A Weak-Constraint-Based Data Assimilation Scheme for Estimating Surface Turbulent Fluxes

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Abstract—Much attention has been focused on the assimilation of satellite data and products into land surface processes. In this letter, a variational data assimilation scheme is developed based on the weak-constraint concept. It assimilates surface skin temperature into a simple land surface model for the estimation of turbulent fluxes. An automatic differentiation technique is used to derive the adjoint codes to evaluate the gradient of the cost function. After the construction of this assimilation system, numerical experiments are conducted to test its performance with different model errors, and the comparison is also made with the strong constraint scheme. The results show that the land surface turbulent fluxes can be retrieved with highly satisfactory accuracy.

Index Terms—Data assimilation, evapotranspiration, land surface temperature (LST), weak constraint.

I. INTRODUCTION

ACCURATE estimation of energy and momentum fluxes, especially sensible and latent heat fluxes, between the land surface and the atmospheric boundary layer is required in a wide variety of agricultural, hydrological, and meteorological applications [1], [2]. Many methods, such as eddy correlation and Bowen ratio, can be used to measure these fluxes at the field scale. Their applicability, however, is limited on the fine spatial scale. At present, the only way to achieve this goal of mapping fluxes on a regional scale is to use remote sensing techniques that can provide various spatial and temporal imageries that cover large areas.

Estimation of surface energy balance components using remote sensing data can be roughly divided into three categories. Empirical methods directly build on the relationship between remote sensing products, such as various vegetation indexes and retrieved land surface temperature (LST) for the estimation. Residual methods of the energy budget couple some empirical formulas and physical mechanisms to realize the estimation of evapotranspiration (ET or LE) and sensible heat flux (H)

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by using remote sensing to directly estimate input parameters, such as the surface energy balance system [2]. In recent years, data assimilation methods have merged remote sensing data and soil–vegetation–atmosphere transfer models for estimating surface fluxes and have achieved encouraging results. This new method has received considerable attention from researchers in recent years [3]–[7], since it combines dynamic models and temporal remote sensing data based on the control theory to accurately retrieve critical parameters for flux estimation. The first two methods more or less use only the instantaneous data and empirical relationships.

A data assimilation system generally comprises the following three components [8]: 1) underlying dynamic model; 2) merging scheme; and 3) observation. Dynamic models are usually different in different disciplines, such as atmosphere, oceanography, and land surfaces. There exist many merging schemes. Some of them [9] are able to handle uncertainties both in models and observations, but others can consider the uncertainty only in observations. As a matter of fact, models are imperfect and always include uncertainties. It is important to consider this kind of uncertainty in the data assimilation scheme to improve the accuracy of estimation and prediction by a model. Kalman filters (KFs) and weak-constraint variational methods have attracted more and more attention from researchers since they can simultaneously handle uncertainties both in models and observations. Among the various kinds of KFs, the ensemble KF is the most popular since its application is relatively easy. However, it is more suitable for state estimation [10], [11]. If there are unspecified parameters in the model, especially time-varying parameters, which need to be estimated together with state variables, its application poses many limitations. Weak-constraint variational methods can estimate both state variables and model parameters. However, it is difficult to develop the adjoint model for the original one to evaluate the derivatives of the cost function with respect to control variables, which are composed of state variables and model parameters to be estimated. However, automatic differentiation (AD) techniques provide powerful tools to efficiently and effectively develop the adjoint of the model at the level of computer language codes.

In this letter, a variational land data assimilation scheme based on the weak-constraint concept [12]–[17] and AD techniques [18], [19] is proposed to assimilate LST to estimate surface turbulent fluxes by retrieving state variables and time-varying parameters at the same time. Numerical experiments are conducted to test the performance of this data assimilation system when different values of model uncertainties are used. Comparisons are also made to show the advantages of this weak-constraint variational scheme over the strong constraint variational scheme that assumes that the model is perfect. Estimation results indicate that this data assimilation

scheme can effectively retrieve LE and H with a satisfactory accuracy.

