1	Toward Improving Drought Monitoring using the Remotely Sensed Soil Moisture
2	Assimilation: A Parallel Particle Filtering Framework
3 4 5 6 7	Hongxiang Yan, Mahkameh Zarekarizi, and Hamid Moradkhani* Center for Complex Hydrosystems research Department of Civil, Construction and Environmental Engineering, The University of Alabama * Corresponding Author
9	Abstract
10	Drought is the costliest hazard among all natural disasters. Despite the significant improvements
11	in drought modeling over the last decade, accurate provisions of drought conditions in a timely
12	manner is still a major research challenge. In order to improve the current drought monitoring
13	skills, this study presents a land data assimilation system by merging the remotely sensed surface
14	soil moisture with the model simulations with the use of a recently developed particle Markov
15	chain Monte Carlo (PMCMC) method. To cope with the computational complexity, a modular
16	parallel particle filtering framework (PPFF) is developed which allows a large ensemble size in
17	PMCMC applications. The implementation of the proposed system is demonstrated with the
18	2012 summer flash drought case study over the Contiguous United States (CONUS). Results
19	from both synthetic and real case studies suggest that the land data assimilation system improves
20	the soil moisture predictions and the drought monitoring skills. Compared with the U.S. Drought
21	Monitoring (USDM), the land data assimilation can better capture the drought onset on May
22	2012 and the drought severity in June and July 2012. This study recommends that the proposed
23	land data assimilation system based on a high-performance computing (HPC) infrastructure can
24	better facilitate the drought preparation and response actions.
25	
26	Keywords: Drought monitoring; Soil moisture; Particle Markov chain Monte Carlo; Remote
27	sensing; Parallel computing
28	

#### 30 1 Introduction

Drought is a complex natural hazard that affects hydrological, environmental, ecological, and 31 social systems in many ways. Currently, no universal definition of drought exists (Lloyd-32 Hughes, 2014). Several drought definitions can be found in Wilhite (2000), Keyantash and 33 Dracup (2002), Mishra and Singh (2010), Sheffield and Wood (2011), and Van Loon (2015). 34 Generally, drought can be described as a deficiency in precipitation, soil moisture, or 35 surface/ground water over an extended period, which can have significant negative impacts on 36 agricultural, ecological, and socio-economic systems. A drought event can be short, lasting for 37 just a few months, or it can persist for multiple years. 38

Among all natural disasters, drought is the most costly hazard (Sheffield et al., 2014). For 39 example, the North American drought in 1988 resulted in nearly \$62 billion loss, which was 40 41 more than the cost of the 1993 Mississippi River flood and Hurricane Andrew combined (Ross 42 and Lott, 2003). The 2012 summertime flash drought event across the Central U.S. caused a major curtailment in crop yields, and resulted in about \$12 billion economic loss (Hoerling et al., 43 2014). One possible reason for such huge losses from a drought event is the lack of prompt 44 preparation and effective response actions due to insufficient knowledge of the drought 45 development behavior. Different from other natural disasters, drought has a slow onset and 46 develops over large areas, which makes it difficult to detect until severe damage has already 47 occurred (Wood et al., 2015). Therefore, a drought monitoring system that can detect drought 48 conditions in a timely manner is essential for drought preparedness and risk reduction 49 (Ahmadalipour et al., 2017; Andreadis et al., 2005; Hao et al., 2014; Maurer et al., 2002; 50 Sheffield et al., 2014). 51

The current operational drought monitoring systems generally use the simulated soil 52 moisture from hydrologic models to monitor drought conditions. For instance, the Climate 53 Prediction Center (CPC) soil moisture data sets operationally used in the U.S. Drought 54 Monitoring (USDM) (Svoboda et al., 2002) is based on a one-layer leaky bucket model. 55 Although model simulations can provide consistent long-term soil moisture data sets at a 56 continental scale, these soil moisture estimates are potentially biased due to the errors in model 57 parameters, forcing data, and deficiencies in the model structure (Chaney et al., 2015; DeChant 58 and Moradkhani, 2014; Moradkhani and Sorooshian, 2008; Samaniego et al., 2013; Yan and 59 Moradkhani, 2016). As a result, the biased soil moisture may lead to sub-optimal drought 60 monitoring skills. 61

A plausible approach to improve simulated soil moisture is to exploit the remotely sensed 62 observations to update the soil moisture states in the model. This method of integrating 63 observations and model simulations is referred to as data assimilation (DA) (Moradkhani, 2008). 64 The assimilation of satellite soil moisture into a hydrologic model has received increasing 65 attention and there have been numerous studies that have investigated the effects of assimilation 66 of remotely sensed data on soil moisture predictions (Brocca et al., 2012; De Lannoy et al., 2007; 67 Draper et al., 2012; Montzka et al., 2011; Reichle et al., 2008; Yan et al., 2015). While these 68 studies have suggested improvements on soil moisture predictions, few of the studies actually 69 quantified the improvements on the end-use application such as drought monitoring skill (Kumar 70 et al., 2014a). Different from the studies focused on the soil moisture predictions, which can be 71 performed at point or watershed scale, drought develops at regional to continental scales and 72 therefore, it generally requires hydrologic modeling at large-scale (DeChant and Moradkhani, 73 2015; Hoerling et al., 2014). Compared to the model forward run, the large-scale DA is far more 74

computationally expensive. Because of this computational complexity, the majority of previous
large-scale satellite soil moisture DA studies were based on the ensemble Kalman filter (EnKF)
with the use of small ensemble size (12–20) (Kumar et al., 2014b, 2009; Pan and Wood, 2010;
Yin et al., 2015).

Although the successful applications of the EnKF have been reported in the above 79 studies, the EnKF technique has some inherent features resulting in sub-optimal performances in 80 hydrologic applications (Abbaszadeh et al., 2018; DeChant and Moradkhani, 2012; Dong et al., 81 2015; Leisenring and Moradkhani, 2011; Lorentzen and Naevdal, 2011; Yan et al., 2017). First, 82 the EnKF uses only the first- and second-order statistical moments and assumes the model and 83 84 observation error distribution to be Gaussian, which is violated in the nonlinear and non-Gaussian hydrologic system. Second, the updating step within the EnKF is based on a linear 85 equation. As is the case in most hydrologic models, the observation model (or observation 86 87 operator) is nonlinear, therefore, such an updating rule may not be correct since the posterior ensemble is not a sample from the posterior probability density function resulted from the Bayes' 88 law (Lorentzen and Naevdal, 2011). Third, the EnKF technique violates mass conservation (not 89 preserving the water balance) because water is removed from or added to the model by the 90 updating formulation, which may lead to non-physical model state values. For drought 91 applications, the closure of the water balance is especially important because a moderate change 92 of soil water due to imbalanced water budget can result in a category change of drought severity. 93 The use of small ensemble size (12-20) in these studies further deteriorates the EnKF 94 performances in drought monitoring because such small ensemble size is insufficient to represent 95 the posterior distributions. 96

To overcome the above EnKF problems, data assimilation by means of particle filter (PF) 97 has been recommended as an alternative approach in hydrologic applications (Dong et al., 2015; 98 Montzka et al., 2011; Moradkhani et al., 2012; Noh et al., 2011; Plaza et al., 2012; Yan et al., 99 2017). In comparison to the EnKF, the PF can preserve the water balance and relaxes the 100 Gaussian assumption of error distributions, which allows the PF to potentially characterize 101 skewed or multimodal posterior distributions. This is accomplished by resampling the model 102 state or state-parameter ensemble, as opposed to the linear updating rule of the EnKF. In other 103 words, the PF can lead to a more complete representation of the posterior distribution for a 104 nonlinear and non-Gaussian hydrologic system. In the literature, a few studies have compared 105 106 the effectiveness and robustness of the EnKF and PF in hydrologic predictions, and they suggested that the PF is a more effective and robust data assimilation technique. For instances, 107 Leisenring and Moradkhani (2011) examined the performances of EnKF and PF on snow water 108 109 equivalent (SWE) predictions with the assimilation of SNOTEL observations. They found out that the PF reduced the root-mean-square-error (RMSE) of SWE predictions from the EnKF by 110 about 33%. DeChant and Moradkhani (2011) assessed both the EnKF and PF techniques on 111 SWE predictions with the assimilation of satellite brightness temperature data. Their results 112 suggested that PF provided more accurate predictions than EnKF. Van Delft et al. (2009) 113 compared the use of EnKF and PF on streamflow predictions and suggested PF approach led to a 114 lower RMSE value. Pasetto et al. (2012) found out that PF is a more robust method in soil 115 moisture assimilation because Gaussian approximation in the EnKF led to a state estimation that 116 is inconsistent with the physics of the model. DeChant and Moradkhani (2012) further provided 117 a comprehensive robust assessment between the EnKF and PF on streamflow predictions. They 118 demonstrated that the PF is a more robust technique because the streamflow predictions from the 119

EnKF were consistently overconfident, and occasional filter divergence was also identified in theEnKF.

Despite the advantages of PF, few satellite soil moisture DA studies used PF approach 122 and the majority of these PF studies were limited to point to watershed scale (Montzka et al., 123 2011; Plaza et al., 2012; Yan et al., 2015; Yan and Moradkhani, 2016), and fewer have attempted 124 to implement PF for large-scale drought analysis (e.g., Yan et al., 2017). The main obstacle for 125 the PF to be applied in large-scale drought application is the limited computational power of 126 modern computers, which means that we cannot have enough model ensembles to simulate the 127 posterior distributions and avoid weight degeneration (filter collapse due to few particles having 128 significant weight). Compared to the EnKF method, the successful application of PF requires a 129 larger ensemble size. The current EnKF based large-scale drought monitoring system (with the 130 use of small ensemble size) is already compute-intensive; while the PF needs to increase that 131 132 demand by 1–2 orders of magnitude. One possible solution allowing the use of PF in large-scale drought applications is to benefit from the parallel computing technique in a high-performance 133 computing (HPC) cluster infrastructure, which requires the parallel implementations of DA 134 algorithm. Currently, open source parallel DA library is available in the community such as the 135 Parallel Data Assimilation Framework (PDAF) (Nerger and Hiller, 2013). The PDAF is 136 developed at the Computing Center of the Alfred Wegener Institute based on Fortran code 137 compilable in the Unix/Linux environment and provides fully implemented and optimized data 138 assimilation based on the Kalman filtering algorithms (Ridler et al., 2014). Although the PDAF 139 can provide parallel simulation for large-scale DA applications on a HPC cluster, the PF 140 technique is not included in the PDAF up to date. 141

Given the above discussions, the main motivation of this study is to advocate the use of PF approach in large-scale drought applications by using the parallel computing technique in the HPC cluster. Specifically, a parallel PF modular is needed to be compatible with modern HPC infrastructure. Therefore, the goals of this study are to:

- develop a modular parallel particle filtering framework (PPFF) which allows a large
   ensemble size in large-scale (continental to global scale) drought applications;
- examine the effectiveness of PPFF by comparing its soil moisture predictions to the
   results from the EnKF based data assimilation system; and
- implement the large-scale assimilation of remotely sensed soil moisture into a distributed
   hydrologic model and provide a quantitative assessment of its impact toward drought
   monitoring skills with the use of PPFF."
- The remaining of the paper is organized as follows: section 2 describes the framework of the proposed PF based drought monitoring system, which includes the dynamical hydrologic modeling, the DA algorithm, and the parallelization of the DA. Section 3 assesses the drought monitoring system over the Contiguous United States (CONUS) for both synthetic and real case studies. Finally, section 4 concludes the paper.
- 158

## 159 2 Drought Monitoring System

In this study, the proposed drought monitoring system is composed of two parts: dynamical hydrologic molding and land data assimilation system. First, the hydrologic model is calibrated for the study region of interest, then the remotely sensed soil moisture observations are assimilated into the calibrated hydrologic model through the land data assimilation system. Figure 1 illustrates the framework of the proposed drought monitoring system.



