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An Integrated Hydrologic Bayesian Multi-Model Combination Framework: Confronting Input, parameter and model structural uncertainty in Hydrologic Prediction

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1	An Integrated Hydrologic Bayesian Multi-Model Combination Framework:
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3	Prediction
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1 Abstract

2 This paper presents a new technique —Integrated Bayesian Uncertainty Estimator 3 (IBUNE) to account for the major uncertainties of hydrologic rainfall-runoff predictions 4 explicitly. The uncertainties from the input (forcing) data — mainly the precipitation 5 observations and from the model parameters are reduced through a Monte Carlo Markov 6 Chain (MCMC) scheme named Shuffled Complex Evolution Metropolis (SCEM) 7 algorithm which has been extended to include a precipitation error model. Afterwards, 8 the Bayesian Model Averaging (BMA) scheme is employed to further improve the 9 prediction skill and uncertainty estimation using multiple model output. A series of case 10 studies using three rainfall-runoff models to predict the streamflow in the Leaf River 11 basin, Mississippi are used to examine the necessity and usefulness of this technique. The 12 results suggests that ignoring either input forcings error or model structural uncertainty 13 will lead to unrealistic model simulations and their associated uncertainty bounds which 14 does not consistently capture and represent the real-world behavior of the watershed.

15 1. Introduction

Various hydrologic rainfall-runoff models have been used to represent the watershed physical processes which control the conversion of precipitation into streamflow and water storage changes. These models include many parameters describing the properties of the watershed that generally need to be estimated through calibration against historical observation data. For many years, research effort has been devoted to develop techniques to find the optimal values of the parameters that enable the model predictions matching the watershed observations. The major weakness of this

1 parameter-calibration approach is that it attributes all sources of uncertainties in the 2 modeling process to parameter errors. In fact, in addition to parameter uncertainty, there are many other uncertainties from various sources to affect the model results, among 3 4 them including the errors in model input (forcing) data such as the precipitation 5 observation data, the description of boundary and initial conditions, and the model 6 structural deficiencies. Because of the highly nonlinear nature of the hydrologic system, it 7 is not feasible to account for all these uncertainties from different sources through model 8 parameter adjustments.

9 Recently, hydrologic research [Bven and Binley, 1992; Kuczera and Parent, 1998; 10 Vrugt et al., 2003] started to analyze various uncertainty sources in hydrological 11 modeling. New techniques have made significant progress in estimating the propagation 12 of confidence bounds from different uncertainty sources to the model output. Among 13 them include the use of data assimilation techniques to tackle uncertainty in boundary 14 and initial conditions [Kitanidis and Bras, 1980 a,b; Beck, 1987; Evenson, 1992; Miller et 15 al., 1994]; simultaneous data assimilation and parameter estimation [Moradkhani et al., 16 2005]; and simultaneous uncertainty estimation of input (forcing) data and parameter 17 estimation [Kavetski et al., 2003]. Most of these studies focus on addressing one or two 18 uncertainty sources based on a selected hydrologic model. However, by using a single 19 model, those techniques (which do not change the model structures) are unable to correct 20 the errors in model output resulting from the structural deficiencies of the specific model.

Lately a new scheme has emerged which seeks to obtain a consensus from a combination of multiple model predictions so that one model's output errors can be

1 compensated by others'. The combination techniques can be categorized into two groups. 2 The first group [e.g., Shamseldin et al., 1997; Abrahart and See, 2002; Georgakakos et 3 al., 2004; Ajami et al., 2005a] uses a set of deterministic weights to combine multiple 4 model outputs. Methods of simple model average (equal weights), linear regression, or 5 artificial neural network (ANN) belong to this category. The consensus prediction from 6 these methods is an alternative deterministic prediction without uncertainty estimates. In 7 addition, the weights in such combination can take any arbitrary real (positive or 8 negative) values that lack physical interpretations.

9 The second group such as Bayesian Model Averaging (BMA), [Madigan et al., 10 1996; *Hoeting et al.*, 1999] employs probabilistic techniques which derive the consensus 11 prediction from competing predictions using likelihood measures as model weights. The 12 likelihood measure (weight) for each member model is based on the success frequency of 13 the predictions that an individual model has made within the observations. For this 14 reason, BMA weights are tied directly to individual model performance. BMA has been 15 applied in a variety of fields including statistics, management science, medicine and 16 meteorology [e.g. Viallefont et al., 2001; Fernandez, et al., 2001; Raftery et al., 2003, 17 2005; Wintle et al., 2003]. In many case studies, the BMA has shown to produce more 18 accurate and reliable predictions than other multi-model techniques [George and 19 McCulloch, 1993; Raftery et al., 1997; Clvde, 1999; Viallefont et al., 2001; Raftery and 20 Zheng, 2003; Ellison, 2004]. Very recently, the BMA method was applied to hydrologic 21 groundwater modeling [Neuman and Wierenga, 2003; Nueman, 2003].

1 This study intends to build a hybrid framework, Integrated Bayesian Uncertainty 2 Estimator (IBUNE), to confront the uncertainties in rainfall-runoff predictions associated 3 with input errors, model parameters estimates, and model structural deficiencies. To 4 accomplish this objective, the paper is divided into three major subsequent parts. First, 5 the SCEM algorithm [Vrugt et al., 2003], which was developed for probabilistic 6 parameter estimation, will be studied. We will demonstrate that ignoring the input and 7 model structural uncertainty, could lead to corrupted parameter estimations as well as 8 unreliable uncertainty bounds on the model predictions. The second part of the paper 9 presents a simple approach to extend SCEM to simultaneously account for the 10 uncertainties originating from both input precipitation data and the model parameters. 11 This is the first step towards building IBUNE. We will prove that the error incorporated 12 within the input (forcing) data is one of the major uncertainty sources in the rainfall 13 runoff modeling system, and by accounting for it within our uncertainty assessment 14 procedure, we will improve the uncertainty bounds in model prediction. We will also 15 show that not assessing model structural uncertainty is still an important limitation of this 16 part of the study.