This letter is organized as follows. In Section II, each component that comprises the data assimilation system is presented. Then, some numerical experiments are carried out to test the system. Finally, the conclusion is given.

II. CONSTRUCTION OF DATA ASSIMILATION SYSTEM

A. Simple Land Surface Model

The land surface model used in the study is similar to the one used by Caparrini *et al.* [5], [6]. However, it differs in two respects: one concerns the deep soil temperature, and the other is the parameterization of the sensible heat. The prognostic equations for LST T_s and deep soil temperature T_d are based on the classical force-restore method described as follows:

$$\frac{dT_s}{dt} = \frac{2\sqrt{\pi\omega}}{P}(R_n - H - LE) - 2\pi\omega(T_s - T_d) \quad (1)$$

$$T_d = \sum_{i=1}^{DN} T_{si} \Big/ DN \quad (2)$$

where R_n is the net radiation, H is the sensible heat, LE is the latent heat, P is the thermal inertia of the land surface, ω is the diurnal frequency, T_{si} is the surface temperature for the ith time step of the previous day, and DN is the number of time steps in a day.

In (1), H and LE are parameterized as

$$H = \rho c_p C_H U(T_s - T_a) \quad (3)$$

$$LE = \frac{EF}{1 - EF} H \quad (4)$$

where T_a is the air temperature, ρ is the air density, c_p is the air specific heat, C_H is the bulk transfer coefficient for heat, U is the wind speed, and EF is the evaporative fraction. A different scheme that was adopted from the biosphere–atmosphere transfer scheme is used for the bulk transfer coefficient C_H, i.e.,

$$C_H = \begin{cases} C_{HN}\left(1 + 24.5(-C_{HN}Ri_B)^{1/2}\right), & Ri_B < 0 \\ C_{HN}/(1 + 11.5Ri_B), & Ri_B > 0 \end{cases} \quad (5)$$

$$Ri_B = \frac{g}{\theta}\frac{\Delta\theta z_{\text{ref}}}{U^2} \quad (6)$$

$$C_{HN} = \frac{\kappa^2}{\ln(z_{\text{ref}}/z_{0m})\ln(z_{\text{ref}}/z_{0h})} \quad (7)$$

where C_{HN} is the bulk heat transfer coefficient under neutral conditions, Ri_B is the bulk Richardson number, g is the gravitational acceleration, θ is the potential temperature of the air, $\Delta\theta$ is the potential temperature difference between the air and the surface, z_{ref} is the measurement height, and z_{0m} and z_{0h} are the roughness lengths for momentum and heat transfer, respectively.

From these formulas, it is noted that C_{HN} and EF are the two main factors [5], [6], [20] that directly affect the estimation of H and LE. Thus, these two parameters will be retrieved as control variables in the process of data assimilation. Since the status of land surface slowly changes relative to meteorological forcing, C_{HN} is assumed to be constant during one assimilation window. In other papers, it was assumed that EF

is kept invariant during 09:00–18:00, local time, based on the analysis of some experimental data [5], [6], [21], [22]. In this study, the daily averaged EF is retrieved. Thus, the original assumption is relaxed. Values of R_n, ρ, U, and T_a are taken from micrometeorological observations.

B. Merging Scheme

The merging scheme plays a key role in the entire data assimilation scheme since it determines how LST and the aforementioned land surface model are coupled. When using the variation method, two merging schemes that minimize a cost function exist. One is the strong constraint scheme, which treats the physical model as perfect, and the other is the weak constraint, which treats the physical model as imperfect. In this study, the weak-constraint method is formulated. In addition to those that were previously mentioned, control variables also include state variables of the model. Thus, a prognostic equation can be represented as after discretization in time, i.e.,

$$T_s(t_i) = M\left(T_s(t_{i-1})\right) + \varepsilon_m(t_i) \quad (8)$$

$$T_s(t_0) = T_s^b + \varepsilon_b \quad (9)$$

$$T_o(t_k) = T_s(t_k) + \varepsilon_o(t_k) \quad (10)$$

where $M(\cdot)$ denotes the discrete dynamic model, T_s^b is the background value for the initial surface temperature, T_o is the observed LST, and ε_m, ε_b, and ε_o are the model error with normal distribution, error for initial value of LST, and observation error, respectively, and they are assumed to be independent of each other. In this letter, $\varepsilon_m(t_i)$ and $\varepsilon_o(t_k)$ are assumed to be temporally independent.