165

Figure 1. The flowchart of the proposed drought monitoring system. The three probability
 distributions associated with the meteorological forcing, remotely sensed soil moisture, and soil
 moisture states represent the corresponding uncertainties.

# 170 2.1 Dynamical Hydrologic Modeling

The Variable Infiltration Capacity (VIC) model is a physically based and semi-distributed 171 macroscale hydrologic model. The VIC model was originally developed by Liang et al. (1994) 172 and later improved by Lohmann et al. (1998) and Liang and Xie (2001). The VIC model includes 173 both water-balance and energy-balance parameterizations and two types of runoff-yielding 174 mechanisms. In this model, the land surface is simulated as a gird of large, flat, and uniform 175 cells. The VIC model balances both surface energy and water over each grid cell. The VIC 176 model represents sub-grid variability in soils, topography, and vegetation, and this allows 177 representation of the non-linear dependence of the partitioning of precipitation into infiltration 178 and direct runoff as determined by soil moisture in the upper layer and its spatial heterogeneity. 179 The VIC model partitions the vadose zone into three soil layers. The first soil layer has a fixed 180 depth of 10 cm and responds quickly to changes in surface conditions and precipitation. The 181 second and third soil layer depths are spatially varied and the same as in the Land Data 182 Assimilation System (LDAS) retrospective simulations (Maurer et al., 2002). Moisture 183 movement between the three soil layers is governed by gravity drainage, with diffusion from the 184

second to the first layer allowed in unsaturated conditions. Water drained from the second layer
to the third layer is entirely controlled by gravity. Base flow is a non-linear function of the soil
moisture content of the third layer (Andreadis et al., 2005; Andreadis and Lettenmaier, 2006;
Shukla et al., 2011). The minimum meteorological forcing data for VIC model are the time series
of daily or sub-daily precipitation, maximum and minimum air temperature, and wind speed. In
this study, the root-zone soil moisture is estimated as the total column soil moisture (the sum of
the three soil layers) as suggested by Shukla et al. (2011).

192

# 193 2.2 Data Assimilation Algorithm

Following Moradkhani (2008), the state-space models that describe the generic earth system areas follows:

$$x_t = f(x_{t-1}, u_t, \theta) + q_t \tag{1}$$

$$y_t = h(x_t) + r_t \tag{2}$$

where  $x_t \in \mathbb{R}^n$  is a vector of the uncertain state variables at current time step,  $y_t \in \mathbb{R}^m$  is a vector of observation data,  $u_t$  is the uncertain forcing data,  $\theta \in \mathbb{R}^d$  is the model parameters,  $h(\cdot)$ is a non-linear function that relates the states  $x_t$  to the observations  $y_t$ ,  $q_t$  represents the model error, and  $r_t$  indicates the observation error. The errors  $q_t$  and  $r_t$  are assumed to be white noise with mean zero and covariance  $Q_t$  and  $R_t$ , respectively.

201

## 202 2.2.1 Ensemble Kalman Filter

The EnKF is an ensemble version of the Kalman filter, which does not require for a liner model and the estimation of priori model covariance (Evensen, 1994). In the EnKF, an ensemble of state vectors is propagated forward in time. Each time an observation becomes available, the
state vector of each ensemble member is updated as follows:

$$x_t^{i+} = x_t^{i-} + K (y_t - H x_t^{i-} + r_t)$$
(3)

where  $x_t^{i+}$  is the posterior state vector for the  $i^{th}$  ensemble member,  $x_t^{i-}$  is the priori state vector, *H* is the linearized observation operator ( $H = \partial h/\partial x$ ) to translate from model space to observation space, and *K* is the Kalman gain factor which is calculated as:

$$K = P^{-}H^{T}(HP^{-}H^{T} + R_{t})^{-1} = C_{xy}(C_{yy} + R_{t})^{-1}$$
(4)

where  $P^-$  is the model state error covariance,  $P^-H^T = C_{xy}$  is the covariance of the state ensembles with the predicted observations, and  $HP^-H^T = C_{yy}$  is the variance of the predicted observations.

213

# 214 2.2.2 Particle Filter Markov Chain Monte Carlo

Under the assumption of independence in time series, the posterior distribution of the state variables  $x_t$  given a realization of the observations  $y_{1:t}$  is as follows:

$$p(x_t|y_{1:t}) = p(x_t|y_{1:t-1}, y_t) = \frac{p(y_t|x_t)p(x_t|y_{1:t-1})}{p(y_t|y_{1:t-1})}$$

$$= \frac{p(y_t|x_t)p(x_t|y_{1:t-1})}{\int p(y_t|x_t)p(x_t|y_{1:t-1})dx_t}$$

$$p(x_t|y_{1:t-1}) = \int p(x_t, x_{t-1}|y_{1:t-1})dx_{t-1} =$$

$$\int p(x_t|x_{t-1})p(x_{t-1}|y_{1:t-1})dx_{t-1} =$$
(6)

where  $p(y_t|x_t)$  is the likelihood,  $p(x_t|y_{1:t-1})$  is the prior distribution, and  $p(y_t|y_{1:t-1})$  is the normalization factor. The marginal likelihood function  $p(y_{1:t})$  can be computed as:

$$p(y_{1:t}) = p(y_1) \prod_{k=2}^{t} p(y_k | y_{1:k-1})$$
(7)

219 where the normalization factor  $p(y_t|y_{1:t-1})$  is:

$$p(y_t|y_{1:t-1}) = \int p(y_t, x_t|y_{1:t-1}) dx_t = \int p(y_t|x_t) p(x_t|y_{1:t-1}) dx_t$$
(8)

Equation (5) shows mathematically that a posterior conditional probability distribution of model predicted states  $x_t$ , given all previous observations  $y_{1:t-1}$  and the current observation  $y_t$ can be computed sequentially in time. In practice, equation (5) does not have an analytic solution except for few special cases. Instead, the posterior distribution  $p(x_t|y_{1:t})$  is usually approximated using a set of Monte Carlo (MC) random samples as:

$$p(x_t|y_{1:t}) \approx \sum_{i=1}^N w_t^{i+} \delta(x_t - x_t^i)$$
(9)

where  $w_t^{i+}$  is the posterior weight of the  $i^{th}$  particle,  $\delta$  is the Dirac delta function, and *N* is the ensemble size. The normalized weights are calculated as follows:

$$w_t^{i+} = w_t^{i-} \frac{p(y_t | x_t^i)}{\sum_{i=1}^N w_t^{i-} p(y_t | x_t^i)}$$
(10)

where  $w_t^{i-}$  is the prior particle weights, and  $p(y_t|x_t^i)$  can be computed from the likelihood  $L(y_t|x_t^i)$ . Generally, a Gaussian distribution is used to estimate  $L(y_t|x_t^i)$ :

$$L(y_t|x_t^i) = \frac{1}{\sqrt{(2\pi)^m |R_t|}} exp\left[-\frac{1}{2}(y_t - h(x_t^i))^T R_t^{-1}(y_t - h(x_t^i))\right]$$
(11)

A resampling operation is necessary to minimize the weight degeneration, where all but few of the importance weights are close to zero. Moradkhani et al. (2005) suggests resampling the particles with a probability greater than the uniform probability. After resampling, all the particle weights are set equal to 1/N.

Regardless of the resampling approach, the successful application of PF still requires a large ensemble size to avoid the potential weight degeneration. For large-scale drought

applications, however, a relatively small ensemble size (50 to maybe 500) can be affordable 235 given the capabilities of the user's HPC resource and study domain. To further reduce the weight 236 degeneration problem in large-scale applications, the particle filter with sampling importance 237 resampling (PF-SIR) algorithm can be combined with Markov chain Monte Carlo (MCMC) 238 (Moradkhani et al., 2012). The particle Markov chain Monte Carlo (PMCMC) was first proposed 239 in statistical literature by Andrieu et al. (2010). Moradkhani et al. (2012) re-designed the 240 PMCMC to address both states and parameters while integrating the variable variance multiplier 241 approach for a more objective perturbation of observation during the assimilation process 242 (Leisenring and Moradkhani, 2012). In comparison to PF-SIR, the PMCMC achieved higher 243 accuracy in hydrologic predictions and required a smaller ensemble size (Moradkhani et al., 244 2012). As such, PMCMC is more robust than PF-SIR as it is less prone to the weight degeneracy 245 246 and sample impoverishment problems (loss of diversity in ensembles) (Abbaszadeh et al., 2018; Andrieu et al., 2010; Moradkhani et al., 2012), which makes the filter more efficient for 247 computationally-intensive large-scale applications. 248

In this paper we just consider the use of PMCMC for state updating (Andrieu et al., 2010). The PMCMC is an extension of the PF-SIR and uses the PF-SIR to design efficient proposal distributions for MCMC algorithm. The PMCMC consists of the following three steps: 1) initialization (j = 0): run PF-SIR targeting  $p(x_t|y_{1:t})$ , sample  $X_t(0) \sim p(x_t|y_{1:t})$  and let  $p(y_{1:t})(0)$  denote the corresponding marginal likelihood estimate, 2) iteration  $(j \ge 1)$ : sample  $X_t^* \sim p(x_t|y_{1:t})$  again and let  $p(y_{1:t})^*$  denote the corresponding marginal likelihood estimate, and 3) calculation of the acceptance ratio as:

$$min\left\{1, \quad \frac{p(y_{1:t})^*}{p(y_{1:t})(j-1)}\right\}$$
(12)

and set  $X_t(j) = X_t^*$  and  $p(y_{1:t})(j) = p(y_{1:t})^*$ ; otherwise set  $X_t(j) = X_t(j-1)$  and  $p(y_{1:t})(j) = p(y_{1:t})(j-1)$ .

258

## 259 2.3 Parallelization of Data Assimilation

Data assimilation with dynamical distributed hydrologic models (such as the VIC model) are computationally expensive and often need to be run on high-performance computing (HPC) architectures. Especially for simulations which are performed at a large-scale with a high spatial resolution, code parallelization is an essential requirement to reduce computational times. Fortunately, the natural parallelism in the 1D ensemble DA algorithm can be used to implement parallel programming, since each ensemble member can be simulated independently from the others.

