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More Efficient Bayesian-based Optimization and Uncertainty Assessment of Hydrologic Model Parameters

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Abstract

An important consideration in assessing the performance of model calibration software is that of run time. Minimizing the number of hydrologic model runs required during the calibration process is nearly always important, but particularly when the objective function landscape contains multiple local minima or hydrologic model run times are high. Minimizing the number of required model runs was one of the primary factors driving the research and development activities encapsulated in this report, such that the resulting optimization and uncertainty tool(s) are more compatible with the computationally expensive physics-based models that are becoming more commonly used within the practice community. SCEM-FA is a modified version of the Markov Chain Monte Carlo sampler SCEM-UA. It is more efficient than the native SCEM-UA algorithm, through employment of function approximation, while effectively inferring the posterior parameter distribution of model parameters and also the most likely parameters within this high probability density region. Based on a summary of thirty random trials, SCEM-FA was able to infer, effectively, the same posterior probability distribution for thirteen SAC-SMA hydrologic model parameters as that of SCEM-UA with an average twenty-one percent savings in total forward model calls.

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Preface

This report describes a Markov Chain Monte Carlo sampler entitled the Shuffled Complex Evolution Metropolis algorithm Function Approximation (SCEM-FA), which is a modification to the original SCEM-UA algorithm. It employs function approximation methods to improve upon the overall efficiency of the Shuffled Complex Evolution Metropolis algorithm (SCEM-UA), while effectively inferring the posterior parameter distribution of model parameters and also the most likely parameters within this high probability density region.

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The work was performed by Dr. Brian E. Skahill of the Hydrologic Systems Branch (HF-H) of the Flood and Storm Protection Division (HF), U.S. Army Engineer Research and Development Center – Coastal and Hydraulics Laboratory (ERDC-CHL) and Dr. Jeffrey S. Baggett of the University of Wisconsin – La Crosse. At the time of publication, Earl V. Edris was Chief, CEERD-HF-H; Bruce A. Ebersole was Chief, CEERD-HF. The Deputy Director of ERDC-CHL was Jose E. Sanchez and the Director was Dr. William D. Martin.

COL Kevin J. Wilson was the Commander and Executive Director of ERDC, and Dr. Jeffery P. Holland was the Director.

1 Introduction

Hydrologic models, regardless of their type (e.g., empirical, physics-based), often contain parameters that cannot be measured directly either because they have no physical basis, it would be impractical, or due to an incompatibility of scales, among other possible reasons. Hence, hydrologic model parameters are inferred by adjusting their values until an acceptable level of agreement is achieved between a set of historical observations of the real world system that the model represents and their simulated counterparts. While manual model calibration is certainly one approach to the problem, it is subjective, labor-intensive, and may also suffer from a lack of consistency and/or repeatability, among others. Moreover, it is difficult to imagine how even an experienced modeler would necessarily manage, in a manual calibration context, the large number of estimable parameters associated with present-day practice- driven complex hydrologic model deployments. Fortunately, the computer-based calibration of hydrologic models (which, in contrast with the manual approach to model calibration, is more objective, repeatable, and better capitalizes on the computational capacity of the modern computer) is an active area of research and development (see; for example, Baggett and Skahill, 2010a, b; Skahill et al. 2009, Skahill and Doherty, 2006; Doherty and Skahill, 2006, and references cited therein) which has resulted in numerous automatic calibration methods that are readily available (see Matott et al. 2009 and references cited therein) for the modern day hydrologic modeler to employ. And the knowledge gained by their application and development has provided the hydrologic modeling community with a better understanding of some of the complications associated with calibrating hydrologic models; viz., among others, the existence of multiple local optima, non-smooth objective function surfaces, and long valleys in parameter space that are a result of excessive parameter correlation or insensitivity (Gupta et al. 2003; Duan et al. 1992).

As mentioned, hydrologic models are typically calibrated by adjusting parameters encapsulated in the simulator until there is an acceptable level of agreement between a set of historical data and their model simulated counterparts. The parameters obtained via calibration are often then used by the model to predict system behavior for one or more pre-defined scenarios of interest to different groups whose life or livelihood is rooted in the local model study area. Regardless of the calibration method

employed and the type (e.g., empirical or physics-based) of model used, some if not all of the parameter values obtained through the calibration process possess a degree of quantifiable uncertainty because the observed data contain measurement errors and also because the model never perfectly represents the watershed system or exactly fits the observation data. And where model parameters are uncertain so too are model predictions. In particular, quantifying uncertainty supports, among others, the following hydrologic modeling activities (Schoups and Vrugt, 2010; Schoups et al., 2010):

1. Model comparison and selection,
2. Identification of the best water management strategies that reflect the likelihood of outcomes,
3. Data collection aimed at improving hydrologic predictions and water management, and
4. Regionalization and extrapolation of hydrologic parameters to ungauged basins.

For example, regarding item four above, to quote Vrugt et al. (2003a), "If we want to be able to regionalize or relate model parameters to easily measurable land or soil-surface characteristics, a prerequisite is that the parameters be unique, preferably having a small variance. From this perspective, it is necessary to infer the parameter uncertainty resulting from calibration studies."

Model uncertainty, characterized by the model covariance matrix calculated using the model Jacobian (Skahill and Doherty, 2006) evaluated at the best estimate for the model, can be quantified by employing a traditional linear analysis. However, this approach is local which does not dovetail well with the understanding that for hydrologic models there may exist many effectively equally acceptable models; i.e., it is difficult to identify a unique best estimate; and moreover, that the set of good models may very well not necessarily even be a closed and bounded set interior to feasible parameter space. In addition, it relies on a linearity assumption that is often violated in hydrologic modeling practice.

Bayesian-based approaches to model calibration, wherein a prior distribution for the model is proposed, and the vector of adjustable model parameters is treated as a random variable with a target probability distribution that is conditioned with observed data, are a formal means to

obtain a realistic and reliable estimate of model uncertainty. In particular, Markov Chain Monte Carlo (MCMC) simulation, which is by far more efficient than other Monte Carlo methods, is used for inference, search, and optimization with hydrologic models (Harmon and Challenor, 1997; Kuczera and Parent, 1998; Campbell et al., 1999; Campbell and Bates, 2001; Makowski et al., 2002; Qian et al., 2003; Kanso et al., 2003; Vrugt et al., 2003a; Vrugt et al., 2003b; Vrugt et al., 2008). With MCMC we are interested in a target probability distribution, and its key elements include exploration of this distribution by way of some sort of random walk or diffusion process that must be initialized in an arbitrary way because we don't know a priori where good places necessarily are in parameter space. The random walk is directed by Markov chain simulation wherein the next step only depends on the previous step, and eventually after a burn in period the target distribution is identified.

