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Advances in the study of uncertainty quantification of large-scale hydrological modeling system

SONG Xiaomeng[1], *ZHAN Chesheng[2], KONG Fanzhe[1], XIA Jun[2]

1. School of Resource and Earth Science, China University of Mining & Technology, Xuzhou 221008, Jiangsu, China;
2. Key Laboratory of Water Cycle & Related Land Surface Processes, Institute of Geographic Sciences and Natural Resources Research, CAS, Beijing 100101, China

Abstract: The regional hydrological system is extremely complex because it is affected not only by physical factors but also by human dimensions. And the hydrological models play a very important role in simulating the complex system. However, there have not been effective methods for the model reliability and uncertainty analysis due to its complexity and difficulty. The uncertainties in hydrological modeling come from four important aspects: uncertainties in input data and parameters, uncertainties in model structure, uncertainties in analysis method and the initial and boundary conditions. This paper systematically reviewed the recent advances in the study of the uncertainty analysis approaches in the large-scale complex hydrological model on the basis of uncertainty sources. Also, the shortcomings and insufficiencies in the uncertainty analysis for complex hydrological models are pointed out. And then a new uncertainty quantification platform PSUADE and its uncertainty quantification methods were introduced, which will be a powerful tool and platform for uncertainty analysis of large-scale complex hydrological models. Finally, some future perspectives on uncertainty quantification are put forward.

Keywords: uncertainty quantification, hydrological model, PSUADE, land-atmosphere coupling model, large scale

Since the 21st century, large-scale land-atmosphere coupling modeling has been regarded as one of the critical issues on the global change research by the International Geosphere-Biosphere Programme (IGBP), the World Climate Research Programme (WCRP), and the Global Energy and Water Cycle Experiment (GEWEX), etc. In these projects and programs, many researches on simulating the land-surface hydrological processes and their coupling studies with climate models have been performed (Chen *et al*., 1997; Lohmann *et al*., 1998; Shao and Henderson, 1996). How to establish a new large-scale hydrological cycle modeling system coupled with atmosphere model, which could both describe the temporal and spatial variations of hydrological cycle effectively and assess water resources partition-

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Author: Song Xiaomeng (1987–), Master Candidate, specialized in hydrology. E-mail: wenqingsxm@126.com
***Corresponding author:** Zhan Chesheng, Ph.D, E-mail: zhancs2006@gmail.com

ing quantitatively at regional or global scale, is a research hot point in the global change research (Yong, 2007; Yong *et al*., 2009). Generally, hydrological model (e.g. conceptual model, distributed hydrological model, large-scale coupled model, etc.) is a principal tool to research the watershed hydrological processes and their evolution laws. Also it is an abstraction, simplification and interpretation of the reality hydrological processes using mathematical formula and physical equations. And there are enormous uncertainties and distortions for hydrological modeling. Therefore, uncertainty quantification of complex hydrological model is also one of the most crucial issues in the hydrological science (Ye and Xia, 2002), especially for the study on uncertainty of large-scale hydrological cycle modeling system.

There are many components in a complex hydrological cycle system model, such as model input, model output, model structure and equations, initial and boundary conditions, and model parameter, etc. The uncertainty sources can be grouped into four categories (Renard *et al*., 2010): 1) uncertainty in the input data, 2) model structure uncertainty, 3) parameter uncertainty, and 4) uncertainty in the output data for model calibration and optimization. There is also great uncertainty in the hydrological modeling, especially for the large-scale land-atmosphere coupled hydrological modeling system. And its uncertainties also consist of the forecasting uncertainty of atmosphere model, land surface model, and the interaction effect of multi-physics processes on the output, and so on.

The much larger scale or more complex land-atmosphere coupled model has been developed with the development of remote sensing (RS), geographic information system (GIS), and computer technology. And also the high-precision and high-resolution observed data and high-performance computer are useful support and facilitation for the model construction. However, how to establish an effective framework of uncertainty quantification techniques for these more complex models become a critical step or issue for the hydrological science research at present.

In this paper, we systematically reviewed the recent advances in the uncertainty analysis approaches and proposed a new framework of uncertainty quantification for complex models. Firstly, the concepts or explanation of uncertainty quantification, uncertainty sources and propagation processes were described. And then, the classical approaches or methods were discussed. Also, the uncertainty analysis of large-scale complex hydrological modeling system was summarized including input uncertainty, model structure uncertainty, parameter uncertainty, analysis approaches uncertainty, and others. Subsequently, a new uncertainty quantification platform PSUADE (**P**roblem **S**olving Environment for **U**ncertainty **A**nalysis and **D**esign **E**xploration) was introduced and proposed to uncertainty analysis of large-scale hydrological cycle modeling system, which can reduce the running computational cost with a good accuracy based on the response surface methodology. Finally, some perspectives and recommendations on uncertainty quantification were put forward and suggested.

1 Uncertainty quantification

Uncertainty quantification is the quantitative characterization and reduction of uncertainties in applications, and it tries to determine how likely certain outcomes are if some aspects of the system are not exactly known. In general, uncertainty quantification has to incorporate research and development efforts in three key, irreducible technical areas: (1) Characterization of uncertainty in system parameters and the external environment; (2) propagation of this uncertainty through large computational models; and (3) verification and validation of the models and incorporating the uncertainty of the models themselves into the global uncertainty assessment. Therefore, according to the propagation processes of uncertainty and the relationship among the uncertainty sources as shown in Figure 1, the thrust of uncertainty quantification to be discussed herein is to determine: 1) the model structure, i.e., how accurately a mathematical model describes the true system for a real-life situation, may only be known approximately, while models are almost always only approximations to reality; 2) the numerical approximation approaches, i.e., how appropriately a numerical method is used in approximating the operation of the system, while most models are too complicated to solve exactly; 3) initial and boundary conditions, i.e., how accurately and really determine the initial and boundary conditions for the models; 4) model input and parameters, i.e., how to enhance the quality of input data and parameter estimation.