For code parallelization, depending on the HPC architecture, either a shared memory or a 267 distributed memory paradigm can be used. The Open Multi-Processing (OpenMP) application 268 programming interface (API) is an implementation of multithreading in a shared memory 269 environment, which means that the memory is accessible by all threads simultaneously. As an 270 alternative, the Message Passing Interface (MPI) is a de facto standardized and portable 271 message-passing system running on a distributed memory system, such as computer clusters. 272 Each processor in the distributed memory system has its own private memory and only the data 273 belonging to a processor itself can be directly accessible. For data belonging to other processors, 274 an explicit communication of data between the processors can be performed via the ethernet 275 networks. 276

Depending on the HPC architecture, two parallelization strategies for the ensemble DA can be devised: the *model decomposition* and the *domain decomposition* (Nerger and Hiller,

2013). The model decomposition schema is to distribute the ensemble members of DA over all 279 available processors, indicating that the study domain grid cell is simulated in sequentially while 280 the ensemble members within each grid cell are simulated in parallel, namely ensemble member 281 simulation is set as a precedent in parallel computing. For instance, if we have a 300 processors 282 cluster and want to run DA on a study domain with 300 grid cells where each grid cell is 283 associated with 300 ensemble members; the *model decomposition* schema first distributes the 284 300 ensemble simulations associated with the first grid cell over the 300 processors. It starts to 285 simulate the second grid cell only if the simulations of the first grid cell are finished. However, 286 the *model decomposition* schema would lead to a significant amount of data communication 287 between different processors in each state updating step of DA. The frequent message-passing 288 between all the processors in each time step may produce a communication overhead in MPI. 289 290 Therefore, the model decomposition schema is more suitable for small-scale DA applications 291 using OpenMP in a computer system with shared-memory (Ridler et al., 2014).

As an alternative, the *domain decomposition* implementation gains more popularity in the 292 community due to the avoidance of the huge amount of message-passing. The domain 293 decomposition distributes the large-scale study domain over all available processors, indicating 294 that the grid cell is simulated in parallel while the ensemble member within each grid cell is 295 simulated sequentially, that is grid cell simulation is set as a precedent in parallel computing. Use 296 297 the same example as the above paragraph, the *domain decomposition* schema first distributes the 300 study domain grid cells over the 300 processors and all the grid cells are simulated 298 simultaneously. Since each grid cell is associated with only one processor, the 300 ensemble 299 simulations are simulated sequentially in each processor. As a result, each processor only 300 updates the grid cell states which belong to its own and other grid cell states can be updated 301

302	concurrently. The huge amount of message-passing at each time step is therefore relaxed in
303	domain decomposition implementation. Currently, the domain decomposition is a standard
304	parallelization strategy in the large-scale dynamical models using MPI.
305	Figure 2 illustrates the <i>domain decomposition</i> implementation in the proposed parallel
306	particle filtering framework (PPFF). The PPFF is processed in the following five steps:
307	1. Initialization of MPI;
308	2. Initialization of the PMCMC;
309	3. Model initialization for VIC;
310	4. For time = start date to end date
311	a. parallel simulation of fluxes and states in each gird cell to the next time step;
312	b. for each grid cell, sequential simulation of fluxes and states for each ensemble
313	member;
314	c. for each grid cell, filtering the fluxes and states by PMCMC;
315	d. for each grid cell, updating the initial conditions for the VIC run in next time step;
316	5. Finishing the VIC simulation and PPFF.



317

Figure 2. The flow diagram of the parallel particle filtering framework (PPFF) using Message Passing Interface (MPI). The *domain decomposition* parallel strategy is used in the PPFF: each grid cell is simulated in parallel while each ensemble member is simulated sequentially.

- 322 **3** Case Study
- 323 *3.1* Study Area and Drought Event

324 The present study aims to implement the drought monitoring framework over the Contiguous

- United States (CONUS). The 2012 summertime (May-August) flash drought over the Central
- 326 U.S. is selected as the case drought event in this study. The 2012 summer drought event

developed rapidly in May and reached peak intensity in August. The two main causes for this drought event were the precipitation deficits and high temperatures (Hoerling et al., 2013). Concurrence of substantial precipitation deficits and high temperatures resulted in decreased soil moisture and propagation of drought from meteorological drought to agricultural drought. According to the USDM, during May–August, over three-quarters of CONUS experienced at least abnormally dry drought conditions and the Central U.S. experienced severe to exceptional drought conditions.

This drought event garnered the attention of stakeholders, water managers, and policy 334 makers due to two reasons. First, it is the most severe seasonal drought event in 117 years with 335 significant economic loss (about \$12 billion) and impacts on food security and commodity prices 336 (PaiMazumder and Done, 2016). Using Arkansas state as an example, until 13 July 2012, the 337 U.S. Department of Agriculture (USDA) had issued a drought disaster declaration for 69 out of 338 339 75 Arkansas counties. Second, the current operational drought monitoring and forecasting systems failed or underestimated the 2012 summer drought event. The National Oceanic and 340 Atmospheric Administration (NOAA) CPC's Seasonal Drought Outlook (SDO) issued on 17 341 May 2012 failed to forecast this event (Hoerling et al., 2014), and the USDM also did not capture 342 this event until late June 2012 (Mo and Lettenmaier, 2015). 343

In addition to the severe 2012 summer drought case, we also examine the performance of the drought monitoring system on a non-drought year of 2010 to check whether the land data assimilation system corrects false positive drought. According to the USDM, the percentage area of CONUS experiencing moderate to exceptional drought were only between 8% and 10% through the 2010 summer. This summer minimum is the smallest percent area in moderate to exceptional drought for the CONUS during the 10-year history of the USDM since 2000. 350

# 351 3.2 Meteorological Forcing Data

The precipitation, maximum and minimum temperature, and wind speed data (January 1, 1979 to 352 present) were acquired from the Phase 2 of the North American Land Data Assimilation System 353 (NLDAS-2) (Xia et al., 2012). The NLDAS-2 was developed upon the first phase of NLDAS 354 (NLDAS-1) project, which was initiated to generate reliable initial land surface states to coupled 355 atmosphere-land models and improve weather predictions. The majority of NLDAS atmospheric 356 forcing data is derived from the North American Regional Reanalysis (NARR) which features a 357 32-km spatial resolution and a 3-hour temporal resolution. Besides the precipitation, temperature, 358 359 and wind speed, the NARR forcing data also includes the specific humidity, surface pressure, incoming solar radiation, and incoming longwave radiation. The NLDAS software is used to 360 interpolate the coarse-resolution NARR data to the finer-scale 1/8° NLDAS grid and to the one-361 hour NLDAS temporal resolution (Xia et al., 2012). In this study, the hourly NLDAS-2 primary 362 forcing data were aggregated into daily time step for DA applications. 363

364

## 365 3.3 Remotely Sensed Soil Moisture

The blended microwave soil moisture climate change initiative (CCI) products v02.2 released on February 2016 are used in this study (Dorigo et al., 2017; Y. Y. Liu et al., 2011). The CCI soil moisture are merged from four passive and two active microwave products, including the Scanning Multichannel Microwave Radiometer (SMMR), Special Sensor Microwave Imager (SSM/I), Tropical Rainfall Measure Mission (TRMM) Microwave Imager (TMI), Advanced Microwave Scanning Radiometer for Earth Observing System (AMSR-E), Advanced Microwave Instrument (AMI), and Advanced Scatterometer (ASCAT). It is noted that more updated CCI
products exist at present, which are expected to provide better performances.

According to Y. Y. Liu et al. (2012), the CCI merged soil moisture products are obtained 374 by rescaling the active and passive retrievals into a common Noah simulated soil moisture 375 climatology in the Global Land Data Assimilation System version 1 dataset (GLDAS-1-Noah), 376 with the use of quantile mapping or cumulative distribution function (CDF) matching approach 377 (Reichle and Koster, 2004). This method consists of three steps: 1) merging the four passive 378 products into one dataset from 1978 to 2014; 2) merging the two active products into one dataset 379 from 1991 to 2014; 3) blending both merged products into one final dataset from 1978 to 2014. 380 In the final blended soil moisture, passive and active merged products are used for sparsely and 381 moderately vegetated regions, separately. For transition areas where passive and active products 382 383 show similar performances, the average of both products are taken. In this way, the blended soil moisture can take advantage of active and passive microwave sensors, as active products have 384 higher accuracy over moderately vegetated regions while passive produces show better 385 performance over sparsely vegetated regions (Albergel et al., 2009; Wagner et al., 2013). 386

The combined CCI soil moisture products are provided at a daily time step with a spatial 387 resolution of 0.25°. Quality flags of both soil moisture have been used to mask pixels affected by 388 snow cover, temperatures below 0 °C, dense vegetation, and pixels where the soil moisture 389 retrieval failed (Dorigo et al., 2015). It is noted that the CCI soil moisture products are selected 390 in this study due to data availability, since this study focuses on the drought event in 2012. In 391 addition, the blended CCI product can have more number of observations (higher temporal 392 resolution) than any single sensor product leading to a better performance of DA application 393 (Yan et al., 2017). The latest Soil Moisture Active Passive (SMAP) L3 radiometer L-band soil 394

moisture products (Das et al., 2011; Entekhabi et al., 2010) issued from 31 March 2015 will be 395 used for future operational drought monitoring. 396

- 397
- 398

#### 3.4 Drought Monitoring Validation

The proposed PPFF LDAS is mainly for agricultural drought monitoring applications. In 399 this study, the simulated drought event is characterized with the root-zone soil moisture 400 percentile. We focus on soil moisture variable because agriculture heavily depends on soil 401 moisture reserves during crop growths. According to the USDM, five drought intensity 402 categories are defined based on the soil moisture magnitude: 403

404	D0—a	bnormally	dry, if	the soil	moisture	percentile	$\leq$ 30%;
-----	------	-----------	---------	----------	----------	------------	-------------

D1—moderate drought, if the soil moisture percentile  $\leq 20\%$ ; 405

D2—severe drought, if the soil moisture percentile  $\leq 10\%$ ; 406

D3—extreme drought, if the soil moisture percentile  $\leq 5\%$ ; and 407

D4—exceptional drought, if the soil moisture percentile  $\leq 2\%$ . 408

One of the main challenges for drought studies is the lack of an objective benchmark for 409 validations, because no "true" drought data exists in real case studies. In this study, the USDM, 410 the USDA's disaster declaration, and the drought economic loss are all used as references to 411 assess the simulated drought monitoring skills. According to the USDM, during May-August 412 2012, over three-quarters of the CONUS experienced at least D0 drought conditions and the 413 Central U.S. experienced D2–D4 drought conditions. The summer drought intensity in Central 414 U.S can be classified as D3-D4 as it resulted in major curtailment of crop yields, and caused 415 nearly \$12 billion economic damage (Hoerling et al., 2014). Further, the USDA's drought 416 disaster declarations are used to quantify the D3-D4 drought extent. USDA declared drought 417

418	disaster in seven Central U.S. states in July and August 2012, including Nebraska, Iowa, Kansas,
419	Missouri, Oklahoma, Arkansas, and Illinois. Table 1 presents the percentages of counties in each
420	state under USDA's drought disaster declarations between July and August 2012. In Table 1, it is
421	noted that in July 2012, over 70% of counties declared drought disaster for four out of the seven
422	Central U.S. states (Arkansas, Kansas, Missouri, and Oklahoma). In August 2012, more than
423	80% of the counties declared drought disaster for the remaining three states (Iowa, Illinois, and
424	Nebraska).

1 4

1.