An obvious advantage of the MCMC method is that no assumptions of model linearity, or even of differentiability of model outputs with respect to parameter values, are required for its implementation; hence it is extremely robust. However, this robustness comes at a cost; this being the high number of model runs required for its implementation. The choice of the proposal distribution, which expresses prior information about the model, can greatly affect the efficiency of an MCMC sampler. A poorly chosen proposal distribution will result in slow convergence to the target distribution. Unfortunately, for complex hydrologic models there is very little a priori knowledge of the high probability density region within parameter space. Hence, with hydrologic models an uninformative prior; wherein all parameters have equal likelihood, may often be the best we can do. Clearly, for hydrologic modeling, there is a need to design efficient MCMC samplers, and this observation was the motivation for the development of the Shuffled Complex Evolution Metropolis algorithm (SCEM-UA), an effective and efficient adaptive MCMC sampler which tunes the proposal distribution during the evolution to the stationary posterior target distribution (Vrugt et al. 2003a).

The SCEM-UA algorithm is a modification to the SCE-UA global optimization algorithm (Duan et al. 1992, 1993). There are two primary modifications, both of which prevent SCEM-UA from collapsing into the region of a single best parameter set. The first modification involves replacement of the downhill simplex method with the Metropolis-annealing scheme (Metropolis et al. 1953). The second modification is that SCEM-UA does not

further subdivide the complex into subcomplexes during the generation of candidate points and it uses a different replacement procedure. In presenting the SCEM-UA algorithm, Vrugt et al. (2003a) noted that their principal focus was algorithm efficiency; viz., the number of simulations needed to converge to the stationary posterior probability distribution. They compared the traditional Metropolis-Hastings sampler (Metropolis et al. 1953; Hastings, 1970) with SCEM-UA to infer the posterior distribution of five parameters associated with a conceptual rainfall-runoff model. It took SCEM-UA approximately 4,000 simulations to converge to the stationary posterior distribution, based on evaluation of the Gelman and Rubin convergence diagnostic (Gelman and Rubin, 1992); whereas, even after 30,000 simulations the Metropolis-Hastings algorithm had not converged to the target distribution when applying the same convergence criteria.

An important consideration in assessing the performance of model calibration software is that of run time. Model calibration software, no matter what its algorithmic basis, must run the hydrologic model to be calibrated many times in the course of minimizing the objective function that is used to characterize model-to-measurement misfit. Minimizing the number of hydrologic model runs required during the calibration process is nearly always important, but particularly when the objective function landscape contains multiple local minima or hydrologic model run times are high. Minimizing the number of required model runs is the primary factor driving the research and development to be discussed herein, such that the resulting optimization and uncertainty tool is compatible with the computationally expensive physics-based models that are becoming more commonly used within the practice community.

Recent research and development activity directed at improving the efficiency of native computer-based model calibration algorithms includes the work of Skahill et al. (2009) and Baggett and Skahill (2010a, b), among others. Skahill et al. (2009) developed an accelerated derivative-based local search algorithm and based on three separate modeling applications demonstrated efficiency gains anywhere from 36-84 percent in comparison with the native algorithm. Baggett and Skahill (2010a, b) reported on an efficiency enhancement to the state-of-the-art covariance matrix adaption evolution strategy (CMAES) (Hansen, 2006) for global parameter identification of difficult problems with noise or other features that make derivatives estimation difficult. The increase in convergence speed was quite dramatic for their modified CMAES algorithm, which uses a local radial

basis function approximation to the objective function to compute approximate first and second derivatives to the objective function surface to propagate a gradient individual alongside the evolving population for possible selection each generation. Based on a summary of thirty trials, it converged with fewer than half of the objective function evaluations required by CMAES when applied to calibrate a hydrologic model.

The primary objective of the research and development encapsulated in this report was to improve upon the already existing documented efficiency of an existing state-of-the-art Bayesian model uncertainty analysis method (Vrugt et al. 2003a). The principal approach that was employed to achieve the stated objective was to simultaneously and adaptively construct an approximation to the objective function.

Background

The hydrologic model f can be written as

$$\hat{\mathbf{y}} = f(\boldsymbol{\theta}; \mathbf{x}) + e \tag{1}$$

where $\hat{\boldsymbol{y}}$, $\boldsymbol{x}$, $\boldsymbol{\theta}$, and $\boldsymbol{e}$ represent, respectively, the vector of model outputs, structural aspects of the model, as well as its input dataset, model parameters that are adjustable through the calibration process, and the vector of statistically independent error terms with zero expectation and constant variance σ^2. Given the vector of observations $\boldsymbol{y}$, the vector of residuals is given by

$$e(\boldsymbol{\theta}) = \hat{\mathbf{y}} - \mathbf{y} \tag{2}$$

Bayesian statistics treats the model parameters $\boldsymbol{\theta}$ as probabilistic variables having a joint posterior probability density function (pdf), $p(\boldsymbol{\theta}|\boldsymbol{y})$. The posterior pdf is a probabilistic statement about the parameters $\boldsymbol{\theta}$ conditioned on the observed data $\boldsymbol{y}$. At the core of Bayesian inference is Bayes' rule, which is given by

$$p(\boldsymbol{\theta}|\mathbf{y}) \propto L(\mathbf{y}|\boldsymbol{\theta}) p(\boldsymbol{\theta}) \tag{3}$$

where $p()$ indicates probability, $p(\boldsymbol{\theta}|\boldsymbol{y})$ is the posterior probability distribution of the parameters $\boldsymbol{\theta}$, $L(\boldsymbol{y}|\boldsymbol{\theta})$ is the likelihood function, and $p(\boldsymbol{\theta})$ is the prior probability density function. The prior pdf, $p(\boldsymbol{\theta})$, represents information about $\boldsymbol{\theta}$ before any data are collected. A critical term in Bayes' rule is

the likelihood term; likelihoods can only be calculated if an error model is available. Assuming that the residuals are mutually independent, Gaussian distributed, with constant variance, and further assuming a non-informative prior of the form $p(\boldsymbol{\theta}) \propto \sigma^{-1}$, Box and