The cost function J can be represented as follows:

$$\begin{aligned} J = &\sum_{i=1}^{N} \left(T_s(t_i) - M\left(T_s(t_{i-1})\right) \cdot Q_m^{-1}\right. \\ &\cdot \left(T_s(t_i) - M\left(T_s(t_{i-1})\right)\right) + \left(T_s(t_0) - T_s^b\right) \cdot Q_b^{-1} \\ &\cdot \left(T_s(t_0) - T_s^b\right) + \sum_{k=1}^{K} \left(T_o(t_k) - T_s(t_k)\right) \cdot Q_o^{-1} \\ &\cdot \left(T_o(t_k) - T_s(t_k)\right) + \left(C_{HN} - C_{HN}^b\right) \cdot Q_c^{-1} \\ &\cdot \left(C_{HN} - C_{HN}^b\right) + \sum_{j=1}^{D} \left(EF_j - EF^b\right) \cdot Q_e^{-1} \\ &\cdot \left(EF_j - EF^b\right) \end{aligned} \quad (11)$$

where N is the total number of time steps, K is the number of observations, D is the number of days in one assimilation window, C_{HN}^b is the background value of C_{HN}, EF^b is the background value of EF, Q_m is the covariance of ε_m, Q_b is the covariance of ε_b, Q_o is the covariance for error of T_o, Q_c is the covariance for error of C_{HN}^b, and Q_e is the covariance for error of EF^b. The setting of these parameters in this letter will be described later.

The objective of the variational data assimilation method is to minimize the cost function J to seek the most optimal control variables and, thus, accurately estimate H and LE. There are two approaches to solve this optimization problem: one is the representer method [15], [17], and the other is the direct derivation of the derivatives of J with respect to control variables and, thus, the use of the optimization algorithm [13]. The representer
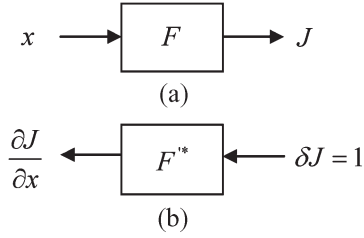
Fig. 1. Illustrations for the evaluation of derivatives of the cost function with AD techniques. F denotes the whole codes for evaluating the cost function. F'^* represents the adjoint codes of the original codes, which can be used to evaluate derivatives with ease.

method derives coupled Euler–Lagrange equations and then solves them. However, its formulation is very complicated. The second approach is easy to use. However, the process of manual derivation is tedious and time consuming. In this letter, AD techniques are used to develop adjoint codes for the evaluation of derivatives of the cost function J at the level of computer source codes. AD is based on two facts [18], [23]. First, any computer code statement can be regarded as a composition of elementary functions. Second, the chain rule can be used to differentiate this composition of elementary functions. Many software packages have been developed in accordance with the principles described above for FORTRAN and C computer languages. In this study, the software package TAPENADE is applied to develop adjoint codes. The illustration of the AD running process is presented in Fig. 1. Provided that the derivatives of the cost function are evaluated, an optimization algorithm has to be chosen to minimize the cost function. In this letter, scaled conjugate gradient algorithms developed by Andrei [24] are used.