425

Table 1. The percentage of counties under drought disaster declarations by U.S. Department ofAgriculture in July and August 2012 for the seven states in Central U.S.

428

States	Percentage of Counties under Drought Declarations issued by USDA				
	July	August	Total		
Arkansas	92.0	8.0	100		
lowa	0	84.8	84.8		
Illinois	19.6	80.4	100		
Kansas	86.7	13.3	100		
Missouri	100	0	100		
Nebraska	15.1	84.9	100		
Oklahoma	72.7	27.3	100		

429

# 430 *3.5 Synthetic Study*

To objectively assess the potential benefit of assimilating satellite surface soil moisture into a hydrologic model, a synthetic study is first conducted through observing system simulation experiment (OSSE) (Moradkhani, 2008). The synthetic study includes the following four steps: 1) a "truth" run of hydrologic model with the pre-calibrated model parameters; 2) simulated satellite surface soil moisture observations, which are generated from the truth run by incorporating the observation errors; 3) an open loop (OL) run with the perturbed forcing data without DA; and 4) the DA step that assimilates the simulated surface soil moisture observations
from step 2 to the model. Then the OL and DA results are compared against the truth simulation
to evaluate the impact of satellite surface soil moisture assimilation. Figure 3 presents the
flowchart of the synthetic study in this study using VIC model.

441



442

Figure 3. The flowchart of the synthetic study using VIC model to assess the potential benefit of
assimilation of satellite surface soil moisture on drought monitoring.

445

# 446 3.5.1 Synthetic Truth Simulations

In this study, the VIC model is performed to simulate the soil moisture and reconstruct the 2012
drought conditions over the CONUS domain, at a 1/8° spatial resolution. The model parameter

files, including the elevations, soil properties, and vegetation cover, are acquired from the VIC retrospective land surface dataset (Maurer et al., 2002). For synthetic truth simulation, the VIC model is run in a daily time step using the NLDAS-2 forcing data from 1 January 1979 to 31 December 2015 to produce long-term girded surface and root-zone soil moisture. In this study, the VIC model is run in water balance mode, which means that the surface temperature is set equal to the surface air temperature rather than iteratively solving the surface energy budget.

455

#### 456 3.5.2 Error Models in Data Assimilation

To account for uncertainties in forcing data due to sensor errors and spatial heterogeneity, both 457 precipitation and wind speed errors are assumed to be heteroscedastic and lognormal with a 458 variance of 25% of the variable's magnitude. Both maximum and minimum temperature are 459 assumed to be homoscedastic and normal with a standard deviation of 3 °C. For both synthetic 460 and the real case studies, the same perturbation errors are used, and the initial state noise is free. 461 The model structure is considered perfect for synthetic study; while for real case study, the 462 model structural error is assumed to be normally distributed with a standard deviation equal to 463 10% of the prediction value. All errors in this study are assumed to be uncorrelated. Error 464 assumptions are applied with the same magnitude in both the EnKF and PMCMC applications. 465 The form and magnitude of these errors are based on previous DA studies, where the values were 466 determined through a manual tuning to achieve reliable predictions (Abbaszadeh et al., 2018; 467 DeChant and Moradkhani, 2014; Yan et al., 2015; Yan and Moradkhani, 2016). We 468 acknowledge that these values may not necessarily be optimum. 469

Following Kumar et al. (2014b), the white noise (standard deviation) for the CCI satellite soil moisture is assumed to be  $0.04 \text{ m}^3/\text{m}^3$  over all grid cells over the CONUS. To account for

spatial correlations in CCI soil moisture errors, the constant CCI soil moisture error standard 472 deviation  $(0.04 \text{ m}^3/\text{m}^3)$  is scaled by the ratio of the soil moisture time series standard deviation of 473 the VIC model to that of the real CCI soil moisture data (separately for each grid cell), resulting 474 in CCI soil moisture error standard deviations that are spatially distributed (Kumar et al., 2014b; 475 Q. Liu et al., 2011; Reichle et al., 2007). The synthetic CCI soil moisture are then generated from 476 synthetic truth simulations by incorporating the scaled CCI soil moisture errors. We 477 acknowledge that the constant soil moisture error (0.04 m<sup>3</sup>/m<sup>3</sup>) assumption before scaling is 478 somewhat arbitrary. More advanced approaches, such as the triple collocation (TC) method, may 479 be used to provide better estimations of satellite soil moisture error structure (Gruber et al., 480 2016). However, successful applications of TC require large numbers of coincident soil moisture 481 from three independent time series (satellite soil moisture, model simulations, and in-situ 482 483 observations), homogeneity of their linear relationships, and error structures. In general, these assumptions are difficult to realize in practice because of the infrequent spatiotemporal sampling 484 of satellite and *in-situ* sensors. (Su et al., 2014). 485

Contrary to the small ensemble size (12–20) used in the majority of previous satellite soil
moisture DA studies (Kumar et al., 2014b, 2009; Pan and Wood, 2010; Yin et al., 2015), a large
ensemble size of 100 is used in this study, in order to fully quantify the soil moisture posteriors.
The PPFF module is written in Python3 script and all the DA simulations are run on the Linux
Hydra Cluster (24 nodes, 384 processors) located at the Office of Information Technology (OIT),
Portland State University (PSU).

#### 493 3.5.3 EnKF versus PMCMC

Before assessing the drought monitoring skill, we first compare the performances of the EnKF 494 and PMCMC for root-zone soil moisture predictions. Both experiments are performed by 495 assimilation of the synthetic satellite surface soil moisture for the period of 1 January 2012 to 31 496 December 2012. Since the main trust of this study is to investigate whether the PMCMC system 497 can improve drought monitoring skill for summer 2012, the EnKF versus PMCMC comparison 498 is based only on one basin as a proof-of-concept. In order to assess the PMCMC performance 499 over the EnKF, the normalized information contribution (NIC) metric (Kumar et al., 2014b) is 500 used in this study. The NIC for root-mean-square-error (RMSE) is defined as follows: 501

$$NIC = \frac{RMSE_{EnKF} - RMSE_{PMCMC}}{RMSE_{EnKF}}$$
(13)

where  $RMSE_{EnKF}$  indicates the RMSE values between EnKF and synthetic truth, and *RMSE<sub>PMCMC</sub>* indicates the RMSE values between PMCMC and synthetic truth. If NIC>0, the PMCMC shows improvement with respect to the EnKF predictions; if NIC<0, the PMCMC shows degraded performance as compared with the EnKF predictions; and if NIC=1, the PMCMC results in perfect predictions.

Figure 4a displays the NIC values in the root-zone soil moisture and their spatial 507 distributions across the Columbia River Basin. The majority of the grid cells show positive NIC 508 values indicating a better performance of the PMCMC over EnKF. The daily domain-averaged 509 root-zone soil moisture RMSE (m3/m3) for the EnKF is 0.0039, and it decreases to 0.0019 with 510 PMCMC (about 51% improvement). To better illustrate this difference, Figure 4b shows the time 511 series of synthetic truth, EnKF, and PMCMC root-zone soil moisture predictions for one grid cell 512 513 with NIC=0.61 (marked as yellow star in Figure 4a). It is observed that though EnKF and PMCMC show similar performances in winter and spring seasons, the EnKF underestimates the 514

soil moisture during summer while the PMCMC predictions are closer to the synthetic truths. As mentioned in the introduction section, this can be explained as the inherent drawbacks of the EnKF technique. It is mainly due to inadequacy of linear updating rule for a nonlinear hydrologic model, leading to over adjustments in the updates (Harlim and Majda, 2010; DeChant and Moradkhani, 2012). These results come as no surprise and are consistent with previous findings which had demonstrated the superiority of the PF DA techniques over the EnKF in hydrologic applications (DeChant and Moradkhani, 2012, 2011; Leisenring and Moradkhani, 2011).

522



523

**Figure 4.** (a) The normalized information contribution (NIC) value between the EnKF and PMCMC root-zone soil moisture predictions (Eq. 13). Positive values indicate that the PMCMC improves soil moisture prediction as compared to the EnKF; negative values indicate the degradation over the EnKF. (b) Time series of the marked (yellow star) grid cell root-zone soil moisture (m3/m3) for the synthetic truth, EnKF, and PMCMC simulation for the period of 1 January 2012 to 31 December 2012. Both NIC values and time series are generated using the posterior means.

531

#### 532 3.5.4 PMCMC Drought Monitoring

Here we examine the potential benefit of assimilating satellite surface soil moisture on drought monitoring skill according to the synthetic study flowchart shown in Figure 3. The OL simulation is run with the perturbed NLDAS-2 forcing data for the period of 1 January 2012 to

31 December 2012. The ensemble size and perturbation errors in the OL simulation are the same 536 as in the DA. Figure 5 presents the NIC values (OL versus DA) in the surface and root-zone soil 537 moisture and their spatial distributions across the CONUS for the 2012. The majority of the grid 538 cells show the positive NIC values indicating the added-value of the DA. Generally, the 539 improvements in the surface soil moisture field are consistent with the improvements in the root-540 zone soil moisture field, with more prominent improvements in the surface soil moisture field. 541 The improvements in surface field are higher than root-zone field, which is mainly caused by the 542 weak and highly non-linear cross covariance between the two layers (Kumar et al., 2014a). For 543 surface soil moisture, the daily domain-averaged RMSE (m3/m3) for the OL is 0.0042, and it 544 545 decreases to 0.0027 with DA (about 36% decrease). Similarly, the daily domain-averaged rootzone soil moisture RMSE (m3/m3) value decreases from 0.0034 in the OL to 0.0024 after DA 546 (about 29% decrease). It is to be noted that several grid cells in Figure 5, show negative NIC 547 values. From a theoretical perspective, the DA is expected to show improvements over the OL 548 skills for all grid cells in a synthetic study framework knowing that the observation errors are 549 synthetically introduced with predefined statistical properties. Here, the negative NIC values can 550 be explained due to suboptimal choice of the uncertainty magnitude in the synthetic CCI soil 551 moisture observations. Specifically, in the particle weight estimation using the Gaussian 552 likelihood function, if the scaled soil moisture observation error is too small (e.g., 0.01 m3/m3), 553 the PF may result in degenerated particles that is a few particles with larger weights dominate the 554 rest of the particles and eventually collapse to one particle which poorly approximates the soil 555 moisture posteriors and eventually resulting in negative NIC values. 556



558

**Figure 5.** The normalized information contribution (NIC) value between the Open-Loop (OL) and Data Assimilation (DA). The NIC values are generated based on posterior means. The positive value indicates that the DA improves soil moisture prediction against OL; negative value indicates the degradation over the OL. (a): Surface soil moisture field. (b): Root-zone soil moisture filed.

