



1	Do surface lateral flows matter for data assimilation of soil moisture observations
2	into hyperresolution land models?
3	Running title: HYPERRESOLUTION LAND DATA ASSIMILATION
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Abstract

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It is expected that hyperresolution land modeling substantially innovates the simulation 14 of terrestrial water, energy, and carbon cycles. The major advantage of hyperresolution 15 16 land models against conventional one-dimensional land surface models is that hyperresolution land models can explicitly simulate lateral water flows. Despite many 17 18 efforts on data assimilation of hydrological observations into those hyperresolution land 19 models, how and when surface water flows driven by local topography matter for data assimilation of soil moisture observations has not been fully clarified. Here I perform two 20 21 minimalist synthetic experiments where soil moisture observations are assimilated into 22 an integrated surface-groundwater land model by an ensemble Kalman filter. A horizontal background error covariance provided by overland flows is important to adjust the 23unobserved state and parameter variables. However, the non-Gaussianity of the 24background error provided by the nonlinearity of a topography-driven surface flow harms 25 the performance of data assimilation. It is difficult to efficiently constrain model states at 26 27 the edge of the area where the topography-driven surface flow reaches by linear-Gaussian filters, which brings the new challenge in land data assimilation for hyperresolution land 28 29 models. This study highlights the importance of surface lateral flows in hydrological data assimilation. 30





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1. Introduction

34 Hyperresolution land modeling is expected to improve the simulation of terrestrial water, energy, and carbon cycles, which is crucially important for meteorological, hydrological 35 36 and ecological applications (see Wood et al. (2011) for a comprehensive review). While 37 conventional land surface models (LSMs) assume that lateral water flows are negligible at the coarse resolution and solve vertical one-dimensional Richards equation for the soil 38 moisture simulation (e.g., Sellers et al. 1996; Lawrence et al. 2011), currently proposed 39 hyperresolution land models, which can be applied at a finer resolution (<1km), explicitly 40 consider surface and subsurface lateral water flows (e.g., Maxwell and Miller 2005; Tian 41 et al. 2012; Shrestha et al. 2014; Niu et al. 2014). The fine horizontal resolution can 42resolve slopes, which are drivers of a lateral transport of water, and realize the fully 43 integrated surface-groundwater modeling. Previous works indicated that a lateral 44 transport of water plays an important role in terrestrial water and energy cycles (e.g., 45 Maxwell and Condon 2016; Ji et al. 2017; Fang et al. 2017) and land-atmosphere 46 interactions (e.g., Williams and Maxwell 2011; Keune et al. 2016). 47





Data assimilation has contributed to improving the performance of LSMs by fusing 49 50 simulation and observation. The grand challenge of land data assimilation is to estimate unobservable variables from observations by propagating observations' information into 5152 model's high dimensional state and parameter space. In previous works on the 53 conventional 1-D LSMs, many land data assimilation systems (LDASs) have been proposed to accurately estimate model's state and parameter variables, which cannot be 54 55 directly observed, by assimilating satellite and in-situ observations. For example, the 56 optimization of LSM's unknown parameters (e.g., hydraulic conductivity) has been 57 implemented by assimilating remotely sensed microwave observations (e.g., Yang et al. 2007; Yang et al. 2009; Bandara et al. 2014; Bandara et al. 2015; Sawada and Koike 2014; 58 Han et al. 2014). Kumar et al. (2009) focused on the correlation between surface and root-59 60 zone soil moistures to examine the potential of assimilating surface soil moisture observations to estimate root-zone soil moisture. Sawada et al. (2015) successfully 61 improved the simulation of root-zone soil moisture by the data assimilation of microwave 62 brightness temperature observations which include the information of vegetation water 63 content. Gravity Recovery and Climate Experiment total water storage observation has 64 65 been intensively used to improve the simulation of groundwater and soil moisture (e.g., Li et al. 2012; Houborg et al. 2012). Improving the simulation of state variables such as 66





soil moisture and biomass by LDASs has contributed to accurately estimating fluxes such 67 68 as evapotranspiration (e.g. Martens et al. 2017) and CO₂ flux (e.g., Verbeeck et al. 2011). 69 However, in most of the studies on the conventional 1-D LDASs, observations impacted 70 state and parameter variables only in a single model's horizontal grid which is identical to the location of the observation. The assumption that the water flows are restricted to 7172 vertical direction in LSMs makes it difficult to propagate observation's information 73 horizontally, which limits the potential of land data assimilation to fully use land hydrological observations. 74 75 The hyperresolution land models, which explicitly solve surface and subsurface lateral 76 77flows, provide a unique opportunity to examine the potential of land data assimilation to 78 propagate observation's information horizontally in a model space and efficiently use land hydrological observations. Previous works successfully applied Ensemble Kalman Filters 79 80 (EnKF) to 3-D Richards' equation-based integrated surface-groundwater models. For 81 example, Camporese et al. (2009) and Camporese et al. (2010) successfully assimilated synthetic observations of surface pressure head and streamflow into the Catchment 82 Hydrology (CATHY). Ridler et al. (2014) successfully assimilated Soil Moisture and 83 Ocean Salinity satellite-observed surface soil moisture into the MIKE SHE distributed 84

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hydrological model (see also Zhang et al. (2015)). Kurtz et al. (2016) coupled the Parallel 85 Data Assimilation Framework (PDAF) (Nerger and Hiller 2013) with the Terrestrial 86 System Modelling Framework (TerrSysMP) (Shrestha et al. 2014). The performance of 87 TerrSysMP-PDAF to assimilate soil moisture observations was evaluated by a simple 88 89 synthetic experiment (see also Zhang et al. (2018)). Those studies have significantly 90 contributed to fully assimilating the new high-resolution soil moisture observations such 91 as Sentinel-1 (e.g., Paroscia et al. 2013) 9293 Although the data assimilation of hydrological observations into hyperresolution land models has been successfully implemented in the synthetic experiments, it is unclear how 94 95 and when topography-driven surface lateral water flows matter for data assimilation of 96 soil moisture observations. Previous studies on data assimilation with high resolution models mainly focused on assimilating groundwater observations (e.g., Ait-El-Fquih et 97 98 al. 2016; Rasmussen et al. 2015; Hendricks-Franssen et al. 2008). There are some 99 applications which focused on the observation of soil moisture and pressure head in 100 shallow unsaturated soil layers. However, in those studies, topography-driven surface flow has not been considered in the experiment (Kurtz et al. 2016) or the role of them in 101

assimilating observations into the hyperresolution land models has not been quantitatively





103 discussed (Camporese et al. 2010; Camporese et al. 2009). This study aims at clarifying if surface lateral flows matter for data assimilation of soil moisture observations into 104 105 hyperresolution land models by a minimalist numerical experiment. 106 107 108 2. Methods 109 2.1. Model ParFlow is an open source platform which realizes fully integrated surface-groundwater 110 flow modeling (Kollet and Maxwell 2006; Maxwell et al. 2015). This parallel simulation 111 112 platform has been widely used as a core hydrological module in hyperresolution land models (e.g., Maxwell and Kollet 2008; Maxwell and Condon 2016; Fang et al. 2017; 113 Kurtz et al. 2016; Maxwell et al. 2011; Williams and Maxwell 2011; Shrestha et al. 2014). 114 A brief description on the method of ParFlow to simulate integrated surface-subsurface 115water flows can be found below and the complete description of ParFlow can be found in 116 117 Kollet and Maxwell (2006), Maxwell et al. (2015) and references therein. 118 In the subsurface, ParFlow solves the variably saturated Richards equation in three 119 120 dimensions.





