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Advancing data assimilation in operational hydrologic forecasting: progresses, challenges, and emerging opportunities

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Abstract

Data assimilation (DA) holds considerable potential for improving hydrologic predictions as demonstrated in numerous research studies. However, advances in hydrologic DA research have not been adequately or timely implemented into operational forecast systems to improve the skill of forecasts to better inform real-world decision making. This is due in part to a lack of mechanisms to properly quantify the uncertainty in observations and forecast models in real-time forecasting situations and to conduct the merging of data and models in a way that is adequately efficient and transparent to operational forecasters.

The need for effective DA of useful hydrologic data into the forecast process has become increasingly recognized in recent years. This motivated a hydrologic DA workshop in Delft, The Netherlands in November 2010, which focused on advancing DA in operational hydrologic forecasting and water resources management. As an outcome of the workshop, this paper reviews, in relevant detail, the current status of DA applications in both hydrologic research and operational practices, and discusses the existing or potential hurdles and challenges in transitioning hydrologic DA research into cost-effective operational forecasting tools, as well as the potential pathways and newly emerging opportunities for overcoming these challenges. Several related aspects are discussed, including (1) theoretical or mathematical considerations in DA algorithms, (2) the estimation of different types of uncertainty, (3) new observations and their objective use in hydrologic DA, (4) the use of DA for real-time control of water resources systems, and (5) the development of community-based, generic DA tools for hydrologic applications. It is recommended that cost-effective transition of hydrologic DA from research to operations should be helped by developing community-based, generic modelling and DA tools or frameworks, and through fostering collaborative efforts among hydrologic modellers, DA developers, and operational forecasters.

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1 Introduction

It is essential to properly characterize and communicate uncertainty in weather, climate, and hydrologic forecasts to be able to effectively support emergency management and water resources decision making (National Research Council, 2006). In hydrology, the importance of accounting for various types of uncertainty involved in the prediction process has been increasingly recognized in recent years, as seen in the emerging global initiatives such as the Hydrologic Ensemble Prediction Experiment (HEPEX, <http://www.hepex.org/>, Schaake et al., 2006). Uncertainty in hydrologic predictions can originate from several major sources, including errors in the model structure and model parameters, as well as model initial conditions and hydrometeorologic forcing (e.g., Ajami et al., 2007; Kavetski et al., 2006a, b; Salamon and Feyen, 2010). Effective quantification and reduction of these uncertainties is necessary to enable the generation of forecast products with accurate and actionable guidance on predictive uncertainty to enable risk-based decision making (e.g., Coccia and Todini, 2010; Weerts et al., 2011). The application of data assimilation (DA), which optimally merges information from model simulations and independent observations with appropriate uncertainty modelling, has proved promising in improving prediction accuracy and quantifying uncertainty (e.g., McLaughlin, 2002; Liu and Gupta, 2007; Reichle, 2008).

Over the last couple of decades, the abundance of new hydrologic observations (in-situ or remotely sensed) has stimulated a great deal of research into the use of these observations for improving hydrologic predictions via model-data infusion applications. Many of these applications rely on assimilating traditional in-situ observations such as discharge, soil moisture and snowpack measurements into hydrologic models to improve predictions of streamflow and other hydrologic variables (e.g., Seo et al., 2003, 2009; Vrugt et al., 2005; Weerts and El Serafy, 2006; Clark et al., 2008a; Komma et al., 2008; Moradkhani, 2008; Thirel et al., 2010a, b). In recent years, increasing availability of satellite observations (e.g., van Dijk and Renzullo, 2011) has generated

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unprecedented research activity into assimilating these remotely sensed retrievals of various quantities, such as soil moisture (e.g., Pauwels et al., 2001; De Lannoy et al., 2007; Moradkhani, 2008; Reichle et al., 2008; Yirdaw et al., 2008; Crow and Ryu, 2009; Kumar et al., 2009; Brocca et al., 2010; Liu et al., 2011b; Montzka et al., 2011; Peters-Lidard et al., 2011), snow water equivalent or snow cover area (e.g., Rodell and Houser, 2004; Lee et al., 2005; Andreadis and Lettenmaier, 2006; Liston and Hiemstra, 2008; Zaitchik et al., 2008; Durand et al., 2009; Kolberg and Gottschalk, 2010; Kuchment et al., 2010; DeChant and Moradkhani, 2011a; De Lannoy et al., 2012), surface water elevation (e.g., Alsdorf et al., 2007; Montanari et al., 2009; Neal et al., 2009; Giustarini et al., 2011), terrestrial water storage (Zaitchik et al., 2008) and land surface temperature (Reichle et al., 2010), among others. These DA applications were developed for a variety of models ranging from physically-based land surface models (LSMs) (e.g., Albergel et al., 2008; Nagarajan et al., 2010) to distributed hydrologic models (e.g., Clark et al., 2008a) and conceptual rainfall-runoff models (e.g., Seo et al., 2003, 2009; Moradkhani et al., 2005a, b; Weerts and El Serafy, 2006), hydraulic models (e.g., Schumann et al., 2009), groundwater models (e.g., Valstar et al., 2004; Hendricks Franssen et al., 2011), coupled surface-subsurface models (e.g., Camporese et al., 2009), biogeochemical models (e.g., Chen et al., 2009), and sediment transport models (e.g., Stroud et al., 2009). Less well-known is the application of DA in the real-time control or operation of various types of water resources systems (e.g., Bauser et al., 2010; Schwanenberg et al., 2011).