In the implementation of the DA, the identifications of model and observation errors are 565 very unintuitive and the inappropriate selections of observation errors may lead to over/under-566 confident soil moisture predictions (Y. Liu et al., 2012; Massari et al., 2015). For small-scale DA 567 applications, such as one soil column DA study (Montzka et al., 2011; Yan et al., 2015), it is 568 straightforward to manually tune the observation error to ensure that the synthetic framework 569 performs well. For large-scale DA applications, however, it is not feasible to conclude on a 570 single ideal manner an optimal error implementation, and some degraded cells are unavoidable. 571 Similar results from a synthetic study using the EnKF-based DA showed the inferior 572 performance of DA with respect to OL) were also reported by Kumar et al. (2014a) using the 573 EnKF method. 574

Leaving the first year as model spin-up period, the soil moisture climatology is the soil 575 moisture simulations from 1 January 1980 to 31 December 2015. Then, the soil moisture 576 percentiles generated from the OL and DA monthly integrations are compared against the 577 corresponding synthetic truth. For instance, to estimate the monthly soil moisture percentile in 578 October 2010, it is first to take all October soil moisture values over 1980-2015 to construct the 579 climatological distribution for each grid cell. Then, for any specific grid cell soil moisture value 580 in October 2010, the corresponding soil moisture percentile can be estimated from the 581 climatological distribution. Drought monitoring skills between the OL and DA are examined 582 using the drought extent bias (%), which is estimated as the absolute difference between the 583 percentage of detected drought area from OL/DA over CONUS and the synthetic true drought 584 area over the CONUS. 585

586 Figures 6 and 7 present the spatial distribution of drought intensities and the drought 587 extent bias (%), respectively, for five drought categories (D0–D4) over CONUS. The severe

drought events from May-August 2012 across Central U.S. (Nebraska, Kansas, Oklahoma, Iowa, 588 Missouri, Arkansas, and Illinois) can be clearly seen in the synthetic truth. In all comparisons of 589 the four-month drought monitoring, the DA estimates show systematic improvements over the 590 OL estimates. For the May 2012 case, the OL underestimates the intensity of drought across the 591 Nevada, Utah, Colorado, and New Mexico whereas DA improves these representations. The 592 drought extent bias (%) for D0–D4 between the OL and synthetic truth is 5.11%, and it decreases 593 to 1.28% (about 75% decrease) with DA. For the June and July 2012 cases, the OL 594 underestimates the intensity of drought across the Central U.S. (i.e., the Kansas, Nebraska, and 595 Colorado), and DA helps to reduce these large biases. Similarly, drought extent biases (%) 596 decrease from 5.25% and 4.69% in the OL to 1.02% (about 81% decrease) and 0.53% (about 597 89% decrease) in the DA, respectively. Although several grid cells in Central U.S. (i.e., Kansas) 598 show relatively high soil moisture values in August 2012, the DA still helps reduce these biases. 599 600 The drought extent bias (%) decrease from 3.02% to 0.34% (about 89% decrease). Overall, these results are consistent with the trends in Figure 5, which shows the improvements obtained by 601 DA. 602



**Figure 6.** Comparison of the drought monitoring skill between Open-Loop (OL) and Data Assimilation (DA) for May–August 2012.



Figure 7. The absolute bias of drought extent (%) against the synthetic truth between Open-Loop
(OL) and Data Assimilation (DA) over the CONUS for the period of May–August 2012.

# 612 3.6 Real Case Study

When assimilating the real satellite soil moisture data, the systematic biases between the 613 satellite-based and model-based soil moisture cannot be avoided (Reichle and Koster, 2004; Su 614 et al., 2014; Yan et al., 2015; Yilmaz and Crow, 2013). Proper treatment of these systematic 615 biases is important, as the DA algorithm is designed to work with errors that are strictly random. 616 The most common approach, the CDF matching (Reichle and Koster, 2004), is implemented in 617 this study to rescale the satellite observations to the model's climatology. The CDF matching 618 approach can correct all the moments of the distribution regardless of its shape. Leaving out the 619 first year as model spin-up period, the CCI soil moisture products are rescaled from 1980-2014. 620 For each model gird cell over the CONUS, the model CDF and the satellite observation CDF are 621 generated for the entire period of 1 January 1980 to 31 December 2014. The CDF matching 622

approach is then used to rescale the satellite observations to the model's climatology, separatelyfor each grid cell.

For real data study, the perturbation errors are the same as the synthetic study except for the model error. As mentioned in section 3.5.2, the model structure error is assumed to be normally distributed with a standard deviation equal to 10% of the prediction value. The DA is performed by assimilation of the rescaled real satellite surface soil moisture for six-month duration from 1 February to 31 August for both 2010 non-drought and 2012 drought years.

630

## 631 3.6.1 2012 Summer Drought Monitoring

Figure 8 presents the OL and DA monthly drought monitoring results across CONUS in 632 May/June/July/August 2012. Note that the drought monitoring from the DA in these 633 634 comparisons are generated using the posterior means. For the purpose of comparison of drought intensity, the USDM weekly monitoring result in the middle of each month is also presented in 635 Figure 8. It is noted that although the USDM maps provide a useful monitoring of current 636 drought conditions, they should not be considered as the "truth" like in the synthetic study since 637 they are largely based on subjective information about drought at multiple time scales and for a 638 wide range of impacts (Otkin et al., 2013). In addition, the USDM did not capture the 2012 639 Central U.S. drought until late June 2012 (Mo and Lettenmaier, 2015; Otkin et al., 2013). 640 Currently, an objective and quantitative measurement of true drought condition is still 641 unconcluded in the community, due to inherent complexity of drought phenomenon. However, 642 the comparisons with USDM are still helpful to assess the capacity of our proposed system to 643 detect drought events at some level (Anderson et al., 2011; Kumar et al., 2016, 2014b; Otkin et 644 al., 2013). 645



Figure 8. Comparison of the 2012 summer drought intensity over the CONUS from Open-Loop
(OL), Data Assimilation (DA), and U.S. Drought Monitoring (USDM).

Because the USDM did not capture the 2012 summertime drought (May–August) until late June (Mo and Lettenmaier, 2015), it is important to investigate whether the proposed DA drought monitoring system can better monitor this drought event, especially in May. It is noted that the OL results in the real case study are the VIC forward model run with the predefined parameters and the unperturbed NLDAS-2 forcing data. These results were treated as the "truth" in the synthetic study. Figure 8 illustrates the added value of assimilating remotely sensed soil moisture for improving drought monitoring skill. For the May 2012 case (the onset of the 2012

646

summer drought), the USDM completely missed the drought onset in Central U.S. (such as 658 Arkansas, Missouri, Oklahoma, and Kansas). Although the OL shows some improvements over 659 the USDM, the soil moisture DA provides a better estimate of drought severity, especially for D0 660 and D1 categories (over Nebraska). For the August 2012 case (the 2012 drought event reached 661 peak intensity in August), this time the USDM successfully captures this severe drought events 662 in Central U.S. whereas the OL underestimates the drought intensity and DA provides similar 663 results as the USDM. For the July 2012 case, since all the counties in Missouri and about 73% 664 counties in Oklahoma had issued drought disaster declaration (due to severe damage to the 665 crops) (Table 1), it is reasonable to conclude that the USDM underestimate the intensity in 666 Missouri and Oklahoma. The USDM only provides D1-D2 drought in these two states, while 667 DA suggests D3–D4 drought, which is more consistent with the USDA drought declaration. 668 Similar pattern can be found for June 2012 case, since the crops were damaged in this month, the 669 670 USDM and OL underestimate the drought intensity and DA provides a better estimate of drought severity. Overall, in all four months, DA estimation predicts more intense drought over Central 671 U.S. and captures the spatial pattern of the intense drought very well relative to the OL and 672 USDM. 673

Figure 9 summarizes the detected drought areas over CONUS based on OL, DA, and USDM. The USDM results are presented in Figure 9 only as a "reference" not "truth". For the May 2012 case, the USDM missed the drought events in parts of Central U.S., however, the DA helps to correct these biases. The detected drought areas over CONUS for OL and DA are 43.82% and 47.91%, respectively. For the August 2012 case, the OL underestimates the drought intensity whereas DA improves these representations. The detected drought areas increase from 48.17% in the OL to 62.66% after the DA, respectively. Similarly, the DA adds the drought monitoring skills for the June and July 2012 cases, from 55.27% and 54.45% by OL to 62.49%
and 65.73% by DA. As a result, compared with OL, the DA provides a more accurate estimate of
drought areas, more consistent with the USDM map of this drought event.

684



685

Figure 9. Comparison of the drought extent (%) over the CONUS from Open-Loop (OL), Data
Assimilation (DA), and U.S. Drought Monitoring (USDM) for May/June/July/August 2012.

After the demonstration of the added-value of DA over OL in Figure 9, Figure 10 examines the drought monitoring skill between DA and USDM in details over Central U.S. Figure 10 shows the percentage area under drought over Central U.S. from the DA and USDM for each drought category. The monthly USDM drought extent is estimated as the average of the four weekly USDM products. It is noted that the drought extents presented in Figure 10 are comprised 7-State region of Nebraska, Iowa, Kansas, Missouri, Oklahoma, Arkansas, and Illinois. In the May 2012 case, the USDM missed the drought onset and detected less than half

(44.39%) of the Central U.S. under drought (D0-D4). While DA improves the detection of 696 drought onset and warns that 78.52% of the Central U.S. is abnormally dry (D0-D4) and more 697 than half (59.50%) of the Central U.S. is under moderate drought or worse (D1–D4). Although 698 the USDM started monitoring the severe (D2) and extreme (D3) droughts since 26 June 2012, 699 the USDM still underestimated the intensity of drought in June and July 2012. Most of the states 700 in Central U.S. issued the drought disaster declaration in July, which indicated that the crop 701 702 plants had been damaged in June (Table 1). For the June 2012 case, only 3.33% of the Central U.S. is under extreme (D3) and exceptional (D4) drought according to the USDM, while DA 703 detects 36% of the Central U.S. under extreme (D3) and exceptional (D4) droughts. Same result 704 705 can also be found for July 2012 case where DA provides a better estimate of drought severity showing 58.77% of the Central U.S. under D3-D4 drought, compared to 38.88% with the 706 USDM. In the August 2012 case, nearly all the counties in Central U.S. issued drought disaster 707 708 declaration (Table 1) and USDM provided a close exceptional drought (D4) monitoring skill as DA. 709



711

Figure 10. Comparison of U.S. Drought Monitoring (USDM) and Data Assimilation (DA)
drought monitoring extent for five different drought categories (D0–D4) over the Central U.S.
The drought extent is comprised of the 7-State region of Nebraska, Iowa, Kansas, Missouri,
Oklahoma, Arkansas, and Illinois.

716

In summary, compared with the OL, the DA systematically improves the drought monitoring skill for 2012 drought event from May to August. Compared with the USDM, the DA could better capture the drought onset in May, and the drought intensity in June and July, and provide similar results in August. These results demonstrate the added-value of DA to facilitate the state drought preparation and effective response actions.

722

# 723 3.6.2 2010 Summer Drought Monitoring

Figure 11 presents the OL and DA monthly drought monitoring results derived based on the root-zone soil moisture posterior means across the CONUS in May/June/July/August 2010. Similar to the 2012 drought results, the USDM weekly monitoring result in the middle of each

month is presented in the figure as a reference. The OL/DA monitoring results and USDM show 727 a general agreement with each other except for the southwest US. For the June 2010 case, the 728 USDM shows D0-D1 drought intensity in Arizona and New Mexico, while both OL and DA 729 results suggest D3–D4 intensities. As the USDM data is a blended product of multiple indicators 730 and data, we do not expect the modeled drought intensities derived based on a single variable 731 (soil moisture) to match the USDM results exactly. Though the DA does not agree with the 732 733 USDM drought intensity, in the southwestern US, it does not over-predict the drought of summer 2010. For the May 2010 case, the percentages of D0-D4 drought extent over the CONUS are 734 25% and 24% from DA and OL, respectively. This result suggests that for a non-drought year 735 event like 2010, the DA performs similar to OL and do not increase false drought detections. 736



737

Figure 11. Comparison of the 2010 summer drought intensity over the CONUS from Open-Loop
(OL), Data Assimilation (DA), and U.S. Drought Monitoring (USDM).

