

Available online at www.sciencedirect.com



Advances in Water Resources

Advances in Water Resources 31 (2008) 1411-1418

www.elsevier.com/locate/advwatres

Data assimilation methods in the Earth sciences

Rolf H. Reichle*

Goddard Earth Sciences and Technology Center, University of Maryland, Baltimore County, Baltimore, MD, USA Global Modeling and Assimilation Office, NASA Goddard Space Flight Center, Code 610.1, Greenbelt, MD 20771, USA

> Received 25 June 2007; received in revised form 21 November 2007; accepted 1 January 2008 Available online 11 January 2008

Abstract

Although remote sensing data are often plentiful, they do not usually satisfy the users' needs directly. Data assimilation is required to extract information about geophysical fields of interest from the remote sensing observations and to make the data more accessible to users. Remote sensing may provide, for example, measurements of surface soil moisture, snow water equivalent, snow cover, or land surface (skin) temperature. Data assimilation can then be used to estimate variables that are not directly observed from space but are needed for applications, for instance root zone soil moisture or land surface fluxes. The paper provides a brief introduction to modern data assimilation methods in the Earth sciences, their applications, and pertinent research questions. Our general overview is readily accessible to hydrologic remote sensing scientists. Within the general context of Earth science data assimilation, we point to examples of the assimilation of remotely sensed observations in land surface hydrology.

© 2008 Elsevier Ltd. All rights reserved.

Keywords: Data assimilation; Remote sensing; Land surface hydrology; Variational methods; Kalman filter

1. Introduction

Hydrologic remote sensing can provide important information about land surface conditions, including surface soil moisture, snow water equivalent, snow cover, and land surface temperature. While hydrologic remote sensing data are not usually sufficient for many applications (such as weather forecast initialization) they can contribute valuable information when used in data assimilation systems. Such systems can also be helpful for the design of new hydrologic remote sensing missions [37] and for the validation of the hydrologic remote sensing observations themselves [8]. Experts in hydrologic remote sensing should thus benefit from a basic understanding of data assimilation theory and applications [51].

Virtually all methods that are currently used for the assimilation of hydrologic remote sensing observations

E-mail address: rolf.reichle@nasa.gov

0309-1708/\$ - see front matter © 2008 Elsevier Ltd. All rights reserved. doi:10.1016/j.advwatres.2008.01.001

have been inspired by and adapted from atmospheric or oceanic data assimilation systems, systems that have evolved over decades, along with a vast literature and a plethora of often confusing jargon. Experts in hydrologic remote sensing who want to use their observations in data assimilation systems may find the assimilation literature and jargon overwhelming. In this paper, we give an introduction to the general concepts of data assimilation in the Earth sciences and, within this general context, point to examples of the assimilation of remote sensing observations in land surface hydrology. Owing to the vast breadth and depth of the topic, we do not provide a formal review or mathematical treatise. Instead, we introduce the reader to data assimilation by describing the central ideas and challenges. The paper is biased towards atmospheric data assimilation systems, which are perhaps the most advanced in their use of remote sensing observations and serve as templates for assimilation efforts in other disciplines. A number of books, survey articles, and lecture notes are recommended for further study [3,4,6,9,17,23, 25,28-30,46,52].

Address: Global Modeling and Assimilation Office, NASA Goddard Space Flight Center, Code 610.1, Greenbelt, MD 20771, USA. Tel.: +1 301 614 5693; fax: +1 301 614 6297.

1.1. Why data assimilation?

Data assimilation methods are designed to merge measurements of any type, including remote sensing observations, with estimates from geophysical models. Here are five reasons why this is a good idea.

1.1.1. Coverage

When compared to the number of in situ measurements of the Earth system, satellite remote sensing observations are truly abundant. Their spatial and temporal coverage, however, is still not sufficient for many applications. Numerical weather forecasts, for example, require initialization of global or regional atmospheric models at 6-h intervals for all prognostic variables in the entire threedimensional domain. Such coverage is not possible with current and future satellite sensors. Data assimilation methods are needed to interpolate and extrapolate the remote sensing data.

1.1.2. Observability

Remote sensing instruments typically observe electromagnetic properties of the Earth system. This implies that most satellite observations are limited to the parts of the Earth system that can be penetrated by electromagnetic radiation at microwave, infrared, or visible frequencies. For example, the temperature, moisture, or salinity of the land or ocean below a thin surface layer remains invisible to typical satellite sensors. Yet these deeper mass and heat reservoirs provide longer-lasting memory in the Earth system and must be accurately initialized in seasonal climate forecasts. Data assimilation systems can spread information from remote sensing observations to all model variables that are in some way connected to the observations.