Finally, the third part of this paper intends to consider model structural uncertainty in addition to input and parameter uncertainty. We present a hybrid approach where we merge the strengths of the Bayesian Model Averaging scheme with the extended SCEM. This is the final step in building the new Framework, called IBUNE. IBUNE further reduces the uncertainties caused by the deficiencies in individual models by using Bayesian Model Averaging, while also accounting for input and parameter uncertainty within individual models by applying extended SCEM. Finally, the IBUNE
 scheme will be applied to a real case study in the Leaf River basin, Mississippi.

The paper is organized as follows. Section 2 investigates the effects of ignoring input uncertainty and model structural uncertainty in model parameters using SCEM. Section 3 describes a new approach for confronting input uncertainty and discusses the performance of this approach. In section 4 we will introduce the logic and architecture of IBUNE and demonstrate how it exploits the strength from extended SCEM-UA and Bayesian Model Averaging to confront multiple sources of uncertainty. Finally in section 5 we summarize the results and conclude with some recommendations.

10 2. Traditional uncertainty assessment in hydrological modeling

11 2.1. Basic Idea in hydrologic modeling uncertainty assessment

12

A typical hydrologic model, M, can be represented as follows:

13
$$y = M(X, \theta) \tag{1}$$

14 where y represents the response matrix of the catchment (e.g., streamflow), M(.) denotes 15 the nonlinear hydrologic model, θ is a set of model parameters and X stands for observed 16 forcing input matrix (e.g., precipitation). In traditional approach, the uncertainty in the 17 catchment response is attributed to parameter estimation uncertainty, while input and 18 model structural uncertainty is ignored. Therefore the residual vector, e, which is the 19 difference between model simulation $y(\theta)$, and measured (observed) catchment response 20 (\tilde{y}) , can be expressed as:

1
$$e(\theta) = \tilde{y} - y(\theta);$$
 (2)

2

3

These residuals are usually assumed to be additive, independent (uncorrelated) and normally distributed noise with mean equal to zero and constant variance, σ :

4
$$y = M(X, \theta) + e(\theta),$$
 $e \sim N(0, \sigma)$ (3)

5 Applying the Bayesian maximum likelihood estimator, the sum of squared errors, 6 over the historical period T, $E = \sum_{t=1}^{T} (e(\theta)_t)^2$, is minimized to identify the most probable 7 parameter set and the associated uncertainty with these estimates as a posterior 8 distribution function, $P(\theta | X, \tilde{y})$. Under Bayes statistics, this term is proportional to the 9 product of likelihood function and the prior distribution function, $P(\theta)$. Assuming that 10 the residuals are normally distributed, *Box and Tio* [1973] described this likelihood 11 function as follows:

12
$$L(\theta \mid X, \tilde{y}) = \exp\left(-\frac{1}{2\sigma^2} \left(\sum_{t=1}^T (e(\theta)_t)^2\right)\right)$$
(4)

13 Further assuming non-informative prior for $P(\theta) \propto \sigma^{-1}$, σ can be integrated out 14 resulting in the following expression [*Box and Tio*, 1973]

15
$$p(\theta \mid X, \tilde{y}) \propto \left[\sum_{t=1}^{T} (e(\theta)_t)^2\right]^{-(\frac{T}{2})}$$
(5)

In practice it is easier to maximize the logarithm of the likelihood function. This
maximization process will identify a set of plausible parameter values given the available

observed data. There are several Bayesian approaches tailored for hydrologic modeling including the Generalized Likelihood Uncertainty Estimation (GLUE) framework [*Beven and Binley*, 1992] and the Shuffled Complex Evolution Metropolis (SCEM-UA) algorithm [*Vrugt et al.*, 2003] that consider model parameters in equation (1) as probabilistic variables and estimate their uncertainty bound based on the posterior PDF. In this study we will further explore the SCEM-UA algorithm for estimating model parameters and their associated uncertainty bounds.

8

2.2. The Shuffled Complex Evolution Metropolis

9 The Shuffled Complex Evolution Metropolis, SCEM, was built upon the 10 principles of the effective and efficient global optimization technique, Shuffled Complex 11 Evolution (SCE-UA) developed by Duan et al. [1992]. Vrugt et al. [2003] combined the 12 strengths of the MCMC sampler with the concept of complex shuffling from SCE-UA, to 13 form an algorithm that not only provides the most probable parameter set, but also 14 estimates the uncertainty associated with estimated parameters. The main difference 15 between SCEM and SCE is that the downhill simplex method in SCE was replaced by 16 Metropolis-Hasting search algorithm [Metropolis et al., 1953; Hastings, 1970] therefore 17 SCEM in every model run, is able to simultaneously identify both the most likely 18 parameter set and its associated posterior probability distribution. SCEM-UA is explained 19 in detail in Vrugt et al. [2003]. The Gelman-Rubin criterion [Gelman and Rubin, 1992] 20 ensures that each parameter converges to a stationary posterior probability distribution.

2.3. Case Study: Use of SCEM for calibration and uncertainty assessment of hydrologic model parameters

In this section we demonstrate the performance and applicability of SCEM-UA to identify and estimate model parameters and their associated uncertainty bounds, by application to three hydrologic models including SAC-SMA [*Burnash et al.*, 1973], HYMOD [*Boyle et al.*, 2000] and SWB model [*Schaake et al.*, 1996].

SAC-SMA is a nonlinear, continuous, conceptual rainfall-runoff model [*Burnash et al.*, 1973] and is being used operationally by many of the United States National
Weather Service River Forecast Centers (NWS-RFC) for flood forecasting. The model
includes two soil moisture layers, an upper and lower zone (Figure 1). This model
includes 16 parameters, three of which were fixed at specified values and remaining 13
parameters need to be determined through optimization process.