C. LST

In this letter, three different concepts of surface temperature occur: 1) radiometric surface temperature retrieved from remote sensing, which is used as the observation to be assimilated; 2) effective vegetated surface temperature, which is the state variable in the simple land surface model; and 3) aerodynamic surface temperature, which is used in the calculation of H and LE. Assumptions have to be made in some studies for using these temperatures, having different physical meanings in a consistent way. Caparrini *et al.* [5] assume that the effective vegetated surface temperature modeled in the land surface model is the radiometric surface temperature, and thus, retrieved C_{HN} is consistent with using radiometric LST in turbulent flux calculations. As a matter of fact, the difference between the physical meanings of these three temperatures can be considered as a part of model and observation errors in the framework of weak constraint. Therefore, no assumptions are needed about the physical meanings of quantities in the entire data assimilation system, and all variables and parameters have their original physical meanings. Observations T_o are derived from the field infrared radiative thermometer in this study. The use of satellite-retrieved LST is the eventual goal.

III. NUMERICAL EXPERIMENTS AND DISCUSSIONS

After setting up the aforementioned data assimilation system, numerical experiments are performed to test its performance by

TABLE I
SETTINGS FOR THE PARAMETERS IN THIS DATA ASSIMILATION SYSTEM

| Symbol	Parameter	Value or average	Variance
P	thermal inertia $[\mathrm{Jm^{-2}K^{-1}s^{-1/2}}]$	1000	-----
ω	diurnal frequency $[\mathrm{s^{-1}}]$	1/86400	-----
C_{HN}^b	background for bulk transfer coefficient for heat	0.004	9.0E-6
EF^b	background for evaporative fraction	0.6	0.25
ε_m	model error [$\mathrm{K^2}$]	0.0	1.0 ~9.0
ε_o	observation error [$\mathrm{K^2}$]	0.0	2.0
T_s^b	background for initial surface temperature [K]	290	9.0
T_d^b	background for initial deep temperature [K]	290	9.0
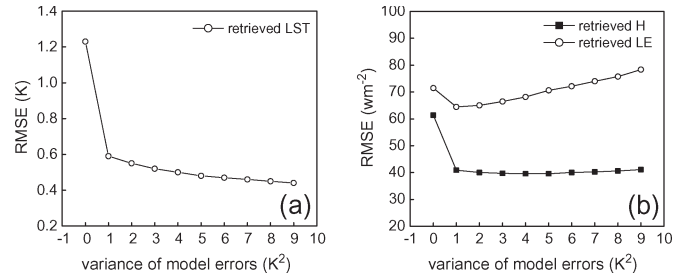
Fig. 2. Inversion results with increasing model errors from 0 to 9 $\mathrm{K^2}$. (a) RMSE of the retrieved LST. (b) RMSE of the retrieved H and LE.

using field data, which are taken from the AmeriFlux Bondvill site. This site is located at $40.00°$ latitude, $-88.29°$ longitude, and its land cover is broadleaf crop. Measured micrometeorological variables and surface fluxes every 30 min from Julian day 231 to 260 in 1999 are used in this study, including air temperature, wind speed, air density, net radiation, temperature by infrared radiative thermometer, and sensible and latent heat fluxes. The length of one assimilation window is ten days, with five days overlap, and the total number of days in this assimilation experiment is 30 days. Parameters needed in this study, which are introduced in the second section, are set in Table I.