#### 741 **4** Conclusion

In this study, a land data assimilation system is proposed through the assimilation of remotely 742 sensed soil moisture into a distributed dynamical hydrologic model to improve the drought 743 monitoring skill. The recent developed PMCMC technique is implemented in this study to 744 quantify the soil moisture posteriors. In order to cope with the large computational demand 745 required by PMCMC, a modular parallel particle filtering framework is developed in this study 746 which allows the use of large ensemble size in the PMCMC applications. The proposed drought 747 monitoring system is assessed based on the 2012 summer flash drought and 2010 non-drought 748 events over the Contiguous United States. The impacts of assimilating remotely sensed surface 749 750 soil moisture on improving soil moisture predictions and drought monitoring are examined. 751 Results from both synthetic and real case studies suggest that the proposed drought monitoring system improves the drought monitoring skill and can facilitate the state drought preparation and 752 declaration. Compared with the state-of-the-art U.S. Drought Monitoring, the proposed system 753 can better capture the drought onset in May, and the drought intensity in June and July 2012. For 754 the 2010 non-drought year case study, the proposed system does not lead to over-detection of 755 false positive drought. 756

A limitation of this study is the short data assimilation periods (two years) due to the limited HPC computational resources. As a result, only two case studies (a drought year and a non-drought year) are presented in this paper to assess the efficiency of this monitoring system. We acknowledge that further examination of the proposed approach with more case studies is desired. A practical path forward that we are currently implementing is to make this system operational monthly scale and compare the results with the U.S. Drought Monitor and otherresources from related agencies.

764

#### 765 Acknowledgement

Partial financial support for this project was provided by the National Oceanic and Atmospheric
Administration (NOAA) Modeling, Analysis, Predictions, and Projections (MAPP) (Grant No.
NA140AR4310234).

769

770 Appendix A. Coupling Data Assimilation with Hydrologic Model

771 Generally, there are two strategies to couple the hydrologic model and DA algorithm: online coupling and offline coupling (Kurtz et al., 2016; Nerger and Hiller, 2013). For online coupling, 772 the DA algorithm is a subroutine of the dynamical model routines and they are all compiled into 773 a single program. Data is exchanged via the main memory. The main advantage of the online 774 *coupling* is that it is computationally more efficient since the exchange of data using files can be 775 avoided. In addition, the model only needs to execute the start-up phase once and there is no 776 additional start-up cost. However, the online coupling schema requires to modify the model 777 source code to make it compatible with the DA subroutine. 778

For *offline coupling* schema, there are two separate programs used for model execution and DA, respectively. Data is then exchanged via the input/output (I/O) files of the model. Obviously, the *offline coupling* is more *ad hoc* since there is no need to modify the model source code. In addition, the *offline coupling* is the only option when the source code of the model is not available or not open source. One limitation of the *offline coupling* is to generate a large amount of files on the local drive and produce a lot of I/O overhead. One possible solution is to use theRAM disk to catch these I/O files.

In general, an ideal parallel DA framework should provide a generic DA environment that can be coupled with any hydrologic model. Therefore, the *offline coupling* schema is used in this study to provide a generic parallel DA framework for the VIC model. Figure A1 describes the detailed PMCMC-VIC *offline coupling* interface in this study. In Figure A1, a one-day VIC model simulation and PMCMC filtering is presented in details.



Figure A1. The flowchart of the *offline coupling* interface of the VIC model and the PMCMC
data assimilation algorithm. The ensemble files indicate the ensemble members of the PMCMC
algorithm. A one-day VIC model simulation and PMCMC updating are shown in this flowchart.

796 From Figure A1, the model grid, parameters, and initial conditions are first prepared in the model initialization phase. The forcing data (precipitation, maximum and minimum 797 temperature, and wind speed) and remotely sensed observations for all the time steps are held in 798 the main memory as one data object waiting for simulation. Subsequently, the PMCMC module 799 initializes the ensemble members and the DA integration is conducted step by step. The remotely 800 sensed observations and ensemble forcing data are perturbed with the Normal Perturb and 801 Lognormal Perturb function routines, respectively. After the VIC model simulation for each 802 ensemble member, the PMCMC module is called again to filter the specified model output (i.e., 803 soil moisture) and also the initial condition files. At this point, the DA integration is finished for 804 one-time step and the users can choose whether or not to output the ensemble members of 805 required variables into the local drive, depending on the available main memory. 806

807

#### 808 **Reference**

- Abbaszadeh, P., Moradkhani, H., Yan, H., 2018. Enhancing hydrologic data assimilation by
  evolutionary Particle Filter and Markov Chain Monte Carlo. Adv. Water Resour. 111, 192–
  204. doi:10.1016/j.advwatres.2017.11.011
- AghaKouchak, A., 2014. A baseline probabilistic drought forecasting framework using
   standardized soil moisture index: application to the 2012 United States drought. Hydrol.
   Earth Syst. Sci. 18, 2485–2492. doi:10.5194/hess-18-2485-2014
- Ahmadalipour, A., Moradkhani, H., Yan, H., Zarekarizi, M., 2017. Remote Sensing of Drought:
  Vegetation, Soil Moisture, and Data Assimilation, in: Lakshmi, V. (Ed.), Remote Sensing of
  Hydrological Extremes. Springer International Publishing Switzerland. DOI: 10.1007/9783-319-43744-6\_7, pp. 121–149. doi:10.1007/978-3-319-43744-6\_7
- Albergel, C., Rüdiger, C., Carrer, D., Calvet, J.-C., Fritz, N., Naeimi, V., Bartalis, Z., Hasenauer,
  S., 2009. An evaluation of ASCAT surface soil moisture products with in-situ observations
  in Southwestern France. Hydrol. Earth Syst. Sci. 13, 115–124. doi:10.5194/hess-13-1152009
- Anderson, M.C., Hain, C., Wardlow, B., Pimstein, A., Mecikalski, J.R., Kustas, W.P., 2011.

Evaluation of Drought Indices Based on Thermal Remote Sensing of Evapotranspiration over the Continental United States. J. Clim. 24, 2025–2044. doi:10.1175/2010JCLI3812.1

- Andreadis, K.M., Clark, E.A., Wood, A.W., Hamlet, A.F., Lettenmaier, D.P., 2005. Twentiethcentury drought in the conterminous United States. J. Hydrometeorol. 6, 985–1001.
  doi:10.1175/JHM450.1
- Andreadis, K.M., Lettenmaier, D.P., 2006. Trends in 20th century drought over the continental
   United States. Geophys. Res. Lett. 33. doi:10.1029/2006GL025711
- Andrieu, C., Doucet, A., Holenstein, R., 2010. Particle Markov chain Monte Carlo methods. J. R.
  Stat. Soc. Ser. B (Statistical Methodol. 72, 269–342. doi:10.1111/j.1467-9868.2009.00736.x
- Brocca, L., Moramarco, T., Melone, F., Wagner, W., Hasenauer, S., Hahn, S., 2012.
  Assimilation of surface- and root-zone ASCAT soil moisture products into rainfall-runoff
  modeling. IEEE Trans. Geosci. Remote Sens. 50, 2542–2555.
  doi:10.1109/TGRS.2011.2177468
- Chaney, N.W., Herman, J.D., Reed, P.M., Wood, E.F., 2015. Flood and drought hydrologic
  monitoring: the role of model parameter uncertainty. Hydrol. Earth Syst. Sci. 19, 3239–
  3251. doi:10.5194/hess-19-3239-2015
- Das, N.N., Entekhabi, D., Njoku, E.G., 2011. An algorithm for merging SMAP radiometer and
  radar data for high-resolution soil-moisture retrieval. Geosci. Remote Sensing, IEEE Trans.
  49, 1504–1512.
- De Lannoy, G.J.M., Reichle, R.H., Houser, P.R., Pauwels, V.R.N., Verhoest, N.E.C., 2007.
  Correcting for forecast bias in soil moisture assimilation with the ensemble Kalman filter.
  Water Resour. Res. 43. doi:10.1029/2006WR005449
- DeChant, C.M., Moradkhani, H., 2015. Analyzing the sensitivity of drought recovery forecasts to
   land surface initial conditions. J. Hydrol. 526, 89–100. doi:10.1016/j.jhydrol.2014.10.021
- DeChant, C.M., Moradkhani, H., 2014. Toward a reliable prediction of seasonal forecast
  uncertainty: Addressing model and initial condition uncertainty with ensemble data
  assimilation and sequential Bayesian combination. J. Hydrol. 519, 2967–2977.
  doi:10.1016/j.jhydrol.2014.05.045
- DeChant, C.M., Moradkhani, H., 2012. Examining the effectiveness and robustness of sequential
   data assimilation methods for quantification of uncertainty in hydrologic forecasting. Water
   Resour. Res. 48, W04518. doi:10.1029/2011WR011011
- DeChant, C.M., Moradkhani, H., 2011. Radiance data assimilation for operational snow and
  streamflow forecasting. Adv. Water Resour. 34, 351–364.
  doi:10.1016/j.advwatres.2010.12.009
- Dong, J., Steele-Dunne, S.C., Judge, J., van de Giesen, N., 2015. A particle batch smoother for
  soil moisture estimation using soil temperature observations. Adv. Water Resour. 83, 111–
  122. doi:10.1016/j.advwatres.2015.05.017
- Dorigo, W., Wagner, W., Albergel, C., Albrecht, F., Balsamo, G., Brocca, L., Chung, D., Ertl,
  M., Forkel, M., Gruber, A., Haas, E., Hamer, P.D., Hirschi, M., Ikonen, J., de Jeu, R., Kidd,
  R., Lahoz, W., Liu, Y.Y., Miralles, D., Mistelbauer, T., Nicolai-Shaw, N., Parinussa, R.,
  Pratola, C., Reimer, C., van der Schalie, R., Seneviratne, S.I., Smolander, T., Lecomte, P.,
  2017. ESA CCI Soil Moisture for improved Earth system understanding: State-of-the art
  and future directions. Remote Sens. Environ. 203, 185–215. doi:10.1016/j.rse.2017.07.001
- Borigo, W.A., Gruber, A., De Jeu, R.A.M., Wagner, W., Stacke, T., Loew, A., Albergel, C.,
  Brocca, L., Chung, D., Parinussa, R.M., Kidd, R., 2015. Evaluation of the ESA CCI soil
  moisture product using ground-based observations. Remote Sens. Environ. 162, 380–395.