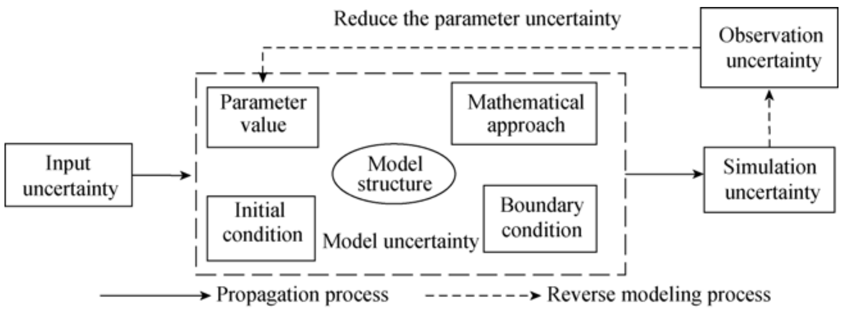

Figure 1 Uncertainty sources and propagation processes

2 Uncertainty analysis methods

Generally, uncertainty assessment methods can be broadly classified into two groups (Li *et al.*, 2010), i.e., the Generalized Likelihood Uncertainty Estimation (GLUE) method and the Bayesian method. The GLUE method, named as the informal Bayesian approach, has been widely used due to its conceptual simplicity, ease of implementation and flexibility of less modification to existing source codes of hydrological models since it was developed by Beven and Binley (1992). The Bayesian method (Engeland *et al.*, 2005; Kavetski *et al.*, 2006a,b; Liang *et al.*, 2010; Thiemann *et al.*, 2001), in contrast, refers to the use of a prior probability over hypotheses to determine the probability of a particular hypothesis given some observed evidence, and then analyze the uncertainty of model. That is, the probability that a particular hypothesis is truely given some observed evidence comes from a combination of the prior probability of the hypothesis and the compatibility of the observed evidence with the hypothesis.

To solve the parameter “equifinality” in the hydrological model, Beven *et al.* (1992, 2001) proposed the GLUE method based on the generalised sensitivity analysis of Hornberger and Spear. It provides tools for sensitivity and uncertainty estimation using the results of Monte Carlo simulations and Bayesian theory, which has been widely applied to various catchments models, such as Xinanjiang model (Shu *et al.*, 2008), TOPMODEL model (Beven *et* *al.*, 1992, 2001), HYMOD model (Montanari, 2005), WASMOD model (Jin *et al.*, 2010), etc. However, the GLUE method has some drawbacks, and a number of questions still remain unresolved. For example, Montanari (2005) stated that the GLUE method relied on some explicit and implicit assumptions, and it was not fully clear how these may affect the uncertainty estimation when referring to large samples of data. And also the prediction limits provided by GLUE do not necessarily include a percentage close to their confidence level of the observed data. Blasone *et al.* (2008) demonstrated that the GLUE derived parameter distributions and uncertainty bounds were entirely subjective and had no clear statistical meaning, and it is incoherent and inconsistent from a statistical point of view. Then, the Latin hypercube sampling (LHS) strategy and SCEM-UA algorithm were used to improve it. And the revised GLUE method was well applied to the NAM model, HYMOD model and SAC-SMA model in the Tryggevalde catchment of Denmark and the Leaf River catchment, located in southern Mississippi. Wei *et al.* (2009) pointed out that the SCEM-UA method excessively depended on the model structure, not accounted for the effect of other uncertainty sources (e.g. input error, model parameters uncertainty, etc.) on the output. Therefore, the Markov Chain Monte Carlo (MCMC) method was used to revise the GLUE, and it can derive more accurate prediction bounds and more proper estimation of the uncertainty in SMAR model.

The Bayesian method was firstly used to analyze the parameter uncertainty problem in the hydrological statistical model by Wood and Rodriguez-Iturbe (1975), and then it has been widely applied to the uncertainty analysis and hydrological forecasting. The Bayesian framework effectively allows for the estimation of model uncertainties by constraining prior information on the parameters in the form of prior distributions using the data available (Khu and Werner, 2003). The posterior parameter distributions which result can be used to make model predictions is shown. Once new data become available, the posterior parameter distributions can be applied again as prior distributions and updated using the new information contained in the additional data (Khu and Werner, 2003). Krzysztowicz *et al.* (1999) proposed Bayesian Forecasting System (BFS) with the foundation of Bayesian theory, and it was an operational framework for probabilistic forecasting via a deterministic hydrological model of an arbitrary complexity. The BFS decomposes the total uncertainty into input uncertainty and hydrological uncertainty, which are quantified independently and then integrated into a predictive distribution. However, the forecasting uncertainty and error sources uncertainty cannot be quantified. The Bayesian total error analysis (BATEA) method was applied to uncertainty analysis of input data, model parameter, model structure and model simulation by Kavetski *et al.* (2006a, b), Kuczera *et al.* (2006), and Thyer *et al.* (2009). And the BATEA method provides a comprehensive framework to hypothesize, infer, and evaluate probability models describing input, output, and model structure error, whose characteristic is that the data and model uncertainty can be incorporated into hydrological modeling. The Bayesian model averaging (BMA) method is also provided to uncertainty analysis, which derives the consensus prediction from competing prediction using likelihood measures as model weights (Hoeting *et al.*, 1999) and has been applied to the hydrological models (e.g., Neuman, 2003; Vrugt and Robinson, 2007; Najafi *et al.*, 2011). Thiemann *et al.* (2001) presented the framework for a Bayesian recursive estimation (BaRE) approach to hydrological prediction that can be used for simultaneous parameter estimation and prediction in an operational setting. The prediction can be described in terms of the probabilities associated with different output values, and this approach could be extremely useful for that ungauged catchments or without adequate observed data. Kuczera and Parent (1998) stated that the Monte Carlo-based approach with Metropolis algorithm provided a quantum advance to deal with parameter uncertainty in hydrological models in the three different conditions or cases. And then, Cheng and Li (2007) developed the parallel adaptive Metropolis (PAM) algorithm based on the Metropolis algorithm to solve the parameter uncertainty and optimization of Xinanjiang model. Also, the integrated Bayesian uncertainty estimator (IBUNE) was developed by Ajami *et al.* (2007), which accounted for the major uncertainties of hydrologic rainfall-runoff predictions explicitly and distinguished between the various sources of uncertainty including parameter, input, and model structural uncertainty.