Tiao (1973) derived the following form for the posterior probability distribution of $\boldsymbol{\theta}$:

$$p(\theta \mid y) \propto [M(\theta)]^{-N(1+\gamma)/2} \tag{4}$$

where

$$M(\theta) = i = 1 N e \theta 2^{(1+\gamma)} \tag{5}$$

2 The Shuffled Complex Evolution Metropolis Function Approximation Algorithm

The goal of the Shuffled Complex Evolution Metropolis (SCEM-UA) algorithm, a Markov Chain Monte Carlo sampler developed by Vrugt et al. (2003a) which is a modified version of the original SCE-UA global optimization algorithm developed by Duan et al. (1992), was to efficiently (and by efficiency, we mean the number of forward model calls necessary to converge to the target posterior distribution) infer the posterior distribution of hydrologic model parameters. The SCEM-UA algorithm is not only able to effectively infer the posterior distribution of hydrologic model parameters but also the most likely parameters within this high probability density region. Function approximation methods have successfully been employed to improve upon the efficiency of native evolutionary strategies utilized for model calibration; for example, see Baggett and Skahill (2010a, b) and references cited therein. By interfacing function approximation methods with the native SCEM-UA algorithm, we further improve upon the already existing reported efficiencies of the SCEM-UA MCMC sampler. The new algorithm presented in full herein, entitled the Shuffled Complex Evolution Metropolis Function Approximation (SCEM-FA) algorithm, is given below and also illustrated in Figures 1 and 2. The SCEM-FA algorithm retains all of the elements of the original SCEM-UA algorithm. We refer the interested reader to Vrugt et al. (2003a) for a thorough description and discussion of the original SCEM-UA algorithm. However, for purposes of completeness, we present the entire SCEM-FA algorithm. We will emphasize those parts which constitute the existing function approximation interface to the original SCEM-UA algorithm. For further clarity regarding the SCEM-FA and SCEM-UA algorithms, we make mention now of the fact that the function approximation interface methodology presented herein is not only possible with SCEM-UA, but likely could also easily be adapted and employed with other MCMC samplers; for example, DREAM (Vrugt et al. 2008).

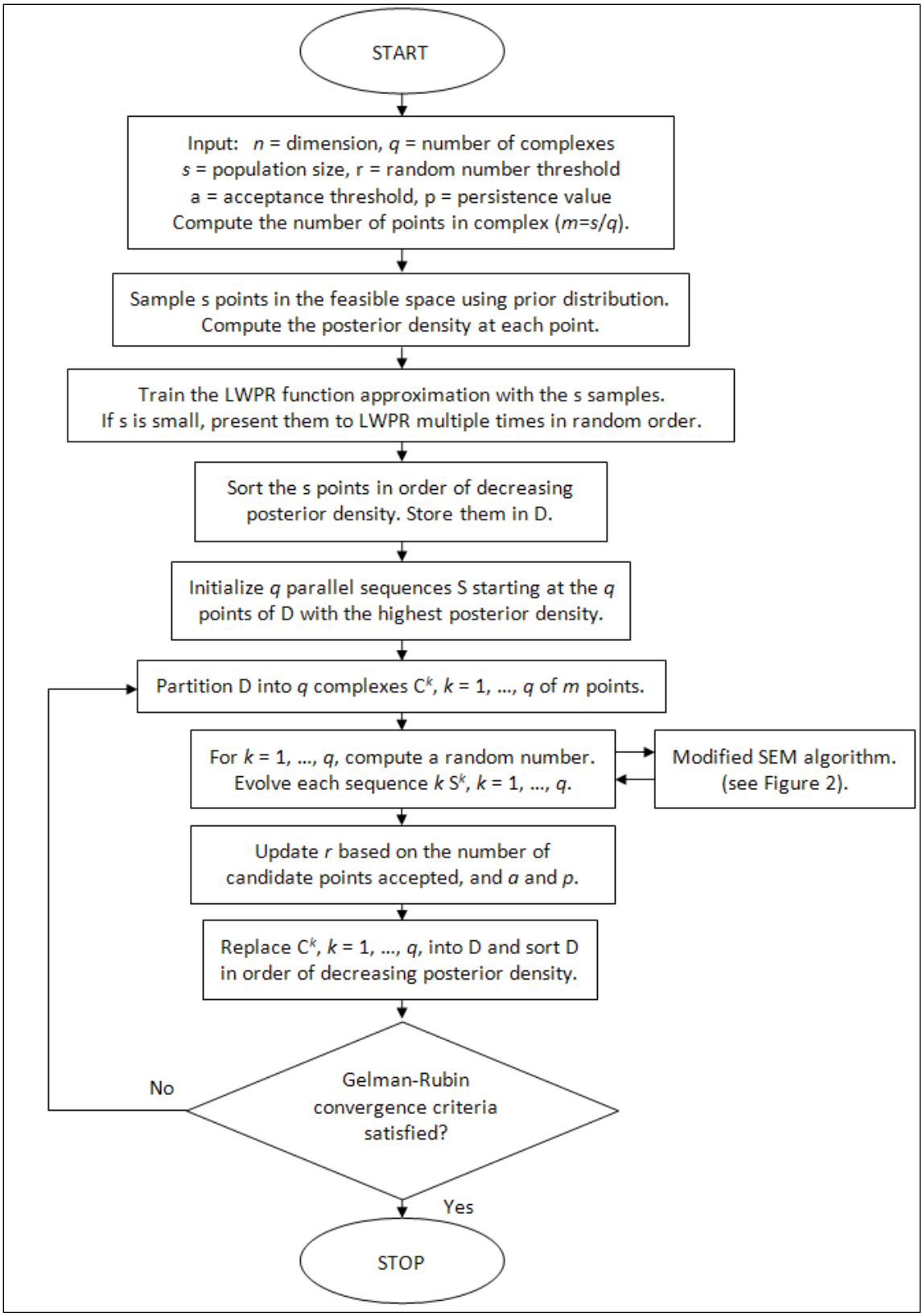

Figure 1. Flowchart of the SCEM-FA algorithm.

