A general probabilistic framework for uncertainty and sensitivity analysis of deterministic models

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Abstract: Uncertainty and sensitivity analysis are valuable tools for the assessment of model applications and several methods were developed in the last decades. However, the applicability of these methods is limited to scalar parameters and in many cases the analysis is still made by One-A-Time methods. These severely constrain the ability of a general assessment of the model in practical applications. In this study a general probabilistic framework for uncertainty and sensitivity analysis of deterministic models is presented. The approach is able to consider all the sources of uncertainty i.e., input, distributed parameters and model structure. In this context a global uncertainty analysis is used as a tool to evaluate the performance of the model. A global sensitivity analysis based on Sobol's method is then used as complementary tool to find the most important sources of uncertainty. The framework is used in a loop to optimize the further activities and improve the performance of the model in a goal-oriented approach. The effectiveness of the framework is demonstrated with an example with SWAP model, a 1D physical-based hydrological model. The procedure is applied in a cropped field in Northern Germany for the year 2011. The simulation results are compared with the soil moisture detected in the root zone and considering the variance of evapotranspiration and bottom fluxes below the root zone simulated by the model. The results show that the errors in the estimation of evapotranspiration and bottom fluxes are negatively correlated. In this way the evaluation of the soil moisture alone can not be seen as a good assessment of the model performance. Finally, the sources of uncertainty are different for each process and improvement of the performance of the model strictly depends on the output considered.

Keywords: Sensitivity analysis, Sobol method, deterministic models.

1   INTRODUCTION

The advances in computer science have taken to a growing number of modeling studies explicitly considering uncertainty analysis (UA) and sensitivity analysis (SA) of model output [e.g., Wagener and Montanari, 2011]. Depending on the fields of application, different definitions can be encountered. Following Saltelli et al. [2006], UA can be defined as a tool to quantify the uncertainty in the model predictions and SA is the complementary tool used to study how the uncertainty in the model output can be apportioned to the different sources of uncertainty. SA methods can be then classified as either Local or Global. Local sensitivity analysis falls generally in the class of the so called One-A-Time (OAT) method, as each factor is perturbed in turn while keeping all other factors fixed at their nominal value. Global Sensitivity Analysis (GSA) studies the effects of input variations on the outputs in the entire allowable ranges of the input space, they can be applied also with non-linear model

and they account for the effects of interactions between different input factors. For these, GSA methods are generally recommended.

Several methods were proposed and compared in practical applications demonstrating the capability to analyze different sources of uncertainty [e.g., Binley and Beven, 2003; Tang et al., 2007; Yang, 2011; Renard et al., 2011]. However, to date, the complexity of models has limited the applicability of GSA methods considering all the sources of uncertainty (i.e., input, distributed parameters and model structure). As a matter of fact, due to these limitations, in many cases this technique is still generally applied in the assessment of scalar parameters. On the other hand, the assessment of other sources of uncertainty is still made by One-A-Time (OAT) method [Saltelli et al., 2006].

In this context, this paper proposes a General Probabilistic Framework (GPF) based on Monte Carlo simulation for the uncertainty (UA) and global sensitivity analysis (GSA) of deterministic models considering the problems mentioned above. In this framework also non-scalar sources of uncertainty can be explicitly considered without any constraint e.g., spatially-distributed parameters and data and alternative models. This framework is based on the approach proposed by Crosetto and Tarantola [2001] and recently revisited in Lilburne and Tarantola [2009]. The utility of the framework is demonstrated with an example from the field of the soil-vegetation-atmospheric systems using SWAP model, a 1D physical-based hydrological model. The proposed framework, however, is readily extendable to a wide variety of distributed hydrological modeling applications.