In the recent research achievement, some new uncertainty analysis techniques based on other assumptions and theories, in addition to the above mentioned methods, have been developed and applied to various catchments, such as the ensemble Kalman filter (EnKF) approach (Vrugt and Robinson, 2007), the shuffled complex evolution Metropolis method (SCEM-UA) (Vrugt *et al.*, 2003a), the multi-objective shuffled complex evolution Metropolis (MOSCEM) (Vrugt *et al.*, 2003b), the fuzzy-based simulation method coupling fuzzy vertex analysis technique with distributed hydrological model (Huang *et al.*, 2010), the meta-Gaussian stochastic approach (Montanari and Brath, 2004), etc.

While the above mentioned approaches are only useful and well applied to the conceptual hydrological model or physically-based distributed hydrological model, not suit to the large-scale complex hydrological modeling system, e.g., a large-scale hydrological model coupled with land surface model and atmosphere model. Uncertainty quantification of coupled models, with complex structure and a large number of parameters involving hydrological model parameters, land-surface model parameters and atmosphere model parameters, adopting only one of the classical methods or approaches may lead to statistical bias and underestimation of the uncertainty, and also it becomes more and more difficult. Also, there is interaction effect among the various modules, and the uncertainty effect of modules on the output cannot be well identified and quantified. The classical analysis methods cannot achieve uncertainty analysis for the complex model with large number of parameters because it is time-consuming and a high-cost computation. For this reason, how to establish an effective uncertainty quantification approach or scheme for large-scale complex hydrodynamics system model becomes one of the crucial efforts and aims in the hydrological science.

3 Uncertainty analysis of large-scale hydrological modeling system

As the atmosphere and hydrosphere are closely connected with various energy and mass exchanges of different scales, the interaction and restraint effects between climate change and hydrological cycle exist (Yu, 2008). Generally, hydrological and atmospheric processes occur over scales that range from microscopic to global, roughly spanning 10^{-10} to 10^{5} meters in space and 10^{-13} to 10^{5} seconds in time. Many poorly understood physical processes in both the hydrosphere and atmosphere (e.g. infiltration and cloud dynamics) exist within this spectrum scales. Some processes may be known and quantifiable under limited conditions, but are difficult to generalize over larger spatial domains. Yet heterogeneous land surfaces dominate the earth and play a key role in land-atmosphere interactions in areas where the surface hydrologic budget may be most affected by climate change. Ideally, models should be able to simulate hydrological and atmospheric processes at any scale, but there are large gaps in the ability of the existing models to do because the nature of some processes may preclude modeling due to lacking sufficient knowledge of the natural processes to model them, or the underlying physics of the processes are too complex to be simulated by computer models. Therefore, the uncertainty effect of the hydrological and atmospheric coupled models or land-atmosphere coupled models on the model output is important, and many hydrologists and meteorologists have paid attention to their uncertainty quantification. And we discussed the uncertainty analysis efforts for the large-scale complex models from the various uncertainty sources.

3.1 Input uncertainty

The uncertainty about model input data is often acknowledged to be one of the main sources of uncertainty in model predictions. There are a large number of input data for large-scale land-atmosphere coupled models, involving the precipitation input, soil input, evapotranspiration input, vegetation cover, air temperature, etc., which could immensely affect on the model output due to various data quality.

To reduce the input data uncertainty, applications of data assimilation arise in many fields of geosciences, perhaps most importantly in atmospheric science, marine science and hydrological science. Several methods have been used to assimilate data into hydrological model, e.g., the linear Kalman filter, variational method (Reichle *et al.*, 2001; Koren *et al.*, 2009), ensemble Kalman filter (Reichle *et al.*, 2002; Ghent *et al.*, 2010), particle filter (Moradkhani *et al.*, 2005; Salamon and Feyen, 2010), etc. Reichle *et al.* (2002) discussed the application of the ensemble Kalman filter to hydrological data assimilation and in particular to the estimation of soil moisture, and compared the performance of the EnKF to an optimal smoother (weak-constraint variational algorithm), and the results showed that the error decreased by 55% from the value obtained without assimilation.