1.1.3. Resolution

The temporal or spatial resolution of remote sensing data is often too coarse or too fine for a given application. Snow cover estimates from the Moderate Resolution Imaging Spectroradiometer (MODIS), for example, are available at 500 m spatial resolution, much finer than the resolution of current global weather and climate models. Conversely, soil moisture retrievals from the Advanced Microwave Scanning Radiometer for the Earth Observing System (AMSR-E) are produced at a resolution of around 50 km, much coarser than the resolution of regional weather models for which soil moisture initial conditions may be required. By merging the satellite data with models that resolve the scale of interest, data assimilation methods are capable of aggregating or downscaling the remote sensing data.

1.1.4. Data volume and redundancy

Some types of remote sensing data are plentiful to the point of overwhelming processing capabilities. Typically, data assimilation systems for numerical weather prediction include sophisticated thinning algorithms for satellite observations, with the consequence that only a small fraction of the available satellite data is actually used in the preparation of a weather forecast. Moreover, there is a great deal of redundancy in satellite observations from different platforms. Polar orbiting satellites, for instance, cross over locations that are simultaneously observed by geostationary platforms carrying similar sensors. Retrievals of land surface temperature may thus be available at the same time and location from two different instruments, but they do not necessarily agree due to measurement errors and errors in the retrieval algorithms. Data assimilation systems can organize and merge potentially redundant or conflicting satellite data and conventional observations into a single best estimate.

1.1.5. Additional information from models

Geophysical and biogeochemical models ranging from global atmosphere–ocean models to local air quality or hydrology models are built on the basic principles of mass, momentum, and energy conservation, well-established chemical equations, or radiative transfer properties. By contrast, remote sensing data alone are not so constrained. In an assimilation system, the physical constraints imposed by models offer additional valuable information. Moreover, models are often forced with boundary conditions that are based on observations (for example, precipitation inputs for land surface models). Such boundary conditions may offer indirect and independent observational information about the remotely sensed fields (for example, soil moisture) – information that can be captured through data assimilation.

1.2. What is data assimilation?

The basic tenet of data assimilation is to combine the complementary information from measurements and models of the Earth system into an optimal estimate of the geophysical fields of interest. In doing so, data assimilation systems interpolate and extrapolate the remote sensing observations and provide complete estimates at the scales required by the application – both in time and in the spatial dimensions. Data assimilation systems thereby organize the useful and redundant observational information into physically consistent estimates of the variables of relevance to data users.

The *optimal* combination of the measurements with the model information rests on the consideration of the respective uncertainties (or error bars) that come with the observations and the model estimates. Whenever and wherever highly accurate remote sensing data are available, the assimilation estimates will be close to these observations. At times and locations that are not observed by any instrument, the assimilation estimates will draw close to the model solution, but will nonetheless be subject to the influence of satellite data in spatial or temporal proximity of the location of interest.

Applications of data assimilation include the study of geophysical and biogeochemical processes, detection of

changes and trends in the Earth system, model improvement, observing system design, and forecast initialization. This last application in particular has driven the development of data assimilation theory and practice. Everyday weather forecasts are simply unthinkable without advanced data assimilation methods.

2. Methods

All data assimilation methods share the basic tenet of merging models and observations, yet the sophistication of the merging algorithm varies widely. Important differences also remain between the specific methods that are most suitable for a given application. Since atmospheric and oceanic dynamics are chaotic (that is, small errors in the initial condition can lead to large differences at later times in the model integration), data assimilation in these areas is very much concerned with the estimation of initial conditions. By contrast, land surface dynamics are damped, and land surface assimilation is all about estimating errors in uncertain meteorological forcing (boundary) conditions and model parameterizations. Clearly, "one size does not fit all" in data assimilation.

The theory of data assimilation in the Earth sciences rests on the mathematical framework of estimation theory [1,7,20,47]. In the Earth sciences, data assimilation involves nonlinear, highly complex, and exceedingly large systems with complicated error structures that defy the straightforward application of classical optimization methods. While general theories exist for nonlinear data assimilation with non-Gaussian error probability distributions, most practical data assimilation methods rely on linear theory and assume Gaussian error distributions, whether or not these assumptions may be true in the application at hand. A judicious selection of the algorithm and a fair number of approximations, ideally based on physical insights, are thus unavoidable [32].

In the following, we restrict our discussion to advanced data assimilation methods that are based on some measure of model and observation error characteristics. Occasionally, simplistic methods such as replacing the model estimate with the observation (*direct insertion*) may be useful, for example for the assimilation of snow cover observations [43].