2   THE GENERAL PROBABILISTIC FRAMEWORK - GPF

The General Probabilistic Framework (GPF) proposed for the uncertainty and sensitivity analysis is shown in Figure 1 and the steps are described as follow. The first step sets the goal of the study, the experimental site and an appropriate scalar objective function [called variable of interest in de Rocquigny et al., 2008]. The second step consists in the collection of all necessary data and the selection of the simulation model for the specific application. In the third step all the sources of

uncertainty U_i, i.e., input data, distributed parameters and alternative model structures, are defined. The uncertainty of each source is characterized using available information, observations, estimations, physical bounds considerations and expert opinion [see Helton 1993 for more details]. If the analysis is exploratory, then also rather crude assumptions may be adequate. In the fourth step, for a given distributed input, n independent realizations are generated. The number of realizations has to be large enough so that the generated sample is statistically representative of the uncertainty associated to that input. Then, in step 5, each realization is associated to an integer number in the range $(1, n)$. If model uncertainty is present, e.g., m alternative model structures are available, each model structure is associated to an integer number in the range $(1, m)$. Therefore, to each distributed
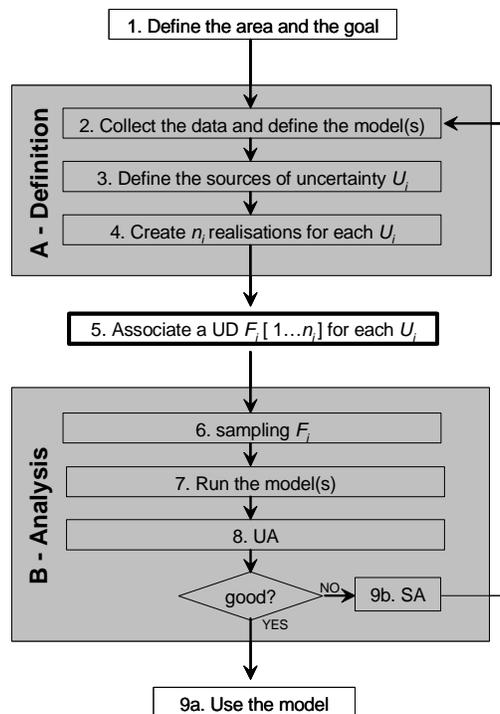

Figure 1. Flowchart of the General Probabilistic Framework (GPF).

input we can associate a discrete uniform distribution $F_i[1…n]$ and, in the presence of model uncertainty with m available alternative models, we can associate a discrete uniform distribution $F_i[1…m]]$. The sampling is carried out for the discrete factors F_i (step 6). In step 7 of the framework the model (or the different models if several structures are considered) is executed considering the combinations created by sampling F_i. Uncertainty analysis (UA) of the model output is then carried out in step 8. If the uncertainty of the model predictions is small it is possible to use directly the results of the model (step 9a). Otherwise (step 9b) the sensitivity analysis is conducted to quantify the contribution of the different sources of uncertainty.

The introduction of this simple trigger factor in the framework (step 5) allows us to describe the sources of uncertainty in a more flexible way, separating the stage of uncertainty set up (Figure 1 box A) from the stage of analysis (Figure 1 box B). In this way also non-scalar sources of uncertainty can be freely considered in the global sensitivity analysis e.g., distributed input and parameters or model structures [Lilburne and Tarantola, 2009]. Finally, the use of the framework in a loop allows the revision and improvement of the model in a goal-oriented approach.

3   SENSITIVITY ANALYSIS AND CODES

The sample generation in step 6 can be accomplished in a number of ways as several sampling designs are available [Saltelli et al., 2000]. Such sampling strategies need their correspondent estimator to obtain sensitivity measures for the inputs in step 9b. In this specific framework proposed, the estimation of the sensitivity indices is done based on the variance decomposition proposed by Sobol' [2001] and further developed by Saltelli [2002] and Saltelli et al [2010]. As shown by Tang et al. [2007], the Saltelli/Sobol' method yields more robust sensitivity rankings than other measurements such as correlation/regression methods or regional sensitivity analysis. Moreover, with this method the estimation of the sensitivity indices does not depend on the order in which the realizations are associated with the scalar input values. For more details about the method we refer further to Lilburne and Tarantola [2009]. The sensitivity indices considered are the so called First sensitivity index (S_i) and Total sensitivity index (S_T) as follows:

$$S_i = \frac{V\left[E\left(Y \mid X_i\right)\right]}{V(Y)} \tag{1}$$

$$S_{T_i} = \frac{E\left[V\left(Y \mid X_{\sim i}\right)\right]}{V(Y)} \tag{2}$$

where the first index is the ratio between the variance of the mean output Y conditioned by all the possible input values X_i and the total variance of the output $V(Y)$. The higher S_i, the higher the importance of the input factor X_i on its own. The total index S_T is the average of the variance of the output Y when this is conditioned by all the possible input values except X_i. The lower S_T, the lower the overall importance of the factor X_i. The difference between the total and the first order index quantifies the effect of the interactions of X_i with all the other input factors. For more details see also Saltelli et al. [2000]. Finally, the evolution of the indexes is evaluated estimating the indexes with increasing sample size.

The framework is implemented using MATLAB and Simlab libraries [SimLab, 2009]. First, a Sobol sequence is generated for each factor X_i (1…n). Then, the model is run in a Monte Carlo approach. The output is stored and then elaborated further. The codes are implemented *ad hoc* for the specific model but they can be easily adapted to all the models without the need to manipulate the original model itself.

4   CASE STUDY

4.1   Model and experimental site

The General Probabilistic Framework is applied to SWAP model, a widely used 1D physical-based hydrological model of soil moisture dynamics in unsaturated soils based on Penman-Monteith and Richards' equations [Kroes and Van Dam, 2003]. In this study the uncertainty in the model structure is not explicitly considered comparing, for instance, models of different complexity [e.g., Baroni et al., 2010]. On the other hand, the framework is applied with the final goal to optimize the monitoring activities and increase the model performance.

The model application is conducted for a cropped flat field of 30 ha located in Bornim (Brandenburg, Germany), where surface run off can be neglected and the 1D vertical fluxes play the most important role. The area situated 40 m a.s.l. is characterized by mean annual precipitation of 595 mm and minimum and maximum daily temperature values of -15ºC (February) and 30ºC (July), respectively (Meteorological Station Potsdam Telegrafenberg - Germany). Soil texture of the site was reported to be dominated up to 1 m by 75% sand content, 17.2% silt content and 7.8% clay content [Gebbers et al., 2009] referring to a loamy-sand soil classification (USDA). The groundwater level is ~ 5 m below the surface as suggested by information from the State Environmental Agency based on a groundwater well nearby. For more details of the experimental site and monitoring activities see also Rivera Villarreyes et al. [2011].

4.2   Data collected and sources of uncertainty

The characterization of the sources of uncertainty is an important step of the analysis [e.g., Beven et al., 2011]. In this case study, during the season, direct monitoring activities were conducted to collect the input and parameters to set up the model and to define the uncertainty in the data available. Table 1 summarizes nominal values and ranges of uncertainty introduced for each of the input data and parameters. In particular, weather data were available from Meteorological Station Potsdam Telegrafenberg. However, the station is located approximately 6 km east of the experimental site. Direct measurements of weather data were also collected in the field during the season and compared to the reference one to define the range of uncertainty for each variable. In 2011 the field was cropped with sunflowers. Crop parameters to set up the model were based on Allen et al. [1998]. Field measurements of crop height H_c (cm) were conducted in the field biweekly to define the uncertainty on the parameter presented in literature. The same range of uncertainty detected for the crop height was considered for the uncertainty of the

Table 1. Ranges of uncertainty defined for Weather data: random error introduced in the time series; Crop parameters: mean and random error introduced at maximum stage; Soil: mean and random error of parameters of Van Genuchten eq. (θ_r and L were fixed to 0.05 (m^3 m^{-3}) and 0.5 (-) respectively).