Another attempts from the efforts of Moradkhani *et al.* (2005) and Koren *et al.* (2009) also showed that the data assimilation techniques could reduce the uncertainties arising from the data and the model. Furthermore, an approach was proposed by Salamon and Feyen (2010) to infer during a calibration process the statistical properties of the principal error sources (i.e. parameter, precipitation, potential evapotranspiration, and model structural uncertainty) by means of sequential data assimilation. It was applied to a large-scale distributed model of the Rhine River to demonstrate its usefulness when characterizing error sources, and the posterior multiplier distributions were used to identify whether a systematic bias exists and to illustrate that uncertainty from those sources can be reduced significantly in comparison to the prior assumptions adopted.

In addition, it is important to notice that the information generated by the atmosphere model is inevitably subject to uncertainties which propagate through the hydrological scheme and eventually influence model results (Kotlarski *et al.*, 2005). Therefore, Kotlarski *et al.* (2005) selected four regional climate models (RCMs, e.g. REMO5.0, REMO5.1, MM5 and CLM) to compare with their effect on the hydrological model output and drive the uncertainty ranges by means of three reference data sets (ERA15, CRU and DWD). And the results showed that differences between RCM results were of the same magnitude as differences between the reference data sets. Other than the climate model simulation results, the radar based quantitative precipitation estimates are also widely used to large-scale distributed hydrological models, and the data obtained remain an important source of uncertainty for hydrological predictions. Schröter *et al.* (2011) demonstrated that the probabilistic use of radar quantitative precipitation estimates may add valuable information to hydrological predictions and reduce the bias of hydrological model parameter estimates.

3.2 Model structure uncertainty

Hydrological cycle model structure is a critical and kernel component for hydrological modeling system, which commonly aggregates the hydrological processes occurring in a catchment into a number of key responses represented by storage components and their interactions. However, any model is an abstraction, simplification and interpretation of reality. The incompleteness of a model structure and the mismatch between the real causal structure of a system and the assumed causal structure as represented in a model always result in uncertainty about model predictions. And also, the discordant scales of hydrological and atmospheric models in the coupled models have become one of the most important sources of uncertainty.

Though the model structure uncertainty is one of the key sources of uncertainty in model predictions, it is frequently neglected and no generic methodology exists for assessing the effects of model structure uncertainty (Refsgaard *et al.*, 2006). Butts *et al.* (2004) addressed the two questions to the model structure uncertainty, i.e., “First, different model structures are expected to perform differently, but is there a trade-off between model complexity and predictive ability? Secondly, how does the magnitude of model structure uncertainty compare to the other sources of uncertainty?”. The results showed that model performance was strong dependent on the model structure, and distributed routing and to a lesser extent distributed rainfall were found to be the dominant processes controlling simulation accuracy. Also, the sensitivities to variations in acceptable model structure were of the same magnitude as uncertainties arising from the other sources. Therefore, he suggested that for practical hydrological predictions there are important benefits in exploring different model structures as part of the overall modeling approach, and the model structure uncertainty should be considered in assessing model uncertainties.

Then Refsgaard *et al.* (2006) presented a framework for assessing the predictive uncertainties of environmental models used for extrapolation, involving the use of multiple conceptual models, assessment of their pedigree and reflection on the extent to which the sampled models adequately represent the space of plausible models. Lin and Beck (2009) demonstrated that the real challenge in dealing with structure error and uncertainty in a model lied in at least two aspects: 1) how to identify this source of uncertainty in models, including unambiguously differentiating it from other sources; 2) how to account for the model error and uncertainty in making forecasting. In their work, the time-varying parameter was proposed to view the parameters of the model’s structure not as random variables, i.e., as constants (albeit known with uncertainty), but as stochastic processes, i.e., quantities that vary with time, in part in a systematic manner and in part in an essentially random manner. The approach is useful to assess the model structure uncertainty.

For a complex coupled model, the discordant resolutions or scales among various models are important error sources (Yu, 2008). To evaluate the effect that the mesoscale meteorological model (MM5) resolution has on the simulation of direct surface runoff in the linked model experiments, and decrease the computational intensity of these experiments, three single storm events and their basin responses were simulated with MM5 using three domain set-ups (i.e. 36-23-4, 36-12 and 36 km) by Lakhtakia *et al.* (1998). And the results showed that the 36-12 km set-up generated similar patterns of precipitation and direct surface runoff to those of the 36-12-4 km domain set-up, and the 36 km domain set-up produced unrepresentative precipitation distributions in time and space. It also was concluded that 12 km precipitation fields may be a suitable compromise, providing sufficient resolution for simulating the basin response to climate variation and change.

With the current emphasis on modeling past and future climate change, the need for better methods for modeling interactions between the hydrosphere and atmosphere has been brought to the forefront of research. A great amount of effort aimed at solving the discordant scale problem and coupled model uncertainty is now being expended by terrestrial, hydrological and atmospheric scientists. In the near future, the coupled model structure uncertainty analysis will become a new hot point.

3.3 Parameter uncertainty

Parameter of model is an important component for a computational model, especially for large-scale coupled model. Also, it is another one of the main sources of uncertainty. Most of the parameters cannot be measured directly but can be inferred by a calibration process that adjusts the parameter values to closely match the input-output behavior of the model to the real system it represents (Vrugt *et al.*, 2003). However, quantification of parameter and predictive uncertainty is not an easy matter. Whilst a number of methodologies are available, none of them are entirely satisfactory (Gallagher and Doherty, 2007). Also, some of them are extremely computationally intensive, requiring many model runs for their implementation, thus making their deployment with many commonly used models difficult, for a large-scale coupled model or a relatively complex model.