2.1. A simple data assimilation system

The basic concept of data assimilation is easily understood by considering a scalar model variable *m* with uncertainty (or error variance) σ_m^2 , and a corresponding scalar observation *o* with uncertainty σ_o^2 . The model estimate *m* represents *prior* or *background* information and may, for example, come from an earlier model forecast that is valid at the time of the newly arrived observation *o*. The goal is to find the least-squares estimate \hat{x} of the true *state x* based on the available information. To this end, an *objective function J* (also known as *cost function, penalty function*, or *mis*- fit) is defined to quantify the misfit between the true state x and the model estimate and the observation, respectively. In our simple case, the objective function J is

$$I = \frac{(x-m)^2}{\sigma_m^2} + \frac{(x-o)^2}{\sigma_o^2}.$$
 (1)

Minimization of J with respect to x (by solving dJ/dx = 0) yields

$$\hat{x} = (\sigma_m^2 + \sigma_o^2)^{-1} (\sigma_o^2 m + \sigma_m^2 o),$$

which is typically rewritten as

$$\hat{x} = (1 - K)m + Ko$$
, where $K = \sigma_m^2 / (\sigma_m^2 + \sigma_o^2)$. (2)

This *best estimate* (or *analysis*) \hat{x} is a weighted sum of the model background *m* and the observation *o*. The weights are determined by the relative uncertainties of the model and the observation and are expressed in the (*Kalman*) gain *K* (note that $0 \le K \le 1$). If the measurement error variance σ_o^2 is small compared to the model uncertainty σ_m^2 , the gain will be large, and the resulting estimate will draw closely to the observation, and vice versa. Equal model and measurement error variances $(\sigma_m^2 = \sigma_o^2)$ produce equal weights (*K* = 0.5), reflecting our equal trust in the model and the observation.

Rewriting (2) as

$$\hat{x} - m = K(o - m) \tag{2a}$$

shows that the assimilation *increment* (difference between the assimilation estimate \hat{x} and the model estimate *m*) is proportional to the *innovation* or *background departure* (difference between the observation *o* and the model estimate *m*). The Kalman gain serves as the constant of proportionality. Eq. (2a) is sometimes called the *update* equation, because the prior model estimate *m* is updated with information from the observation *o*. If the errors in the model forecast and the observation are uncorrelated, the error variance of the assimilation estimate is

$$\sigma_{\hat{x}}^2 = (1 - K)\sigma_m^2 = K\sigma_o^2 \tag{3}$$

and is smaller than the error variances of either the model estimate or the observation alone (recall that $0 \le K \le 1$), reflecting the increased knowledge about the true state x after data assimilation.

2.2. Variational data assimilation

In a realistic application, the first right-hand-side term of (1) consists of a large sum of model states, including for example pressure, temperature, humidity and winds at all grid points in a global three-dimensional domain, arranged into a long state vector with possibly 10^8 components. The error variance σ_m^2 then becomes the error covariance matrix of these model states. Similarly, the second right-hand-side term of (1) becomes a large sum over the individual conventional and satellite observations – typically upward of 10^6 observations per assimilation step in a global weather prediction application – weighted by the

inverse measurement error covariance. Because of the immense size of the vectors and matrices and because of nonlinearities, analytic solutions such as (2) are impossible. Instead, *variational* data assimilation algorithms employ advanced numerical methods to minimize J directly.

The two terms of the simple objective function (1) are representative of the main ingredients of most current, large-scale atmospheric data assimilation systems. If both terms correspond to a single instant in time, the resulting static data assimilation methods include common techniques such as *Optimal Interpolation*, *Physical-Space Statistical Analysis System (PSAS)*, *1DVAR*, and *3DVAR* (where 1D and 3D refer to one or three spatial dimensions, respectively). Fig. 1a shows a schematic of 3DVAR, which is still widely used in operational weather forecasting centers worldwide. An example of 1DVAR is the satellite data retrieval problem. A satellite sounding of radiances, for instance, may be assimilated into a vertical column of the atmospheric model to retrieve physical temperatures along the column.

If the objective function J contains measurements at several different times within an *assimilation interval*, and if the minimum of J is sought for this interval (by varying the model initial condition), the assimilation method is known as 4DVAR (where 4D refers to three spatial dimensions



Fig. 1. Schematic of continually operating data assimilation systems based on (a) filtering (for example 3DVAR, Kalman filter) and (b) smoothing (for example 4DVAR, representers).

plus the time dimension). 4DVAR thus includes dynamic features such as the propagation of the model to the exact time of the observation, and the evolution of the back-ground error covariance within the assimilation interval (Fig. 1b). In 4DVAR, the error covariance evolution is sometimes referred to as *implicit* because the assimilation estimates can be obtained without ever explicitly computing their full error covariance matrix. The 4DVAR data assimilation step is thus more flow-dependent than in 3DVAR and the quality of the estimates improves. The European Centre for Medium-Range Weather Forecasts (ECMWF) and the Japan Meteorological Agency, for example, currently use 4DVAR in their global data assimilation systems.