13 We have selected the Leaf River basin to demonstrate the performance of SCEM-UA. This 1949 km² basin is located north of Collins, Mississippi. Five years of daily 14 including 15 historical data (1953-1957) Precipitation (mm/6hours). Potential Evapotranspiration (mm/day), and streamflow (m^3/s) were used for calibration and 16 17 uncertainty assessment. Since many other studies were conducted over the period of 18 1953-1957 [Yapo et al., 1996; Boyle et al., 2001; Misirli et al., 2003, Vrugt et al., 2003], 19 for comparison purposes we selected the same period for this study. To reduce the 20 sensitivity to initial state variables, a 365-day (through year 1952) warm-up period was 21 used, during which no calibration and uncertainty estimation was performed.

1 Since the Leaf River Basin has been studied extensively for optimization purposes 2 [e.g. Yapo et al., 1996; Boyle et al., 2001; Misirli et al., 2003], we have gained a very 3 good knowledge of what SAC-SMA parameter values should be for this basin. For the 4 sake of simplicity, we decided to fix five percolation parameters (Figure 1) to pre-5 specified values. Further, we also maintained the relative values of the parameters 6 associated with the lower zone and upper zone. Consequently the number of parameters 7 in the SAC-SMA model that needs to be identified was decreased to five: UZTWM, 8 upper zone tension water maximum storage, UZFWM, upper zone free water maximum 9 storage, UZK, upper zone free water lateral depletion rate, LZTM, Lower Zone Total 10 Maximum storage and finally LZSK, lower zone supplementary free water depletion rate. 11 LZTM represents summation of all lower zone storages. Lower zone primary free water 12 depletion rate, LZPK is estimated based on LZPK is 3% of lower zone supplemental free 13 water depletion rate (LZSK).

14 Input forcing data and model structure were assumed perfect in this section and 15 all the uncertainty in the streamflow simulation was attributed to parameter estimation 16 uncertainty. We used a 2000 initial population size. Figure 2 illustrates the marginal 17 posterior probability distribution for the estimated SAC-SMA model parameters. These 18 distributions are generated using 20,000 samples after the algorithm converged to the 19 final posterior distribution. This figure illustrates two points. The first point is that the 20 posterior distributions for three of the five parameters (UZTWM, LZTM and LZSK) are 21 approximately normal, however the posterior distribution of UZFWM depicts the 22 existence of two modes (multi-modality). The posterior distribution of UZK is very close 23 to the upper boundary of the predefined parameter range. This can be an indication that

1 the adopted upper limit for the UZK parameter, which had been used in all of the 2 previous studies [Yapo et al., 1996; Boyle et al., 2001; Vrugt et al., 2003], might need to 3 be reevaluated and modified. The second observation is that the final converged samples 4 for all the parameters capture only a small space of the predefined range for the 5 parameters (Table 1). This indicates that the algorithm has high confidence on the 6 parameters. However, this confidence is not justified since the hydrograph uncertainty 7 bounds associated with these parameter ranges do not cover the expected number of 8 observed streamflow values (dark-gray region in the Figure 3). The light-gray region in 9 the Figure (3) shows the 95% hydrograph prediction uncertainty associated with the total 10 error in the hydrologic system in terms of model residuals (calculated based on predictive 11 variance of SCEM). Even though the 95% total prediction uncertainty range captures all 12 the observations, it is very wide compared to uncertainty bounds associated with 13 parameter uncertainty, revealing a considerable amount of uncertainty in both the data 14 and structure of the model under study.

15 To further demonstrate the applicability of SCEM, we used this algorithm to 16 estimate optimal parameter sets and assess their associated uncertainty boundaries for 17 two other hydrologic models, HYdrologic MODel (HYMOD), [Boyle et al., 2000] and 18 Simple Water Balance model (SWB), [Schaake et al., 1996]. These are both simple and 19 conceptual rainfall-runoff models. The HYMOD model consists of a simple rainfall 20 excess model, which is connected to two series of linear reservoirs to route surface and 21 subsurface flow (three quick flow reservoirs and a single slow flow reservoir). This 22 model includes five parameters: C_{max} (L) is the maximum storage capacity in the 23 catchment, b_{exp} (-) is the shape factor of the main soil water storage tank that represent the degree of spatial variability of the soil moisture capacity within the catchment, *Alpha* (-), the factor distributing flow between two series of reservoirs, and finally R_q (T) and R_s (T) are the residence time of linear quick and slow flow reservoirs, respectively. Figure 4 illustrates the schematic of this model and Table 2 represents the parameters and their initial uncertainty bounds.

6 The Simple Water Balance model is a conceptual, parametric water balance 7 model with two soil layers. A thin upper layer represents the vegetation canopy and the 8 soil surface while a lower layer represents the vegetation root zone and groundwater 9 system. Five parameters controlling the SWB model processes are: $D_{b,max}$, the maximum 10 soil moisture deficit of bottom layer of the soil, Q_{max} , the potential subsurface runoff, Q_{max} 11 $/S_{max}$, the ratio of the lower level posture that produce subsurface flow (S_{max} is the 12 minimum threshold that guaranties subsurface flow), $D_{u,max}/D_{b,max}$, the upper layer deficit 13 proportion ($D_{u,max}$ is the maximum soil moisture deficit of upper layer) and finally K_{dt} , the 14 time scale factor. Table 3 lists the SWB model parameters and their initial uncertainty 15 bounds.

Figure 5 exhibits the final estimated marginal posterior distributions of the HYMOD model parameters, after 20000 samples. The results reveal that the distributions for all HYMOD parameters are approximately normal. These parameter distributions cover a very small range of predefined parameter ranges, therefore indicating the model's over-confidence on the final estimated parameter set. However in Figure 6 we can see that even though the algorithm shows high probability for these parameter sets, the estimated hydrograph prediction uncertainty bounds (dark-gray) does not include many of the observed streamflow values. Similar results are presented in Figures 7 and 8 for
 SWB model.

The examples presented above reveal that no model can capture all the processes within the watershed. Attributing all uncertainties in hydrologic models to model parameters and ignoring input and model structural uncertainties leads to an inaccurate, biased and inconsistent simulation of the system processes and their associated uncertainty bounds. Therefore there is a need for a more accurate uncertainty estimator which addresses other sources of uncertainty in conjunction with the parameter estimation uncertainty.