Chen and Dudhia (2001) introduced the sensitivity of coupled model with land surface model (LSM) and Penn State-NCAR MM5 model, and stated that soil moisture parameters were important, i.e., the soil thermal, hydraulic conductivities and surface energy balance were very sensitive to soil moisture changes. Hence, it was necessary to establish an appropriate soil moisture data assimilation system to improve the soil moisture initialization at fine scales.

The GLUE method and Sobol approach were applied to the global routing model in the HTESSEL-TRIP2 coupled model by Pappenberger *et al.* (2010). In their work, the ground water delay parameter is identified as being the most sensitive calibration parameter, and its uncertainty effect on output is significant. And also, the application results showed that the global runoff routing model was fit for the purpose although there were significant uncertainties in the modeling system, whose uncertainties came from meteorological inputs, hydrological model and the observations, not from the routing component itself. It will have the potential to be used for alternative purpose such as flood early warning or climate studies.

A primary limitation in using the GLUE method is the prohibitive computational burden imposed by uniform random sampling of the parameter distributions, especially for a large-scale complex model (Hossain and Anagnostou, 2005). Therefore, a revised GLUE method was proposed using stochastic modeling of the parameters' response surface to recognize the inherent non-linear parameter interactions. The results showed that it can reduce computational burden by at least 15%–25%, and demonstrated the potential for increasing efficiency of GLUE uncertainty estimation for rainfall-runoff models as it does not impose any additional structural or distributional assumptions.

At present, response surface methodology (RSM) as a surrogate model of complex model arouses a great concern by some scholars. When the model simulation is very expensive, as in any large-scale complex model (e.g. land surface model) applications, it is not easy to employ the traditional model calibration techniques. It acquired succeed application in the common land surface model (Duan *et al.*, 2009).

The multi-criteria algorithm, the multi-objective generalized sensitivity analysis (MOGSA) (Bastidas *et al.*, 1999), was used to investigate the parameter sensitivity of five different land surface models with increasing levels of complexity in the physical representation of the vegetation (BUCKET, CHASM, BATS1, Noah, and BATS2) at five different sites representing crop land/pasture, grassland, rain forest, cropland, and semidesert areas (Bastidas *et al.*, 2006). The methodology allowed for the inclusion of parameter interaction and did not require assumptions of independence between parameters, while at the same time allowing for the ranking of several single-criterion and a global multi-criteria sensitivity indices. However, the analysis required on the order of 50 thousand model runs. Also, this approach has been applied to parameter estimates, which was found to be effective in constraining the parameter estimates into physically plausible ranges when observations on at least one appropriate heat flux and one properly selected state variable are available (Gupta *et al.*, 1999).

A large-scale coupled model (revised AVIM model), which had been coupled to GCM, between hydrological model (Xinanjiang model) and land surface processes was proposed by Su (2001). In order to evaluate the surface water budgets of AVIM and to evaluate the ability to simulate runoff, the implementation of AVIM to Xilinhe basin (in Inner Mongolia of China) and daily streamflow simulations from the year 1991 to 1994 were presented. The results of sensitive experiments indicated that runoff direactly affected the change of soil moisture states, thus affecting sensible and latent heat fluxes and other energy terms.

3.4 Uncertainty approaches

The uncertainty quantification is much expensive for a large-scale land-atmosphere coupled model due to its large number of parameters, complex structure, and many components. Therefore, the traditional and classical uncertainty analysis approaches are not useful to the complex models. Recently, there are some approaches or attempts applied to the complex models.

The SCEM-UA algorithm was attempted to be applied to uncertainty analysis of the large-scale BIGMOD model by Fernando *et al.* (2007), and the results indicated a high level of uncertainty for each of the 16 parameters modeled. However, this variation was likely to be due to the fact that measured flow and salinity data were only available at one location each, and that different combinations of model parameters can achieve the same output. That highlighted the importance of incorporating as much a prior knowledge into the calibration as possible. Also, to reduce the computational cost, such knowledge was required to choose the physically most plausible set of parameter values generated.

The Gaussian error propagation (GEP) approach was used to assess uncertainty of state variables and fluxes in the CoLM model (Liang, 2008), and the results showed that the uncertainties in soil parameters affected more remarkably compared to plant parameters, meanwhile, soil hydraulic parameters (e.g., porosity -η_S, saturated matrix potential -Ψ_S, pore-size distribution index-b, and saturated hydraulic conductivity -k_S) contributed much more than thermal parameters (e.g., saturated soil albedo -α_S, and volumetric heat capacity -$\rho_S c_S$). Also, uncertainty in b dominated uncertainty of all state variables and fluxes under most conditions, followed by η_S on sand and loam and k_S on clay. The GEP method can identify critical parameters and parameterization, and also could form a scientific basis for model parameter determination and parameterization improvement.

The MOGSA approach based on multi-criteria calibration procedure, which provided an objective determination of the multicriteria sensitivity of the modeled variables to the parameters and thereby allowing the number of calibration parameters and hence the computational effort to be reduced, was proposed and used to sensitivity analysis of BATS (Biosphere-Atmosphere Transfer Scheme) model (Bastidas *et al.*, 1999). And the results were found to be consistent with the physical properties of the different environments, and also there was little degradation in the quality of the model description and little change in the preferred range of the remaining parameters when the insensitive parameters were omitted from the calibration process (Bastidas *et al.*, 1999), that is to say, the approach can reduce the uncertainty of parameters via decreasing the number of parameters.