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$$S_S S_W(h) \frac{\partial h}{\partial t} + \phi S_W(h) \frac{\partial S_W(h)}{\partial t} = \nabla \cdot \mathbf{q} + q_r$$
 (1)

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$$\mathbf{q} = -\mathbf{K}_{s}(\mathbf{x})k_{r}(h)[\nabla(h+z)\cos\theta_{x} + \sin\theta_{x}]$$
(2)

- 123 In equation (1), h is the pressure head [L]; z is the elevation with the z axis specified as
- upward [L]; S_S is the specific storage [L⁻¹]; S_W is the relative saturation; ϕ is the
- porosity [-]; q_r is a source/sink term. Equation (2) describes the flux \mathbf{q}
- 126 [LT⁻¹] by Darcy's law, and K_s is the saturated hydraulic conductivity tensor [LT⁻¹]; k_r
- is the relative permeability [-]; θ is the local angle of topographic slope (see Maxwell et
- al. 2015). In this paper, the saturated hydraulic conductivity is assumed to be isotropic
- 129 and a function of z:

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$$K_s = K_s(z) = K_{s,surface} \exp\left(-f\left(z_{surface} - z\right)\right)$$
(3)

- where $K_{s,surface}$ is the saturated hydraulic conductivity at the surface soil, and $z_{surface}$
- 132 is the elevation of the soil surface. The saturated hydraulic conductivity decreases
- 133 exponentially as the soil depth increases (Beven 1982). A van Genuchten relationship
- 134 (van Genuchten 1980) is used for the relative saturation and permeability functions.

Overland flow is solved by the two-dimensional kinematic wave equation. The dynamics

of the surface ponding depth, h [L], can be described by:

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$$\mathbf{k} \cdot [-K_s(z)k_r(h) \cdot \nabla(h+z)] = \frac{\partial \|h,0\|}{\partial t} - \nabla \cdot \|h,0\| \mathbf{v}_{sw} + q_r$$
(4)





In equation (4), **k** is the unit vector in the vertical and ||h,0|| indicates the greater value of the two quantities following the notation of Maxwell et al. (2015). If h < 0, equation (4) describes that vertical fluxes across the land surface is equal to the source/sink term q_r (i.e., rainfall and evapotranspiration). If h > 0, the terms on the right-hand side of equation (4), which indicate water fluxes routed according to surface topography, are active. v_{sw} is the two-dimensional depth-averaged water flow velocity [LT⁻¹] and estimated by the Manning's law:

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$$v_{sw} = \frac{\sqrt{S_{f,x}}}{\binom{n}{n}} h^{\frac{2}{3}}$$
 (5)

where $S_{f,x}$ and $S_{f,y}$ are the friction slopes [-] for the x- and y-direction, respectively; n is the Manning's coefficient [TL^{-1/3}]. In the kinematic wave approximation, the friction slopes are set to the bed slopes. The methodology of discretization and numerical method to solve equations (1-5) can be found in Kollet and Maxwell (2006).

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2.2. Data Assimilation

In this paper, the ensemble Kalman filter (EnKF) was applied to assimilate soil moisture observations into ParFlow. The general description of the Kalman filter is the following:

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$$\mathbf{x}^f(t) = \mathcal{M}[\mathbf{x}^a(t-1)]$$
 (6)





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$$\mathbf{x}^{a}(t) = \mathbf{x}^{f}(t) + \mathbf{K}[\mathbf{y}^{o} - \mathcal{H}\mathbf{x}^{f}(t)]$$
 (7)

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$$\mathbf{K} = \mathbf{P}^f \mathbf{\mathcal{H}}^T (\mathbf{\mathcal{H}} \mathbf{P}^f \mathbf{\mathcal{H}}^T + \mathbf{R})^{-1}$$
(8)

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$$\mathbf{P}^a = (\mathbf{I} - \mathbf{K}\mathbf{\mathcal{H}})\mathbf{P}^f$$
(9)

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I follow the notation of Houtekamer and Zhang (2016). In equation (6), a forecast model \mathcal{M} (ParFlow in this study) is used to obtain a prior estimate at time t, $x^f(t)$, from the 161 estimation at the previous time $x^a(t-1)$. In equation (7), a prior estimate $x^f(t)$ is 162 163 updated to the analysis state, $x^a(t)$, using new observations y^o . The Kalman gain matrix K, calculated by equation (8), gives an appropriate weight for the observations with an 164 error covariance matrix \mathbf{R} , and the prior with an error covariance matrix \mathbf{P}^f . To calculate 165 \mathbf{K} , the observation operator $\boldsymbol{\mathcal{H}}$ is needed to map from model space to observation space. 166 It should be noted that the equations (6-9) give an optimal estimation only when the model 167 and observation errors follow the Gaussian distribution. When the probabilistic 168 distribution of the error in either model or observation has a non-Gaussian structure, 169 results of the Kalman filter are suboptimal. This point is important to interpret the results 170 171 of this study.

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EnKF is the Monte Carlo implementation of equations (6-9). To compute the Kalman gain

matrix, **K**, ensemble approximations of $P^f \mathcal{H}^T$ and $\mathcal{H} P^f \mathcal{H}^T$ can be given by: 174





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$$\mathbf{P}^{f} \mathcal{H}^{T} \equiv \frac{1}{k-1} \sum_{i=1}^{k} \left(\mathbf{x}_{i}^{f} - \overline{\mathbf{x}^{f}} \right) (\mathcal{H} \mathbf{x}_{i}^{f} - \overline{\mathcal{H} \mathbf{x}^{f}})^{T}$$
 (10)

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$$\mathcal{H}P^f\mathcal{H}^T \equiv \frac{1}{k-1}\sum_{i=1}^k \left(\mathcal{H}x_i^f - \overline{\mathcal{H}x^f}\right) \left(\mathcal{H}x_i^f - \overline{\mathcal{H}x^f}\right)^T$$
 (11)

where x_i^f is the ith member of a k-member ensemble prior and $\overline{x^f} = \frac{1}{k} \sum_{i=1}^k x_i^f$ and

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$$\overline{\mathcal{H}x^f} = \frac{1}{k} \sum_{i=1}^k \mathcal{H}x_i^f$$
.

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Once $\overline{x^a} = \sum_{i=1}^k x_i^a$ (x_i^a is the ith member of a k-member ensemble analysis) and $P^a =$

181 $\frac{1}{k-1}\sum_{i=1}^k (x_i^a - \overline{x^a}) (x_i^a - \overline{x^a})^T$ are computed by equations (6-11), there are many

choices of an analysis ensemble. Although equations (6-11) can calculate the mean and

variance of the ensemble members, they do not tell how to adjust the state of the ensemble

members in order to realize the estimated mean and variance. There are many proposed

185 flavors of EnKF and one of the differences among them is the method to choose the

analysis x_i^a . In this paper, the Ensemble Transform Kalman Filter (ETKF; Bishop et al.

187 2001; Hunt et al. 2007) was used to transport forecast ensembles to analysis ensembles.

Please refer to Hunt et al. (2007) for the complete description of the ETKF and its

localized version, the Local Ensemble Transform Kalman Filter (LETKF). The open

source available at https://github.com/takemasa-miyoshi/letkf was used in this study as

the ETKF code library.

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In many ensemble Kalman filter systems, the ensemble spread tends to become

underdispersive without any ensemble inflation methods (Houtekamer and Zhang, 2016).

In this paper, the relaxation to prior perturbation method (RTPP) of Zhang et al. (2004)

was used to maintain an appropriate ensemble spread. In the RTPP, the computed analysis

197 perturbations are relaxed back to the forecast perturbations:

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$$\mathbf{x}_{i,new}^a = (1 - \alpha)(\mathbf{x}_i^a - \overline{\mathbf{x}^a}) + \alpha(\mathbf{x}_i^f - \overline{\mathbf{x}^f}), \ 0 \le \alpha \le 1 \ (12)$$

where α was set to 0.975 in this study.

In the data assimilation experiments, I adjusted pressure head by data assimilation so that

 x^f is pressure head. Since the surface saturated hydraulic conductivity was also adjusted,

 x^f includes log-transformed $K_{s,surface}$. Since I assimilated volumetric soil moisture

204 observations (y^o are observed volumetric soil moisture), the van Genuchten relationship

works as an observation operator \mathcal{H} in order to transport the model estimated pressure

head into the observable volumetric soil moisture in this study.