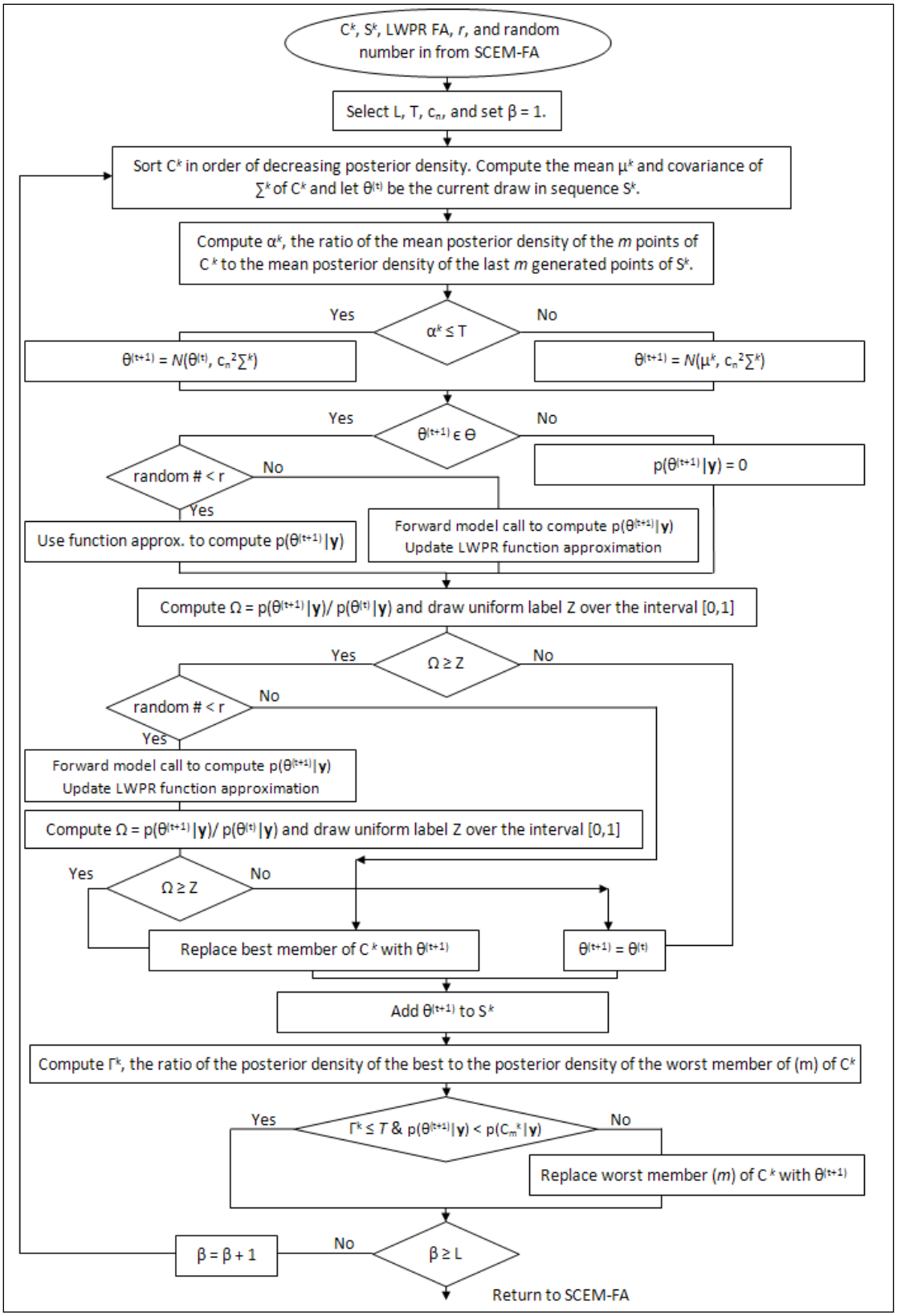

Figure 2. Flowchart of the SEM-FA algorithm employed in the SCEM-FA algorithm.

1. Generate sample. Sample s $\{\theta_1, \theta_2, ..., \theta_s\}$ points randomly from the prior distribution and computes the posterior density of each point $\{p(\theta^{(1)}|\boldsymbol{y}), p(\theta^{(2)}|\boldsymbol{y}), ..., p(\theta^{(s)}|\boldsymbol{y})\}$ using equation (4).
2. Rank points. Sort the s points in order of decreasing posterior density and store them in array $D[1:s, 1:n + 1]$ where n is the number of parameters, so that the first row of D represents the point with the highest posterior density.
3. Build function approximation. Train a locally weighted projection regression function (LWPR) approximation (Vijayakumar et al. 2005) using the s points randomly sampled from the prior distribution. If the sample is small, then present the sample to LWPR multiple times in random order.
4. Initialize parallel sequences. Initialize the starting points of the parallel sequences, $S^1, S^2, ..., S^q$, such that S^k is $D[k, 1:n + 1]$, where $k = 1, 2, ..., q$.
5. Partition into complexes. Partition the s points of D into q complexes $C^1, C^2, ..., C^q$, each containing m points, such that the first complex contains every $q(j-1)+1$ ranked point, the second complex contains every $q(j-1)+2$ ranked point of D, and so on, where $j = 1, 2, ..., m$.
6. Evolve each sequence. Evolve each of the parallel sequences according to the Sequence Evolution Metropolis Function Approximation (SEM-FA) algorithm outlined below.
7. Adjust SEM-FA input value r. Based on the monitored acceptance rate in SEM-FA, and predefined input values for an acceptance rate threshold for SEM-FA, and the occurrence frequency for SEM-FA input parameter adjustment, update the SEM-FA input, r, a number in the interval (0,1) which effectively dials in or out the employment of function approximation in SEM-FA.
8. Shuffle complexes. Unpack all complexes C back into D, rank the points in order of decreasing posterior density, and reshuffle the s points into q complexes according to the procedure specified in step 5.
9. Check convergence. Check the Gelman and Rubin convergence statistic (Gelman and Rubin, 1992). If convergence criteria are satisfied, stop; otherwise, return to step 6.

Items 3, 6, and 7 above are specific to the SCEM-FA algorithm while the other elements are a restatement of the native SCEM-UA algorithm originally presented in Vrugt et al. (2003a). The first modification, listed in item 3 above, uses the initial random sample to build a function approximation model which is later used in SEM-FA as a surrogate for the objective function. While locally weighted progression regression (Vijayakumar et al.

2005) was the function approximation method used for the current modifications to the SCEM-UA algorithm documented in this report, alternative function approximation methods, such as radial basis functions (Powell, 1992), could also have been used. Item 6 above refers to the SEM-FA algorithm which is presented and discussed below while item 7 above refers to the current method that is employed to regulate the degree to which the function approximation model is utilized in SEM-FA. Both items 6 and 7 will be discussed further below.

As Vrugt et al. (2003a) mentioned, one of the essential elements of the SCEM-UA algorithm is the Sequence Evolution Metropolis (SEM) algorithm, wherein new candidate points are produced in each of the parallel sequences S^k and the Metropolis algorithm is used to test whether or not the candidate point should be added to the current sequence. As part of the overall effort to further improve upon the already existing reported efficiencies of the SCEM-UA MCMC sampler, the SEM algorithm was adapted to include a function approximation model which is used as a surrogate for the objective function. It is named SEM-FA for Sequence Evolution Metropolis Function Approximation and it is presented below and also in Figure 2. As with the previously mentioned comparison of the SCEM-UA and SCEM-FA algorithms, the SEM-FA algorithm retains all of the elements of the original SEM algorithm. And we refer the interested reader to Vrugt et al. (2003a) for a thorough description and discussion of the original SEM algorithm. However, for purposes of completeness, we present the entire SEM-FA algorithm. We will emphasize those parts which constitute the existing function approximation interface to the original SEM algorithm.

I. Compute the mean, μ^k, and covariance structure $\sum^k$ of the parameters of C^k. Sort the m points in complex C^k in order of decreasing posterior density and compute I^k, the ratio of the posterior density of first ("best") to the posterior density of the last ("worst") member of C^k.
II. Compute α^k, the ratio of the mean posterior density of the m points in C^k to the mean posterior density of the last m generated points in S^k.
III. If α^k is smaller than a predefined likelihood ratio, T, generate a candidate point, $\theta^{(t+1)}$, by using a multinormal distribution centered on the last draw, $\theta^{(t)}$, of the sequence, S^k, and covariance structure $c_n^2 \sum^k$, where c_n is a predefined jumprate. Go to step V, otherwise, continue with step IV.
IV. Generate offspring, $\theta^{(t+1)}$, by using a multinormal distribution with mean μ^k and covariance structure $c_n^2 \sum^k$, and go to step V.