Uncertainty quantification for a large-scale model is a challenging activity that requires a different approach to uncertainty analysis at a relatively small scale (Bijlsma *et al.*, 2007). And Bijlsma *et al.* (2007) stated that the some limitations and inherent subjectivity existed, and it was not always valid when the practice of uncertainty analysis approach at a large scale was derived from a small scale. Also, the current restriction of uncertainty assessment was mostly based the given structurally conservative estimates, and the unknown bias was usually not assessed though it may easily outweigh the effects of variability.

3.5 Others

Hou *et al.* (2009) discussed the effect of large-scale atmospheric uncertainty on the streamflow predictability. The global ensemble forecast system (GEFS) of NCEP was evaluated following an approach, in which its hydrological component was considered free of errors and the initial conditions in the hydrological variables were assumed to be accurate. And the results suggested that the coupled system was capable of generating useful gridded streamflow forecast when the land surface model and the river routing model can successfully simulate the hydrological processes, and the ensemble strategy significantly improve the forecast. Also, the expected forecast skill increased with the increasing size of the river basin.

A land-surface hydrological model TOPX based on the saturated runoff generation mechanism of the improved SIMTOP with topography concept of TOPMODEL model, in association with the water budget calculation principle of the Xinanjiang model was proposed by Yong (2007) to be coupled with regional climate model RIEMS to improve the parameterization scheme of the hydrological processes in regional climate model. The uncertainty effect of regional climate model RIEMS on the land surface hydrological processes was also discussed, and the results showed that the precipitation estimated from the regional climate model was an important effect factor on the streamflow forecasting.

Gao *et al.* (2006) improved the Noah land surface model, in which the evaporation of pond water and re-infiltration were taken into account in the land surface model, and the overland routing and subsurface routing parameterization were added into land surface scheme. Routing module was linked with MM5 through the disaggregating or aggregating method. Then, the high-resolution atmosphere-hydrology coupling model was applied to simulate the feedback of land surface water cycle in atmosphere in the Heihe River basin. The results indicated that the atmospheric fields were influenced by land surface water cycle process at large extent, involving the soil moisture, evaporation, boundary layer stability, cloud water and rain water.

The fully-coupled, stochastic simulation was used by Williams and Maxwell (2011) to demonstrate the uncertainty propagation between land surface and atmosphere in the coupled model. Feedbacks between the land surface and the atmosphere, manifested as mass and energy fluxes, are strongly correlated with soil moisture, making soil moisture an important factor in land-atmosphere interactions. The results state that a reduction of the uncertainty in hydraulic conductivity creates a reduction in uncertainty in land-atmosphere feedbacks that yields more accurate atmospheric predictions. Also, by reducing uncertainty associated with land-atmosphere feedback mechanisms, they reduce uncertainty in both spatially distributed and domain-averaged wind speed magnitudes, thus improving simulation ability to make more accurate forecasts.

All in all, although many efforts and achievements have been devoted to quantify the uncertainty of large-scale land-atmosphere coupled models, there are also many problems or puzzles to solve. Because of the highly nonlinear nature of the hydrological cycle system, it is not feasible to account for all these uncertainties from different sources through model calibration, verification and validation (e.g. parameter adjustments) (Ajami *et al.*, 2007). For examples, regarding to the errors or uncertainty in model input data, there is no perfect method to assess the sensitivity of input data spatial distribution because no enough information can be used to describe the spatial relationship of each unit or cell, such as the temporal and spatial distribution of precipitation, soil moisture, and so on. In addition to that, usually, the interpolation uncertainty effect of input data on the output is neglected. The model structure is another source of uncertainty for a hydrological model, especially for a large-scale land-atmosphere coupled model. A large-scale complex model consists of many sub-modules or sub-models, in which the uncertainties come from the abstraction, simplification and interpretation of reality system, and lack of knowledge to the natural processes, etc. Therefore, an effective approach or method has not been accomplished and applied to a complex computational model, and it will be a research hot point for hydrological science. Also, the parameter estimation is important for model constructing and simulation. Many approaches or algorithms have been widely applied to calibrate and optimize these parameters of models. However, it is difficult to seek the global optimization value or achieve the identification and calibration processes because there are various peak values for the parameter response surface and interaction effect among parameters. Also it makes the calibration process exist inherent subjectivity due to large number of parameters and some without physical meanings, i.e., it cannot be observed in the reality system and can only be calibrated from the model. Apart from that, the uncertainties of initial and boundary conditions are rarely considered in the existing literatures. But for a large-scale land-atmosphere model, these conditions could affect on the forecasting and simulation output, which should be taken account into the uncertainty quantification of complex models in the future research.

4 A new effective uncertainty quantification approach

An effective uncertainty quantification system for a large-scale complex hydrological cycle modeling system has not been established at present. For classical analysis approaches, there is some insufficiency (e.g., high computational cost, etc.) for complex hydrological cycle system. To improve the simulation accuracy and well understand the uncertainty of large-scale hydrological cycle models, a new tool or platform called PSUADE can be selected to solve that problem, and applied to the uncertainty quantification of large-scale hydrological model.

4.1 PSUADE

The PSUADE is a software toolkit developed by the Lawrence Livermore National Laboratory to facilitate uncertainty quantification for large-scale complex modeling system. It has a rich set of tools or approaches involving the sampling design, uncertainty analysis, sensitivity analysis, numerical/statistical optimization, model calibration, etc. In particular, PSUADE provides a surrogate model (response surface methodology) to simplify the original computational model, and make the uncertainty quantification more tractable with reducing the computational cost. Also, it enables to assess the uncertainty of complex computational model or system, and offers beneficial reference and experience for uncertainty quantification of large-scale land-atmosphere coupled hydrological cycle modeling system.