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2.3. Kullback-Leibler divergence





To evaluate the non-Gaussianity of the background error sampled by an ensemble, I used

211 the Kullback-Leibler divergence (KLD) (Kullback and Leibler 1951):

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$$D_{KL}(p,q) = \sum_{i} p(i) log \frac{p(i)}{q(i)}$$
 (13)

where $D_{KL}(p,q)$ is the KLD between two probabilistic distribution functions (PDFs), p

and q. If two PDFs are equal for all i, $D_{KL}(p,q) = 0$. A large value for $D_{KL}(p,q)$

215 indicates that the two PDFs, p and q, substantially differ from each other. Therefore,

the KLD can be used as an index to evaluate the closeness of two PDFs. It should be

217 noted that the KLD is not symmetric $(D_{KL}(p,q) \neq D_{KL}(q,p))$.

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3. Synthetic experiments

221 3.1. Simple 2-D slope with homogeneous hydraulic conductivity

222 3.1.1. Experiment Design

The synthetic experiment was implemented to examine how topography-driven surface lateral flows contribute to efficiently propagating observation's information horizontally in the data assimilation of soil moisture observation. Two synthetic reference runs were created by Parflow. The 2-D domain has a horizontal extension of 4000m and a vertical extension of 5m. The domain of the virtual slope was horizontally discretized into 40 grid





cells with a size of 100m and vertically discretized into 50 grid cells with a size of 0.10m. 228 229 The domain has a 25% slope. In two synthetic reference runs, it heavily rains only in the 230 upper half of the slope (2000m<x<4000m). A constant rainfall rate of 50mm/h was 231 applied for 3 hours and then the period with no rainfall and evaporation of 0.075mm/h 232lasted for 117 hours. This 120-hour rain/no rain cycle was repeatedly applied to the 233 domain. There is no rainfall in the lower half of the slope (0m<x<2000m). The 234 configurations described above were schematically shown in Figure 1a. The parameters of the van Genuchten relationship, alpha and n, were set to 1.5 [m⁻¹] and 1.75, respectively. 235The porosity, ϕ in equation (1), was set to 0.40. The Manning's coefficient, n in equation 236 (5), was set to 5.52×10^{-6} [m^{-1/3}h]. These clayey soil properties described above are 237 applied to the whole domain. The groundwater table was located at z=3m and the 238 239 hydrostatic pressure gradient was assumed for the initial pressure heads in the unsaturated 240 soil layers.

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The difference between two synthetic reference runs is the value of saturated hydraulic conductivity. The surface saturated hydraulic conductivity, K_{s,surface} in equation (3), was set to 0.005 [m/h] in one reference, and 0.02 [m/h] in the other. These surface saturated hydraulic conductivities described above are applied to the whole domain.





Figure 1 shows the difference of the response to heavy rainfall between the two synthetic reference runs. In the case of the low saturated hydraulic conductivity (hereafter called the LOW_K reference), larger surface lateral flows are generated than the case of the high saturated hydraulic conductivity (hereafter called the HIGH_K reference). In the LOW_K reference, the topography-driven surface lateral flows reach the left edge of the domain (Figure 1b). In the HIGH_K reference, supplied water moves vertically rather than horizontally and the topography-driven surface flow reaches around x = 1000~1500m (Figure 1d).

For the data assimilation experiment, an ensemble of 50 realizations was generated. Each ensemble member has different saturated hydraulic conductivity and rainfall rate. Lognormal multiplicative noise was added to surface saturated hydraulic conductivity and rainfall rate of the synthetic reference runs. This specification of uncertainty in rainfall was also adopted in Crow et al. (2011). The two parameters of the lognormal distribution, commonly called μ and σ , were set to 0 and 0.15, respectively. The initial groundwater depth of each ensemble member was drawn from the uniform distribution from 2.0m to 3.5m. The hydrostatic pressure gradient was assumed for the initial pressure heads in the unsaturated soil layers.





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The virtual hourly observations were generated by adding the Gaussian white noise whose mean is zero to the volumetric soil moisture simulated by the synthetic reference runs. The observation error (the standard deviation of the added Gaussian white noise) was set to 0.05 m³/m³. It was assumed that the volumetric soil moistures can be observed in every model's soil layer from surface to the depth of 1m at the specific location. The two scenarios of the observation's location are provided. In the first scenario (hereafter called the UP_O scenario), the volumetric soil moisture at the upper part of the slope (x = 2500m) was observed. In the UP O scenario, I could observe the volumetric soil moisture in the upper part of the slope where it heavily rains and tried to infer the soil moisture in the lower part of the slope where it does not rain by propagating the observation's information downhill. In the second scenario (hereafter called the DOWN O scenario), the volumetric soil moisture at the lower part of the slope (x = 1500m) was observed. In the DOWN O scenario, I could observe the volumetric soil moisture in the lower part of the slope where it does not rain and tried to infer the soil moisture in the upper part of the slope where it heavily rains by propagating the observation's information uphill.





281 Since I had the two synthetic reference runs (the HIGH K and LOW K references) and 282 the two observation scenarios (the UP_O and DOWN_O scenarios), I implemented totally 283 four data assimilation experiments. Table 1 summarizes the data assimilation experiments implemented in this study. For instance, in the HIGH K-UP O experiment, I chose the 284285 HIGH K reference and generated an ensemble of 50 realizations from the HIGH K 286 reference. The soil moisture observations were generated from the HIGH K reference at 287 the location of x = 2500m and assimilated into the model every hour. The simulated 288 volumetric soil moisture of the data assimilation experiment was compared with that of 289 the HIGH K reference.

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In addition to the data assimilation (DA) experiments, I implemented the NoDA experiment (also called the open-loop experiment in the literature of the LDAS study) in which the ensemble was used but no observation data were assimilated. As evaluation metrics, root-mean-square-error (RMSE) was used:

295 RMSE =
$$\sqrt{\frac{1}{k} \sum_{i=1}^{k} (F_i - T)^2}$$
 (14)

where k is the ensemble number, F_i is the volumetric soil moisture simulated by the i-th member in the DA or NoDA experiment, T is the volumetric soil moisture simulated by the synthetic reference run.





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To evaluate the impact of data assimilation, the improvement rate (IR) was defined and

301 calculated by the following equation:

$$302 IR = \frac{\overline{RMSE_{DA}} - \overline{RMSE_{NODA}}}{\overline{RMSE_{NODA}}} (15)$$

303 where $\overline{RMSE_{DA}}$ and $\overline{RMSE_{NoDA}}$ are time-mean RMSE of the DA and NoDA

304 experiments, respectively. The negative IR indicates that data assimilation positively

305 impacts the simulation of soil moisture. The metrics described above was calculated in

306 the whole domain. In the DA experiment, soil moisture values before the update by ETKF

307 (i.e. initial guess) were used to calculate the metrics.

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Four of 120-hour rain/no rain cycles were applied so that the computation period was 480

hours. The spin-up results in the first 120 hours were not used to calculate the evaluation

metrics. Since the steady state of groundwater level is not the scope of this paper, the long

312 spin-up is not absolutely necessary.

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3.1.2. Results





Figure 2a shows the IR of the LOW K-UP O experiment. The time series of the DA and 316 NoDA experiment and the synthetic reference run in the LOW_K-UP_O experiment can 317 318 be found in Figure S1. The data assimilation efficiently propagates the information of the 319 observations located in the upper part of the slope (see the black arrow in Figure 2a) both 320 horizontally and vertically. RMSE is reduced by data assimilation not only directly under 321 the observation but also the lower part of the slope where it does not rain. The optimized 322 $K_{s,surface} \approx 0.00508$ [m/h] is also accurate. However, the increase of RMSE by data 323 assimilation can be found at the left edge of the domain, which is far from the location of 324 the observation. The impact of data assimilation on the surface soil moisture simulation is small because the RMSE of the NoDA experiment is already small ($\leq 0.01 \text{m}^3/\text{m}^3$) there 325326 in the case of the LOW K reference so that any improvements there do not make sense. 327 Figure 2b shows the IR of the LOW_K-DOWN_O experiment (see also Figure S2 for 328 time series). The IR's spatial pattern of the LOW K-DOWN O experiment is similar to 329 330 that of the LOW_K-UP_O experiment. It is promising that I can accurately infer soil 331 moisture in the region where it heavily rains from the shallow soil moisture observations in the region where it does not rain. The optimized $K_{s,surface} \approx 0.00512$ [m/h] is also 332 333 accurate.