In the meantime, DA algorithms are becoming increasingly sophisticated, from simple ruled-based, direct insertion methods to advanced smoothing and sequential techniques, as well as the various variants of these techniques. These include, for example, the one-, two-, three- and four-dimensional variational algorithms (1-D-, 2-D-, 3-D, and 4-D-VAR, e.g., Seo et al., 2003, 2009; Valstar et al., 2004), extended or ensemble Kalman filtering (EKF or EnKF, e.g., Moradkhani et al., 2005b, Slater and Clark, 2006; Weerts and El Serafy, 2006; Shamir et al., 2010), particle filtering (e.g., Moradkhani et al., 2005a; Weerts and El Serafy, 2006; Matgen et al., 2010), H-infinity filters (Wang

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and Cai, 2008), hybrid EnKF or 4-D-VAR approaches (e.g., Zhang et al., 2009), and other Bayesian approaches (e.g., Reggiani and Weerts, 2008; Todini, 2008; Reggiani et al., 2009). While most DA applications have focused on updating hydrologic model states (e.g., soil moisture and snow water equivalent), recent research has also examined the benefits of estimating models states and model parameters simultaneously (e.g., Moradkhani et al., 2005a, b; Vrugt et al., 2005; Hendricks Franssen and Kinzelbach, 2008; Lu et al., 2010; Leisenring and Moradkhani, 2011; Nie et al., 2011), as well as the possibility of model structure identification and uncertainty estimation (e.g., Neuman, 2003; Bulygina and Gupta, 2010; Hsu et al., 2009; Parrish et al., 2012).

It is worth noting that many of the hydrologic DA studies reported in the literature focused on advancing the theoretical development of DA techniques using, for example, identical or fraternal twin synthetic experiments (e.g., Andreadis et al., 2007; Kumar et al., 2009; Crow and Ryu, 2009). This is especially the case when it comes to assimilating satellite data. The synthetic experiments are useful for diagnostic and design purposes such as assessing the impact of improper characterization of model and observation errors (e.g., Crow and Van Loon, 2006; Reichle et al., 2008) and evaluating the potential benefits of future satellite missions (e.g., Matgen et al., 2010). Nevertheless, despite the overwhelming research into hydrologic DA, only a few studies (e.g., Seo et al., 2003, 2009; Thirel et al., 2010a, b; Weerts et al., 2010; DeChant and Moradkhani, 2011a, b) formulated DA in an operational setting and attempted to evaluate the performance gain from DA in a forecast mode (e.g., as a result of better characterized initial conditions). The application of advanced DA techniques for improving hydrologic forecasts by operational agencies is even rarer, especially when it comes to assimilating new observations from multiple sources across a range of spatiotemporal scales. In operational practice, the correction of model inputs, states, initial conditions and parameters is often conducted in a rather empirical and subjective way (Seo et al., 2009). Generally speaking, hydrologic DA as an objective tool for reducing predictive uncertainty is not yet technically ready for operational hydrologic forecasting and water resources management. This is due in part to a lack of mechanisms to properly

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quantify the uncertainty in observations and forecast models in real-time forecasting situations and to conduct the merging of data and models in a way that is adequately efficient and transparent to operational forecasters.

Nevertheless, the need for implementing effective DA in the forecast process to
5 bridge the immense gap between the theory and operational practice is increasing. For example, Welles et al. (2007) reported that the hydrologic forecasting skill for some river basins at the US National Weather Service (NWS) River Forecast Centers has hardly improved over the past decade, with above flood-stage hydrologic forecasts beyond three days having very poor skill. This highlights the potential, as well as
10 the need, of assimilating new observations into the operational hydrologic forecasting process to improve the predictive skill and extend the forecast lead time. For many parts of the world, remotely-sensed observations (e.g., satellite images) are the only observations available and their optimal use in hydrologic forecasting via DA needs to be fully explored (National Research Council, 2007). In meteorological and atmo-
15 spheric sciences, steady improvements in numerical weather forecasting and climate prediction over the last couple of decades have been enabled to a large degree by the development of community-based models and DA systems (e.g., Reichle, 2008; Pappenberger et al., 2011). While satellite DA has not been adequately explored in operational hydrology, the improvement of performance in operational weather fore-
20 cast has been attributed (at least partially) to the incorporation of satellite data whose quality and spatiotemporal resolutions have been steadily improving in recent years (Rabier, 2005). The hydrologic community should learn from the experiences of the meteorological and atmospheric communities by accelerating the transition of hydro-
25 logic DA research into operations to better utilize new observations and by developing community-supported, open-source modelling systems (e.g., Werner et al., 2004; Mcenery et al., 2005) and DA tools (e.g., van Velzen and Verlaan, 2007; Kumar et al., 2008b; Weerts et al., 2010a).

The assimilation of various types of observations into operational hydrologic forecasting offers ample research opportunities and poses substantial challenges such as

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satellite retrieval algorithm development, bias correction, error estimation, downscal-
ing, model diagnosis and improvement, new DA algorithm development, efficient or
effective performance evaluation, computational efficiency enhancement, among oth-
ers. To address these challenges and identify potential opportunities in the context of
5 improving operational hydrologic forecasting and water resources management via DA, an international workshop was held in Delft, The Netherlands on 1–3 November 2010 (Weerts and Liu, 2011). The overall goal of the workshop was to develop and fos-
ter community-based efforts for collaborative research, development and synthesis of
10 techniques and tools for hydrologic DA, and the cost-effective transition of these techniques and tools from research to operations. The workshop was attended by a mix of senior scientists and graduate students from a range of entities including universities, government agencies, operational centers, and non-profit research institutions from 12
different countries representing 23 different organizations.