In 4DVAR, only the model state at the beginning of the interval – the initial condition – is uncertain, and the model is otherwise considered perfect. In other words, the model physics are imposed as a *strong-constraint* in the minimization of the objective function. Adding another term to the objective function that represents errors in the model dynamics or time-varying boundary conditions yields the so-called *weak-constraint* methods, which include the *representer* or *general inverse* techniques [4]. The latter has been used for soil moisture assimilation [42].

In practice, the "best" estimate obtained from the data assimilation system is only a reasonable approximation of the truly "optimal" estimate. Coarse-resolution versions of the model are frequently used in the minimization to ease the computational burden. For numerical stability, nonlinear problems are tackled by iterations that use tangent-linear and adjoint models – essentially linearized versions of the dynamic model that can be efficiently integrated forward or backward in time.

2.3. The Kalman filter

Data assimilation algorithms known as Kalman filters [16] share the static update (2) with some of the variational techniques, but Kalman filter algorithms also explicitly compute the error covariances through an additional matrix equation (not shown) that propagates error information from one update time to the next, subject to possibly uncertain model dynamics (Fig. 1a). The error covariance propagation in the traditional Kalman filter and its nonlinear variant, the Extended Kalman filter (EKF), however, is prohibitively expensive for large-scale applications - the size of the error covariance matrices would be on the order of $10^8 \times 10^8$ for global weather prediction applications. It goes without saying that - even if the computational aspects could somehow be handled there is simply not enough information about error structures to fill such large matrices with meaningful numbers. Like variational methods, the Kalman filter can be derived from an objective function, given a number of additional assumptions about the error structure, including model and observation errors that are uncorrelated in time and mutually uncorrelated. For linear problems that satisfy

these additional assumptions, the Kalman filter and weakconstraint variational methods therefore produce identical estimates at the end of the assimilation interval. The EKF has been demonstrated successfully for soil moisture data assimilation [41,44,50] and is currently being integrated into the land surface analysis of the ECMWF global data assimilation system.

Reduced-rank approximations such as the Ensemble Kalman filter (EnKF) [15,18,48] are designed to reduce the number of degrees of freedom to a manageable level. The idea behind the EnKF – a Monte-Carlo variant of the Kalman filter – is that a comparably small ensemble of model trajectories captures the relevant parts of the error structure. The error covariance matrices that are required for the update (2) can then be diagnosed from the spread of the ensemble at the update time. The EnKF is flexible in its treatment of errors in model dynamics and parameters. It is also very suitable for modestly nonlinear problems. Experimental versions of the EnKF have been implemented at the Canadian Meteorological Centre [19] and for ocean assimilation within the NASA seasonal forecasting system [26]. The EnKF is also frequently used for assimilating hydrologic remote sensing observations [40,2,33,45,53,13,14,35].

2.4. Filtering, smoothing, and continually operating assimilation algorithms

In a continually operating (or *cycling*) data assimilation system, all observations can never be processed at once. If observations at a single point in time are processed separately, and if some information about the state estimate and its covariance is propagated from one update time to the next, the assimilation method is called a *filtering* (or *sequential*) algorithm (Fig. 1a). In this case, information from measurements at previous time steps is accumulated in the assimilation estimates at the latest time. In other words, the assimilation sup to that time, but not on "future" observations. Examples of such sequential algorithms include 3DVAR and the Kalman filter.

4DVAR is an example of a *smoothing* (or *batch*) algorithm in which measurements at different times within an assimilation interval are processed simultaneously (Fig. 1b). The estimate at the initial time is therefore based on "future" observations from the entire assimilation interval. For most applications, such a smoothing solution can only cover a relatively short time interval – typically just 12 h in data assimilation systems used for weather prediction. The practical solution is to restart the assimilation for each forecast initialization. This implies that each time, the initial background error covariance must be reinitialized.

A fundamental difference between the Kalman filter and 4DVAR is that the former *explicitly* evolves the covariance matrix without interruption, whereas the covariance propagation in 4DVAR is implicit and only applies within the

assimilation interval (see above). In a continually operating assimilation system, the Kalman filter offers both an initial model (or background) state estimate and its covariance matrix at each assimilation time step, while 4DVAR does not propagate error covariance information from one assimilation interval to the next.

3. Ongoing research activities

Depending on the application, the sophistication of and research in data assimilation varies tremendously. Established atmospheric assimilation systems are transitioning to more advanced algorithms such as 4DVAR, the EnKF, or hybrid approaches. Recently, the development of assimilation systems in biogeochemistry [25] and land surface hydrology [31,49,50] has attracted a lot of attention. In this section, we summarize a few topics that are common to most data assimilation research, including radiance assimilation, input error parameters, quality control, bias, and validation.