Daily weather data (W)	
Parameter	Range
Air Temperature (ºC)	± 1.0
Air humidiy (hPa)	± 0.2
Wind (m/s)	± 1.0
Glob.Radiation (W m^{-2})	± 20
Rain (mm)	± 2.0

Crop parameters (C)		
Parameter	mean	CV
H_c max (cm)	130	8%
R_d max (cm)	40	8%
LAI max (-)	2.5	8%

Soil parameters (S)		
Parameter	mean	CV
θ_s (m^3 m^{-3})	0.37	5%
n (-)	1.55	4%
α (cm^{-1})	0.05	25%
K_{sat} (cm d^{-1})	195	40%

other crop parameters necessary to set up the model, i.e., Leaf Area Index *LAI* (-) and Root depth R_d (cm).

Direct soil samples were also sampled in the field at different depths, for analysis of the soil texture and bulk density. Then, Pedotransfer Functions (PTFs) were used for the estimation of the soil hydraulic parameters. In particular, considering the ranges of the soil texture in the field, a homogeneous soil profile was considered and PTFs of Zacharias and Wessolek [2007] and PTFs of Rawls and Brakensiek [1989] were applied for the estimation of the parameters of the soil retention curve and for the estimation of the hydraulic conductivity K_{sat} (cm d^{-1}), respectively. The uncertainty of each parameter was then fixed considering a range in the parameters estimated as proposed by the authors of the PTFs. At the experimental site the interaction between root zone and groundwater can be neglected and free drainage was set as bottom boundary condition without introduce an error. Finally a warm-up period was used to eliminate the sensitivity to the initial conditions.

4.2   Set up of the model and of the General Probabilistic Framework - GPF

The simulation was run from May to September 2011, and the analysis was focused on the temporal variability of evapotranspiration, soil moisture in the root zone and bottom fluxes below the root zone simulated by the model. The model performance is evaluated considering the variance of the model outputs in case of evapotranspiration and bottom fluxes. The performance of the soil moisture dynamic simulated is done comparing the soil moisture measured by calibrated Theta Probes (Delta-T Devices, Cambridge, UK) installed in the field at three depths (0, 20 and 40 cm). In this case the RMSE (m^3 m^{-3}), between simulated and measured mean soil moisture in the root zone (50 cm) is calculated for the period considered.

Considering the monitoring activities described above, the sources of uncertainty were grouped in three main classes: meteorological data (W), crop parameters (C) and hydraulic soil parameters (S). Taking into account the range of uncertainty defined for each of the sources, a number of realizations n_i were defined, which cover the space of variability introduced. In particular, 64 realizations of meteorological data were created, 64 realizations of daily series of crop parameters were considered (i.e., *LAI*, H_c and R_d) and 64 realizations of hydraulic soil properties were generated. The realizations were sampled from the range defined in Table 1 and considering the correlation between parameters as detected in the data. The simulations were run using a sampling number N = 1024. In concordance to the method proposed in Saltelli et al [2010], a total number of runs $N_R = N(k+2)$ = 5120 was carried out, where k = 3 is the number of input factors (i.e., W, S, C). The evolution of the indexes is evaluated estimating the indexes with increasing sample size.

4.3   Results

In figure 2 the RMSE between mean soil moisture in the root zone measured in the field and simulated is plotted for each run. As we can see, the soil moisture shows a general agreement even without a specific model calibration underlining the good capability of the model to simulate the process. However, especially in the first period (results not shown), when soil is relatively dry due to the high evapotranspiration rate and the low precipitation, the model has a tendency to overestimate the process.