This paper reviews the status of DA applications in hydrology from several important
15 aspects and summarizes the discussion and findings from the workshop regarding the progresses, challenges, and opportunities in advancing DA applications in operational forecasting. It is noted that the current paper does not seek to perform a compre-
hensive assessment of the state of the hydrologic DA research; rather, it presents the knowledge, experience, and best judgments of the workshop participants in rele-
20 vant areas of applying DA to operational hydrologic forecasting and water resources management, and makes corresponding recommendations for advancing these applications (where possible or relevant). Since DA applications for both hydrologic models and LSMs are relevant for operational hydrologic forecasting or water resources man-
agement across various spatiotemporal scales, advances in both research areas will
25 be discussed (albeit currently conceptual rainfall-runoff models are more commonly used in operational hydrologic forecasting than physically-based LSMs).

The paper is organized as follows. Theoretical and mathematical aspects of hydro-
logic DA applications are reviewed in Sect. 2, followed by a discussion on the mod-
elling and quantification of model and data uncertainties in DA applications in Sect. 3.

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Section 4 discusses the challenges and new opportunities related to the objective utilization of new and existing sources of data (in-situ or remotely-sensed) for hydrologic DA applications. Section 5 is devoted to the discussion of using DA for the real-time control and operation of water resources systems, an area of research and development less well-known to the general hydrologic community. The development and potential benefits of open-source and community-based tools for hydrologic DA is presented in Sect. 6. A summary of the discussions is presented in Sect. 7.

2 Theoretical aspects

Broadly speaking, operational hydrologic forecasting presents three types of DA problems. The first is the state updating problem in which data such as stage, streamflow, rainfall, snow water equivalent, snow depth, potential or actual evapotranspiration, soil moisture and piezometric heads are assimilated into lumped or distributed hydrologic, hydraulic or land surface models to update the models' dynamic states. The second is the parameter estimation or optimization problem, referred to often as calibration, in which the data are used to estimate or optimize the model parameters that may be considered static or time-varying. The third, termed the error updating problem, refers to using DA to revise the predictions of an error model representing the difference between the hydrologic forecasts and corresponding observations. These three types of DA problems are not mutually exclusive since a forecasting system can utilize any combination (see e.g., Young, 2002; Moradkhani et al., 2005b). The focus here is largely on the first and third types, while referring the readers to the vast literature on calibration for the second type (e.g., Beven and Binley, 1992; Vrugt et al., 2003).

Below, we briefly review the theoretical basis of the existing DA techniques with the aim of identifying limitations, perceived or demonstrated, for application specifically in operational hydrologic forecasting. We then describe significant challenges from theoretical considerations in applying them in operational hydrologic forecasting.

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2.1 State updating

The aim of this form of DA is to render the model states (as translated through the model dynamics) consistent with the observations. The model parameters could be augmented to this in a form of joint estimation (e.g., Moradkhani et al., 2005b). The most direct form of assimilating data into a model in operational hydrologic forecasting is the manual correction of the internal states of the model by human forecasters based on their expert interpretation of the discrepancy between the recent model simulations and the observed data. While such techniques are widely practiced in operational forecasting, their effectiveness is scantily reported (Seo et al., 2009). It is reasonable to presume that the successful application of such manual techniques requires an experienced forecaster along with an interpretable and preferably simple lumped hydrologic model. The latter condition is considered necessary since it is probably impractical to manually apply hydrologically consistent corrections to a distributed hydrologic model or land surface model without simplifying rules. The formulation of such simplifying rules can be extended to provide an automated system of deterministic DA. Operational examples of such rule-based DA include the Grid2Grid rainfall runoff model operational in the UK flood forecasting centre (Cole et al., 2009) and the Probability Distributed Model (PDM, Moore, 2007) operational in the Environment Agency National Flood Forecasting System, which utilizes a flow partitioning to correct the upstream storage volumes in a grid-based distributed hydrologic model. Other schemes (e.g., Rungo et al., 1989) utilize similar concepts to assimilate data into hydraulic models.

A more common framework is to consider the state space model in Eqs. (1) and (2) (Evensen, 1994; Liu and Gupta, 2007),

$$\mathbf{x}_{k+1} = \mathbf{M}_{k+1}(\mathbf{x}_k, \boldsymbol{\theta}, \mathbf{u}_{k+1}) + \boldsymbol{\eta}_{k+1} \quad (1)$$

$$\mathbf{z}_{k+1} = \mathbf{H}_{k+1}(\mathbf{x}_{k+1}, \boldsymbol{\theta}) + \boldsymbol{\varepsilon}_{k+1} \quad (2)$$

where \mathbf{M}_{k+1} represents the forward model that propagates the system states \mathbf{x} from time t_k to t_{k+1} in response to the model input \mathbf{u}_{k+1} (with an error term $\boldsymbol{\zeta}_{k+1}$) and

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parameters θ ; \mathbf{H}_{k+1} is the observation function that relates model states and parameters to observations \mathbf{z}_{k+1} ; $\boldsymbol{\eta}_{k+1}$ denotes the model error with mean $\bar{\boldsymbol{\eta}}_{k+1}$ and covariance \mathbf{Q}_{k+1} ; and $\boldsymbol{\varepsilon}_{k+1}$ denotes the observation error with mean $\bar{\boldsymbol{\varepsilon}}_{k+1}$ and covariance \mathbf{R}_{k+1} . The predictive distribution of \mathbf{z}_{k+1} (or more generally prediction n time steps ahead \mathbf{z}_{k+n}) arises from the mapping of the stochastic noise terms through Eqs. (1) and (2). The operational usefulness of the forecast summarized by the predictive distribution is dependent upon two main factors. The first of these is the ability of the modeller to appropriately define the distributions of $\boldsymbol{\zeta}_{k+1}$, $\boldsymbol{\eta}_{k+1}$ and $\boldsymbol{\varepsilon}_{k+1}$ to characterize the various sources of uncertainty, including errors in the model input, measurement errors in the observations, conceptual discrepancies between observed and model states, and the inadequacy of the model in representing the dynamics of the system. The second of these is the computational approximation of the predictive distribution (see relevant discussions below).