10 3. Extended SCEM-UA to include the input error model: Simultaneous Parameter 11 and Input Uncertainty Estimation

12 Results from previous section indicate that the dealing only with model parameter 13 uncertainty is not enough to accurately estimate the true uncertainty in hydrologic 14 simulation. Uncertainties from other sources must be dealt more directly. There have 15 been a few studies in hydrological modeling that explicitly account for input uncertainty 16 within the system through input error models. One such approach is the BAyesian Total 17 Error Analysis (BATEA) by Kavetski et al. [2003]. BATEA is the only method which 18 explicitly considers input error in the development of the likelihood function in 19 hydrological modeling. They introduce rainfall depth multipliers as some latent variable 20 to the system and introduce an explicit term to the likelihood function to estimate these variables. If \tilde{r}_t represent the true rainfall depth $\tilde{X} = [\tilde{r}_1, \tilde{r}_2, \dots, \tilde{r}_t, t=1:T]$; and r_t is the 21 22 observed rainfall depth, their input error model has the following form:

1
$$r_j = m_j \tilde{r}_j;$$
 $m \sim N(0, \sigma_m^2)$ (6)

2 where, j indicates the storms within the rainfall series, m_i is the random noise from a normal distribution with zero mean and known (pre-specified) variance σ_m^2 in the form of 3 multiplier from that corrupts the true rainfall depth and yields the observed rainfall depth. 4 5 Kavetski et al. [2003] assumed the rainfall multipliers, m_t , as latent variables and 6 estimated both them and the model parameters through their probabilistic calibration 7 procedure called BATEA. They considered these multipliers just for the storm events in 8 the historical period to decrease dimensions of the system. Considering Bayes' law, and 9 assuming that, (1) X (observed input) and \tilde{y} (true catchment response) are statistically independent since catchment response, \widetilde{y} , depends only on the true input forcing, \widetilde{X} , not 10 11 necessarily observed forcing, and (2) X is statistically independent of θ (model parameter 12 set), since observed input is uncorrelated to the hydrologic model parameters, Kavetski et 13 al. [2003] derived the final form of their likelihood function as follows:

14
$$p(\theta, \tilde{X} \mid X, \tilde{y}) \propto L(\tilde{y} \mid \theta, \tilde{X}) \times L(X \mid \tilde{X}) \times p(\theta, \tilde{X})$$
 (7)

15 where $L(\tilde{y} | \theta, \tilde{X})$ is the likelihood of observing \tilde{y} given a parameter set θ and 16 the true input forcing \tilde{X} , $L(X | \tilde{X})$ is the likelihood based on input error model, and 17 $p(\theta, \tilde{X})$ represent the prior distribution of parameters and true input forcing.

18 *Kavetski et al.* [2003] applied their BATEA framework to a series of synthetic case 19 studies and demonstrated that considering an input error model explicitly and adding a 20 new term to the likelihood function can improve the response surface and assessment of 1 uncertainty bounds. Nonetheless even though equation (7) allows the use of explicit input 2 error models, it has two drawbacks. First there is no way to know what the true input 3 forcing is and therefore it is impossible to assess the input error model 4 likelihood, $L(X | \tilde{X})$. Second in some cases, the number of these latent variables can 5 increase considerably and cause some dimensionality issues. To circumvent these two 6 problems, we decided to change the input error model as follows:

Instead of introducing latent variables to the system, we considered a multiplier in the following form:

9
$$\widetilde{r}_t = \phi_t r_t; \qquad \phi \sim N(m, \sigma_m^2)$$
 (8)

where ϕ_t represents a random multiplier with mean equal to $m, m \in [0.9, 1.1]$ and 10 variance equal to σ_m^2 , $\sigma_m^2 \in [1e-5, 1e-3]$. In this implementation we assume, true 11 rainfall depth, \tilde{r}_t , is corrupted at all times by random multipliers from the 12 identical distribution with mean *m* and variance σ_m^2 . Therefore instead of 13 searching for every single multiplier as a latent variable, we introduce two new 14 15 parameters to the system including mean and variance of error model multiplier (instead of additive) distribution, $\eta = \{m, \sigma_m^2\}$. Considering the error term in the 16 form of the multiplier helps to maintain the heteroscedastic (non-homogeneous) 17 18 nature of the error, (higher deviation in higher rainfall depths), [Sorooshian and 19 Dracup, 1980].

• To deal with the issue of not having true observation of input forcing data, we decided to keep the likelihood function in the original format and integrate the input error model into model error term and change the equation (2) as follows:

$$e(\theta) = \tilde{y} - y(\theta, \eta) \tag{9}$$

5 Therefore the likelihood function will have the following form:

4

6
$$p(\theta, \eta \mid X, \tilde{y}) \propto L(X, \tilde{y} \mid \theta, \eta) \times p(\theta, \eta)$$
 (10)

7 These changes were implemented into the hydrologic input-output system and the
8 SCEM-UA was used to estimate the model parameters and input error model parameters
9 simultaneously.

3.1. Case Study: Use of extended SCEM for calibration and uncertainty assessment of Hydrologic model parameters and input error model parameters

Here by means of a case study, we illustrate the performance of SCEM-UA while considering an input error model to specify the hydrologic system. Again we applied SCEM-UA to calibrate and assess uncertainty bounds for SAC-SMA, HYMOD and SWB model parameters along with input error model parameters on the Leaf River Basin. The idea is to compare the results from this part of the study to those from section 2.3.