V. If the random number from the interval (0,1), input from SCEM-FA, is less than r, then use the function approximation to compute the posterior density, $p(\theta^{(t+1)}|\boldsymbol{y})$, of $\theta^{(t+1)}$ using equation (4). If the generated candidate point is outside the feasible parameter space, then set $p(\theta^{(t+1)}|\boldsymbol{y})$ to zero.

VI. If the random number from the interval (0,1), input from SCEM-FA, is greater than or equal to r, then perform a forward model call, compute the posterior density, $p(\theta^{(t+1)}|\boldsymbol{y})$, of $\theta^{(t+1)}$ using equation (4), and update the LWPR function approximation with the new data point $\theta^{(t+1)}$. If the generated candidate point is outside the feasible parameter space, then set $p(\theta^{(t+1)}|\boldsymbol{y})$ to zero.

VII. Randomly sample a uniform label Z over the interval 0 to 1.

VIII. If the random number from the interval (0,1), input from SCEM-FA, is less than r, then go to step IX; otherwise, go to step XII.

IX. Compute the ratio $\Omega = p(\theta^{(t+1)}|\boldsymbol{y})/\ p(\theta^{(t)}|\boldsymbol{y})$. If Z is smaller than or identical to Ω, then perform a forward model call, compute the posterior density, $p(\theta^{(t+1)}|\boldsymbol{y})$, of $\theta^{(t+1)}$ using equation (4), and update the LWPR function approximation with the new data point $\theta^{(t+1)}$. If the generated candidate point is outside the feasible parameter space, then set $p(\theta^{(t+1)}|\boldsymbol{y})$ to zero.

X. However, if Z is larger than Ω, reject the candidate point and remain at the current position in the sequence, that is, $\theta^{(t+1)} = \theta^{(t)}$. Go to step XIII.

XI. Recompute the ratio $\Omega = p(\theta^{(t+1)}|\boldsymbol{y})/\ p(\theta^{(t)}|\boldsymbol{y})$. If Z is smaller than or identical to Ω, then accept the new candidate point. However, if Z is larger than Ω, reject the candidate point and remain at the current position in the sequence, that is, $\theta^{(t+1)} = \theta^{(t)}$. Go to step XIII.

XII. Compute the ratio $\Omega = p(\theta^{(t+1)}|\boldsymbol{y})/\ p(\theta^{(t)}|\boldsymbol{y})$. If Z is smaller than or identical to Ω, then accept the new candidate point. However, if Z is larger than Ω, reject the candidate point and remain at the current position in the sequence, that is, $\theta^{(t+1)} = \theta^{(t)}$.

XIII. Add the point $\theta^{(t+1)}$ to the sequence S^k.

XIV. If the candidate point is accepted, replace the best member of C^k with $\theta^{(t+1)}$, and go to step XV; otherwise replace the worst member (m) of C^k with $\theta^{(t+1)}$, provided that Γ^k is larger than the predefined likelihood ratio, T, and $p(\theta^{(t+1)}|\boldsymbol{y})$ is higher than the posterior density of the worst member of C^k.

XV. Repeat the steps I – XIII L times, where L is the number of evolution steps taken by each sequence before complexes are shuffled.

Items I – IV, VI, VII, and XII – XV (with the SCEM-FA input value r set to zero) are a restatement of the native SEM algorithm originally presented in Vrugt et al. (2003a). The SCEM-FA algorithm is equivalent to the original SCEM-UA algorithm when the SCEM-FA input parameter r is set

to a value of zero. Items I – XV directly above list the existing modification to the original SEM algorithm.

The basic reasoning behind SEM-FA is that if the function approximation prediction, which is used as a surrogate for the objective function, suggests that the candidate point should be selected, by way of evaluation of the Metropolis algorithm criterion (Metropolis et al. 1953), then proceed ahead with a forward model call and re-evaluation of the Metropolis algorithm criterion to determine if in fact the candidate point is to be accepted or not. And if the Metropolis algorithm criterion computed using the function approximation prediction indicates otherwise, then reject the candidate point. In effect, the function approximation prediction serves as a screening device in that forward model calls are only performed when it suggests that it would be beneficial. And the degree to which the filter is applied is based on a SCEM-FA input parameter, *r*, which is dynamically adjusted during SCEM-FA execution, and its comparison (see Figure 2) with a unique randomly sampled uniform label over the interval 0 to 1 that is passed to SEM-FA for the evolution of each sequence (see Figure 1).

If the SCEM-FA input value for r is greater than zero, then the function approximation adaptations described above and also shown in Figures 1 and 2 will be active. In this case, the value for r is reset to zero at the beginning of SCEM-FA execution and dynamic adjustment is subsequently based not only on a comparison of the candidate point acceptance rate within SEM-FA with a user specified acceptance rate threshold, but also the integer value for a persistence parameter which determines the frequency for updating the value for *r*. In particular, at present, if it is an opportunity to update *r* and the SEM-FA acceptance rate is less/greater than the user specified acceptance rate threshold, then decrease/increase the value for *r* by one-tenth. The minimum possible value for *r* is zero, and its maximum is equivalent to its specified input value. At present, an input value is specified for *r*. However, it could possibly be effectively removed as an input for SCEM-FA by altering the existing dynamic adjustment process to simply allow the value for *r* to vary between zero and one. Testing is needed to explore this potential opportunity. If it is not already clear to the reader, decreasing/increasing the value for *r* increases/decreases the number of forward model calls within SEM-FA.

Guidance for the proper selection of SCEM-UA algorithmic input parameter values can be found in Vrugt et al. (2003a). The SCEM-FA

algorithm contains three additional parameters that at present need to be specified by the user. These are (1) the random number threshold, r, (2) the acceptance rate threshold, a, and (3) the parameter, p, an integer value which determines the update frequency for r. The increment/decrement value embedded in the dynamic adjustment process for r could also be viewed as a parameter that could possibly impact SCEM-FA performance. Further exploration in terms of how these parameters affect the reliability (i.e., the capacity to converge to the same posterior probability distribution as the native SCEM-UA algorithm) and efficiency of SCEM-FA is needed before any recommendations can be provided for default values. However, optimal acceptance rates for MCMC samplers range anywhere from 20 – 70 percent in the literature (Gallagher and Doherty, 2007).

Additional opportunities exist, of course, for further exploration in terms of their potential capacity to yield additional efficiency gains beyond those already achieved and documented below with the existing SCEM-FA implementation. These include, among others, (1) relaxing the current requirement to perform a forward model call every time the function approximation suggests that the candidate point is to be accepted, and (2) comparing the current function approximation model with an alternative model, such as radial basis functions (Powell, 1992). Both of these opportunities would be modest development efforts.