For state updating, the state space model outlined above may be solved as a filtering or smoothing problem. For problems with non-linear \mathbf{M} and/or non-linear \mathbf{H} , the solution is not trivial. A number of computational techniques are available to provide approximate solutions. The commonly applied methodologies for solving the problem via filtering are non-linear extensions to the Kalman Filter (KF, Kalman, 1960). Three extensions to the KF are widely known, namely, the Extended Kalman filter (EKF, e.g., Georgakakos, 1986a, b; Kitanidis and Bras, 1980), Ensemble Kalman Filter (EnKF, Evensen, 1994) and Unscented Kalman Filter (UKF, Julier and Uhlmann, 1997). The key difference between the nonlinear Kalman filters lies in the methods of propagating the expected value and covariance of the state space through the non-linear operators \mathbf{M} and \mathbf{H} . The EKF linearises (sometimes unrealistically) these operators based on local derivatives, which are often difficult to compute reliably; hence, the EKF technique has fallen out of favour (Da Ros and Borga, 1997). The two remaining techniques propagate the state space using a sample. In EnKF, the state space is presumed to be multivariate Gaussian while the UKF presumes the state space is unimodal, symmetric and unbound. Despite the more relaxed assumptions of the UKF, it has received little

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attention in the hydrologic literature to date. The EnKF technique, however, has become the most frequently used DA technique in the hydrologic community, due largely to its easy implementation and its robustness in solving most DA problems encountered in hydrologic applications.

The size of the sample used in the EnKF or UKF may prove computationally burdensome in an operational environment. Another limitation of the EnKF is that its optimal performance is restricted to multi-Gaussian distributed states and parameters. In the operational weather forecasting community, the local ensemble transform Kalman filter (LETKF) was introduced to overcome the issue of prohibitively large dimensionality by solving the analysis independently in a local region around every model grid point using only local observations (e.g., Szunyogh et al., 2008; Ott et al., 2004). Similarly, Sun et al. (2009) applied grid-based localization and a Gaussian mixture model (GMM) clustering technique to improve the performance of EnKF for states and parameters which are not multi-Gaussian distributed. Zhou et al. (2011) illustrated how a normal score transformation for both states and parameters improved the performance of EnKF drastically for bimodal distributed parameter fields. It has yet to be investigated in more detail under which conditions, and for which types of problems, such transformations could significantly outperform the classical EnKF. Alternatively, more sophisticated transformations could also be explored. For all these extensions, $\boldsymbol{\varepsilon}_{t+1}$ and $\boldsymbol{\eta}_{t+1}$ are considered symmetric, unimodal, and unbounded zero-mean random variables which are independent (both in time and of each other). This means that great care should be taken in constructing \mathbf{M} and \mathbf{H} if there is belief that systematic biases or phase errors in the data or model exist (e.g., Crow and Van Loon, 2006; Dee, 2005). It is also noted that the common assumption that the distribution of the states is unbounded is rarely satisfied in real-world problems; hence some mathematical transformation is often necessary.

Another flexible (but potentially more computationally expensive) approach to solving the above filtering problem includes the sequential Monte Carlo (SMC) methods such as particle filtering (PF) (e.g., Arulampalam et al., 2002; Moradkhani et al., 2005a;

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imperfection of the model structure itself, due to the parameterization of physical processes or unresolved scale issues. Even with an assumption of having a perfect model structure, the estimates of model parameters could also be uncertain given the observational uncertainties that affect the model calibration. Therefore, the “optimality” of a DA scheme depends critically on the reliability of error estimates for the inputs and the model itself, as well as proper consideration of interdependencies and interaction of the uncertain model components and/or observations (e.g., Crow and Van Loon, 2006; Moradkhani et al., 2006; Hong et al., 2006). This is because the weight assigned to observations in a DA scheme is computed based on estimates of the relative error in the model and in the observations. The discussion now turns to critically examine different methods to estimate these errors.

3.1 Uncertainty in model inputs – the problem of precipitation

Precipitation is often viewed as the most uncertain model input (e.g., Huard and Mailhot, 2006; Kavetski et al., 2006a, b; Bárdossy and Das, 2008; Renard et al., 2010). This is because precipitation typically has short correlation length scales (in both space and time), and the reliability of basin-average (or gridded) precipitation estimates is constrained by the poor spatial representativeness of most station networks (e.g., Willems, 2002; Clark and Slater, 2006; Bárdossy and Das, 2008; Villarini and Krajewski, 2008; Volkmann et al., 2010). The uncertainty in precipitation is difficult to reduce, as alternative methods for estimating precipitation, such as radar, satellite, and numerical weather prediction models, have errors that are at least as large as those in many operational station networks (e.g., Hossain and Huffman, 2008; Volkmann et al., 2010.), and substantial errors in basin-average rainfall still exist in well-instrumented watersheds. Given the impact of errors in precipitation on the model response (e.g., Bárdossy and Das, 2008), obtaining more reliable estimates of precipitation uncertainty is critical to the success of DA applications.