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Figure 3a shows the difference of time-mean RMSEs ($\overline{RMSE_{DA}}$ in equation (15)) 335 336 between the LOW K-UP O and LOW K-DOWN O experiments. Although observing 337 the lower part of the slope slightly improves the soil moisture simulation at the left edge 338 of the domain compared with observing the upper part of the slope, there are few 339 differences between the UP_O and DOWN_O scenarios in the case of the LOW_K 340 reference. The soil moisture observations have large representativeness and I can 341 efficiently infer soil moisture in the soil columns which are horizontally and vertically far 342 from the observations. 343 Figure 2c shows the IR of the HIGH K-UP O experiment (see also Figure S3 for time 344 345 series). The data assimilation significantly reduces RMSE of the soil moisture simulation 346 directly under the observations (see the black arrow in Figure 2c), which indicates that 347 the data assimilation efficiently propagates the information of the observations vertically. 348 The saturated hydraulic conductivity is also accurately optimized ($K_{s,surface} \approx 0.0204$ 349 [m/h]. However, the impact of the data assimilation on the soil moisture simulation in the 350 lower part of the slope around x=1500m is marginal although there are large RMSE in





the NoDA experiment (>0.05m³/m³) at the edge of the area where topography-driven 351 surface flow reaches in the HIGH_K reference (see Figure 1d). 352353 Figure 2d shows the IR of the HIGH K-DOWN O experiment (see also Figure S4 for 354 355 time series). Although the observations in the lower part of the slope (see the black arrow 356 in Figure 2d) significantly improve the soil moisture simulation in the downstream area 357 of the observation and accurately optimize $K_{s,surface} \approx 0.0208$ [m/h], the impact of the data assimilation on the shallow soil moisture simulation around x=500~1000m is 358 marginal. As I found in the LOW K-DOWN O experiment, the shallow soil moisture 359 360 observations in the region where it does not rain can improve the soil moisture simulation in the region where it heavily rains. However, the IR of the HIGH K-DOWN O 361 experiment in the upper part of the slope is smaller than that of the LOW K-DOWN O 362 experiment (see Figure 2b and 2d). 363 364 365 The high representativeness of the observations which I found in the case of the LOW K 366 reference cannot be found in the case of the HIGH K reference. Figure 3b shows the difference of time-mean RMSEs ($\overline{RMSE_{DA}}$ in equation (15)) between the HIGH_K-367 368 UP O and HIGH K-DOWN O experiments. Compared with the LOW K reference case





(Figure 3a), there are significant differences between the UP_O and DOWN_O scenarios in the case of higher saturated hydraulic conductivity. In this case, the vertical propagation of the observations' information is more efficient than the horizontal propagation.

The relatively low efficiency of the data assimilation and the low representativeness of the soil moisture observations in the case of the HIGH_K reference are caused by the non-Gaussian background error distribution. I calculated KLD by comparing the PDF of the NoDA ensemble (p in equation (13)) with the Gaussian PDF which has the mean and variance of the NoDA ensemble (q in equation (13)). Figure 4 shows that the NoDA ensemble in the case of the HIGH_K reference has stronger non-Gaussianity than the case of the LOW_K reference especially in the shallow soil layers. The strong non-Gaussianity of the NoDA ensemble generated from the HIGH_K reference can be found at the edge of the area where the topography-driven surface flow reaches (Figure 1d). Figure 5 shows that there is the bifurcation of the ensemble in this region when the ensemble is generated from the HIGH_K reference. The process of topography-driven surface flows is switched on if and only if the surface soil is saturated (see equation (4)) so that the ensemble tends to be bifurcated into the members with surface flows and without surface flows. As I mentioned in section 2.2, in the ETKF, the state and parameter variables are adjusted





assuming the Gaussian PDF of the model's error and the linear relationship between observed variables and unobserved variables. Therefore, the non-Gaussianity of the prior ensemble induced by the strong non-linear dynamics of surface lateral flows makes the ETKF inefficient. It is more difficult to reconstruct 3-D fields of soil moisture in high conductivity soils since the 1-D vertical water movement is more dominant. The absolute RMSE of the NoDA experiment in the HIGH_K reference is larger than the LOW_K reference in many places (not shown). Please note that the non-Gaussianity can also be found in the LOW_K reference at the edge of the domain (x=500m) due to the non-linear dynamics, which causes the degradation of the soil moisture simulation in the LOW_K-UP O experiment (see Figure 2a).

One of the major simplifications in this experiment is spatially homogeneous surface saturated hydraulic conductivity. The optimization of it can efficiently improve the soil moisture simulation in the whole domain. However, the optimization of this homogeneous surface saturated hydraulic conductivity has a limited impact on the soil moisture simulation. Figure S5 shows the IR of the HIGH_K-DOWN_O experiment where the parameter optimization by ETKF is switched off. Even if I do not optimize the surface saturated hydraulic conductivity, I could obtain the similar IR to the original





405 experiment and the shallow soil moisture observations in the region where it does not rain 406 can improve the soil moisture simulation in the region where it heavily rains. The 407 horizontal propagation of the observations' information shown in this experiment was 408 brought out not only by the optimization of spatially homogeneous saturated hydraulic 409 conductivity but also by the horizontal error correlation due to topography-driven surface 410 flows. 411 Please note that the improvement of the soil moisture simulation cannot be found if the 412 topography-driven surface flow is neglected. Figure S6 shows the IR of the LOW-413 K DOWN-O experiment where the topography-driven surface flow is neglected in the 414 ParFlow simulation. The imperfect model physics of ParFlow substantially degrades the 415 416 skill to simulate soil moisture and data assimilation cannot compensate this degradation. This point will also be discussed in the section 3.2 more deeply. 417 418 419 3.2. Simple 3-D slope with heterogeneous hydraulic conductivity 3.2.1. Experiment design 420 To further demonstrate how land data assimilation works with topography-driven surface 421 422 lateral flows, I implemented another synthetic experiment which is more realistic than

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424 and a vertical extension of 3m. The domain was horizontally discretized into 40×40 grid cells with a size of 100m×100m and vertically discretized into 30 grid cells with a size 425 426 of 0.1m. The domain has a 10% slope in both x and y directions (see Figure 6a). The 427 parameters of the van Genuchten relationship, porosity and Manning's coefficient were 428 set to the same variables for the synthetic experiment in section 3.1. 429 430 The spatially heterogeneous surface saturated hydraulic conductivity was generated following Kurtz et al. (2016). The field of $log_{10}(K_{s,surface})$ was generated by two-431 432 dimensional unconditioned sequential Gaussian simulation. A Gaussian variogram with nugget, sill, and range values of $0.0 \log_{10}(m/h)$, $0.1 \log_{10}(m^2h^2)$, and 12 model 433 grids (1200m), respectively was used to simulate the spatial distribution of 434 $log_{10}(K_{s,surface})$. A constant value of -2.30 $log_{10}(m/h)$ (i.e. 0.005 (m/h)) was added 435 436 to the generated field. Subsurface saturated hydraulic conductivity was calculated by 437 equation (3). An ensemble of 51 realizations of $log_{10}(K_{s,surface})$ was generated and one of them was chosen as a synthetic reference (Figure 6a). The remaining 50 members were 438

that shown in section 3.1. The 3-D domain has a horizontal extension of 4000 m×4000m

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used for data assimilation experiments.