With respect to the first opportunity noted directly above, at present, SCEM-FA is biased conservatively in that we completely trust the function approximation prediction to reject candidate points; whereas, if the function approximation prediction suggests that the candidate point is to be accepted, then we go to additional measures to ensure that is in fact the case. One alternative would be to simply accept the candidate point when the function approximation prediction suggests it should; however, that approach may be too aggressive and impair the reliability of SCEM-FA. A relatively simple easily implementable approach would be to monitor the success rate of the function approximation prediction and use that as a basis for deciding whether to perform a forward model call after the function approximation prediction suggests the candidate point is to be accepted. The second opportunity mentioned directly above would be a fairly modest effort because early SCEM-FA development utilized a k-nearest neighbor cubic radial basis function (RBF) local function approximation model rather than locally weighted projection regression (LWPR).

3 Case Study

To comprehensively demonstrate the efficiency gains that can be achieved with the SCEM-FA development efforts to date, all the while maintaining consistency with respect to convergence to the same target distribution, thirty unique instances of SCEM-UA and SCEM-FA were each employed to infer the posterior distribution of thirteen Sacramento soil moisture accounting (SAC-SMA) hydrologic model parameters using hydrologic data from the 1944 km^2 Leaf River watershed near Collins, MS. The SAC-SMA hydrologic model is used by the National Weather Service (NWS) for flood forecasting throughout the United States. While it has 16 parameters that need to be specified by the user, consistent with previous work (see Vrugt et al. 2003b and references cited therein), 13 were specified as adjustable. The prior uncertainty ranges of the specified adjustable SAC-SMA hydrologic model parameters are defined in Table 1. The reader is referred to (see Vrugt et al. 2003b and references cited therein) for comprehensive discussions regarding the SAC-SMA hydrologic model, the Leaf River watershed, and also its related hydrologic data (viz., mean areal precipitation (mm/day), potential evapotranspiration (mm/day), and streamflow (m^3/s)) that was used to support the effective inference of the posterior distribution of the SAC-SMA adjustable model parameters and also the most likely parameters within this high probability density region.

Table 1. Prior uncertainty ranges of the SAC-SMA model parameters.

Parameter	Minimum	Maximum	Unit
UZTWM	1	150	[mm]
UZFWM	1	150	[mm]
UZK	0.1	0.5	day^{-1}
PCTIM	0	0.1	[-]
ADIMP	0	0.4	[-]
ZPERC	1	250	[-]
REXP	1	5	[-]
LZTWM	1	500	[mm]
LZFSM	1	1000	[mm]
LZFPM	1	1000	[mm]
LZSK	0.01	0.25	day^{-1}
LZPK	0.0001	0.025	day^{-1}
PFREE	0	0.6	[-]

Results associated with the thirty trials are summarized in Tables 2 – 8 and Figure 3. The results presented in Tables 2 – 5 are associated with an earlier version of SCEM-FA wherein the input parameter *r* was fixed and not dynamically adjusted as it is now, based on the candidate point acceptance rate, an acceptance rate threshold, and the persistence parameter, *p*, which dictates the update frequency for *r*. Examining the results in Table 2, we clearly see as one would expect, improved efficiency for SCEM-FA relative to SCEM-UA as the value for *r* increases. However, the improved efficiency that is obtained through more aggressive utilization of the function approximation prediction comes at the cost of decreased effectiveness in terms of convergence to the same posterior probability distribution as SCEM-UA, evidenced upon inspection of the lower order statistics for the objective function and SAC-SMA parameter values that are presented in Tables 3 – 5.

Table 2. Summary of efficiency for an earlier version of SCEM-FA, relative to SCEM-UA, for fixed values of r. Results are based on thirty unique instances of the earlier version of SCEM-FA and also SCEM-UA.

Total Model Calls						
		SCEM-FA				
		Random Number Threshold in SEM-FA				
	SCEM-UA	0.1	0.3	0.5	0.7	0.9
Average	87253	79379	70602	66852	55158	50090
% reduction		9.0	19.1	23.4	36.8	42.6

Table 3. Summary of objective function value lower order statistics for an earlier version of SCEM-FA, relative to SCEM-UA, for fixed values of r. Each individual result if based on thirty unique instances for the earlier version of SCEM-FA and also SCEM-UA, in particular, 15,000 (500 for each of the 30 trials) samples generated after convergence to a posterior distribution has been achieved with either the SCEM-FA or SCEM-UA.

	Objective Function Values	
Method	Average	Standard Deviation
SCEM-UA	13.31669413	0.02331727
SCEM-FA (r=0.1)	13.3073988	0.030142989
SCEM-FA (r=0.3)	13.35390347	0.21756169
SCEM-FA (r=0.5)	13.3382782	0.218278563
SCEM-FA (r=0.7)	13.42101667	0.325857754
SCEM-FA (r=0.9)	13.6533664	0.252643413

Table 4. Summary of SAC-SMA average parameter values obtained from an earlier version of SCEM-FA, for fixed values of r, and also SCEM-UA. Each individual result is based on thirty unique instances for the earlier version of SCEM-FA and also SCEM-UA, in particular, 15,000 (500 for each of the 30 trials) samples generated after convergence to a posterior distribution has been achieved with either the SCEM-FA or SCEM-UA.

Method	Adjustable Model Parameters Average Values												
	UZTWM	UZFWM	UZK	PCTIM	ADIMP	ZPERC	REXP	LZTWM	LZFSM	LZFPM	LZSK	LZPK	PFREE
SCEM-UA	26.8812	29.5574	0.3811	0.0040	0.2722	203.3623	3.7797	250.7199	48.1212	105.5772	0.2364	0.0200	0.1502
SCEM-FA (r=0.1)	26.8277	29.2832	0.3798	0.0037	0.2762	206.1732	3.7819	249.4870	48.6453	105.7939	0.2367	0.0199	0.1472
SCEM-FA (r=0.3)	34.7161	35.9214	0.3805	0.0057	0.2845	204.0555	3.7810	248.0950	97.5675	136.9293	0.2387	0.0191	0.1571
SCEM-FA (r=0.5)	35.2474	36.3110	0.3848	0.0058	0.2847	209.6409	3.8505	249.8837	97.2791	136.5281	0.2402	0.0198	0.1629
SCEM-FA (r=0.7)	51.8347	45.8982	0.3906	0.0098	0.3013	204.0789	3.9138	239.9127	187.4767	199.7868	0.2422	0.0177	0.1851
SCEM-FA (r=0.9)	111.4248	66.9965	0.4062	0.0214	0.3526	185.1139	4.1644	200.3526	218.5091	212.8119	0.2413	0.0182	0.2908

Table 5. Summary of standard deviations associated with SAC-SMA parameter values obtained from an earlier version of SCEM-FA, for fixed values of r, and also SCEM-UA. Each individual result is based on thirty unique instances for the earlier version of SCEM-FA and also SCEM-UA, in particular, 15,000 (500 for each of the 30 trials) samples generated after convergence to a posterior distribution has been achieved with either the SCEM-FA or SCEM-UA.