In a DA context, uncertainty in precipitation is quantified either by stochastically perturbing the precipitation inputs or through conditional simulation methods. The

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stochastic perturbation approach is the most common (e.g., Steiner, 1996; Crow and Van Loon, 2006; Pauwels and De Lannoy, 2006; Weerts and El Serafy, 2006; Clark et al., 2008a; Komma et al., 2008; Turner et al., 2008; Pan and Wood, 2009). In this approach the size of the precipitation perturbations is typically based only on order-of-magnitude considerations. For example, Reichle et al. (2002) assumed the standard deviation of precipitation errors is equal to 50 % of the precipitation total at each model time step. However, uncertainty in precipitation estimates tends to vary both spatially and temporally (e.g., Tian and Peters-Lidard, 2010; Sorooshian et al., 2011), and therefore estimates of precipitation uncertainty from such order-of-magnitude based approaches may be statistically unreliable. Conditional simulation methods have the potential to provide more reliable uncertainty estimates (e.g., Clark and Slater, 2006; Göttinger and Bárdossy, 2008). For example, the regression-based ensemble spatial interpolation methods used by Clark and Slater (2006) provide an error estimate (i.e., the spread of the precipitation ensemble) that is connected to the error in the regression equations. This approach – and others, such as geostatistically based conditional simulation techniques (Göttinger and Bárdossy, 2008) – provides statistically reliable precipitation ensembles by explicitly linking the error in precipitation estimates to the adequacy of the station network. While conditional simulation methods can be data-intensive to parameterize and computationally expensive to run (McMillan et al., 2011), their potential to provide statistically reliable uncertainty estimates suggests that the implementation costs may be worthwhile.

3.2 Uncertainty in the model itself

Here we define a model as a simplified representation of reality, in which the structure of the model includes the selection of model equations and the time stepping scheme used to integrate the model equations forward in time (e.g., Clark and Kavetski, 2010). Model structure uncertainty is associated with the assumptions that act on the development of the model conceptualization and mathematical structure. An unfortunate truth in model development is that no matter how many resources are invested

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3.3.4 Constructing reliable multi-model ensembles

The multi-model ensemble strategy is a means to address model structure uncertainty by synthesizing outcomes from multiple models representing different parameterizations of underlying physical processes and has been demonstrated to offer better predictability (Hagedorn et al., 2005). The success of a multi-model strategy requires constructing a reliable model ensemble such that the differences among the individual models represent the uncertainty in simulating natural processes. This can be accomplished by using multi-physics model toolboxes such as the Framework for Understanding Structural Errors (FUSE) approach, which provides an effective means to construct multiple unique models by combining the different options for the model architecture and the flux equations (Clark et al., 2008b). For example, to develop an empirically-based surface water model, multiple options are available for the choice of state variables in the unsaturated and saturated zones, as well as the choice of flux equations describing surface runoff, interflow, vertical drainage from the unsaturated zone, base flow, and evaporation (Clark et al., 2008b). Niu et al. (2011) recently reported a similar multi-parameterization approach within the Noah land surface model framework (Noah-MP).

One typical challenge in a multi-model ensemble approach is concerned with developing an effective strategy to optimally combine the individual models to achieve enhanced predictive skill and uncertainty estimation. This can be addressed by simple approaches such as equal weighting (Palmer et al., 2000) or optimal weighting (Regonda et al., 2006). Statistics-based approaches such as linear regression (Krishnamurti et al., 1999) and canonical variate analysis (Mason and Mimmack, 2002) can also be employed to improve the predictive skill of multi-model ensembles. Recent investigations into combining the strengths of DA and multi-model ensembles provide another promising opportunity for simultaneously addressing model and data uncertainties (e.g., Parrish et al., 2012). Further developments along these lines should help to enhance the ability to quantify and reduce uncertainties in hydrologic DA applications.

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4 New measurements

Hydrologic forecasting can potentially benefit from assimilating relevant observations, especially those not used in developing the models. This section discusses the application of several types of newly emerging hydrologic observations and the challenges and opportunities therein.

4.1 Remote sensing data

Recent advances in remote sensing technologies have enabled a large suite of terrestrial observations from satellites and various remote sensing platforms. These observations can be used to derive information on rainfall, evapotranspiration, snow, soil moisture, topography, vegetation dynamics, flooding, and the total water storage, all of which play an important role in the hydrologic cycle. While in-situ measurements contain little information on the spatial variability of these important quantities, remote sensing data are able to provide continuous spatial distributions of these variables (albeit sometimes at a very coarse resolution) that are needed to perform distributed hydrologic modelling and DA.

4.1.1 Hydrologic observations from remote sensing

Remotely-sensed snow observations are among the most investigated measurements in the hydrologic research community. The Rutgers University Global Snow Lab (RUCL) has been generating snow cover measurements at varying temporal and spatial resolutions, from 1966 to present using the snow cover dataset of the National Oceanic and Atmospheric Administration (NOAA). Since early 2000, the Moderate Resolution Imaging Spectroradiometer (MODIS) instrument of the National Aeronautics and Space Administration (NASA) has been providing daily snow maps at a variety of temporal and spatial resolutions (Hall et al., 2002). Passive microwave radiometry-based estimates of SWE and snow depth from several satellites have been generated

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in the past 30 yr. The Advanced Microwave Scanning Radiometer (AMSR-E) sensor, launched in 2002 on board the Aqua satellite, is the most recent addition to the passive microwave suite of instruments (Kelly, 2009). A blended snow product, known as the AFWA NASA snow algorithm (ANSA), has also been developed by combining the retrievals from both MODIS and AMSR-E retrievals (Foster et al., 2011). DA of remote sensing snow products has been explored in numerous studies (e.g., Rodell and Houser, 2004; Parajka and Blöschl, 2008; Hall et al., 2010; Kuchment et al., 2010).