It is difficult to estimate the model errors, which are normally assigned according to experiences from researchers and *a priori* information. In this study, measurements of 1–9 $\mathrm{K^2}$ are taken with an increment of 1 $\mathrm{K^2}$ to investigate their effects on estimation results, as listed in Table I. In fact, the weak-constraint scheme will be close to the strong one when the model error takes a very minor value. Thus, the strong constraint scheme can be considered as a special case with a model error that is equal to 0 $\mathrm{K^2}$. Fig. 2 indicates the changes of the root mean square errors (RMSE) of LST, H,
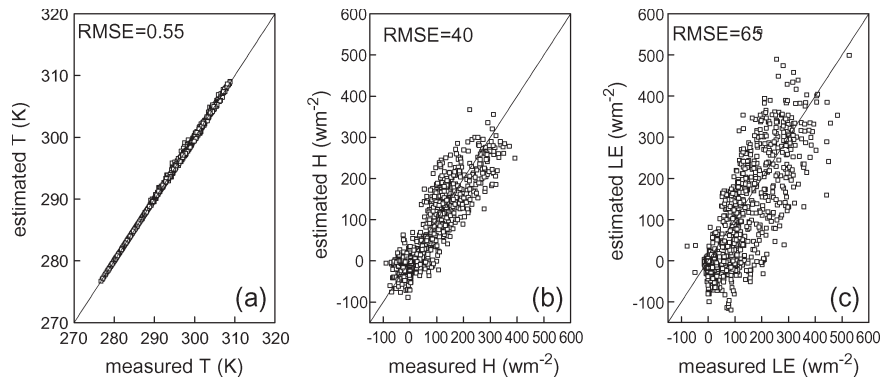
Fig. 3.   Scatter plots for estimation results from data assimilation experiments. Measured versus estimated (a) surface temperature, (b) sensible heat flux, and (c) latent heat flux.
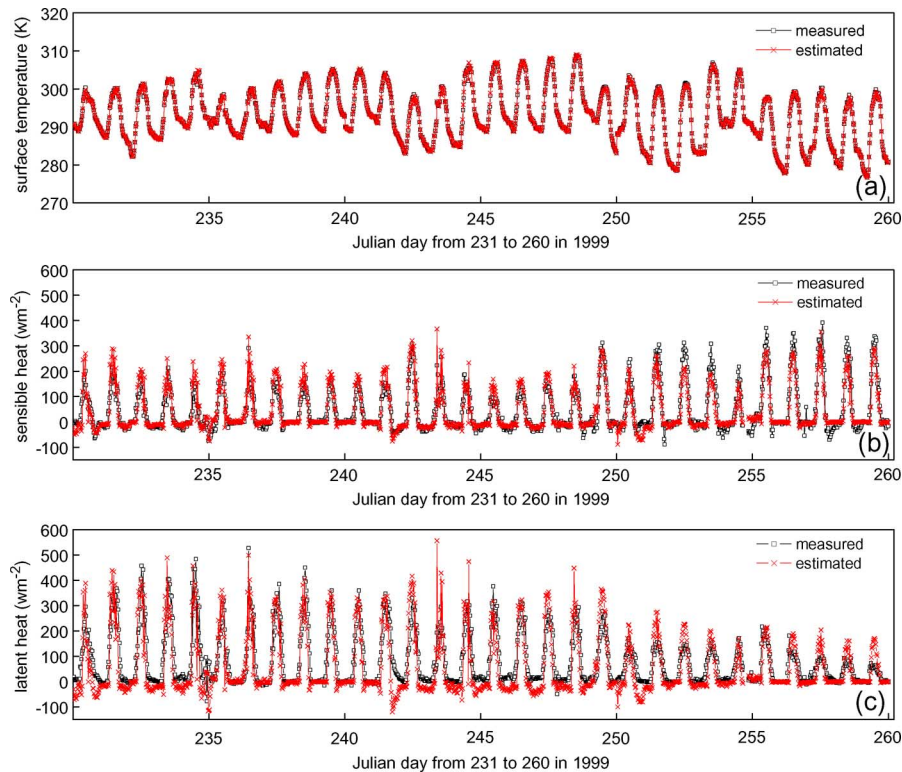

Fig. 4.   Time profiles for estimation results and measurements. (a) Surface temperature. (b) Sensible heat flux. (c) Latent heat flux.

and LE, with increasing model errors from 0 to 9 K^2. As seen, the weak-constraint scheme performs generally better than the strong one. The RMSE of the retrieved LST drops down with the variance of model errors ranging from 0 to 9 K^2. The RMSE of the retrieved H largely declines when the model error is considered and then becomes stable when the model error increases. The RMSE of the retrieved LE first declines and then rises while the model error increases. This illustrates that the choice of the magnitude of the model error has an apparent effect on the retrieved latent heat flux. However, influences are not clear as far as other retrieved parameters are concerned.