3.1. Observation operators and radiance assimilation

As written, Eq. (1) assumes that the model state variable is directly observed. This is, however, rarely the case for satellite observations, which typically come in the form of radiances and are only indirectly related to the geophysical quantities of interest (such as atmospheric humidity, soil moisture, or trace gas concentrations). Radiative transfer modeling is required to link the satellite observations and the geophysical variables. An observation operator (for example, a forward radiative transfer model) is then introduced that transforms the model variables and permits a direct comparison with satellite observations. (The observation operator also maps the model variables to the observations.) Alternatively, a retrieval algorithm – essentially an inverse observation operator - can be used to process the satellite radiances into model variables that are subsequently assimilated into the geophysical model. (Recall that the retrieval problem can itself be cast within the framework of data assimilation; Section 2.2.)

The assimilation of satellite radiances (as opposed to retrievals) is attractive because all relevant models, including the geophysical model and the radiative transfer model, are then part of the same data assimilation system and share information directly. Consider, for example, the assimilation of microwave radiobrightness temperatures for soil moisture estimation. If retrievals of soil moisture are assimilated, they are based on external estimates of soil temperature. These external estimates, however, are not consistent with the soil temperature that is available from the land surface model within the assimilation system. By combining all modeling as part of the data assimilation system, such inconsistencies are avoided. Satellite radiance assimilation has lead to undeniable improvements in weather forecast skill [23]. But it is also more complex as it requires a detailed knowledge of radiative transfer models, expertise that assimilation developers may lack.

3.2. Input error covariances

If the input error covariances for the model and the observations are known, minimizing the objective function is a fairly technical aspect and can be accomplished with existing engineering solutions. The science of data assimilation and the key to success are largely in the accurate specification of the input error parameters. This can be a tremendously difficult task. Observation error covariances must not only take into account instrument errors, but also errors in the observation operator (such as radiative transfer models) and errors in the interpolation of the observations. The latter two are also called *errors of representativeness*.

Determining error covariances for the model fields presents an even greater challenge and is typically based on (i) comparisons of model simulations with observations outside of the data assimilation system, (ii) comparisons of model forecasts with different lead times at the same verifying time, (iii) analysis of the assimilation increments or innovations, or (iv) ensemble integrations. Adaptive techniques for estimating error covariances during data assimilation may also be used and permit some measure of automation [10]. Such techniques are based on the stream of new information that is continually provided by the innovations and have been used successfully in soil moisture data assimilation [36]. Ultimately, the specification of input error covariances remains largely subjective.

3.3. Quality control

Quality control algorithms that weed out particularly poor observations are an integral part of any assimilation system. If an observational data set is contaminated by bad data whose errors are not well represented by the input error parameters, the data assimilation system will fail in estimating the true fields. For example, soil moisture retrieval from passive microwaves during rain events should not be assimilated. Elementary quality control is typically included in satellite data sets. AMSR-E soil moisture retrievals, for instance, are flagged for pixels known to be contaminated by radio-frequency interference. However, such a priori quality control is rarely sufficient for the success of data assimilation. On-line quality control routines need to be added as part of the assimilation system. Such (possibly adaptive) routines cross-compare observations, incorporate information from the geophysical model, and discard inconsistent observations [12].

3.4. Bias

Unbiased errors are a key assumption in all data assimilation methods – that is, errors must be strictly random, and on average the model estimates and the observations must agree with the true fields. Unfortunately, this is almost never the case in practice. The proper treatment of bias is therefore critically important to the success of a data assimilation system – otherwise the assimilation estimates will not be the desired "best" estimates.

It is important to distinguish between biased observations and bias in the model. If observations are biased, and if the bias is known a priori, the observations can be preprocessed and the bias removed prior to data assimilation. In practice, however, it is difficult to obtain the necessary bias estimates, in particular for remote sensing data. Satellite observations from different platforms are usually biased against each other due to differences in calibration. Because of orbital drift, the bias in observations even from a single platform may change over time. Similarly, geophysical models are never perfect and usually produce biased estimates, with biases varying in time and in space. Provided that unbiased observations are available for assimilation, a model for the bias can be formulated and the bias model parameters can be added to the state vector (state augmentation). The data assimilation system then also produces model bias estimates [11]. Variants of this approach have been used for the assimilation of land surface (skin) temperature [5] and for the assimilation of field-scale in situ observations of soil moisture [13].