Figure 9 shows the new marginal posterior distribution estimated for each parameter of the SAC-SMA model while considering an input error model's first two moments as two additional parameters in the system, using SCEM-UA. Looking at Figure 9 and comparing the results with Figure 2, two observations can be made from

1 these results. One is that considering input error model, the final estimated marginal 2 distribution for the model parameters moved over the possible parameter range and 3 assigned the mode of the probability distribution to different parameter values. The 4 second observation is that the mean of the input error model has a mode different than 5 one. These two observations prove that it is necessary to account for the uncertainty in 6 the input forcing. If the input forcing was correct, the mean of the input error model 7 would concentrate around one and the final marginal distribution of the parameters would 8 be the same as if we did not account for input uncertainty. Figure 10 shows the estimated 9 uncertainty bounds for the hydrograph associated with input and model parameter 10 uncertainty. The 95% prediction intervals are narrower here compared to the original case 11 (just considering uncertainty in model parameters). This reveals that the final uncertainty 12 bounds associated with both input and model parameters are more accurate and variance 13 of the residuals at each point is smaller compared to the original scenario.

14 Table 4 confirms these abovementioned results for the SAC-SMA model. The 15 observation coverage for the estimated uncertainty bounds for the simulation has 16 increased by 14% when we account for input uncertainty. The same results are presented 17 in the table for the HYMOD and SWB model, which reveals that accounting for input 18 uncertainty improved the final streamflow simulation of these models as well. These 19 results illustrate that not accounting for input uncertainty can lead to biased parameter 20 estimates, which are compensating for other sources of uncertainty. Figure 11 shows that 21 accounting for input uncertainty improves the Daily Root Mean Square error (DRMS) for 22 all three models across all of their ensembles. We can also see that this improvement is 23 more significant for the SAC-SMA model and less significant for the SWB models. The reason is that the SWB has a higher model structural uncertainty than the SAC-SMA, this
 can corrupt the final estimated parameters therefore weakens the gain from accounting
 for input uncertainty.

4 One of the important observations from the set of experiments presented in this 5 section was that the estimated mean and variance of input error model and their 6 associated uncertainty bound are different from one hydrological model to the other one. 7 This is an inevitable result since we are still ignoring model structural uncertainty. 8 Therefore all the model parameters as well as input error model parameter are still 9 compensating for model structural uncertainty. The next section focuses on this important 10 source of uncertainty in hydrologic system simulation.

4. Uncertainty Assessment in Hydrological Modeling: Simultaneous Parameter and Input and model structural Uncertainty Estimation

13 4.1. Classical Model structural error

14 The dominant approach in hydrological modeling and streamflow forecasting has 15 been the use of a single model. However, dependence on a single hydrological model, 16 which presumably does not adequately represent all of the physical processes of the 17 watershed well, results in unreliable, uncertain and overconfident forecast. This is the 18 case even if we account for all other sources of uncertainty such as parameter estimation 19 and input forcing uncertainty [Geogakakos et al., 2004]. So far all the approaches set 20 forth to identify model structural inadequacy focused on a single model structure and 21 how it can be improved to more adequately represent the system [e.g. see Vrugt et al.,

1 2004]. One major drawback of this kind of approach is that no matter how much we 2 improve a structure of a model, each model is still a simplification of the real world. Also 3 every hydrologic model was originally developed and designed for a specific purpose, 4 hence contains certain assumptions that might not hold in other circumstances. This was 5 demonstrated earlier in the paper, by illustrating dissimilar performance of three 6 hydrologic models in capturing observed streamflow for the same basin.

7 A new kind of approach that recently emerges to identify model structural 8 uncertainty is to use multi-model combination techniques, which provides a better 9 understanding of the watershed by investigating multiple model structures. Examples of 10 multi-model combination techniques which have been applied in hydrologic models, 11 include Weighted Average Model (WAM) [Shamseldin et al., 1997], MLBMA [Neuman, 12 2003], Bayesian Recursive Model Combination (BRMC) [Ajami et al., 2005b, Duan et 13 al., 2005], and M3SE [Ajami et al., 2005a]. The MLBMA and BRMC algorithms, based 14 on Bayesian Model Averaging (BMA), [Hoeting et al., 1999], were developed for 15 hydrological applications. Even though these BMA algorithms consider model parameter 16 and model structural uncertainties, they typically do not explicitly account for input 17 forcing uncertainty.

18

4.2. Bayesian Model Averaging

Bayesian Model Averaging is a probabilistic scheme for model combination. It is a coherent technique for accounting for model structural uncertainty [*Madigan et al.*, 1996]. Below is a brief description of the essence of the BMA scheme. Let's consider a quantity \tilde{y} to be the forecasted variable and $M=[M_1, M_2, ..., M_K]$ the set of all considered

models. p_k(y | M_k, X, ỹ) is the posterior distribution of y which represent the quantity to
be forecasted, under model M_k, given a discrete data set, X (Input forcing data) and
ỹ (observed system processes, here streamflow). The posterior distribution of the BMA
prediction is therefore given as:

5
$$p(y \mid M_1, \dots, M_k, X, \widetilde{y}) = \sum_{k=1}^{K} p(M_k \mid X, \widetilde{y}) \cdot p_k(y \mid M_k, X, \widetilde{y})$$
(11)

6 where $p(M_k | X, \tilde{y})$ is the posterior probability of model M_k . This term is also known as 7 the likelihood of model M_k being the correct model. If we denote $w_k = p(M_k | X, \tilde{y})$, we 8 should obtain $\sum_{k=1}^{K} w_k = 1$. $p_k(y | M_k, X, \tilde{y})$ is represented by the normal distribution 9 with mean equal to M_k and standard deviation σ . Suppose that y_k is a prediction made by 10 model M_k . Weights can be estimated through Expectation –Maximization algorithm 11 [*Dempster et al.*, 1977].