Generally, uncertainty quantification will help: 1) tune a simulation model to match better with experiments, 2) establish the integrity of (validate) a simulation model, 3) assess the region of the validity of a simulation model, 4) characterize the output uncertainties of a simulation model, 5) identify the major sources of uncertainties of a model, and 6) provide information on which additional experiments are needed to improve the understanding of a model, and others. To accomplish the goal of uncertainty quantification, many design and analysis tools are needed. In the PSUADE, there are a set of sampling design methods including Monte Carlo sampling (MC), Latin Hypercube sampling (LHS), orthogonal array sampling (OA), quasi-random sampling (LPTAU), central composite designs (CCD), Morris one-at-a-time designs (MOAT), fourier amplitude sensitivity test designs (FAST), factorial designs (FACT), fractional factorial design (FF), Placket-Burman design, etc. Also, it provides many methodologies to construct the response surface, such as polynomial regression model, multivariate adaptive regression splines (MARS), artificial neural network (ANN), Gaussian process model (GP), and support vector machines (SVM), and so on. Furthermore, it supports a lot of global sensitivity analysis methodologies for models with large number of parameters and complex constraints, i.e. qualitative analysis methods (e.g. LH-OAT method, MOAT screening method, and FAST method) and quantitative analysis methods (e.g. Sobol method, Extend FAST, main effect, two-way interaction effect, and RSM-based method). Take the sensitivity analysis as a case, the flowchart for running the PSUADE is as shown in Figure 2.

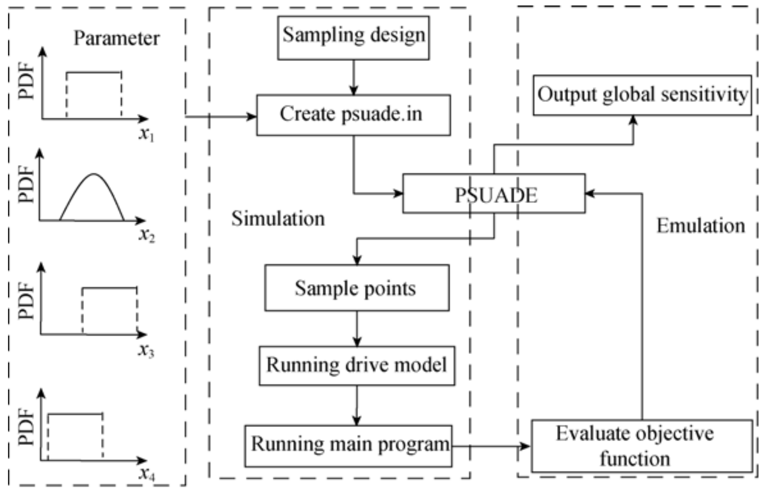

Figure 2 Operation framework in PSUADE (after Tong Charles. Uncertainty quantification methodologies and methods for multi-physics applications [PPT])
Note: PDF means probability density function.

4.2 Response surface model

Response surface methodology (RSM), which is also known as a meta-model or surrogate model, is a collection of statistical and mathematical techniques useful for developing, improving, and optimizing processes. In the PSUADE, a good response surface model, which is used to approximate and simplify the complex and high-dimension nonlinear input-output relationship, has been constructed with sufficient accuracy via rigorous validation or cross validation. Subsequent all the analysis can rely on this response surface model which is inexpensive to evaluate. And it will facilitate the efficacy of the more quantitative analysis that requires a large number of evaluations. The original definition of RSM pertains to linear and polynomical regression analyses. The kernel for response surface involves appropriate sample data (such as the input-output data and the space-filling data) and fitting method. PSUADE provides a number of response surface methods ranging from parametric regression methods to non-parametric methods, such as Friedman's multivariate adaptive regression splines (MARS), artificial neural network (ANN), Gaussian process model, support vector machines (SVM). Take the land-atmosphere coupled hydrological cycle system model as a case, the procedure (as shown in Figure 3) for creating the response surface is as follows: 1) Choose a sampling design method, such as LPTAU, Metis, LH, etc.; 2) run the simulator with the sample; 3) use response surface check to see goodness of fit, e.g. examine training errors and cross validation errors; 4) if errors are not acceptable, add more points; 5) create a FF IV design to sample some corners, to test the robustness against extrapolation; 6) use "rstest" to examine extrapolation errors; 7) if good, add FF design and create new response surface.

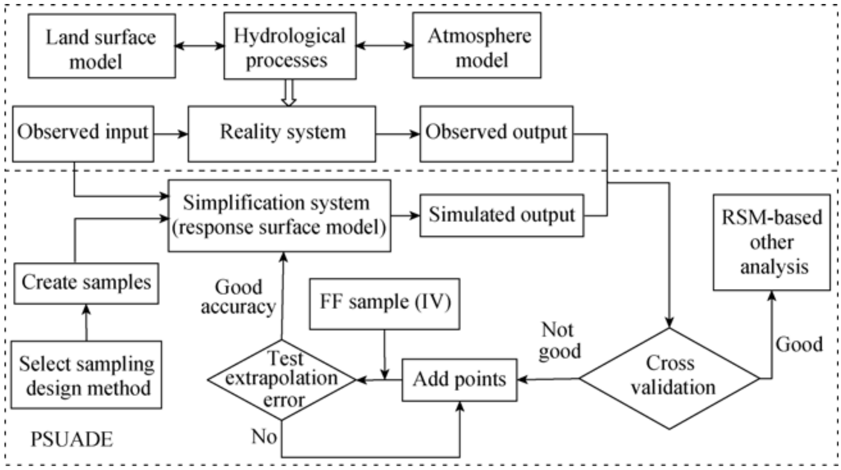

Figure 3 The procedure for structure of response surfaces and generalization of complex system