In practice, however, it is extremely difficult, if not impossible to attribute the bias conclusively to either the model or the observations, and subjective assumptions need to be made. The bias problem is particularly acute for *reanalysis* projects that retrospectively assimilate observations spanning multiple decades [21,22,24]. Long time series of conventional and satellite observations from a multitude of different platforms and sensors exhibit many jumps and trends due to changes in the observing system, making the production of a long and homogeneous climate time series a formidable challenge. In some cases, it must even be argued that the climatology is practically unknown at present, as is the case for global soil moisture fields [38]. If anomaly information is all that is needed, for example for forecast initialization, normalized deviates or percentiles may be assimilated by scaling observations to the model's climatology [34,35].

3.5. Validation of data assimilation systems

Given the numerous assumptions about nonlinearities, error properties, and the like – most of which are anyway violated in the application at hand – it might be surprising that data assimilation has been so very successful. Yet there are a number of ways in which the success of a data assimilation system can be assessed, and the system can be steadily improved.

In forecast initialization problems, verification of forecasts provides a straightforward measure of the impact of the assimilation system. Weather forecasts, for example, have improved dramatically with advances in satellite technology and the assimilation of satellite observations. This is exemplified by large increases in forecast skill in the Southern Hemisphere, where few conventional observations are available and the observing system relies primarily on satellites. Another metric for success is provided by a careful analysis of the innovations that are available from any data assimilation system. If the system operates in accordance with its underlying assumptions, the innovations exhibit certain statistical properties (including mean zero and temporal decorrelation). Testing for such properties can show up deficiencies in the system. See [35] for a soil moisture assimilation example.

Further validation of a data assimilation system is possible through comparisons with independent data, for example from intensive field campaigns or other high-quality in situ data that have not been assimilated. Additional tests can also be conducted by withholding some observations from the assimilation and subsequently comparing the resulting assimilation estimates to the portion of the data that was withheld from the assimilation. Thorough and ongoing validation efforts that use all applicable metrics will steadily improve the performance of a data assimilation system. Improvements will include model refinements, a better observing system that is tailored to the needs of the application, and more accurate input and output error information.

4. Conclusions

Much can be learned from continually confronting models with observations within a data assimilation system. Data assimilation remains a vibrant and active area of research across many disciplines of Earth science, including atmospheric and oceanic sciences. More and more Earth science disciplines make great strides in satellite data assimilation, among them atmospheric chemistry and land surface hydrology.

Hydrologic remote sensing observations are typically assimilated into land data assimilation systems. Considerable progress has already been made in the development of a community software infrastructure for the integration of land surface models and accompanying data assimilation modules [27; this issue]. But there is a lot more work to be done. To date, land data assimilation systems have mostly assimilated a single data type, for example satellite retrievals of surface soil moisture. Future developments will undoubtedly require a multi-variate approach in which many different types of observations are assimilated as part of the same system. Because hydrologic remote sensing provides observations at a range of scales, efficient algorithms for the assimilation at multiple scales are being developed [54].

Another grand challenge is the assimilation of hydrologic remote sensing observations into coupled models of the land surface and the atmosphere. Only in such coupled systems can the hydrologic remote sensing observations fully contribute to improved estimates of land-atmosphere coupling and forecast skill. Moreover, the generally damped dynamics of land surface processes imply a special challenge for the assimilation of hydrologic remote sensing observations. The focus on model errors (as opposed to initial condition errors) puts a strong emphasis on the characterization of errors in the land surface model dynamics and parameters and errors in the surface meteorological forcing data. Ensemble filtering methods provide a convenient way to address this challenge but require sophisticated tools for the generation of perturbations that are suitably correlated in time and space [39] and across variables [35].

The great success of sophisticated assimilation systems that use remote sensing observations is evident in the dramatic improvements in weather forecast skill over the past decade, particularly in the Southern Hemisphere. As remote sensing data become increasingly diverse and plentiful, and as computing resources become more powerful and at the same time more affordable, data assimilation is bound to remain a lively field of research that holds great promise for achieving improvements in our understanding, modeling, and prediction of the Earth system.

Acknowledgements

Thanks to Randal Koster and Gilberto Vicente for many helpful comments.