Method	Adjustable Model Parameters Standard Deviation Values												
	UZTWM	UZFWM	UZK	PCTIM	ADIMP	ZPERC	REXP	LZTWM	LZFSM	LZFPM	LZSK	LZPK	PFREE
SCEM-UA	4.2085	2.6528	0.0512	0.0026	0.0262	26.5712	0.4820	10.9419	11.6494	11.3510	0.0085	0.0025	0.0242
SCEM-FA (r=0.1)	4.2885	3.3627	0.0526	0.0024	0.0295	25.2751	0.4926	11.2260	11.6630	11.1780	0.0088	0.0027	0.0345
SCEM-FA (r=0.3)	29.4503	25.9629	0.0580	0.0085	0.0396	32.0259	0.5540	15.1575	182.9817	122.1159	0.0075	0.0054	0.0478
SCEM-FA (r=0.5)	29.4968	26.4420	0.0573	0.0081	0.0369	32.2464	0.5393	14.8277	180.8541	124.1650	0.0066	0.0053	0.0386
SCEM-FA (r=0.7)	47.2430	40.4975	0.0677	0.0133	0.0486	40.5929	0.7078	23.1352	299.4427	209.2608	0.0053	0.0078	0.0717
SCEM-FA (r=0.9)	47.1152	56.9383	0.0962	0.0130	0.0391	46.5461	0.7981	33.2429	297.6354	208.1662	0.0090	0.0080	0.0967

Table 6. Summary of objective function value lower order statistics for SCEM-FA, relative to SCEM-UA. Each individual result is based on thirty unique instances for SCEM-FA and also SCEM-UA, in particular, 15,000 (500 for each of the 30 trials) samples generated after convergence to a posterior distribution has been achieved with either the SCEM-FA or SCEM-UA.

	Objective Function Values	
Method	Average	Standard Deviation
SCEM-UA	13.31669413	0.02331727
SCEM-FA	13.27271167	0.02663205

Table 7. Summary of SAC-SMA average parameter values obtained from SCEM-FA and also SCEM-UA. Each individual result is based on thirty unique instances for SCEM-FA and also SCEM-UA, in particular, 15,000 (500 for each of the 30 trials) samples generated after convergence to a posterior distribution has been achieved with either the SCEM-FA or SCEM-UA.

Method	Adjustable Model Parameters Average Values												
	UZTWM	UZFWM	UZK	PCTIM	ADIMP	ZPERC	REXP	LZTWM	LZFSM	LZFPM	LZSK	LZPK	PFREE
SCEM-UA	26.8812	29.5574	0.3811	0.0040	0.2722	203.3623	3.7797	250.7199	48.1212	105.5772	0.2364	0.0200	0.1502
SCEM-FA	27.3790	29.1978	0.3919	0.0033	0.2780	216.8556	3.9589	252.2889	50.7311	105.1115	0.2408	0.0212	0.1565

Table 8. Summary of standard deviations associated with SAC-SMA parameter values obtained from SCEM-FA and also SCEM-UA. Each individual result is based on thirty unique instances for SCEM-FA and also SCEM-UA, in particular, 15,000 (500 for each of the 30 trials) samples generated after convergence to a posterior distribution has been achieved with either the SCEM-FA or SCEM-UA.

Method	Adjustable Model Parameters Standard Deviation Values												
	UZTWM	UZFWM	UZK	PCTIM	ADIMP	ZPERC	REXP	LZTWM	LZFSM	LZFPM	LZSK	LZPK	PFREE
SCEM-UA	4.2085	2.6528	0.0512	0.0026	0.0262	26.5712	0.4820	10.9419	11.6494	11.3510	0.0085	0.0025	0.0242
SCEM-FA	3.2647	2.6198	0.0493	0.0020	0.0228	19.6017	0.4135	9.8273	11.2531	10.1219	0.0060	0.0020	0.0198