4.3 Application

At present, there are few case studies of PSUADE to the hydrological model or hydrological cycle system, but which has been applied to other complex computational model. For example, Tong and Graziani (2008) proposed a global sensitivity analysis methodology using the PSUADE for general multi-physics applications that are characterized by strong nonlinearities and interactions in their input-output relationships, expensive simulation runs, and large number of input parameters. And they present a four-step approach consisting of (1) prescription of credible input ranges, (2) parameter screening, (3) construction of response surfaces, and (4) quantitative sensitivity analysis on the reduced set of parameters. The numerical results show that it obtains a good accuracy compared with the classical method, and reduce the computational cost. Furthermore, it is also applied to quantification of parameter uncertainty of the Common land model (CoLM), and the results demonstrate the usefulness of the response surface technique as a potential calibration tool. Hsieh (2007) focuses on using PSUADE as a tool for global sensitivity analysis and uncertainty quantification to an engineering model. In addition, Tong (2008) applied a spectrum of uncertainty quantification techniques to the study of a two-dimensional soil-foundation-structure-interaction (2DSFSI) system subjected to earthquake excitation. Also, Wemhoff and Hsieh (2007) used the code PSUADE to calibrate Prout-Tompkins kinetic parameters for pure recrystallized TNT. The results stated the methodology based on response surface using PSUADE provided a basis for future calibration studies.

The PSUADE software package integrates many uncertainty quantification approaches with a rich collection of sampling methods. And it also supports a flexible runtime environment, e.g., serial and asynchronously parallel execution modes, non-intrusive to user codes, a user-friendly interface via input and output filters. In particular, the response surface methodologies based on statistical and mathematic theory can be widely applied to many complex computational model to facilitate the uncertainty quantification, and it will be well applied to the complex hydrological modeling system.

5 Future prospects

There are many uncertainty sources for a large-scale hydrological cycle modeling system, involving the uncertainties of the both-way transmission and feedback of the input-output information via inter-coupling between land surface model with atmosphere model, which become a crucial factor to model simulation accuracy or reliability (Yong *et al.*, 2006). How to reduce or decrease the uncertainty effect of large-scale hydrological modeling system has become a hot point and frontier issue for hydrological and atmospheric sciences (Yin *et al.*, 2006). Currently, an effective framework of uncertainty quantification of complex hydrodynamics system has been not constructed yet. Also, many problems of uncertainty quantification should be solved urgently, such as, how to quantify the effect of the uncertainty of model input, parameter, and structure on the output, how to develop and establish an effective approach framework to reduce the cost of uncertainty quantification for complex system model, and how to construct the integration assessment platform or tool package to support complex model, and so on. Therefore, the following aspects on uncertainty quantification should be emphasized in the future.

(1) Uncertainty methods

The uncertainty methods are the basis of model uncertainty quantification. Now, although many methods or approaches have been widely used and applied to hydrological model, the classical methods have limitations for large-scale physically-based distributed hydrological models or complex land-atmosphere coupled models. Consequently, an effective assessment and quantification method system should be formed and constructed based on the classical approaches integrating with their strong points and advantages, so that they are also suitable to the uncertainty quantification of complex computational models, and quantitatively distinguish the effect of various uncertainty sources on the output without increasing the computational cost and reducing the model simulation accuracy. The PSUADE is a relatively effective platform for uncertainty quantification, which integrates many uncertainty analysis methods, and can emulate the complex model using a response surface (or surrogate model) to reduce the uncertainty computational cost. It will be a new hot point issue to uncertainty quantification of complex models, especially for multi-parameters and multi-processes coupled models.

(2) Parameter optimization methods

Model parameter is a crucial component for computational models, and also is the external representation and explanation of model structure. In a great many situations, the model parameters are conceptual representations of abstract watershed characteristics and must be determined through a trial-and-error process or an optimization algorithm with population-evolution-based search strategy which adjusts the parameter values so that the model response matches the historical input-output data (Yapo *et al.*, 1998). However, many optimization algorithms have several shortcomings, i.e., being dependent on the parameter initial values, optimization ranges, quality of the historical input-output data, and parameter distribution, also being extremely time consuming when comprehensive assessment is carried out on the model structure and others, and the optimization parameter values are usually not best ones. Therefore, a multi-objective global optimization algorithm should be enhanced to reduce the uncertainty effect of model parameters on model output, and it will be another key hot point.

(3) Model structure and mechanism

The theory of hydrological science is a basis and foundation for constructing the model structure and system. However, the water cycle processes are complex considering the hydrological processes, land surface processes, atmospheric processes, etc., and a computational model is abstracted from reality system, and has great uncertainty if we do not have a good and comprehensive knowledge for inherent laws of reality system. In addition, the uncertainty of coupled processes between the land surface model and atmosphere model has been also not well known (e.g., the scale transformation). So, the research on model structure and mechanism should be enhanced based on the existing models, to make the modeling system well represent the reality system and then reduce the forecasting uncertainty.

(4) Data source and quality control

Model input is one of the unavoidable uncertainty sources. Model input data based on various techniques with different precisions exists extreme errors, which can propagate the error from the modeling system to the output. To reduce the effect of input error on the output, many new techniques or approaches controlling data quality should be widely used to hydrological science, such as remote sensing, data assimilation, etc.

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