12 The posterior mean and variance of the BMA prediction for variable, y, are:

13
$$E[y | y_1..., y_K, X, \tilde{y}] = \sum_{k=1}^{K} w_k y_k$$
 (12)

14
$$Var[y | y_1..., y_K, X, \tilde{y}] = \sum_{k=1}^{K} w_k \left(y_k - \sum_{i=1}^{K} w_i y_i \right)^2 + \sigma^2$$
(13)

15 where σ^2 measures the expected uncertainty conditional on one of the models being best. 16 In essence, the BMA prediction is the average of predictions weighted by the likelihood 17 that an individual model is correct. There are several attractive properties to the BMA predictions. First the BMA prediction receives higher weights from better performing models as the likelihood of a model is essentially a measure of the agreement between the model predictions and the observations. Second, the BMA variance is a measure of the uncertainty of the BMA prediction. This measure is a better description of predictive uncertainty than that in a non-BMA scheme, which estimates uncertainty based only on the model ensemble spread (i.e., only the between-model variance is considered), and consequently results in under-dispersive predictions [*Raftery et al.*, 2003 & 2005].

8 4.3. Combination of global optimization and Bayesian multi-model combination: An

9 Integrated Bayesian Uncertainty Estimator

10 Since the Bayesian multi-model combination framework offers an excellent 11 statistical approach to account for model structural uncertainty we combined the BMA 12 framework with the SCEM-UA to form a hybrid framework to exploit the strengths of 13 these two techniques for integrated scheme for quantification of input, parameter 14 estimation and model structural uncertainty. This framework should provide a more 15 precise measure of uncertainty in system simulations. Throughout the remainder of this 16 paper we will refer to this Integrated Bayesian UNcertainty Estimator framework as 17 IBUNE.

18 IBUNE first estimates the two terms in the right hand side of the equation (11), 19 $p(M_k | X, \tilde{y})$ and $p_k(y | M_k, X, \tilde{y})$ for each model. $p_k(y | M_k, X, \tilde{y})$, which represents 20 the posterior distribution of estimated hydrologic response (e.g. streamflow), *y*, under 21 model M_k , is directly related to the input and parameter uncertainty under model M_k , as 22 expressed as follows:

$$p(y \mid M_k, X, \tilde{y}) \propto p(y \mid M_k, \theta_k, \eta_k, X, \tilde{y})$$
(14)

2 and

1

3
$$p(y | M_k, \theta_k, \eta_k, X, \tilde{y}) \propto p(\theta_k, \eta_k | M_k, X, \tilde{y})$$
(15)

If we can plug equation (15), which is the outcome of SCEM-UA into equation (11) directly. The first term of equation (11), $p(M_k | X, \tilde{y})$, which represents the posterior probability of the model M_k being a correct model, reflects how well model M_k matches the observed quantity of interest. This term under Bayes' theorem is defined as:

8
$$p(M_k \mid X, \tilde{y}) = \frac{p(X, \tilde{y} \mid M_k) p(M_k)}{\sum_{l=1}^{K} p(X, \tilde{y} \mid M_l) p(M_l)}$$
(16)

9 where

10
$$p(X, \tilde{y} \mid M_k) = \int p(X, \tilde{y} \mid \theta_k, \eta_k, M_k) p(\theta_k, \eta_k \mid M_k) d(\theta_k, \eta_k)$$
(17)

11 is the marginal likelihood of model M_k . $p(M_k)$ represents the prior probability that 12 M_k is a correct model. As we mentioned in model the previous section $p(M_k | X, \tilde{y})$ represents the model weight, w_k for model M_k . To approximate 13 14 equation (17) and estimate the model weights as Raftery et al. [2003] suggested, we 15 maximized the logarithm of this equation (17) and performed the Expectation-16 Maximization technique to solve this maximization problem. All the conditional densities 17 were described as Gaussian distribution for computational simplicity however the BMA 18 scheme can be applied by assuming other probability distributions. The EM algorithm is

applied to estimate w_k and σ^2 (which is the summation of the expected variance of each 1 2 model being the best) for each model. In brief, the Expectation-Maximization [Dempster 3 et al., 1977] algorithm casts the maximum likelihood problem as a "missing data" problem. The missing data here is introduced as a latent variable $Z_{k,t}$ that needs to be 4 5 estimated. If the kth model ensemble is the best prediction at time t, $Z_{k,t}=1$; otherwise 6 $Z_{k,t}=0$. At any time t, there is only one $Z_{k,t}$ equal to 1 and the rest is equal to 0. The EM algorithm starts with an initial guess for w_k and σ^2 and then alternates between the E (or 7 expectation) step which estimates $Z_{k,t}$ based on the current value of w_k and σ^2 and the M 8 (or maximization) step where new values for w_k and σ^2 are estimated based on the 9 current value of $Z_{k,t}$. The EM algorithm is described in Figure 12. For more detailed 10 11 description of the EM algorithm, readers are referred to McLachlan and Krishnan [1997]. 12 After convergence of this algorithm we will have specified weights for each 13 model. Therefore equation (11) can be derived and the posterior mean and variance of the 14 forecast can be estimated through equations (12) and (13), respectively. 15 In brief, the IBUNE framework can be implemented as follows: 16 (1) Select the number of hydrologic models 17 (2) Assign prior probability to each model (we assume non-informative 18 prior which gives uniform weights to all the models) 19 (3) Define an input error model. 20 (4) Obtain posterior distribution of model parameters and input error 21 model parameters for each model applying SCEM [Vrugt et al., 2003].

- (5) Estimate the posterior probability of each model (model weights)
 using the results from step (2) and (4) and performing EM algorithm
 [Dempster et al., 1977].
- 4 (6) Combine the results over all models.

5

(7) Assess predictive mean and variance using equation (12) and (13).

6 The following section provides a case study on the applicability and robustness of
7 IBUNE for reliable assessment of predictive uncertainty propagated through the system
8 from all the important sources of uncertainty.