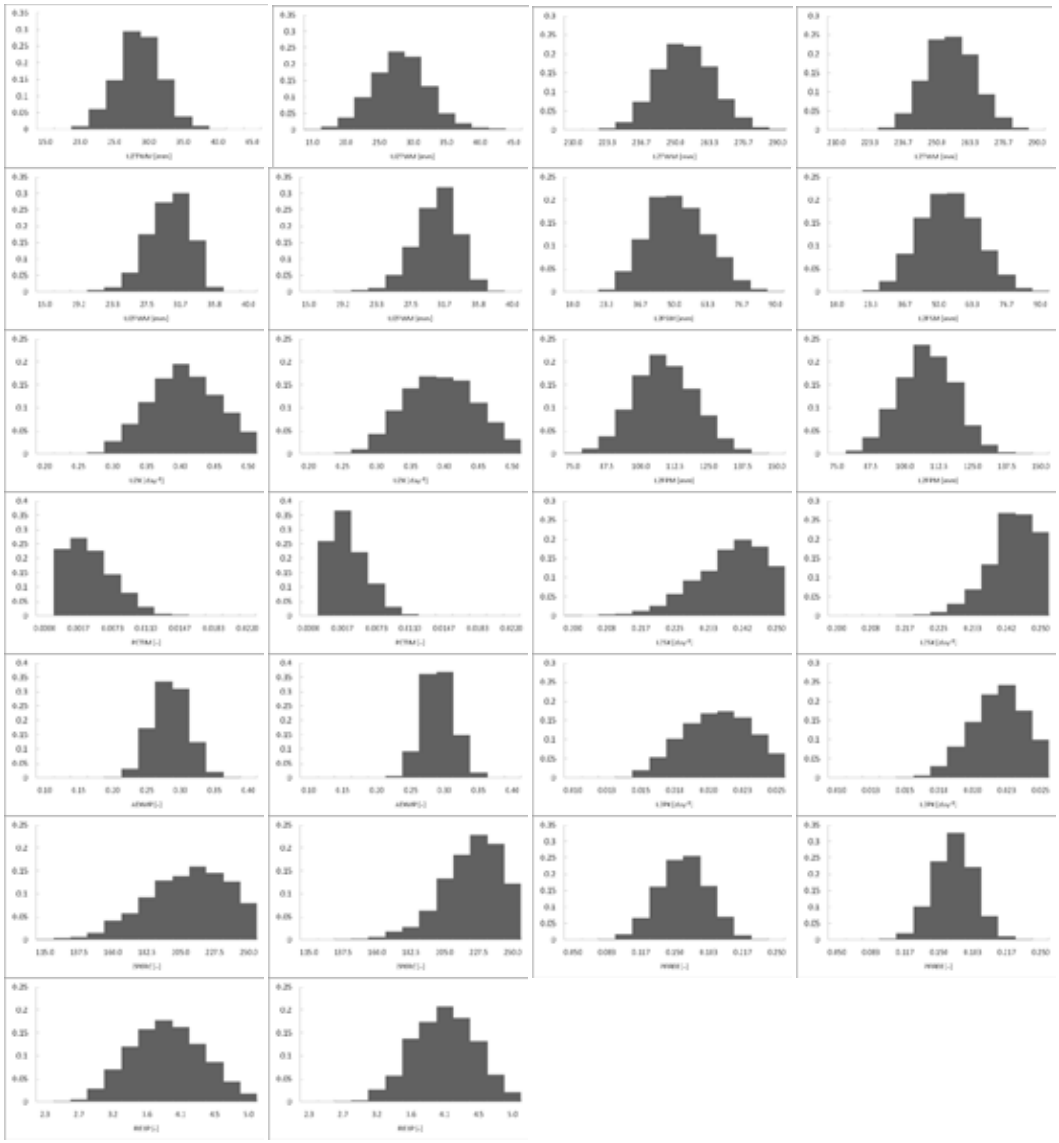

Figure 3. The marginal posterior probability distributions of the SAC-SMA model parameters inferred for the Leaf River watershed using the 15,000 (500 for each of the 30 trials) samples generated with the SCEM-UA (1st and 3rd columns) and SCEM-FA (2nd and 4th columns) algorithms after convergence has been achieved with SCEM-UA and SCEM-FA.

In attempts to balance efficiency with effectiveness, different heuristics for controlling the activation of the function approximation prediction within SCEM-FA were subsequently implemented, resulting in the existing SCEM-FA implementation documented in this report. Based on the thirty trials, the average number of forward model calls for SCEM-UA was 87,253; whereas, it was 68,642 with SCEM-FA, resulting in an approximate 21 percent reduction in total forward model calls. Comparing lower order statistics associated with the objective function and related parameter values obtained from samples generated after convergence to a posterior distribution has been achieved with either the SCEM-FA or SCEM-UA, as shown in Tables 6 – 8, it is clear that the existing SCEM-FA algorithm converged to the same target distribution as SCEM-UA. The results presented in Figure 3, marginal posterior probability distributions of the SAC-SMA model parameters based on 15,000 (500 for each of the 30 trials) samples generated with the SCEM-UA and SCEM-FA algorithms after convergence has been achieved with SCEM-UA and SCEM-FA, further confirm this observation. The results presented in Tables 6 – 8 and Figure 3 were obtained with SCEM-FA input parameters set to r = 0.9, a = 0.35, and p = 3.

4 Summary

This report began by outlining the need for hydrologic model calibration and, related, the realistic assessment of hydrologic model uncertainty, which has many benefits, including model comparison and selection, identification of the best water management strategies that reflect the likelihood of outcomes, data collection aimed at improving hydrologic predictions and water management, and regionalization and extrapolation of hydrologic parameters to ungauged basins. Bayesian-based approaches to model calibration, in particular Markov Chain Monte Carlo (MCMC) simulation methods, are a formal means to obtain a realistic and reliable estimate of model uncertainty. However, their application comes at a computational cost. For hydrologic modeling, it was noted that there is a need to design efficient MCMC samplers, and this observation was in fact the motivation for the development of the Shuffled Complex Evolution Metropolis algorithm (SCEM-UA) (Vrugt et al. 2003a). The primary objective of the research and development encapsulated in this report was to improve upon the already existing documented efficiency of the state-of-the-art Bayesian model uncertainty analysis method SCEM-UA (Vrugt et al. 2003a). As with other recent research and development activity that was directed to enhancing the efficiency to the state-of-the-art covariance matrix adaption evolution strategy (CMAES) (Baggett and Skahill, 2010a, b), the principal approach that was employed to achieve that stated objective was to simultaneously and adaptively construct an approximation to the objective function.

The report followed with some brief background material and then a description of the current methodology that is employed for interfacing a function approximation model with the native SCEM-UA algorithm to improve upon its already existing documented efficiency. Thereafter, based on a comprehensive set of thirty trials using the SAC-SMA soil moisture accounting hydrologic model and local hydrologic data for the Leaf River watershed near Collins, MS, it was clearly demonstrated that SCEM-FA was able to achieve, on average, a 21 percent reduction in total model calls while inferring the same posterior probability distribution as that obtained with SCEM-UA.

Several opportunities exist for future development (and likely additional efficiency gains) and also application. Numerical experiments are needed to explore how the random number threshold, *r*, the acceptance rate threshold, *a*, the parameter, *p*, an integer value which determines the update frequency for *r*, and the increment/decrement value embedded in the dynamic adjustment process for *r* impact overall SCEM-FA performance, relative to SCEM-UA, in terms of efficiency and reliability. A relatively simple and easily implementable approach that would likely yield additional efficiency gains for the current implementation of SCEM-FA would be to monitor the success rate of the function approximation prediction and use that as a basis for deciding whether to perform a forward model call after the function approximation prediction suggests the candidate point is to be accepted. Early SCEM-FA development utilized a k-nearest neighbor cubic radial basis function (RBF) local function approximation model rather than locally weighted projection regression (LWPR). It would be interesting to explore how the two different function approximation models impact overall SCEM-FA performance, relative to SCEM-UA, in terms of efficiency and reliability. Moreover, it could be of potential benefit to explore ways in which the confidence estimate associated with the LWPR function approximation prediction could be beneficially used to improve overall SCEM-FA performance, relative to SCEM-UA, in terms of efficiency and reliability. Additional case studies are needed to further document SCEM-FA performance in terms of efficiency relative to SCEM-UA. And future applications need to focus on model prediction uncertainty. As was mentioned earlier, the methods reported upon in this report should be relatively easy to transfer to other MCMC methods. It is our intent to explore just that with the DREAM MCMC sampler, particularly in light of potential balance issues that have been presented regarding the SCEM-UA algorithm (Vrugt et al. 2008). The code for the SCEM-FA algorithm is available from the first author.

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14. ABSTRACT

An important consideration in assessing the performance of model calibration software is that of run time. Minimizing the number of hydrologic model runs required during the calibration process is nearly always important, but particularly when the objective function landscape contains multiple local minima or hydrologic model run times are high. Minimizing the number of required model runs was one of the primary factors driving the research and development activities encapsulated in this report, such that the resulting optimization and uncertainty tool(s) are more compatible with the computationally expensive physics-based models that are becoming more commonly used within the practice community. SCEM-FA is a modified version of the Markov Chain Monte Carlo sampler SCEM-UA. It is more efficient than the native SCEM-UA algorithm, through employment of function approximation, while effectively inferring the posterior parameter distribution of model parameters and also the most likely parameters within this high probability density region. Based on a summary of thirty random trials, SCEM-FA was able to infer, effectively, the same posterior probability distribution for thirteen SAC-SMA hydrologic model parameters as that of SCEM-UA with an average twenty-one percent savings in total forward model calls.

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