- doi:10.1016/j.rse.2014.07.023
- B71 Draper, C.S., Reichle, R.H., De Lannoy, G.J.M., Liu, Q., 2012. Assimilation of passive and
  active microwave soil moisture retrievals. Geophys. Res. Lett. 39, L04401.
  doi:10.1029/2011GL050655
- Entekhabi, D., Njoku, E.G., O'Neill, P.E., Kellogg, K.H., Crow, W.T., Edelstein, W.N., Entin,
  J.K., Goodman, S.D., Jackson, T.J., Johnson, J., Kimball, J., Piepmeier, J.R., Koster, R.D.,
  Martin, N., McDonald, K.C., Moghaddam, M., Moran, S., Reichle, R., Shi, J.C., Spencer,
  M.W., Thurman, S.W., Tsang, L., Van Zyl, J., 2010. The soil moisture active passive
  (SMAP) mission. Proc. IEEE 98, 704–716. doi:10.1109/JPROC.2010.2043918
- Evensen, G., 1994. Sequential data assimilation with a nonlinear quasi-geostrophic model using
  Monte Carlo methods to forecast error statistics. J. Geophys. Res. 99, 10143–10162.
  doi:10.1029/94JC00572
- Gruber, A., Su, C.-H., Zwieback, S., Crow, W., Dorigo, W., Wagner, W., 2016. Recent advances
  in (soil moisture) triple collocation analysis. Int. J. Appl. Earth Obs. Geoinf. 45, 200–211.
  doi:10.1016/j.jag.2015.09.002
- Hao, Z., AghaKouchak, A., Nakhjiri, N., Farahmand, A., 2014. Global integrated drought
  monitoring and prediction system. Sci. Data 1, 1–10. doi:10.1038/sdata.2014.1
- Harlim, J., Majda, A.J., 2010. Catastrophic filter divergence in filtering nonlinear dissipative
  systems. Commun. Math. Sci. 8, 27–43.
- Hoerling, M., Eischeid, J., Kumar, A., Leung, R., Mariotti, A., Mo, K., Schubert, S., Seager, R.,
  2014. Causes and predictability of the 2012 Great Plains drought. Bull. Am. Meteorol. Soc.
  95, 269–282. doi:10.1175/BAMS-D-13-00055.1
- Hoerling, M., Schubert, S., Mo, K., 2013. An Interpretation of the Origins of the 2012 Central
   Great Plains Drought, Assessment Report. NOAA Drought Task Force.
- Keyantash, J., Dracup, J.A., 2002. The quantification of drought: An evaluation of drought
  indices. Bull. Am. Meteorol. Soc. 83, 1167–1180. doi:10.1175/15200477(2002)083<1191:TQODAE>2.3.CO;2
- Kumar, S. V., Harrison, K.W., Peters-Lidard, C.D., Santanello, J. a., Kirschbaum, D., 2014a.
  Assessing the impact of L-band observations on drought and flood risk estimation: A
  decision-theoretic approach in an OSSE environment. J. Hydrometeorol. 15, 2140–2156.
  doi:10.1175/JHM-D-13-0204.1
- Kumar, S. V., Peters-Lidard, C.D., Mocko, D., Reichle, R., Liu, Y., Arsenault, K.R., Xia, Y., Ek,
  M., Riggs, G., Livneh, B., Cosh, M., 2014b. Assimilation of remotely sensed soil moisture
  and snow depth retrievals for drought estimation. J. Hydrometeorol. 15, 2446–2469.
  doi:10.1175/JHM-D-13-0132.1
- Kumar, S. V., Reichle, R.H., Koster, R.D., Crow, W.T., Peters-Lidard, C.D., 2009. Role of
  subsurface physics in the assimilation of surface soil moisture observations. J.
  Hydrometeorol. 10, 1534–1547. doi:10.1175/2009JHM1134.1
- Kumar, S. V., Zaitchik, B.F., Peters-Lidard, C.D., Rodell, M., Reichle, R., Li, B., Jasinski, M.,
  Mocko, D., Getirana, A., De Lannoy, G., Cosh, M.H., Hain, C.R., Anderson, M., Arsenault,
  K.R., Xia, Y., Ek, M., 2016. Assimilation of gridded GRACE terrestrial water storage
  estimates in the North American Land Data Assimilation System. J. Hydrometeorol. 17,
  1951–1972. doi:10.1175/JHM-D-15-0157.1
- Kurtz, W., He, G., Kollet, S.J., Maxwell, R.M., Vereecken, H., Franssen, H.J.H., 2016.
   TerrSysMP-PDAF (version 1.0): A modular high-performance data assimilation framework for an integrated land surface-subsurface model. Geosci. Model Dev. 9, 1341–1360.

- 916 doi:10.5194/gmd-9-1341-2016
- Leisenring, M., Moradkhani, H., 2012. Analyzing the uncertainty of suspended sediment load
  prediction using sequential data assimilation. J. Hydrol. 468–469, 268–282.
  doi:10.1016/j.jhydrol.2012.08.049
- Leisenring, M., Moradkhani, H., 2011. Snow water equivalent prediction using Bayesian data
   assimilation methods. Stoch. Environ. Res. Risk Assess. 25, 253–270. doi:10.1007/s00477 010-0445-5
- Liang, X., Lettenmaier, D.P., Wood, E.F., Burges, S.J., 1994. A simple hydrologically based
  model of land surface water and energy fluxes for general circulation models. J. Geophys.
  Res. 99, 14415–14428. doi:10.1029/94JD00483
- Liang, X., Xie, Z., 2001. A new surface runoff parameterization with subgrid-scale soil
  heterogeneity for land surface models. Adv. Water Resour. 24, 1173–1193.
  doi:10.1016/S0309-1708(01)00032-X
- Liu, Q., Reichle, R.H., Bindlish, R., Cosh, M.H., Crow, W.T., de Jeu, R., De Lannoy, G.J.M.,
  Huffman, G.J., Jackson, T.J., 2011. The contributions of precipitation and soil moisture
  observations to the skill of soil moisture estimates in a land data assimilation system. J.
  Hydrometeorol. 12, 750–765. doi:10.1175/JHM-D-10-05000.1
- Liu, Y., Weerts, a. H., Clark, M., Hendricks Franssen, H.J., Kumar, S., Moradkhani, H., Seo,
  D.J., Schwanenberg, D., Smith, P., Van Dijk, a. I.J.M., Van Velzen, N., He, M., Lee, H.,
  Noh, S.J., Rakovec, O., Restrepo, P., 2012. Advancing data assimilation in operational
  hydrologic forecasting: Progresses, challenges, and emerging opportunities. Hydrol. Earth
  Syst. Sci. 16, 3863–3887. doi:10.5194/hess-16-3863-2012
- Liu, Y.Y., Dorigo, W.A., Parinussa, R.M., De Jeu, R.A.M., Wagner, W., McCabe, M.F., Evans,
  J.P., Van Dijk, A.I.J.M., 2012. Trend-preserving blending of passive and active microwave
  soil moisture retrievals. Remote Sens. Environ. 123, 280–297.
  doi:10.1016/j.rse.2012.03.014
- Liu, Y.Y., Parinussa, R.M., Dorigo, W. a., De Jeu, R. a M., Wagner, W., M. Van Dijk, a. I.J.,
  McCabe, M.F., Evans, J.P., 2011. Developing an improved soil moisture dataset by
  blending passive and active microwave satellite-based retrievals. Hydrol. Earth Syst. Sci.
  15, 425–436. doi:10.5194/hess-15-425-2011
- Lloyd-Hughes, B., 2014. The impracticality of a universal drought definition. Theor. Appl.
  Climatol. 117, 607–611. doi:10.1007/s00704-013-1025-7
- Lohmann, D., Raschke, E., Nijssen, B., Lettenmaier, D.P., 1998. Regional scale hydrology: I.
  Formulation of the VIC-2L model coupled to a routing model. Hydrol. Sci. J. 43, 131–141.
  doi:10.1080/02626669809492107
- Lorentzen, R.J., Naevdal, G., 2011. An Iterative Ensemble Kalman Filter. IEEE Trans. Automat.
   Contr. 56, 1990–1995. doi:10.1109/TAC.2011.2154430
- Luo, L., Wood, E.F., 2007. Monitoring and predicting the 2007 U.S. drought. Geophys. Res.
   Lett. 34, L22702. doi:10.1029/2007GL031673
- Madadgar, S., Moradkhani, H., Garen, D., 2014. Towards improved post-processing of
   hydrologic forecast ensembles. Hydrol. Process. 28, 104–122. doi:10.1002/hyp.9562
- Massari, C., Brocca, L., Tarpanelli, A., Moramarco, T., 2015. Data assimilation of satellite soil
  moisture into rainfall-runoff modelling: A complex recipe? Remote Sens. 7, 11403–11433.
  doi:10.3390/rs70911403
- Maurer, E.P., Wood, A.W., Adam, J.C., Lettenmaier, D.P., Nijssen, B., 2002. A long-term
   hydrologically based dataset of land surface fluxes and states for the Conterminous United

- 962
   States\*.
   J.
   Clim.
   15,
   3237–3251.
   doi:10.1175/1520 

   963
   0442(2002)015<3237:ALTHBD>2.0.CO;2
   0442(2002)015<3237:ALTHBD>2.0.CO;2
   0442(2002)015<3237:ALTHBD>2.0.CO;2
- Mishra, A.K., Singh, V.P., 2010. A review of drought concepts. J. Hydrol. 391, 202–216.
   doi:10.1016/j.jhydrol.2010.07.012
- Mo, K.C., Lettenmaier, D.P., 2015. Heat wave flash droughts in decline. Geophys. Res. Lett. 42, 2823–2829. doi:10.1002/2015GL064018
- Montzka, C., Moradkhani, H., Weihermüller, L., Franssen, H.-J.H., Canty, M., Vereecken, H.,
  2011. Hydraulic parameter estimation by remotely-sensed top soil moisture observations
  with the particle filter. J. Hydrol. 399, 410–421. doi:10.1016/j.jhydrol.2011.01.020
- Moradkhani, H., 2008. Hydrologic remote sensing and land surface data assimilation. Sensors 8,
   2986–3004. doi:10.3390/s8052986
- Moradkhani, H., Dechant, C.M., Sorooshian, S., 2012. Evolution of ensemble data assimilation
   for uncertainty quantification using the particle filter-Markov chain Monte Carlo method.
   Water Resour. Res. 48, W12520. doi:10.1029/2012WR012144
- Moradkhani, H., Hsu, K.-L., Gupta, H., Sorooshian, S., 2005. Uncertainty assessment of
   hydrologic model states and parameters: Sequential data assimilation using the particle
   filter. Water Resour. Res. 41, W05012. doi:10.1029/2004WR003604
- Moradkhani, H., Sorooshian, S., 2008. General review of rainfall-runoff modeling: model
   calibration, data assimilation, and uncertainty analysis, in: Hydrological Modelling and the
   Water Cycle. Springer Berlin Heidelberg, pp. 1–24.
- Nerger, L., Hiller, W., 2013. Software for ensemble-based data assimilation systems Implementation strategies and scalability. Comput. Geosci. 55, 110–118.
   doi:10.1016/j.cageo.2012.03.026
- Noh, S.J., Tachikawa, Y., Shiiba, M., Kim, S., 2011. Applying sequential Monte Carlo methods
  into a distributed hydrologic model: lagged particle filtering approach with regularization.
  Hydrol. Earth Syst. Sci. 15, 3237–3251. doi:10.5194/hess-15-3237-2011
- Otkin, J.A., Anderson, M.C., Hain, C., Mladenova, I.E., Basara, J.B., Svoboda, M., 2013.
  Examining Rapid Onset Drought Development Using the Thermal Infrared–Based
  Evaporative Stress Index. J. Hydrometeorol. 14, 1057–1074. doi:10.1175/JHM-D-120144.1
- PaiMazumder, D., Done, J.M., 2016. Potential predictability sources of the 2012 US drought in
   observations and a regional model ensemble. J. Geophys. Res. Atmos.
   doi:10.1002/2016JD025322
- Pan, M., Wood, E.F., 2010. Impact of accuracy, spatial availability, and revisit time of satellitederived surface soil moisture in a multiscale ensemble data assimilation system. IEEE J.
  Sel. Top. Appl. Earth Obs. Remote Sens. 3, 49–56. doi:10.1109/JSTARS.2010.2040585
- Pasetto, D., Camporese, M., Putti, M., 2012. Ensemble Kalman filter versus particle filter for a physically-based coupled surface–subsurface model. Adv. Water Resour. 47, 1–13. doi:10.1016/j.advwatres.2012.06.009
- Plaza, D.A., De Keyser, R., De Lannoy, G.J.M., Giustarini, L., Matgen, P., Pauwels, V.R.N.,
  2012. The importance of parameter resampling for soil moisture data assimilation into
  hydrologic models using the particle filter. Hydrol. Earth Syst. Sci. 16, 375–390.
  doi:10.5194/hess-16-375-2012s
- Reichle, R.H., Crow, W.T., Keppenne, C.L., 2008. An adaptive ensemble Kalman filter for soil
   moisture data assimilation. Water Resour. Res. 44, W03423. doi:10.1029/2007WR006357
- 1007 Reichle, R.H., Koster, R.D., 2004. Bias reduction in short records of satellite soil moisture.