441 A rainfall rate R(x,y) (mm/h) was modelled by a logistic function:

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$$R(x,y) = \frac{R_{max}}{1+100\exp(-0.2 \times \frac{x+y}{2})}$$
 (16)

443 where x and y are horizontal grid numbers $(1 \le x \le 40, 1 \le y \le 40)$. In the synthetic reference, the maximum rainfall rate in the domain, R_{max} , was set to 50 (mm/h) (Figure 444 445 6b). This rainfall rate was applied for 3 hours and then the period with no rainfall and 446 evaporation of 0.075mm/h lasted for 117 hours. For data assimilation experiment, an 447ensemble of 50 realization of R(x,y) was generated by adding a lognormal 448 multiplicative noise to R_{max} of the synthetic reference. The two parameters of the 449 lognormal distribution, commonly called μ and σ , were set to 0 and 0.15, respectively. 450 451 Figure 6c shows the distribution of surface soil moisture in the synthetic reference run. 452 Strong rainfall rate applied in the upper part of the slope generates the topography-driven surface lateral flows. The virtual hourly observations were generated by adding the 453 Gaussian white noise, whose mean is zero and standard deviation is 0.05 m³/m³, to the 454 volumetric surface soil moisture simulated by the synthetic reference run. Unlike the 455 456 experiment in section 3.1, only surface soil moisture can be observed in this synthetic 457 experiment, which makes this experiment more realistic since satellite sensors can observe only surface soil moisture. Three different observing networks with different 458





observation densities were used (Figure 7). The observing networks shown in Figure 7a,

7b, and 7c have totally 1, 9, and 361 observations and are called obs1, obs9, and obs361,

respectively.

In the DA experiments, those virtual observations of surface soil moisture were assimilated every hour to adjust pressure head and saturated hydraulic conductivity. As I did in the section 3.1, the NoDA experiments were also implemented. The two different configurations of ParFlow were used for both DA and NoDA experiments. In the first configuration, called OF, Parflow explicitly solves overland flows. In the second configuration, called noOF, Parflow assumes the flat terrain for surface flows so that no overland flows are generated. Since the synthetic reference run explicitly considers the topography-driven surface flow, the configuration of noOF assumes that the model physics is imperfect. I implemented 8 numerical experiments which are summarized in Table 2. For example, the OF_DA_obs9 experiment is the data assimilation experiment with the observing network shown in Figure 7b, in which Parflow explicitly solves the topography-driven surface flow. The noOF_NoDA is the model run without assimilating observations, in which Parflow does not consider the topography-driven surface flow.





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3.2.2. Results

479 Figure 8a shows the RMSE of soil moisture simulation of a second soil layer (i.e. 10-480 20cm soil depth) in all 8 experiments (the same conclusion described below can be 481 obtained by analyzing all of shallow soil layers). When Parflow explicitly solves the 482 topography-driven surface flow, data assimilation substantially reduces RMSE of the soil 483 moisture simulation (green bars in Figure 8a). The OF_DA_obs361 experiment has the 484 smallest RMSE so that a denser observing network is beneficial to estimate soil moisture. 485 Figure 8b shows the RMSE of the estimation of saturated surface hydraulic conductivity 486 in all 8 experiments. Data assimilation also reduces the uncertainty in model's parameters 487 (green bars in Figure 8b). However, the OF DA obs361 experiment has larger RMSE 488 than the other DA experiments. This is because the adjustment of hydraulic conductivity 489 in the OF_DA_obs361 experiment is overfitting to observations. In the OF configuration, 490 there are two sources of errors, rainfall rate and hydraulic conductivity. However, data 491 assimilation can adjust only hydraulic conductivity so that the assimilation of a large 492number of observations causes overfitting to mitigate the impact of errors in rainfall rate.





494 The noOF NoDA experiment has larger RMSE than the OF NoDA experiment due to the negligence of the topography-driven surface flow. In the noOF configuration, data 495496 assimilation also improves the soil moisture simulation (red bars in Figure 8a). The 497 noOF DA obs361 experiment outperforms the OF NoDA experiment so that data 498 assimilation with a dense observing network can compensate the negative impact of 499 neglecting the topography-driven surface flow. Although data assimilation positively 500 impacts the parameter estimation, the denser observing network cannot reduce RMSE of 501 hydraulic conductivity estimation (red bars in Figure 8b). The negative impact of the 502 dense observations in the noOF DA obs361 experiment on the parameter estimation is 503 larger than in the OF DA obs361 experiment. In addition to rainfall rate and hydraulic 504 conductivity, the imperfect model physics (i.e., no topography-driven surface flow) is the 505 source of error in the noOF configuration. The assimilation of a large number of 506 observations causes overfitting because it mitigates the impact of all systematic errors 507 which comes from three different sources only by adjusting hydraulic conductivity. 508 509 Figure 9 shows the difference of RMSE of the soil moisture simulation between the DA 510 experiments and the OF_NoDA experiment. In the DA configuration, the improvement 511 of the soil moisture estimation can be found in a large area even if there is a single

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observation in the center of the domain (Figure 9a). Figure 9b shows that the increase of the number of observations substantially improves the soil moisture simulation in the region which is affected by topography-driven surface flow (see also Figure 6c). However, the skill to simulate soil moisture is severely degraded in the lower-left corner of the domain, which causes the stalled improvement from the OF DA obs1 experiment to the OF DA obs9 experiment shown in Figure 8a. Figure 9c shows that although the far denser observing network can slightly mitigate this degradation, increasing the number of observations cannot efficiently solve this issue. This degradation is caused by the bifurcation of ensemble members at the edge of the area where topography-driven surface flow reaches (Figure S7). Figure 10 shows KLD in the OF NoDA and noOF NoDA experiments. Figure 10a clearly shows that the ensemble simulation generates the strong non-Gaussianity at the edge of the area where topography-driven surface flow reaches, which harms the efficiency of the ETKF. This finding is consistent to what I found in the previous experiment in section 3.1. In the noOF configuration, there are large errors in the area around 500<=x, y <=1500

since the increase of soil moisture in this area is caused by the topography-driven surface

flow which is neglected in the noOF configuration. Figures 9d and 9e show that the sparse





observations cannot completely remove this degradation caused by imperfect model physics. Figure 9f shows that the noOF_DA_obs361 can outperform the OF_NoDA experiment in exchange for the degradation of the parameter estimation as I found in Figure 8. The unstable behavior of the ETKF found in the OF configuration does not occur when the topography-driven surface flow is neglected since the ensemble simulation does not generate the non-Gaussian background distribution (Figure 10b).

4. Discussion

In this study, I revealed that the hyperresolution integrated surface-subsurface hydrological model gives the unique opportunity to effectively use soil moisture observations to improve the soil moisture simulation in terms of a horizontal propagation of observation's information in a model space. I found that the explicit calculation of the topography-driven surface flow has an important role in propagating the information of soil moisture observation horizontally by data assimilation even if there is considerable heterogeneity of meteorological forcing. It is possible that the soil moisture observations





in the area where it does not heavily rain can improve the soil moisture simulation in the severe rainfall area.

This potential cannot be brought out in the conventional 1-D LSM where sub-grid scale surface runoff is parameterized and the surface flows in one grid do not move to the adjacent grids. Neglecting the topography-driven surface flow causes significant bias in the soil moisture simulation and this bias cannot be completely mitigated by data assimilation especially in the case of a sparse observing network. However, I found that even if the model uses imperfect physics which neglects the interaction between topography-driven surface lateral flows and subsurface soil moisture, assimilating soil moisture observations into the model's three-dimensional state and parameter space can improve the skill to estimate soil moisture and hydraulic conductivity. This finding implies that the conventional 1-D LSM with full 3-D data assimilation may be a computationally cheap and reasonable choice in some cases although many land data assimilation systems with the conventional 1-D LSM currently update state variables only in a single model's horizontal grid which is identical to the location of the observation.