In figure 2 the evolution of the estimated first order sensitivity indices are also plotted. The Sobol method shows a clear ranking of the input factors considered even with a relatively low number of runs. As we expected, the results show that the soil properties (S) play the major role in the variability of the simulation results. Thus, calibration should be firstly made on these parameters for the subsequent improvement of the model performance in the simulation of the soil moisture dynamics. No particular differences are detected between first and total sensitivity indices underlining the general additivity of the model (results not shown).
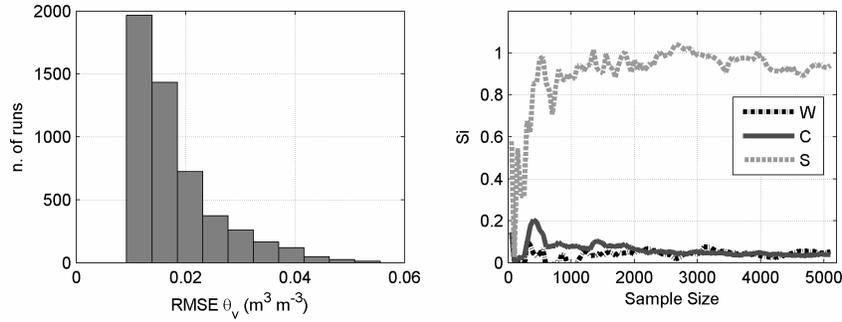
Figure 2. Histograms of the RMSE calculated between simulated and measured mean soil moisture θ_v (-) and sensitivity indexes.

In figure 3 the histograms of the cumulative evapotranspiration (ET_a) and of the bottom fluxes (Q_{bot}) below the root zone (50 cm) are plotted with the corresponding first order sensitivity indices. The uncertainty in the estimation of the evapotranspiration is relatively low with mean value and range of ~ 275 ± 40 mm respectively. On the other hand, the bottom fluxes are quite limited in the period considered but the relative error becomes more important with mean value and range of ~ -55 ± 40 mm, respectively. For both processes the ranges are comparable.

Also for these processes, Sobol method shows a clear ranking of the input factors even if, in particular for the evapotranspiration, the absolute values of the sensitivity indexes are not stable. However, it is interesting to see that soil properties (S) for these processes are not important sources of uncertainty (figure 3, right). In this way, the results show how a better calibration of the soil properties would not improve the performance of the simulation of these processes. For this goal, reduction of uncertainty has to be obtained with a better definition of the upper boundary condition driven by the weather data (W). Differences between first and total indices are also not detected for these fluxes, underlining a general independency between the input factors (results not shown).
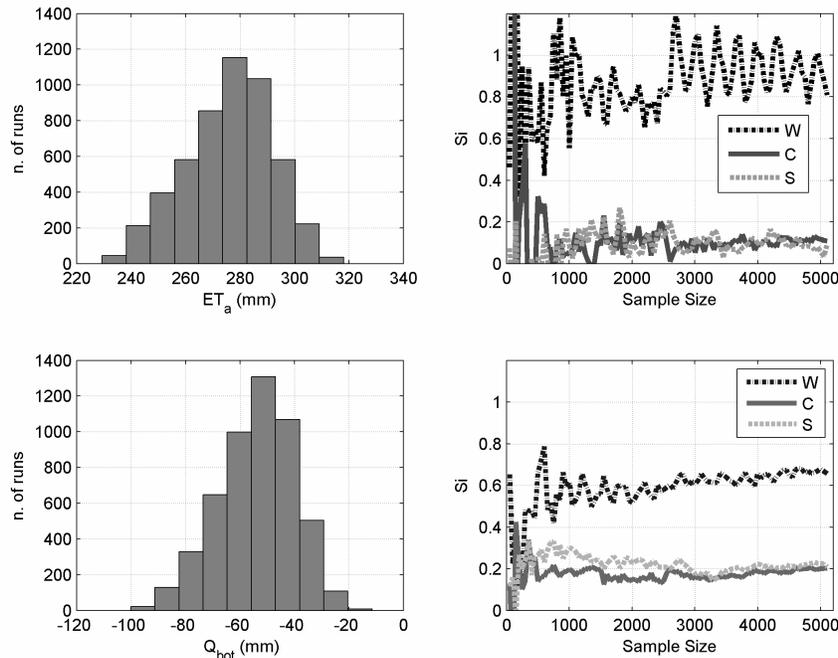

Figure 3. Histograms of the cumulative values of the evapotranspiration (ET_a) and bottom flux (Q_{bot}). On the right, sensitivity indices are plotted.