9 4.4. Case Study: Use of IBUNE: uncertainty assessment of Hydrologic model 10 parameters and input error model parameters and model structure

11 The IBUNE scheme holds the promise of better assessment of total uncertainty 12 since it accounts for model parameters, input and model structural uncertainty. In this 13 section we will present the results for IBUNE and compare it to all other scenarios. 14 Figure 13 illustrates the estimated uncertainty bound using SCEM, associated with input 15 and model parameters for the three abovementioned models for the year 1957. The dots 16 in this figure represent observed streamflow. It is interesting to notice that different 17 models include different observation values. This can be interpreted as skill of the model 18 to capture different processes within the watershed. Based on step five of IBUNE 19 (presented in the previous section) the posterior probability distribution of each model in 20 capturing observations, (i.e., the weight) for each model was estimated. The weights are 21 presented in Figure 13. As expected the model with the higher skill (SAC-SMA) was 22 assigned the highest weight while the model with the lowest skill (SWB) was assigned

1 the lowest weight. Both HYMOD and SWB gain very small weights. However their 2 contribution in final results is considerable since they represent different spectrum of the 3 watershed processes which was well represented in the SAC-SMA. Figure 14 shows the 4 final IBUNE predictive probability which was estimated based on the probability of 5 contributing model in the combination. The width of this final probability can be 6 calculated through equation (13), however the shape and intensity of the distribution can 7 be captured through summation of posterior probability distribution of contributing 8 models in the combination (Figure 14-a). The connected dots depict the IBUNE 9 predictive mean which was estimated through equation (12) using the estimated weights 10 and model simulations at each point. Another interesting observation from this figure is 11 that in some parts of the hydrograph, the final posterior probability of the three 12 contributing model do not meet and therefore cause discontinuity in the final posterior 13 probability distribution at these parts of the hydrograph (Figure 14-a). These areas are 14 presented in light gray color in the Figure 14. Figure 14-a shows the profile of a cross-15 section in the hydrograph for clarification. Notice that there is the posterior probability 16 distribution at this time step is discontinuous with three distinct modes. This is a clear 17 indication that these three models do not represent the model space well and more models 18 are needed to avoid this problem. Figure 15 shows the distribution of Daily root mean 19 square error as well as Daily Absolute error for all three contributing models and 20 simulation generated through IBUNE. These distributions were estimated based on the 21 ensemble of simulation generated by each model through their input and model parameter 22 distributions. The figure illustrates that IBUNE improved DRMS more than DABS.

These results indicate that IBUNE improved simulation of the high flow values more
 than the low flow values.

We also used the Brier Score (BS) to compare the skill of the individual model ensembles (considering both parameter and input uncertainty) with IBUNE. The Brier skill (BS) score is a scalar measure of the quality of probabilistic forecast and has been commonly used in literature. BS is defined as follows [*Georgakakos et al.*, 2004]:

7
$$BS = 1 - \frac{1}{N} \sum_{t=1}^{N} (f(t) - o(t))^2$$
(18)

8 Where f(t) is frequency of target event at time step t estimated by the fraction of model 9 ensemble simulations which are larger than pre-specified threshold; o(t) is equal to one if 10 observation at that time step is larger than threshold and equal to zero otherwise; and N is 11 the number of time step in the record. Usually BS is a negatively oriented score, in that a 12 smaller value is better, however by adding the one behind the equation we made it 13 positively oriented, therefore in the figure the higher the BS the better. Figure 16 shows 14 the BS for all the models and IBUNE. Figure 16 confirms the findings in Figure 15 that 15 IBUNE produces superior predictions than individual member models. One can see that 16 IBUNE gained a higher score in most of the thresholds. Another observation from this 17 figure is that IBUNE outperformed other models over the low flow periods as well as 18 high flow periods. This suggests that IBUNE is a promising flood forecasting framework 19 since is has higher skills in capturing higher flows.

Figure 17 reveals the percentage of observations which are bracketed by the estimated uncertainty bounds. Uncertainty bounds estimated through IBUNE cover 72%

of the observation over the whole study period which is significantly higher than any single model. This 72% excludes the points which are in the discontinuity sections with zero probability. However just considering the minimum and maximum of the uncertainty bounds at each time step will give us a percent converge equal to 77% (Figure 17).

6 5. Summary and conclusions

7 The prevailing approach in hydrological modeling and assessment of related 8 uncertainty has been the use of sophisticated calibration techniques to estimate an optimal 9 set of parameters for a single model. Through these processes all other sources of 10 uncertainty including input and model structural uncertainty, are generally ignored and 11 the uncertainty in the model estimation of the system is primarily assigned to the 12 uncertainty in model parameters. Nevertheless, we know that a single model structure is 13 incapable of representing all the hydrological processes within a watershed and all of the 14 system observation including input forcing contains measurement error. Consequently 15 these assumptions lead to incorrect estimation of total uncertainty in the model 16 predictions.

The objectives of this paper were three-fold, one to demonstrate that the classic uncertainty assessment approach in hydrology that relays all the uncertainty within the system on the parameter estimation, is not reliable and accurate, two to introduce a new approach to simultaneously address model parameter estimation and input forcing uncertainty and finally three to propose a new framework that tackles three major sources

of uncertainty including uncertainty inherited in input forcings, parameter estimation and
 model structure. The conclusion of this work can be summarized as follows:

3 The underlying approach for uncertainty assessment in hydrological (a) 4 modeling has been to treat the model and observation data unbiased and precise 5 and treat the uncertainty in the modeling processes as being explicitly attributed to 6 the uncertainty in the parameter estimates. In this study we verified that such an 7 assumption will lead to biased and corrupted parameter estimates therefore 8 unrealistic model simulations and their associated uncertainty bounds which does 9 not consistently capture and represent the real-world behavior of the watershed. 10 This was demonstrated through two separate case studies using Shuffled Complex 11 Evolution Metropolis, SCEM, [Vrugt et al, 2003], the newly developed 12 probabilistic parameter estimation algorithm, to calibrate three selected 13 hydrologic models for the Leaf River Basin in Mississippi. The under study 14 models were included SACramento soil Moisture Accounting model (SAC-15 SMA), Soil Water Balance model (SWB) and HYdrologic MODel (HYMOD).