Results, which correspond to the case where the model error is equal to 2 K^2, are presented in Figs. 3(a) and 4(a). They show that measured and estimated surface temperatures match very well and that the RMSE is 0.55 K. Figs. 3(b) and 4(b) indicate that the data assimilation method developed can estimate the

sensible heat flux with satisfactory accuracy; the RMSE is about $40 \, \text{W} \cdot \text{m}^{-2}$, considering the error in LE and H measured in the field to be around $50 \, \text{W} \cdot \text{m}^{-2}$. Retrieved latent heat fluxes are not as good as sensible heat fluxes, as shown in Figs. 3(c) and 4(c), with an RMSE equal to about $65 \, \text{W} \cdot \text{m}^{-2}$. In particular, estimated LE values are systematically biased low largely during the nighttime of Julian days 242 and 251, and several LE values during the daytime of Julian days 244 and 249 are biased high. Control variables, including modeling effective surface temperature, bulk transfer coefficient for heat, and daily averaged evaporative fraction, are adjusted to minimize mostly the misfit between modeling surface temperature and its observed counterpart. As a result, accurate surface temperatures are retrieved and so do sensible heat fluxes in accordance with (3). Since daily averaged EF are retrieved in this study and approximate constant EF are held only around the local noon [21], [22], large biases will occur when patterns greatly differ
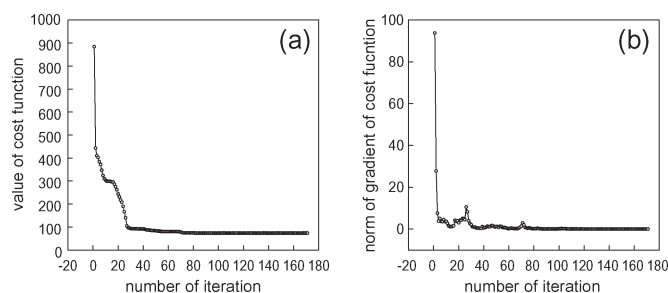
Fig. 5. Performance of cost function and its gradient in the course of minimization for a period from Julian day 231 to 240. (a) Value of the cost function. (b) Norm of the gradient of the cost function.

between LE and H. The discussions above indicate that the relatively high RMSE of the retrieved latent heat flux stems from some systematic errors since the parameterization for water balance processes that are closely related to evapotranspiration is rather simple in this letter. However, the whole retrieved results are encouraging, although the RMSE of the retrieved latent heat flux is a little high compared to the aforementioned measurement uncertainties since there is no additional information introduced, such as soil texture and land cover type, in addition to the observed LST and a few meteorological variables.

Fig. 5 shows the performance of minimization of the cost function for a period from Julian day 231 to 240 in the case above. It can be seen that the optimization works effectively and efficiently. Both the value of the cost function and the norm of its gradient rapidly decline with the increase in the number of iteration cycles and reach stability after roughly 80 iterations. Minimizations in other assimilation windows show similar patterns.

IV. CONCLUSION

Quantitative estimation of turbulent fluxes between atmospheric boundary layer and land surface plays an important part in a wide range of applications. The data assimilation method has received more and more attention because of its advantages over other estimation methods. In this study, a simple land surface model has been developed based on the work by Caparrini *et al.* The variational data assimilation method was developed using the weak-constraint concept. Rather than using the representer method or manual derivation, direct evaluation of derivatives of the cost function through AD techniques was applied. This can greatly accelerate the speed of the data assimilation system. After the construction of the data assimilation system, different model errors were used to test it. The retrieval values were validated against the field measurements, and the results were very encouraging. The RMSEs for sensible and latent heat fluxes were around 40 and 60 W $\cdot$ m^{-2}, respectively. The eventual goal was to use this algorithm with satellite data on a regional scale. Much work needs to be done to improve this data assimilation system, such as the comparison between different optimization algorithms and the replacement of the land surface model used in this study with a more advanced and complex one. Research along these lines is on the way.

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