To further investigate the results, in figure 4 the deviations from the mean evapotranspiration and bottom fluxes are compared (left) and the marginal influence of soil properties on the RMSE is represented by a scatter plot (right). As example, K_{sat} values are plotted but similar results are obtained with the other soil parameters. For each graph, the gray dots represent all runs and the black dots the runs that achieve the best performance in the simulation of the soil moisture (RMSE < 0.01). The results show an uncertainty of the same order of magnitude in the fluxes, i.e., ± 40 mm and negative correlation (R^2 ~ 0.8). These errors compensate each other and they cannot be captured by the error in the simulation of the mean soil moisture since also the best set of soil properties are still affected by the same behavior. This reflects a general non-identifiability of the soil parameters and the need of multi-criteria for a proper assessment of the model.
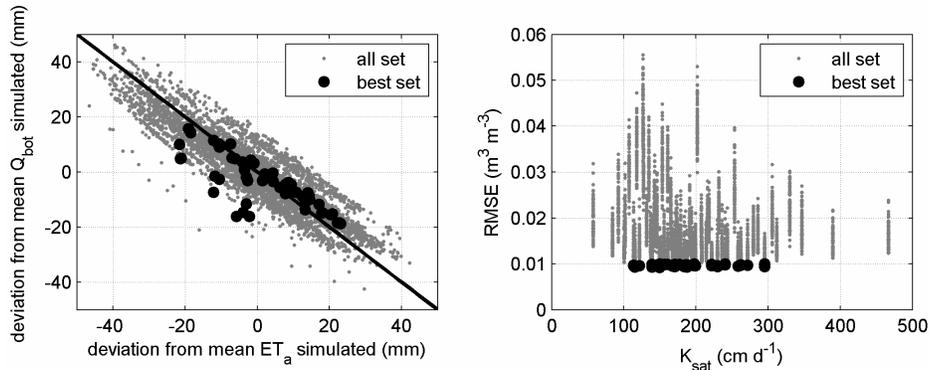

Figure 4. correlation between the deviation from the mean of evapotranspiration (ET_a) and bottom fluxes (Q_{bot}) (left); scatter plot of K_{sat} and RMSE (right).

5   CONCLUSIONS

The General Probabilistic Framework (GPF) used in this study is a useful approach to consider in a global sensitivity analysis also non-scalar sources of uncertainty (e.g., input, distributed parameters or model structure). Such information can be useful for purposes of model improvement, parameter estimation, or model simplification. This approach can be then used in a loop to optimize further activities to improve the performance of the output considered. The framework is conceptually simple and relatively easy to implement. In this study the codes are developed *ad hoc* in MATLAB environment using SimLab libraries for the specific hydrological model but they can be easily adapted to other models.

In the specific model application, input (weather data - W), time-dependent parameters (crop parameters - C) and scalar parameters (soil properties - S) are considered with the 1D-physical based hydrological model SWAP. The results show a general good performance of the model and that the sources of uncertainty are different for each process considered. In particular, the soil moisture pattern is quite well simulated and improvement could be done, as expected, by calibration of soil properties (S). However, the evapotranspiration and bottom flux at 50 cm depth simulated by the model show an uncertainty of the same order of magnitude (i.e., ± 40 mm and negative correlation). These errors compensate each other and cannot be captured by the error in the simulation of the mean soil moisture. The major sources of uncertainty related to these processes are the weather data (W) and the crop parameters (C). In this way, an improvement of the model by calibrating the soil properties will not reduce the uncertainty in these outputs. On the other hand, an improvement can be done by focusing further activities on the reduction of the uncertainty at the upper boundary condition (e.g., installing a new meteorological station close to the experimental site or improving the extrapolation of the existing weather data). Finally, the Sobol method show good ranking of the sensitivity of the input factors considered even with a relatively low number of simulations.

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