(b) In the second attempt to estimate more accurate and less corrupt uncertainty bounds for the hydrologic model simulation, we proposed a new approach to account for associated uncertainty in the input forcings. We simply introduced an input error model which assumed a random Gaussian error as a multiplier for every input observation. The common ground for these multipliers is that they are all from an identical distribution with unknown first two moments (mean and variance). Therefore we extended SCEM to estimate these two new unknown

parameters with the hydrologic model parameters and their associated uncertainty.
 We demonstrated that undertaking such a simple approach to address input
 uncertainty, improved the accuracy and reliability of the hydrologic simulations
 and their associated uncertainty bounds, significantly.

5 (c) Even though, accounting for the input uncertainty generated more reliable 6 results, but these results were still suffering from a very common limitation in 7 hydrologic modeling attitude that the model under study is the best model in hand. 8 However the most sophisticated models are still simple representation of real 9 world and can not capture all the processes with the catchments. In order to take 10 into account this source of uncertainty, we exploit the newly developed technique, 11 called Bayesian Model Averaging (BMA), [Hoeting et al., 1999], which 12 disregards the traditional believe in hydrological modeling and explores multiple 13 model structures to represent the processes within the system. We merged this 14 method (BMA) with the extended SCEM presented in this paper which accounts 15 for both input and parameter uncertainty and proposed a new hybrid framework 16 entitled, Integrated Bayesian UNcertainty Estimator (IBUNE). IBUNE combines 17 and exploits the strengths of the SCEM as an efficient and effective probabilistic 18 model parameter estimator algorithm and the introduced input error model as well 19 as Bayesian model combination techniques, to provide an integrated assessment 20 of uncertainty propagating through the system from parameter estimation, input 21 forcing and model structure.

To demonstrate the usefulness and applicability of IBUNE, we used the same hydrologic models considered earlier. The strength of these three models was combined through IBUNE. We showed that IBUNE is a very useful and applicable technique which accounts for all different sources of uncertainty within the hydrologic system and results in improved model prediction uncertainty bounds that brackets higher percentage of system observations.

7 IBUNE is a flexible framework which can be expanded by including many more 8 hydrologic models. All three major components of the framework, SCEM, Input error 9 model and BMA investigate different limitations in hydrologic modeling processes and 10 provide more precise estimation of uncertainty bounds by confronting all these different 11 sources of uncertainty.

12 The results presented here were obtained through simulation experiment however 13 it would be very interesting to test the performance of this framework through a set of 14 forecast experiments which uses forecasted inputs such as precipitation to force the 15 hydrologic models. Even though accounting for all sources of uncertainty is very 16 important in forecasting future devastating events, but all the at hand techniques 17 including the work was presented here are still to expensive to be used for real-time 18 operational application. However, ever increasing pace of computational power will soon 19 provide the opportunity for operational communities to take advantage of these state-of-20 the-art methods to address uncertainty associated with their forecast in a more reliable 21 and accurate manner.

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Table 1. Parameters of modified SAC-SMA	model and their initial uncertainty ranges
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Parameters	Description	Initial ranges
UZTWM	Upper zone tension-water capacity (mm)	1.00-150.0
UZFWM	Upper zone free-water capacity (mm)	1.00-150.0
UZK	Upper zone recession coefficient (day ⁻¹)	0.10-0.5
LZTM	Total Lower zone water capacity (mm)	1.00-1000.0
LZSK	Lower zone supplementary recession coefficient (day ⁻¹)	0.01-0.25

Parameters	Description	Initial ranges
C _{max}	Maximum storage capacity in catchment (mm)	1.0-500.0
b_{exp}	Factor distributing flow between two series of reservoirs (-)	0.1-2.0
ALPHA	Shape factor for the main soil water storage tank (-)	0.1-0.990
R_s	Residence time of linear slow flow reservoirs (day)	0.0-0.1
R_q	Residence time of linear quick flow reservoirs (day)	0.1-0.99

 Table 2. Parameters of HYMOD model and their initial uncertainty ranges

Parameters	Description	Initial ranges
$D_{b,max}$	Maximum soil moisture deficit of bottom layer of the soil (mm)	10.0-800.0
Q_{max}	Potential subsurface runoff (mm/day)	5.0-100.0
Q_{max}/S_{max}	Ratio of the lower level posture that produce subsurface flow (-)	0.1-0.90
$D_{u,max}/D_{b,max}$	Upper layer deficit proportion (-)	0.01-0.5
K_{dt}	Time scale factor (day)	1.0-20.0

Table 3. Parameters of SWB model and their initial uncertainty ranges

	SAC-SMA	HYMOD	SWB
SCEM (hydrologic model parameters)	16%	10%	6%
SCEM (hydrologic +Input model Parameters)	30%	14%	11%

Table 4. Percentage of observations being in uncertainty range



Figure 1. Schematic of SAC-SMA model



Figure 2. Marginal Posterior probability distribution of the SAC-SMA parameters, using 20,000 samples generated after convergence of SCEM-UA algorithm.



Figure 3. Streamflow hydrograph prediction uncertainty associated with estimated parameters (shown in darker gray) for SAC-SMA model and 95% confidence interval for prediction of observed streamflow (shown in lighter gray) for the water year 1957.



Figure 4. Schematic of HYMOD model



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Figure 10. Streamflow hydrograph prediction uncertainty associated with estimated parameters and input error model parameters (shown in darker gray) for SAC-SMA model and 95% confidence interval for prediction of observed streamflow (shown in lighter gray) for the water year 1957.



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and input uncertainty



Figure 12. EM flowchart



Figure 13. Streamflow hydrograph prediction uncertainty associated with estimated parameters and input error model parameters for all three models for the water year 1957 and estimated combination weights for each model using IBUNE.



Figure 14. Streamflow hydrograph prediction uncertainty associated with estimated parameters and input error model parameters as well as model structural uncertainty (in shaded gray) for the water year 1957. The lighter patches in the uncertainty bounds represent the discontinuity of the final model distributions. (a) illustrates profile of the selected cross section which includes the final distribution of each member model and the final IBUNE predictive PDF.



Figure 15. Distribution of DRMS and DABS for individual models and IBUNE.



Figure 16. Brier Score for IBUNE and three Member models



Figure 17. Percentage of observation in uncertainty range of different models and IBUNE