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The conventional ensemble data assimilation (i.e. ETKF) severely suffers from the non-Gaussian background error PDFs caused by the strongly nonlinear dynamics of the topography-driven surface flow. The efficiency of ETKF to propagate the information of observations horizontally in the model space is limited in the edge of the area where the topography-driven surface flow reaches. Please note that the low representativeness of the soil moisture observations in the case of the HIGH K reference shown in section 3.1 is due to the core assumption of the Kalman filter that the error PDFs follow the Gaussian distribution so that the increase of the ensemble size cannot solve this issue. I implemented the data assimilation experiment in the case of the HIGH K reference with an ensemble size of 500, which is 10 times larger than the original experiments shown in section 3.1, and found no significant improvement of the soil moisture simulation (not shown). Some studies revealed that volumetric soil moisture distributions follow the Gaussian distribution better than pressure head so that they recommend to update soil moisture as a state variable (e.g., Zhang et al. (2018)). However, in this study, I found that volumetric soil moisture distributions have bimodal structure and do not follow the Gaussian distribution. The limitation of ensemble Kalman filters found in this study does not depend on the updated state variables.





The spatially dense soil moisture observations are needed to efficiently constrain state variables at the edge of surface flows. High resolution soil moisture remote sensing based on satellite active and passive combined microwave observations at the 1 km spatial resolution (e.g., He et al. 2018) and the assimilation of those data (Lievens et al. 2017) may be important in the era of the hyperresolution land modeling. High resolution observations of surface inundated water from satellite imagery with a spatial resolution finer than 100 m (e.g., Sakamoto et al. 2007; Arnesen et al. 2013) may also be useful. However, the numerical experiment in section 3.2 implies that the dense observing network of surface soil moisture cannot completely remove the negative impact of the non-Gaussian background PDF.

Since there is a nonlinear relationship between observed and unobserved variables sampled by an ensemble, a localization method, which spatially restricts the impact of assimilating observations, is crucially needed for real-world applications. The results of this study imply that the optimal localization radius strongly depends on the model parameter (i.e. saturated hydraulic conductivity). Rasmussen et al. (2015) successfully applied the adaptive localization method (Anderson 2007; Bishop and Hodyss 2009) to the data assimilation of groundwater observations into a hydrological model. It is





600 appropriate to adaptively determine the localization radius considering the lack of prior 601 knowledge of how soil moisture simulated by an ensemble is horizontally correlated. 602 603 Reducing the uncertainty in rainfall positively impacts the efficiency of data assimilation 604 since the bifurcation of simulated soil moisture found in Figure 5c is originally induced 605 by the uncertainty in rainfall. Although assimilating land hydrological observations to 606 improve the rainfall input has been intensively investigated (e.g., Sawada et al. 2018; Herrnegger et al. 2015; Crow et al. 2011; Vrugt et al. 2008), it has yet to be applied to 607 608 hyperresolution land models. Please note that the parameters of the lognormal distribution 609 to model the uncertainty in rainfall were specified to make the rainfall PDF similar to the 610 Gaussian distribution. I chose the lognormal distribution in order not to generate negative 611 rainfall values and I intended not to introduce non-Gaussianity into the external forcing. 612 The rainfall input which follows the Gaussian PDF was transformed into the non-613 Gaussian PDF of the background error by the strongly nonlinear dynamics of the 614 topography-driven surface flow. 615 616 To explicitly consider non-Gaussianity and non-linear relationship between observed and unobserved variables induced by the topography-driven surface flow, the particle filters 617





may be useful. The particle filter can represent a probability distribution (including non-Gaussian distributions) directly by an ensemble. Particle filters have been intensively applied to conventional 1-D LSMs (e.g., Sawada et al. 2015; Qin et al. 2009) and lumped hydrological models (e.g., Yan and Moradkhani 2016; Vrugt et al. 2013). Although particle filtering in a high dimensional system suffers from the "curse of dimensionality" (e.g., Snyder et al. 2008), the applicability of particle filtering to 3-D hyperresolution land models should be assessed in the future.

Since the synthetic numerical experiments in this paper adopted the simple and minimalistic setting, the findings of this paper may be exaggerated. There are no river channels in the synthetic experiment so that the skill to simulate river water level and discharge cannot be discussed, which is the major limitation of this study. The simple representation of soil properties is also a limitation of this study. In future work, the contributions of the topography-driven surface runoff process to the data assimilation of hydrological observations should be quantified in real-world applications. In addition, in the virtual experiment of this paper, I neglected some of the important land processes such as transpiration, canopy interception, snow, and frozen soil. Although they are generally not primary factors in the propagation of overland flows generated by extreme rainfall,

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which has a shorter timescale than the neglected processes, those processes should be considered in the future.

5. Conclusions

The simplified synthetic experiments of this study indicate that topography-driven lateral surface flows induced by heavy rainfalls do matter for data assimilation of hydrological observations into hyperresolution land models. Even if there is extreme heterogeneity of rainfall, the information of soil moisture observations can be propagated horizontally in the model space and the soil moisture simulation can be improved by the ensemble Kalman filter. However, the nonlinear dynamics of the topography-driven surface flow induces the non-Gaussianity of the model error, which harms the efficiency of data assimilation of soil moisture observations. It is difficult to efficiently constrain model states at the edge of the area where the topography-driven surface flow reaches by linear-Gaussian filters, which brings the new challenge in land data assimilation for hyperresolution land models.

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Table 1. Configuration of the data assimilation experiments in section 3.1.

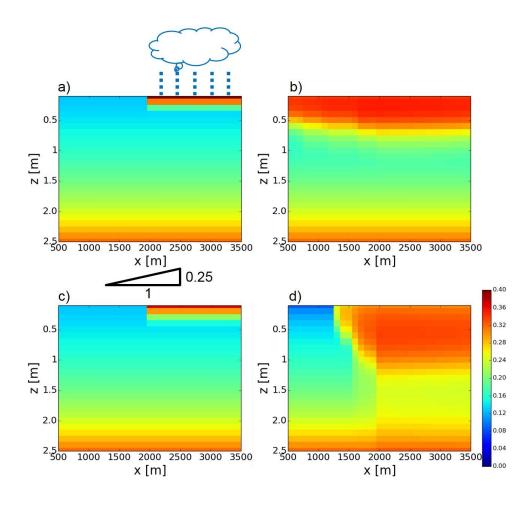
	hydraulic conductivity	observation's location	
	[m/h]	[m]	
LOW_K-UP_O	0.005	2500	
LOW_K-DOWN_O	0.005	1500	
HIGH_K-UP_O	0.02	2500	
HIGH_K-DOWN_O	0.02	1500	

Table 2. Configuration of the data assimilation experiments in section 3.2

	overland flows	observing network	
noOF_NoDA	none	no data assimilation	
noOF_DA_obs1	none	Figure 7a	
noOF_DA_obs9	none	Figure 7b	
noOF_DA_obs361	none	Figure 7c	
OF_NoDA	simulated	no data assimilation	
OF_DA_obs1	simulated	Figure 7a	
OF_DA_obs9	simulated	Figure 7b	
OF_DA_obs361	simulated	Figure 7c	

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Figure 1. Distributions of volumetric soil moisture simulated by the synthetic reference runs. (a) The distribution of volumetric soil moisture $[m^3/m^3]$ simulated by the LOW_K synthetic reference run at t=0h. The schematic of the configuration of the synthetic reference runs is also shown (see also section 3). (b) same as (a) but at t=130h. (c,d) same as (a,b) but for the HIGH_K synthetic reference run.