Remote sensing products of soil moisture are also become increasingly available in recent years. Global soil moisture products are (or will be) available from the current European Space Agency (ESA) Soil Moisture and Ocean Salinity mission (SMOS, Kerr and Levine, 2008) and the upcoming NASA Soil Moisture Active passive mission (SMAP, Entekhabi et al., 2010). Surface soil moisture retrievals based on these sensors have been generated (Jeu, 2003; Owe et al., 2008; Li et al., 2010) and demonstrated in various hydrologic DA applications (e.g., Pauwels et al., 2001; Liu et al., 2011b). Other space-borne microwave window-channel radiometers with significant soil moisture sensitivity include the Scanning Multichannel Microwave Radiometer (SMMR, 1978–1987), the AMSR-E, the Tropical Rainfall Measuring Mission (TRMM) Microwave Imager (TMI, launched in 1997), and the Windsat radiometer (launched in 2003). The NASA/German Gravity Recovery and Climate Experiment (GRACE) satellite (launched in 2002) can map Earth's gravity field with enough accuracy to discern month to month changes in the distribution of the total terrestrial water storage on Earth (Tapley et al., 2004). Despite its coarse spatial ($>150\,000\text{ km}^2$ at mid-latitudes) and temporal (\sim monthly) resolutions, GRACE has been used to effectively measure changes in groundwater, deep soil moisture, as well as snowpack (e.g., Su et al., 2010; Forman et al., 2012).

Hydraulic information, such as river water levels and bathymetry, can also be observed from space (e.g., with radar altimetry). The international Surface Water Ocean Topography mission (SWOT) will be launched in 2019 to produce high-resolution observations of water elevations of the earth surface (Alsdorf et al., 2007). Information on water elevation as well as its spatial and temporal variability is critical for

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short-term hydrologic forecasting, especially during flooding situations. The potential of assimilating space-born water level information for improved discharge and water depth estimation has been explored in a few studies (e.g., Andreadis et al., 2007; Neal et al., 2009; Matgen et al., 2010).

In addition, satellite and airborne remote sensing data have also been used to develop model inputs, such as precipitation (e.g., Tian and Peters-Lidard, 2010; Sorooshian et al., 2011), land classification maps, digital elevation models, land surface property maps and spatial model parameterizations, and to evaluate the outputs of hydrologic models – some of which are used in operational systems (see van Dijk and Renzullo (2011) for a review). In summary, there can be little doubt that remote sensing provides information relevant to hydrologic forecasting.

Operationally, satellite observations have been routinely assimilated into numerical weather prediction models since the early 1970s (Tracton and McPherson, 1977). The first operational remote sensing application in hydrology occurred in the 1980s (Ramamoorthi, 1983). However, despite the recent increasing availability of remote sensing data, their application in operational hydrologic forecasting is still very limited.

4.1.2 Challenges and opportunities

Many experimental studies exploring the use of satellite data have been reported in recent literature. However, most such studies either merely referred to the potential or utility of satellite DA, or were focused on the development of approaches to assimilate hydrologic observations into LSMs used in numerical weather forecasting models. A major difference between LSMs and “conventional” hydrologic models is that the former include a full description of the radiation and coupled surface water and energy balance at diurnal time scales and – when coupled to an atmospheric model – are able to consider the effect of atmospheric transmissivity on sensor observations. These features make it easier to assimilate satellite land surface temperature and microwave brightness temperature observations. A conventional hydrologic model normally requires considerable modifications or extensions to be amenable for assimilating “raw”

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satellite observations. This can include, for example, the coupling of a radiative transfer and energy balance model to assimilate remotely-sensed thermal and microwave emissions. One of the first studies attempting assimilation of satellite observations into such a “conventional” hydrologic model was Ottlé and Vidal-Madjar (1994), who used
5 Land Surface Temperature (LST) and Normalized Difference Vegetation Index (NDVI) products derived from Advanced Very High Resolution Radiometer (AVHRR) observations to update a rainfall-runoff model. Houser et al. (1998) was one of the first to use brightness temperature to improve soil moisture estimation in a distributed hydro-
10 logic model. More straightforward for hydrologic models is the assimilation of satellite derived products. Published examples include the assimilation of satellite-derived soil moisture, evapotranspiration, vegetation properties and GRACE-derived terrestrial water storage (see van Dijk and Renzullo, 2011 for references).

A big challenge in assimilating remotely-sensed hydrologic data is concerned with the “mapping” between observed and modelled variables. The spatial and temporal
15 characteristics of these variables are rarely identical, and therefore aggregation or disaggregation of either (or both) is required. A specific problem arises when the remote sensing resolution is much coarser than that of the model, a particular issue for the assimilation of passive microwave and GRACE observations. As another example, satellite observations of surface radiances may not help estimate hydrologic processes
20 that occur within small areas below satellite resolution (such as runoff from saturated zones). While approaches can and have been developed to deal with such issues (e.g., Zaitchik et al., 2008) they tend to be observation specific and hence not generically available. Conceptual “mapping” can also be a problem. For example, most remote sensing soil moisture products reflect the water status of a very shallow top
25 layer of the soil, whereas hydrologic models typically simulate the water storage of a deeper soil column. Li et al. (2012) introduced a mass conservation component into the EnKF-based assimilation of AMSR-E soil moisture retrievals, resulting in improved estimates of moisture contents in deep soil layers. Further developments along similar (or other innovative) lines would be helpful.

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Another challenge is the specification of uncertainty in remote sensing observations, which is a prerequisite for formal DA. Because of a general lack of accurate information on the magnitude and structure of these errors, usually simplistic assumptions are made. This is a pragmatic solution but can lead to large errors. Such errors are more
5 likely if retrieved variables (e.g., soil moisture) are used rather than primary observations (e.g., brightness temperature). This pleads for the assimilation of primary data, which however shifts the potential for inappropriate error specification to the biophysical and observation models. A promising intermediary approach might be to produce spatially and temporally explicit error estimates, either as part of the remote sensing product retrieval process (Pathe et al., 2009) or through statistical comparison to alternative
10 estimates where errors are independent (Dorigo et al., 2010; Tian and Peters-Lidard, 2010; Liu et al., 2011b).