1008 Geophys. Res. Lett. 31, L19501. doi:10.1029/2004GL020938

- Reichle, R.H., Koster, R.D., Liu, P., Mahanama, S.P.P., Njoku, E.G., Owe, M., 2007.
  Comparison and assimilation of global soil moisture retrievals from the Advanced
  Microwave Scanning Radiometer for the Earth Observing System (AMSR-E) and the
  Scanning Multichannel Microwave Radiometer (SMMR). J. Geophys. Res. 112, D09108.
  doi:10.1029/2006JD008033
- Ridler, M.E., van Velzen, N., Hummel, S., Sandholt, I., Falk, A.K., Heemink, A., Madsen, H.,
  2014. Data assimilation framework: Linking an open data assimilation library (OpenDA) to
  a widely adopted model interface (OpenMI). Environ. Model. Softw. 57, 76–89.
  doi:10.1016/j.envsoft.2014.02.008
- 1018 Ross, T., Lott, N., 2003. A climatology of 1980-2003 extreme weather and climate events.
   1019 National Ocanic and Atmospheric Administration.
- Samaniego, L., Kumar, R., Zink, M., 2013. Implications of parameter uncertainty on soil
   moisture drought analysis in Germany. J. Hydrometeorol. 14, 47–68. doi:10.1175/JHM-D 12-075.1
- 1023 Sheffield, J., Wood, E.F., 2011. Drought: past problems and future scenarios. Routledge.
- Sheffield, J., Wood, E.F., Chaney, N., Guan, K., Sadri, S., Yuan, X., Olang, L., Amani, A., Ali,
  A., Demuth, S., Ogallo, L., 2014. A drought monitoring and forecasting system for subsahara african water resources and food security. Bull. Am. Meteorol. Soc. 95, 861–882.
  doi:10.1175/BAMS-D-12-00124.1
- Shukla, S., Steinemann, A.C., Lettenmaier, D.P., 2011. Drought monitoring for Washington
  State: indicators and applications. J. Hydrometeorol. 12, 66–83.
  doi:10.1175/2010JHM1307.1
- Su, C.H., Ryu, D., Crow, W.T., Western, A.W., 2014. Beyond triple collocation: Applications to
  soil moisture monitoring. J. Geophys. Res. Atmos. 119, 6419–6439.
  doi:10.1002/2013JD021043
- Svoboda, M., LeComte, D., Hayes, M., Heim, R., Gleason, K., Angel, J., Rippey, B., Tinker, R.,
  Palecki, M., Stooksbury, D., Miskus, D., Stephens, S., 2002. The drought monitor. Bull.
  Am. Meteorol. Soc. 83, 1181–1190. doi:10.1175/15200477(2002)083<1181:TDM>2.3.CO;2
- van Delft, G., El Serafy, G.Y., Heemink, A.W., 2009. The ensemble particle filter (EnPF) in
  rainfall-runoff models. Stoch. Environ. Res. Risk Assess. 23, 1203–1211.
  doi:10.1007/s00477-008-0301-z
- 1041 Van Loon, A.F., 2015. Hydrological drought explained. Wiley Interdiscip. Rev. Water 2, 359–
   1042 392. doi:10.1002/wat2.1085
- Wagner, W., Hahn, S., Kidd, R., Melzer, T., Bartalis, Z., Hasenauer, S., Figa-Saldaña, J., de
  Rosnay, P., Jann, A., Schneider, S., 2013. The ASCAT soil moisture product: A review of
  its specifications, validation results, and emerging applications. Meteorol. Zeitschrift 22, 5–
  33.
- Wagner, W., Naeimi, V., Scipal, K., Jeu, R., Martínez-Fernández, J., 2007. Soil moisture from
  operational meteorological satellites. Hydrogeol. J. 15, 121–131. doi:10.1007/s10040-0060104-6
- Wilhite, D.A., 2000. Drought as a natural hazard: concepts and definitions, in: Wilhite, D.A.
  (Ed.), Drought: A Global Assessment. Routledge, London, pp. 3–18.
- Wood, E.F., Schubert, S.D., Wood, A.W., Peters-Lidard, C.D., Mo, K.C., Mariotti, A., Pulwarty,
   R.S., 2015. Prospects for advancing drought understanding, monitoring, and prediction. J.

- 1054 Hydrometeorol. 16, 1636–1657. doi:10.1175/JHM-D-14-0164.1
- Xia, Y., Mitchell, K., Ek, M., Sheffield, J., Cosgrove, B., Wood, E., Luo, L., Alonge, C., Wei,
  H., Meng, J., Livneh, B., Lettenmaier, D., Koren, V., Duan, Q., Mo, K., Fan, Y., Mocko, D.,
  2012. Continental-scale water and energy flux analysis and validation for the North
  American Land Data Assimilation System project phase 2 (NLDAS-2): 1. Intercomparison
  and application of model products. J. Geophys. Res. Atmos. 117, D03109.
  doi:10.1029/2011JD016048
- Yan, H., DeChant, C.M., Moradkhani, H., 2015. Improving Soil Moisture Profile Prediction
  With the Particle Filter-Markov Chain Monte Carlo Method. IEEE Trans. Geosci. Remote
  Sens. 53, 6134–6147. doi:10.1109/TGRS.2015.2432067
- Yan, H., Moradkhani, H., 2016. Combined assimilation of streamflow and satellite soil moisture
  with the particle filter and geostatistical modeling. Adv. Water Resour. 94, 364–378.
  doi:10.1016/j.advwatres.2016.06.002
- Yan, H., Moradkhani, H., Zarekarizi, M., 2017. A probabilistic drought forecasting framework:
  A combined dynamical and statistical approach. J. Hydrol. 548, 291–304.
  doi:10.1016/j.jhydrol.2017.03.004
- Yilmaz, M.T., Crow, W.T., 2013. The optimality of potential rescaling approaches in land data
   assimilation. J. Hydrometeorol. 14, 650–660. doi:10.1175/JHM-D-12-052.1
- Yin, J., Zhan, X., Zheng, Y., Liu, J., Fang, L., Hain, C.R., 2015. Enhancing Model Skill by
  Assimilating SMOPS Blended Soil Moisture Product into Noah Land Surface Model. J.
  Hydrometeorol. 16, 917–931. doi:10.1175/JHM-D-14-0070.1
- 1075

1076 5 List of Captions

1077 Figure 1 The flowchart of the proposed drought monitoring system. The three probability 1078 distributions associated with the meteorological forcing, remotely sensed soil moisture, and soil 1079 moisture states represent the corresponding uncertainties

1080

Figure 2. The flow diagram of the parallel particle filtering framework (PPFF) using Message
Passing Interface (MPI). The domain decomposition parallel strategy is used in the PPFF: each
grid cell is simulated in parallel while each ensemble member is simulated sequentially.

1084

Figure 3. The flowchart of the synthetic study using VIC model to assess the potential benefit ofassimilation of satellite surface soil moisture on drought monitoring.

1087

Figure 4. (a) The normalized information contribution (NIC) value between the EnKF and PMCMC root-zone soil moisture predictions (Eq. 13). Positive values indicate that the PMCMC improves soil moisture prediction as compared to the EnKF; negative values indicate the degradation over the EnKF. (b) Time series of the marked (yellow star) grid cell root-zone soil moisture (m3/m3) for the synthetic truth, EnKF, and PMCMC simulation for the period of 1 January 2012 to 31 December 2012. Both NIC values and time series are generated using the posterior means

1095

Figure 5. The normalized information contribution (NIC) value between the Open-Loop (OL) and Data Assimilation (DA). The NIC values are generated based on posterior means. The positive value indicates that the DA improves soil moisture prediction against OL; negative value indicates the degradation over the OL. (a): Surface soil moisture field. (b): Root-zone soilmoisture filed.

1101

Figure 6. Comparison of the drought monitoring skill between Open-Loop (OL) and DataAssimilation (DA) for May–August 2012.

1104

1105 Figure 7. The absolute bias of drought extent (%) against the synthetic truth between Open-Loop

1106 (OL) and Data Assimilation (DA) over the CONUS for the period of May–August 2012.

1107

1108Figure 8. Comparison of the 2012 summer drought intensity over the CONUS from Open-Loop

1109 (OL), Data Assimilation (DA), and U.S. Drought Monitoring (USDM).

1110

1111 Figure 9. Comparison of the drought extent (%) over the CONUS from Open-Loop (OL), Data

1112 Assimilation (DA), and U.S. Drought Monitoring (USDM) for May/June/July/August 2012.

1113

Figure 10. Comparison of U.S. Drought Monitoring (USDM) and Data Assimilation (DA)
drought monitoring extent for five different drought categories (D0–D4) over the Central U.S.
The drought extent is comprised of the 7-State region of Nebraska, Iowa, Kansas, Missouri,
Oklahoma, Arkansas, and Illinois.

1118

Figure 11. Comparison of the 2010 summer drought intensity over the CONUS from Open-Loop(OL), Data Assimilation (DA), and U.S. Drought Monitoring (USDM).

1121

Figure A1. The flowchart of the offline coupling interface of the VIC model and the PMCMC data assimilation algorithm. The ensemble files indicate the ensemble members of the PMCMC algorithm. A one-day VIC model simulation and PMCMC updating are shown in this flowchart.