributions, in principle being able to accommodate every probability distribution functions, including multimodal ones. However, PF techniques typically require larger ensembles to characterize the full probability distribution of the state variables and consequently their uncertainties *via* resampling sets of state variables. Due to this disadvantage, PF applications in physics-based hydrological models have been limited to a few cases (Pasetto et al., 2012; Zhang et al., 2017).

Interesting new developments for non-Gaussian DA applications in physics-based hydrological modeling could derive from applications of the transport theory (Villani, 2009). Ning et al., 2014 showed how transportation metrics in the framework of optimal mass transport can be used with variational data assimilation to obtain optimal estimates of the system state in the presence of systematic model errors or bias, for which no prior knowledge is available. More recently, Ramgraber et al. (2021) introduced their work on non-linear smoothing, whereby transport methods are applied as a pathway for non-linear/non-Gaussian generalization of two different ensemble Kalman-type smoothers.

Compared to traditional EnKF implementations, DA algorithms based on PF or transport methods require additional computational effort. However, due to the increased availability of ever more powerful computers, we expect this is going to be less of an issue in the near future.

Conclusions

Physics-based integrated hydrological modeling have been declined in different ways by two scientific communities. On one hand, integrated surface-subsurface hydrological models (ISSHMs), solving flow and transport processes in detail, are typically applied to local to meso-scale catchments. On the other hand, land surface and global hydrological models (LSMs/GHMs) focus on continental to global scale applications, paying more attention to hydrological processes at the land-atmosphere interface and representing subsurface processes with simplified approaches. Accordingly, data assimilation has long been used by the two communities in different ways, exploiting data types consistent with their respective scales, i.e., ground-based measurements for ISSHMs and remote sensing observations for LSMs/GHMs.

In this mini review, we advocate for the two communities to find common ground for advancing data assimilation at intermediate scales (Figure 1). This can be done by pursuing new hydrological modeling approaches that can result in less computational requirements for ISSHMs and more accurate process representation for LSMs/GHMs. Also, we gave an overview of opportunities for exploiting state-of-the-art technologies providing data types at intermediate scales that can be of interest for assimilation in both categories of models. Finally, as non-gaussianity is a common issue in hydrological models and makes the most used DA algorithms sub-optimal, we suggest exploring alternative and innovative DA methods that can lead to a more plausible representation of parameter and process spatial variability.

Ultimately, these developments can contribute to bridge the gap between the two DA and modeling communities, with obvious benefits for both.

Author contributions

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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.

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