References

- Anderson BDO, Moore JB. Optimal filtering. Englewood Cliffs, NJ: Prentice-Hall; 1979. 357 pp.
- [2] Andreadis K, Lettenmaier D. Assimilating remotely sensed snow observations into a macroscale hydrology model. Adv Water Resour 2006;29:872–86.
- [3] Bennett AF. Inverse methods in physical oceanography. New York: Cambridge University Press; 1992. 346 pp.
- [4] Bennett AF. Inverse modeling of the ocean and atmosphere. New York: Cambridge University Press; 2002. 234 pp.
- [5] Bosilovich M, Radakovich J, da Silva A, Todling R, Verter F. Skin temperature analysis and bias correction in a coupled land–atmosphere data assimilation system. J Meteorol Soc Jpn 2007;85A:205–28.
- [6] Bouttier F, Courtier P. Data assimilation concepts and methods. ECMWF lecture notes. Reading, England: European Centre for Medium-Range Weather Forecasts; 1999. 59 pp.
- [7] Cohn SE. An introduction to estimation theory. J Meteorol Soc Jpn 1997;75:257–88.
- [8] Crow WT. A novel method for quantifying value in spaceborne soil moisture retrievals. J Hydrometeorol 2007;8(1):56–67.
- [9] Daley R. Atmospheric data analysis. New York: Cambridge University Press; 1991. 457 pp.
- [10] Dee DP. On-line estimation of error covariance parameters for atmospheric data assimilation. Mon Weather Rev 1995;123:1128–45.
- [11] Dee DP, da Silva AM. Data assimilation in the presence of forecast bias. Q J R Meteorol Soc 1998;124:269–95.
- [12] Dee DP, Rukhovets L, Todling R, da Silva AM, Larson JW. An adaptive buddy check for observational quality control. Q J R Meteorol Soc 2001;127:2451–71.
- [13] De Lannoy GJM, Reichle RH, Houser PR, Pauwels VRN, Verhoest NEC. Correcting for forecast bias in soil moisture assimilation with the ensemble Kalman filter. Water Resour Res 2007;43:W09410. <u>doi:10.1029/2006WR005449</u>.

- [14] Durand M, Margulis SA. Correcting first-order errors in snow water equivalent estimates using a multifrequency, multiscale radiometric data assimilation scheme. J Geophys Res – Atmos 2007;112:D13121. doi:10.1029/2006JD008067.
- [15] Evensen G. Data assimilation: the ensemble Kalman filter. New York: Springer-Verlag; 2006. 279 pp.
- [16] Gelb A, editorApplied optimal estimation. Cambridge, MA: The MIT Press; 1974. 374 pp.
- [17] Ghil M, Malanotte-Rizzoli M. Data assimilation in meteorology and oceanography. Adv Geophys 1991;33:141–266.
- [18] Heemink AW, Verlaan M, Segers AJ. Variance reduced ensemble Kalman filtering. Mon Weather Rev 2001;129:1718–28.
- [19] Houtekamer PL, Mitchell HL, Pellerin G, Buehner M, Charron M, Spacek L, et al. Atmospheric data assimilation with an ensemble Kalman filter: results with real observations. Mon Weather Rev 2005;133:604–20.
- [20] Jazwinski AH. Stochastic processes and filtering theory. New York: Academic Press; 1970. 376 pp.
- [21] Kallberg P, Berrisford P, Hoskins B, Simmmons A, Uppala S, Lamy-Thépaut S, et al. ERA-40 atlas. ERA-40 project report series 19. Reading, England: European Centre for Medium-Range Weather Forecasts; 2005. 191 pp.
- [22] Kalnay E et al. The NCEP/NCAR 40-year reanalysis project. Bull Am Meteorol Soc 1996;77:437–71.
- [23] Kalnay E. Atmospheric modeling, data assimilation and predictability. New York: Cambridge University Press; 2003. 364 pp.
- [24] Kanamitsu M, Ebisuzaki W, Woolen J, Yang S-K, Hnilo JJ, Fiorino M, et al. NCEP-DOE AMIP-II reanalysis (R-2). Bull Am Meteorol Soc 2002;77:437–71.
- [25] Kasibhatla P, Heimann M, Rayner P, Mahowald N, Prinn RG, Hartley DE, editorsInverse methods in biogeochemical cycles. AGU geophysical monograph series, vol. 114. Washington, DC: American Geophysical Union; 2000. p. 324.
- [26] Keppenne CL, Rienecker MM, Kurkowski NP, Adamec DA. Ensemble Kalman filter assimilation of temperature and altimeter data with bias correction and application to seasonal prediction. Nonlinear Proc Geophys 2005;12:491–503.
- [27] Kumar SV, Reichle RH, Peters-Lidard CD, Koster RD, Zhan X, Crow WT, et al. A land surface data assimilation framework using the land information system: description and applications. Adv Water Resour, 2008, in press, <u>doi:10.1016/j.advwatres.2008.01.013</u>.
- [28] Lewis JM, Lakshmivarahan S, Dhall S. Dynamic data assimilation: a least squares approach. New York: Cambridge University Press; 2006. 654 pp.
- [29] Malanotte-Rizzoli P, editorModern approaches to data assimilation in ocean modeling. New York: Elsevier; 1996. 455 pp.
- [30] McLaughlin D. Recent developments in hydrologic data assimilation. Rev Geophys 1995;33(Part 2, Suppl. S):977–84.
- [31] McLaughlin D. An integrated approach to hydrologic data assimilation: interpolation, smoothing, and filtering. Adv Water Resour 2002;25:1275–86.
- [32] McLaughlin D, Zhou YH, Entekhabi D, Chatdarong V. Computational issues for large-scale land surface data assimilation problems. J Hydrometeorol 2006;7:494–510.
- [33] Pan M, Wood EF. Data assimilation for estimating the terrestrial water budget using a constrained ensemble Kalman filter. J Hydrometeorol 2006;7:534–47.
- [34] Reichle RH, Koster RD. Bias reduction in short records of satellite soil moisture. Geophys Res Lett 2004;31:L19501. <u>doi:10.1029/</u> 2004GL020938.