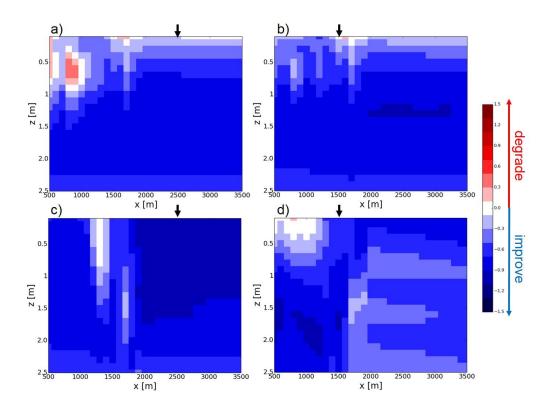


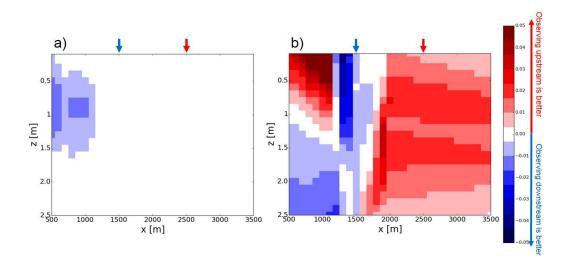
Figure 2. The improvement rates of the (a) LOW_K-UP_O, (b) LOW_K-DOWN_O, (c) HIGH_K_UP_O, (d) HIGH_K-DOWN_O experiments (see Table 1 and section 3). Black arrows show the locations of the soil moisture observations in each experiment.

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Figure 3. (a) The difference of time-mean RMSEs between the LOW_K-UP_O and LOW_K-DOWN_O experiments (see Table 1 and section 3). Red (blue) color indicates that the observations in the upper (lower) part of the slope reduce time-mean RMSE by data assimilation better than those in the lower (upper) part of the slope (see also arrows which are the locations of the observations). (b) same as (a) but for the difference between the HIGH_K-UP_O and HIGH_K-DOWN_O experiments.

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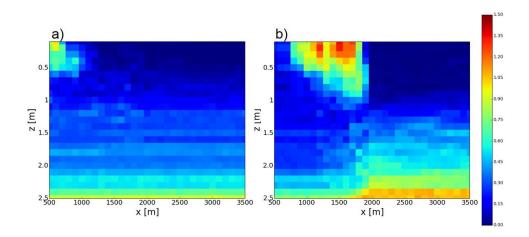


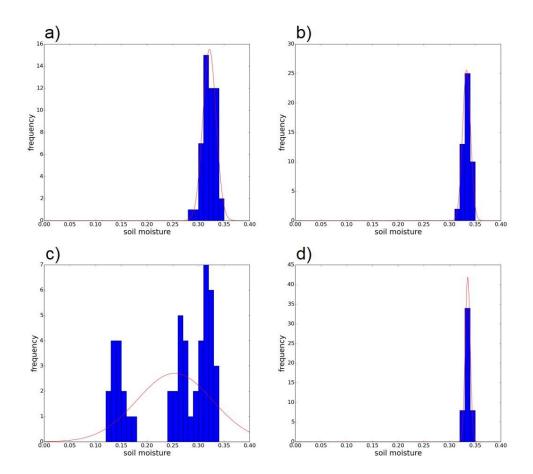
Figure 4. The Kullback-Leibler divergence of the NoDA experiment generated by (a) the LOW_K reference

and (b) the HIGH_K reference at t = 130h (see also Figure 1b and 1d).

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Figure 5. (a) The histogram (blue bars) of the volumetric soil moisture simulated by the NoDA experiment (see section 3) with the LOW_K reference at x=1500m, z=0.5m, and t=130h (see also Figure 4). Red line shows the Gaussian distribution with the mean and variance sampled by the ensemble. (b) same as (a) but at x=2500m, z=0.5m, and t=130h. (c) same as (a) but for the HIGH_K reference. (d) same as (c) but at x=2500m, z=0.5m, and t=130h.





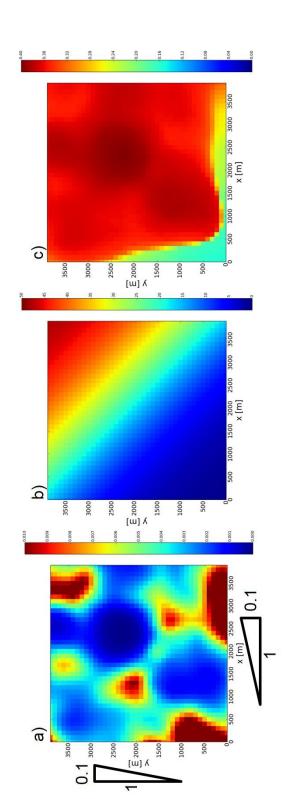


Figure 6. (a) Distribution of surface saturated hydraulic conductivity [m/h] in the synthetic reference. (b) Distribution of rainfall rate [mm/h] in the synthetic

reference. (c) Surface volumetric soil moisture $[m^3/m^3]$ at t=5 [h] in the synthetic reference.

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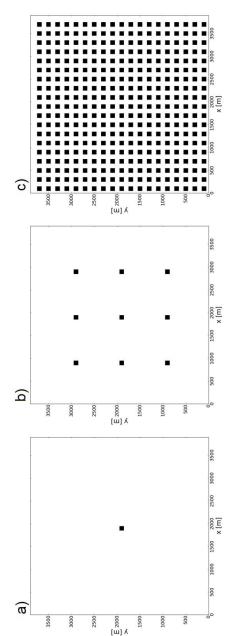
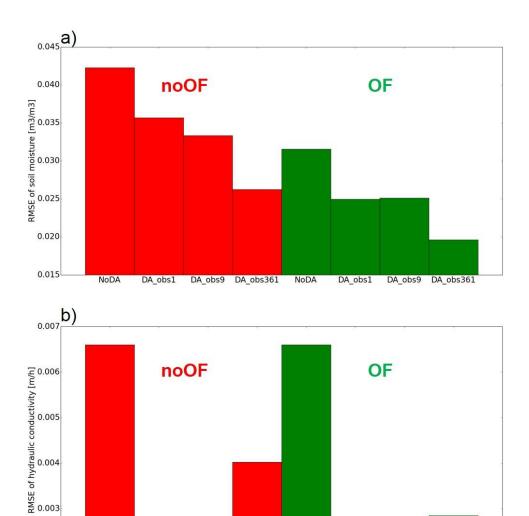


Figure 7. Observing networks. Black boxes are observed grids. (a) obs1, (b) obs9, (c) obs361 See also section 3.2.1.







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Figure 8. Time-mean RMSEs of the estimation of (a) soil moisture and (b) hydraulic conductivity. Red and green bars are results of the noOF and OF configuration, respectively (see section 3.2.1 and Table 2).

DA_obs9 DA_obs361

DA_obs9 DA_obs361

DA_obs1

NoDA





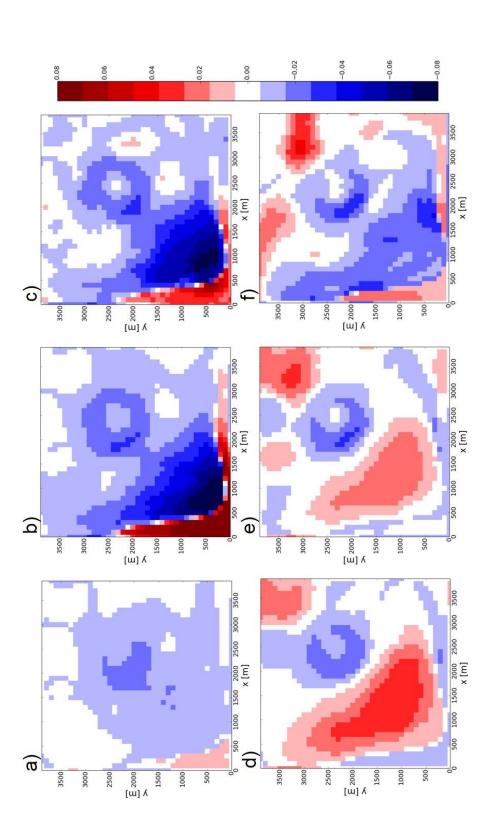


Figure 9. Differences of time-mean soil moisture RMSEs between the DA experiments and the OF_NoDA experiment. (a) OF_DA_obs1, (b) OF_DA_obs9 (c) OF_DA_obs361 (d) noOF_DA_obs1, (e) noOF_DA_obs9, (f) noOF_DA_obs361. 966 997

