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Quantifying Drought Propagation from Soil Moisture to Vegetation Dynamics Using a Newly Developed Ecohydrological Land Reanalysis

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Supplement Material: Formulations of Coupled Land and Vegetation Data Assimilation System (CLVDAS)

S1. Land surface model

The LSM of CLVDAS, EcoHydro-SiB solves vertical interlayer flows using the one-dimensional Richards equation. Capillary suction and hydraulic conductivity are calculated by the van Genuchten's water retention model [1]. Transpiration is estimated by the photosynthesis-conductance model of Simple Biosphere model version 2 (SiB2) [2] which simultaneously calculates transpiration and net primary production (carbon assimilation). The other fluxes are also estimated using the parameterizations of SiB2. No groundwater module is included in EcoHydro-SiB.

EcoHydro-SiB can explicitly solve carbon balance. EcoHydro-SiB simulates carbon-pool dynamics by the following equations:

$$\frac{dC_{leaf}}{dt} = a_{leaf}NPP - (d_{leaf} + \gamma + \lambda)C_{leaf} \quad (1)$$

$$\frac{dC_{stem}}{dt} = a_{stem}NPP - d_{stem}C_{stem} \quad (2)$$

$$\frac{dC_{root}}{dt} = a_{root}NPP - d_{root}C_{root} \quad (3)$$

where C_{leaf}, C_{stem}, and C_{root} are the carbon pools of leaves (photosynthetically active part), stems (photosynthetically inactive part), and roots, respectively [g/m^2]. a_{leaf}, a_{stem}, and a_{root} are the carbon allocation fractions of leaves, stems, and roots, respectively, and $a_{leaf} + a_{stem} + a_{root} = 1$. NPP is the net primary production (mol m^{-2} s^{-1}) estimated by the SiB2 photosynthesis-conductance model, and d_{leaf}, d_{stem}, and d_{root} are the normal turnover rates of leaves, stems, and roots, respectively. γ and λ are the water- and temperature-related stress factors for leaves, respectively. The carbon allocation fractions are the function of water-related stress and light availability and are calculated by a parameterization proposed by [3]. The water-related stress factor is calculated from the vertical distribution of soil moisture:

$$\beta_T(i) = \min[1, \max(0, \frac{\theta_i - \theta_w}{\theta_o - \theta_w})], \quad (4)$$

$$\beta_{TOT} = \sum_{i=1}^{N} \beta_T(i) \times \left[Y(\Delta z_i \times i) - Y(\Delta z_i \times (i-1))\right], \quad (5)$$

$$Y(d) = 1 - B^d \quad (6)$$

$$\gamma = \gamma_{\max}(1 - \beta_{TOT})^4, \quad (7)$$

where β_T (i) is the Soil Moisture Index (SMI) of the *i*-th soil layer, θ_i is the volumetric soil moisture of the *i*-th soil layer, θ_w is the wilting point, and θ_o is the point of stress onset. To obtain θ_w and θ_o, we specify the corresponding suction pressure values and inversely solve the van Genuchten's water retention model. β_{TOT} is calculated by aggregating the SMI in the soil layers, weighted by the root biomass fraction, *Y*, which is estimated using the empirical relationship found by [4] (equation 6). *N* is the number of soil layers and Δz_i is the depth of each soil layer. *Y(d)* is the cumulative root fraction from the surface to depth *d* (cm) and *B* is the empirical parameter. $\gamma_{\max}$ is the maximum stress loss. Since the water-related stress factor affects the carbon pool dynamics, our simulated root-zone soil moisture is strongly related to vegetation dynamics. This parameterization of water-related stress was proposed by [5]. In EcoHydro-SiB, the empirical linear relationship between a carbon pool of leaves and LAI suggested by [6] is used:

$$LAI = SLA \times C_{leaf}, \quad (8)$$

where *SLA* is the specific leaf area which indicates leaf thickness (m^2/kg).

S2. Radiative transfer model

To directly assimilate brightness temperature observations into a LSM instead of assimilating derived soil moisture and vegetation products, a RTM is needed to convert the land surface condition to microwave brightness temperature. The input data of the RTM are surface soil moisture, surface soil temperature, and LAI, which is calculated by EcoHydro-SiB.

The microwave radiative transfer of a land surface and a vegetation canopy is calculated by the tau-omega model proposed by [7]:

$$T_b^{p,f} = T_{bs}^{p,f}\exp(-\tau_c) + (1-\omega_c)T_c(1-\exp(-\tau_c)) + R_{p,f}(1-\omega_c)T_c(1-\exp(-\tau_c))\exp(-\tau_c) \quad (9)$$