- [35] Reichle RH, Koster RD, Liu P, Mahanama SPP, Njoku EG, Owe M. Comparison and assimilation of global soil moisture retrievals from the Advanced Microwave Scanning Radiometer for the Earth Observing System (AMSR-E) and the Scanning Multichannel Microwave Radiometer (SMMR). J Geophys Res – Atmos 2007;112:D09108. <u>doi:10.1029/2006JD008033</u>.
- [36] Reichle RH, Crow WT, Keppenne CL. An adaptive ensemble Kalman filter for soil moisture data assimilation. Water Resour Res 2008; in press. <u>doi:10.1029/2007WR006357</u>.
- [37] Reichle RH, Crow WT, Koster RD, Sharif HO, Mahanama SPP. The contribution of soil moisture retrievals to land data assimilation products. Geophys Res Lett 2008;35:L01404. <u>doi:10.1029/</u> 2007GL031986.
- [38] Reichle RH, Koster RD, Dong J, Berg AA. Global soil moisture from satellite observations, land surface models, and ground data: implications for data assimilation. J Hydrometeorol 2004;5(3):430–42.
- [39] Reichle RH, Koster RD. Assessing the impact of horizontal error correlations in background fields on soil moisture estimation. J Hydrometeorol 2003;4(6):1229–42.
- [40] Reichle RH, McLaughlin DB, Entekhabi D. Hydrologic data assimilation with the ensemble Kalman filter. Mon Weather Rev 2002;130:103–14.
- [41] Reichle RH, Walker JP, Koster RD, Houser PR. Extended versus ensemble Kalman filtering for land data assimilation. J Hydrometeorol 2002;3:728–40.
- [42] Reichle RH, McLaughlin DB, Entekhabi D. Variational data assimilation of microwave radiobrightness observations for land surface hydrology applications. IEEE Trans Geosci Remote Sensing 2001;39(8):1708–18.
- [43] Rodell M, Houser PR. Updating a land surface model with MODISderived snow cover. J Hydrometeorol 2004;5:1064–75.
- [44] Seuffert G, Wilker H, Viterbo P, Drusch M, Mahfouf JF. The usage of screen-level parameters and microwave brightness temperature for soil moisture analysis. J Hydrometeorol 2004;5:516–31.
- [45] Slater A, Clark M. Snow data assimilation via an ensemble Kalman filter. J Hydrometeorol 2006;7:478–93.
- [46] Swinbank R, Shutyaev V, Lahoz WA, editorsData assimilation for the Earth system. NATO science series IV, vol. 26. Boston: Kluwer Academic Publishers; 2003. 377 pp.
- [47] Tarantola A. Inverse problem theory: methods for data fitting and model parameter estimation. New York: Elsevier; 1987. 613 pp.
- [48] Tippett MK, Anderson JL, Bishop CH, Hamill TM, Whitaker JS. Ensemble square root filters. Mon Weather Rev 2003;131:1485–90.
- [49] Viterbo P, van den Hurk B, editorsECMWF/ELDAS workshop on land surface assimilation (8–11 November 2004). ECMWF workshop proceedings. Reading: European Centre for Medium-Range Weather Forecasts; 2005.
- [50] Walker JP, Houser PR. Hydrologic data assimilation. In: Aswathanarayana U, editor. Advances in water science methodologies. Netherlands: A.A. Balkema; 2005.
- [51] Walker JP, Houser PR, Reichle RH. New remote sensing technologies require advances in hydrologic data assimilation. EOS, Am Geophys Union 2003;84(49):545–51.
- [52] Wunsch C. The ocean circulation inverse problem. New York: Cambridge University Press; 1996. 442 pp.
- [53] Zhou Y, McLaughlin D, Entekhabi D. Assessing the performance of the ensemble Kalman filter for land surface data assimilation. Mon Weather Rev 2006;134:2128–42.
- [54] Zhou Y, McLaughlin D, Entekhabi D, Ng G-HC. An ensemble multiscale filter for large nonlinear data assimilation problems. Mon Weather Rev, in press.