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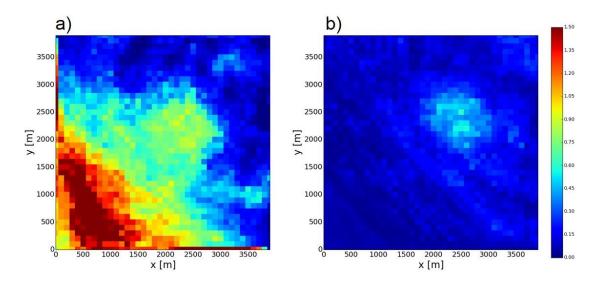
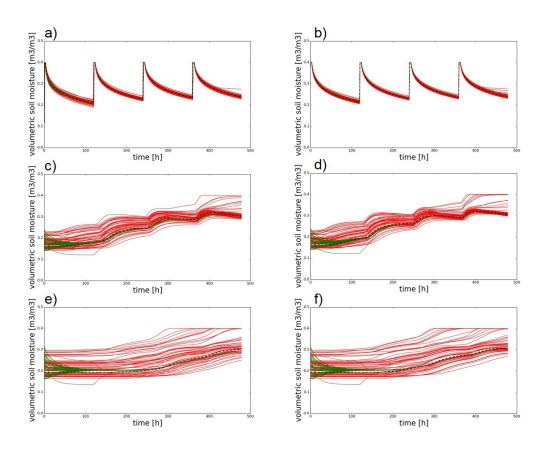


Figure 10. The Kullback-Leibler divergence of ensemble members generated by the (a) OF_NoDA and (b) noOF_NoDA experiments at t = 4 [h].





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Figure S1. Time series of volumetric soil moisture simulated by the synthetic reference run (black dashed line), the NoDA experiment (red lines), and the DA experiment (green lines) in the LOW_K-UP_O experiment at a) x=1500m, z=0.05m; (b) x=2500m, z=0.05m; c) x=1500m, z=1.0m; (d) x=2500m, z=1.0m; e) x=1500m, z=1.5m; (f) x=2500m, z=1.5m. In the DA experiment, initial guesses are used for this figure.

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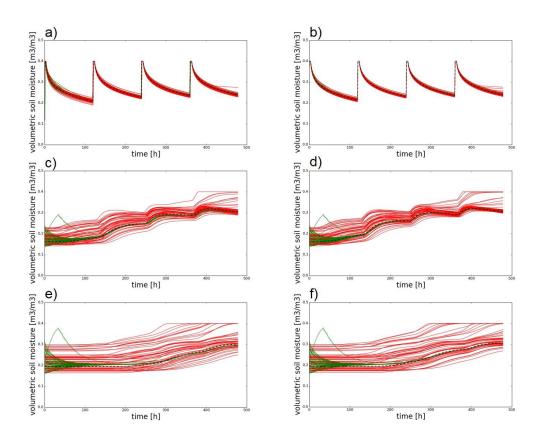


Figure S2. Same as Figure S1 but for the LOW_K-DOWN_O experiment.

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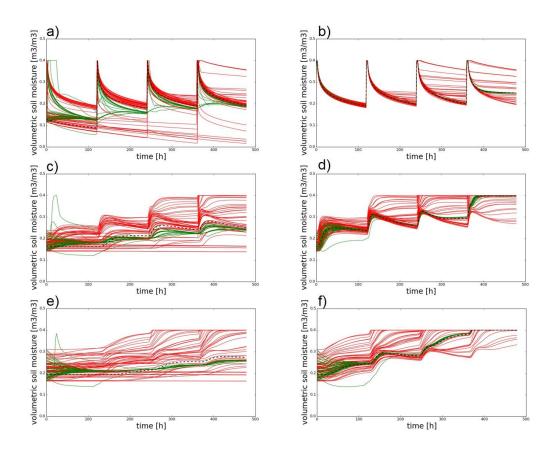


Figure S3. Same as Figure S1 but for the HIGH_K-UP_O experiment.

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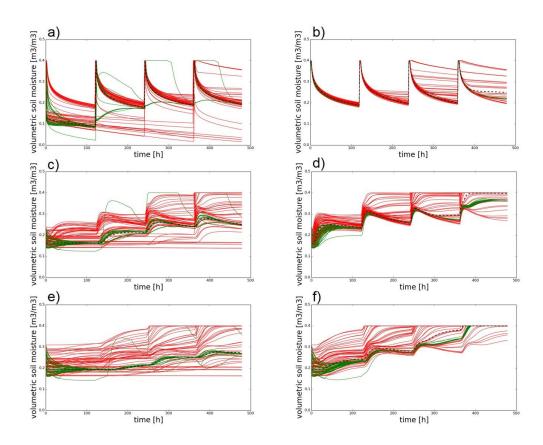


Figure S4. Same as Figure S1 but for the HIGH_K-DOWN_O experiment.

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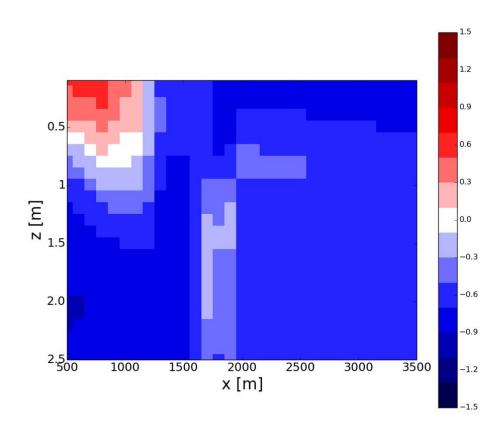


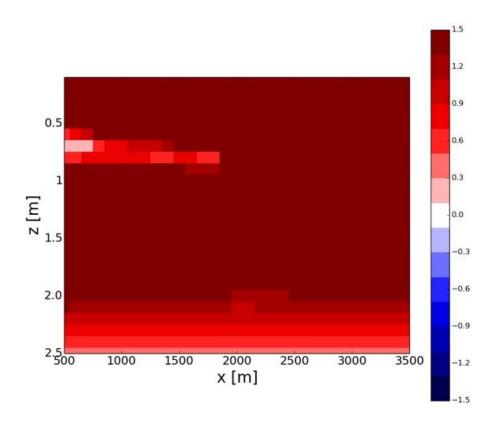
Figure S5. The improvement rates of the HIGH_K-DOWN_O experiment without a parameter optimization. 022

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Figure S6. The improvement rates of the LOW_K-DOWN_O experiment where the topography-driven

028 029 surface flow is neglected in ParFlow.





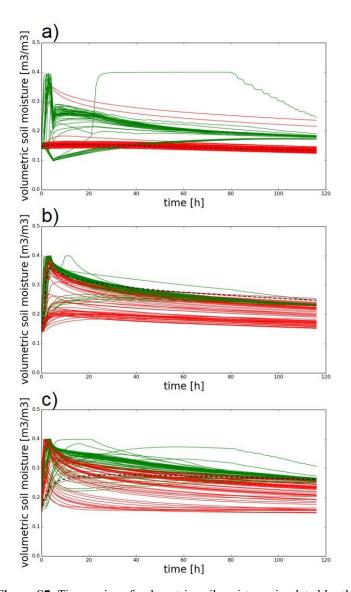


Figure S7. Time series of volumetric soil moisture simulated by the synthetic reference run (black dashed line), the OF_NoDA experiment (red lines), and the OF_DA_obs361 experiment (green lines) at a) x=200m, y=200m. z=0.15m; b) x=1200m, y=1200m, z=0.15m; c) x=2200m, y=2200m, z=0.15m.

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