where $T_b^{p,f}$ is the brightness temperature at radiometer level (note that we can neglect atmospheric contribution), $T_{bs}^{p,f}$ is the brightness temperature at ground level and $T_{bs}^{p,f} = (1-R_{p,f})T_s$, T_s and T_c are the physical land surface temperature and canopy temperature, respectively, ω_c is the single scattering albedo of the canopy, $R_{p,f}$ is the reflectivity of the land surface, and subscripts *p* and *f* reveal the polarization (vertical or horizontal), and the frequency, respectively. The first, second, and third terms on the right-hand side of (9) describe the emission from the land surface attenuated by the canopy, the emission from the canopy, and the emission from the canopy reflected by the land surface, respectively. The reflectivity of the land surface is the function of surface soil moisture and calculated by an Advanced Integral Equation Model (AIEM) with the incorporation of a shadowing effect [8]. τ_c is the vegetation optical depth (VOD), which is calculated using:

$$\tau_c = \frac{b'\lambda_c{}^x VWC}{\cos\theta}, \quad (10)$$

where b' is the vegetation parameter which is independent of wavelength (λ_c), *x* is a parameter which depends on wavelength (in shorter wavelength, microwave is easier to be attenuated by vegetation water) and θ is the incident angle. VWC is the vegetation water content. VWC can be directly related to LAI using the function proposed by [9]:

$$VWC = \exp(LAI / y) - 1 \quad (11)$$

with the empirical parameter y. Equations (8-11) relate vegetation dynamics calculated by Ecohydro-SiB to microwave brightness temperature. The RTM has been validated by in-situ observation experiments [8,10,11].

S3. Data assimilation

The PF is an ensemble data assimilation method. Ensemble data assimilation is a Monte Carlo estimation of Bayes' theorem:

$$p(x_t \mid y_{1:t}) \propto p(y_t \mid x_t) p(x_t \mid y_{1:t-1}) \quad (12)$$

where $p(x_t \mid y_{1:t})$ is the probability of the model state *x* at time *t*, given all observations up to time *t*. In the PF, the two factors in the right hand side of (12) are obtained by an ensemble calculation of a numerical model *f*:

$$p(x_t \mid y_{1:t-1}) \approx \frac{1}{N_e} \sum_{i=1}^{N_e} \delta(x_t - f(x_{t-1}^i)) \quad (13)$$

$$p(y_t \mid x_t) = g(y_t \mid x_t) \quad (14)$$

where *Ne* is the ensemble size, x^i is the realization of the model state provided by the ensemble member (or particle) *i*,, $\delta()$ is the Direc delta function. The function g is the potential function. In this study, the Gaussian distribution of observation errors is assumed and the conditional probability can be estimated as the following equation:

$$g(y_t \mid x_t) \propto \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2} \frac{(y_t - h(x_t))}{\sigma^2} \right] \quad (15)$$

where σ is an observation error and h is an observation operator which projects the model state onto the observation space. In CLVDAS, the RTM works as the observation operator. Please note that we show the conditional probability in the case that a single observation is assimilated for brevity. If there are multiple observations to be assimilated, which is the case of this study, σ should be replaced with a variance-covariance error matrix.

In CLVDAS, the sampling-importance-resampling filter (e.g., [12,13,14,15]) is used to do the analysis update of equation (12). This type of PF is widely applied to a LSM and a hydrological model (e.g., [12,16]). First, particles which are far from observations are rejected in the analysis step. We calculate the probability of the selections (survival rate $P_S(x_t^i)$) for each particle. The survival rate of the particle i is defined as (Remy et al. 2012):

$$P_s(x_t^i) = \frac{g(x_t^i)}{\max\limits_{j\in A} g(x_t^j)} \quad (16)$$

where A is the set which includes all prior particles. We select survived particles according to their survival rates.

Resampling particles is needed to replace rejected particles. Resampling is applied by copying the surviving particles based on the weights of the particles:

$$w_t^i = \frac{g(x_t^i)}{\sum\limits_{j\in S} g(x_t^j)} \quad (17)$$

where w_t^i is the weight of the particle i and S is the set which includes the surviving particles. The weights are calculated only for the surviving particles and $\sum\limits_{i\in S} w_t^i = 1$. In this resampling step, the posterior given by (12) is approximated as:

$$p(x_t \mid y_{1:t}) \approx \sum_{i\in S} w_t^i \delta(x_t - f(x_{t-1}^i)) \quad (18)$$

The surviving particles are resampled according to their weights using multinomial draws until the original number of particles is recovered. After the resampling, we add the fluctuations to soil moisture in all soil layers and LAI of the particles to maintain the diversity of the particles. Perturbing particles contributes to preventing the filter degeneracy, in which all but one particles have extremely small weights. Please note that the resampling step inevitably breaks water balance in the LSM, which is the case of most of conventional data assimilation methods, such as ensemble Kalman filter and variational methods. Uncertainty in model parameters and meteorological forcings is not considered in our PF framework.

In CLVDAS, the model state vector for PF, x_t^i has soil moisture in all soil layers, biomass pools (including LAI), and temperature. Although satellite microwave remote sensing can observe only surface soil moisture (θ_1) and vegetation dynamics (LAI), we can adjust the unobservable variables in x_t^i (i.e. subsurface soil moisture) by the PF. Using the correlations between vegetation dynamics and subsurface soil moisture sampled by particles, CLVDAS can improve the skill of EcoHydro-SiB to simulate subsurface soil moisture which is not directly observed by satellites [17].

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