Finally, the engineering requirements and infrastructure required for operational satellite DA are currently probably prohibitive for many applications. For example, the
15 observation matrix might become very large for remote sensing data, making inversion of the observation matrix a challenge. Also, parameter optimization and state updating can introduce considerable computational overheads, even more so when large satellite data volumes are involved and iterative solution is required. In these cases, the LETKF method (Ott et al., 2004) used in the meteorological community
20 may represent a viable candidate for dimension reduction to facilitate implementation in operational hydrologic forecasting. The current generation of computing infrastructure in most operational weather forecast centres can support intensive calculations required by satellite DA. Most operational hydrologic forecast centres, however, lack the required computing support to implement such intensive calculations. Moreover,
25 there is currently no computer software to support spatiotemporal grid-based DA to the extent that it only requires “minor” software engineering investment to achieve the coupling of models, data, DA techniques and exploitation of high performance computing solutions in the operational forecasting process. Several potential components of a future solution have been or are being developed, through such initiatives as the

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Traditionally, the common technique for supervisory control of water resources systems is the definition of offline, reactive operating rules that optimizes the controls to minimize cost of operations. An alternative to the offline technique is the application of online optimization. The main representative of this approach is Model Predictive Control (MPC), also referred to as Receding Horizon Control (RHC). MPC makes use of a process model of the dynamic system for predicting future trajectories of the state vector over a finite time horizon in order to determine the optimal set of controlled variables by minimizing a cost function. Like hydrologic forecasting, MPC can benefit from proper DA techniques (e.g., Kalman filtering) for improving estimates of the current system states that are the basis for enhanced accuracy in forecasting future system states. A common DA technique jointly used with MPC is the Moving Horizon Estimation (MHE) approach that looks back into the past for updating current system states by modifying historical inputs, states or model parameters. The optimization problem of nonlinear MPC and MHE schemes can be solved by nonlinear programming algorithms such as Sequential Quadratic Programming (SQP) (e.g., Wächter and Biegler, 2006).

A DA-based MPC framework typically adopts either a “simultaneous” or “sequential” approach. In a simultaneous approach, optimization and simulation (with state updating) are performed simultaneously. In a sequential approach, each iteration of the optimization consists of a sequential simulation of the system with an appropriate numerical integration and optimization (or state updating). In this case, the optimization problem has a reduced variable space compared to the simultaneous approach and leads to valid state trajectories in each iteration step of the optimization. Using one or the other approach has certain advantages which are discussed in Diehl et al. (2009). To make connections to common hydrologic DA applications, the simultaneous approach to control optimization and state updating in MPC is equivalent to the dual state-parameter estimation methodology presented in Moradkhani et al. (2005b), while the sequential approach of MPC is analogous to the SODA methodology introduced in Vrugt et al. (2005).

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5.2 DA applications in MPC

Although the application of MPC to water resources systems has been subject of research for at least 15 yr, stakeholders have been conservative in applying the technique for full automation of their systems. Ackermann et al. (2000) presented one of the early examples on the control of a run-of-river hydropower plant. In this approach, a linearised one-dimensional Saint-Venant model in combination with quadratic objective functions is used for balancing the damping of discharge peaks against the deviation of a water level in the head barrage of the German river Moselle. The approach is reported to be running successfully for more than 10 yr. Other applications of MPC to run-of-river hydropower plant were investigated by Glanzmann et al. (2005), and more recently by Setz et al. (2008) and Sahin (2009). Most applications represent the river section by simple pool models, where the need for sophisticated DA methods is relatively low.

Low-land water systems with highly interconnected and highly regulated river and canal networks have been the focus of several studies in recent years and DA-based MPC seems to be a promising candidate for coordinated control of these systems. Van Overloop et al. (2008) present the application of MPC to the drainage of Dutch polder systems using MHE for state updating. Several DA techniques were applied to the control of a river weir in the Dutch delta of the rivers Rhine and Meuse in Schwanenberg et al. (2011); due to the small extension of the modelled river system, simple Auto-regressive (AR) error correction models in combination with MHE were found to outperform state updating techniques. Breckpot et al. (2010) and Blanco et al. (2010) applied MPC in combination with MHE to a regional water system in Belgium. Bauser et al. (2010) applied EnKF to update the model states in the real-time control of a groundwater well field, using a groundwater flow-mass transport model and a cost function that was based on fuzzy decision rules and minimized with genetic algorithms. Furthermore, MPC has been used in the short-term decision-support and supervisory control of reservoir systems, as well as the automation of irrigation systems (e.g., van Overloop et al., 2008; Negenborn et al., 2009; Kearney et al., 2011).

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The reason for this unbalance between generic tools for calibration and state updating is probably that state updating requires a high level of interaction with the numerical model. Model calibration can often be performed via relatively simple alterations of a model parameter file. One potential means of dealing with the high level interaction between model and DA algorithms is via the use of the open Model Interface (openMI, Moore and Tindall, 2005; Gregersen et al., 2007). The openMI allows models to exchange data with each other on a time step by time step basis as they run, facilitating the modelling of process interactions. This bears similarity with the exchange of model states between model and DA algorithms, although the focus of openMI is normally not to exchange the complete state vectors but geared towards exchange of model states or fluxes at specific locations.

Another challenge in developing generic DA tools lies in the definition of model noise, which often depends on the model and requires a great deal of model specific knowledge and interactions that are difficult to generalize. However, one could argue that this generalization is not necessary, since the model noise description is part of the model itself so that the responsibility of providing the tools and methods for error estimation lies with the model and not with the interfaces that deal with connecting model-algorithm-observations.

Finally, although parallelism can be easily implemented to deal with the heavy model computation needed by the DA algorithm, the optimal parallelization of the DA update algorithm requires a different distribution of the data over the processors (distributing rows of a matrix) than the optimal parallelization of model computations (distributing columns of a matrix). Optimal results are therefore to be expected with a hybrid form of parallelization of the data (Roest and Vollebregt, 2002). Parallel computing is used in DA systems like DART, PDAF, and OpenDA. DART allows the parallelization of the update algorithm which is useful when a large amount of observations needs to be assimilated. The model steps can be performed in parallel as well in DART but the data interaction between the model and filter is still sequential by files. PDAF is implemented as an extension to the model code; the update algorithm is therefore parallelized using

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the same approach as the model without any exchange by files. OpenDA automatically parallelizes the model computations and allows parallel models to be used without file interaction; implementation of the parallelization of the update algorithms is planned for the near future.

7 Summary and discussions

The need for transitioning hydrologic DA research into effective operations has become increasingly recognized in the wake of frequent occurrences of extreme events in recent years and increasing availability of new observations. This paper reviews the current status of DA applications in hydrologic research, and discusses the existing or potential challenges and emerging opportunities in transitioning hydrologic DA research into effective and efficient operational forecasting tools. The discussion focuses on several critical aspects related to hydrologic DA and is briefly summarized below.

Several theoretic or mathematical challenges need to be addressed before hydrologic DA can fully benefit operational forecasting (Sect. 2). Issues include the high non-linearity in hydrologic processes, the high dimensionality of the state or parameter vectors of hydrologic models, the skewness and heteroscedasticity in the probabilistic distribution of hydrologic variables, the need for impractically large samples in ensemble approaches, and the limited observations of extreme events. Emerging opportunities include localized and transformation-based ensemble approaches and decomposing of the hydrologic forecast system into smaller subcomponents for separate DA solutions. It is recommended that bias correction precede or accompany DA applications.

The success of a DA application depends critically on the characterization of uncertainties (Sect. 3). Uncertainty in precipitation can be quantified by stochastically perturbing precipitation inputs or through conditional simulation methods. Determining model uncertainty can be complicated by interactions among uncertainty sources, poorly constrained inference problems, and difficulty in constructing a reliable

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multi-model ensemble. These issues can be addressed by detangling uncertainty sources, intelligent use of available data for inverse modelling, using integrated multi-model and multi-parameterization frameworks, and combining the strength of DA and multi-model ensembles.

5 Hydrologic forecasting can potentially benefit from integrating, via DA, newly emerging observations such as remote sensing data (Sect. 4). Some of the difficulties (or emerging opportunities) in effectively assimilating these data include, for example, developing proper modifications of an operational hydrologic model to assimilate “raw” satellite data, constructing proper “mapping” relationships between remotely observed and modelled variables, providing appropriate specification of uncertainty in remote
10 sensing data, and building an efficient computing infrastructure for retrieving remote sensing data to support satellite DA in operational forecasting.

Although less well known in the hydrologic community, DA has played an important role in real-time control of water resources systems and hydraulic structures (Sect. 5).
15 DA for real-time control is often conducted within a parameter optimization framework and uses optimization-based techniques (rather than sophisticated DA approaches such as EnKF) for state updating. It is recommended that the hydrologic and control communities work together to learn from each other’s experiences to more efficiently address issues encountered in DA applications.

20 Besides the computational and technical aspects already discussed, other operational aspects like transparency and clearness of the outcomes of DA applications are at least as important for the implementation of automated DA methods in operational practice. For operational forecasters who are used to manual interactions with the forecast system, automated DA of the black-box type may be too adventurous a step to take
25 in the short run. Hence, efforts are needed to speed up the operational implementation of automated DA, by enabling the operational control (with manual interaction) over noise models and observations to be used in DA, and developing DA-guided systems, where the DA results will be presented next to the current forecast to guide operational forecasters.

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It is important to note that comprehensive and robust verification of DA results is necessary to demonstrate the value of DA for operational forecasting and to build trust in DA among operational forecasters. One important goal of DA in operational forecasting is to provide an improved analysis of the model initial conditions to produce improved
5 hydrologic forecasts. However, the link between the accurate characterization of the initial conditions and the sensitivity of forecast skill at different lead times to this characterization is still uncertain, largely due to lack of proper verification of the potential gain from DA in a forecast context. Some have also argued that statistically based post-processing of hydrologic forecasts may outperform DA, since the latter aims at
10 improving initial conditions that may not have a sufficiently long memory to improve forecast skill at longer lead times. All of these point to the need for robust forecast verification (e.g., Demargne et al., 2010) that will identify and quantify the sensitivity of forecast skill to accuracy of initial conditions and hence help quantify the value of DA for operational hydrologic forecasting.

15 The various issues described above calls for the need of a community-based approach to hydrologic DA, which aims at providing a set of generic modelling, DA, and verification tools to serve diverse needs of the community and to facilitate effective and efficient advances through community contribution and feedback (Sect. 6). This also opens a promising pathway for the cost-effective transition of hydrologic DA research
20 into operational forecasting, while at the same time facilitating the communication of new hurdles encountered in operational DA back to the research community. In summary, it is recommended that cost-effective transition of hydrologic DA from research to operations should be helped by developing community-based, generic modelling and DA tools, and through fostering collaborative efforts among modellers, DA researchers,
25 and operational forecasters.

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