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Calibration of simulation platforms including highly interweaved processes: the MAELIA multi-agent platform

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Abstract: The MAELIA project develops an agent-based modeling and simulation platform to study the environmental, economic and social impacts of various regulations regarding water use and water management in combination with climate change. An integrated modelling approach has been used to model the investigated social-ecological system. MAELIA combines spatiotemporal models of ecologic (e.g. water flow and plant growth) and human decision-making processes (e.g. cropping plan), socio-economic dynamics (e.g. land cover changes). Due to the diversity and the interweaving of the processes considered, the calibration and evaluation of such a multi-agent platform is a scientific challenge. Indeed, many parameters can reveal to be influential on the model outputs, with a high level of interactions between parameters impacts. In order to get an overview of the model behaviour and to screen influential parameters, multiple sensitivity analyses were performed, while considering some sub-sets of processes or not. This step-by-step sensitivity analyses enabled to disentangle the different influences and interactions, and was a preliminary step to the calibration process. In our case, the calibration, which is a multi-objective (e.g. reproducing water flows and anthropic dynamics, traduced by different numerical criteria such as joint use of L2-norm with variance-covariance matrix and indices of squared errors on water crisis temporality) optimization problem, was achieved thanks to metamodels built on an appropriated design of experiments.

Keywords: multi-objective calibration; sensitivity analysis; multi-agent platform, integrated modelling

1. INTRODUCTION

Water is a critical resource for a number of social and human activities and for the sustainability of ecosystems. To study such question, integrated assessment and modelling has been playing an increasing role since last decades (Jakeman et al., 2006). The MAELIA project developed a high-resolution agent-based modeling and simulation platform to study the environmental, economic and social impacts of various regulations regarding water use and water management in combination with climate change. An integrated modelling approach has been used to model the investigated social-ecological system (Gaudou et al., 2013). MAELIA combines spatiotemporal models of ecologic (e.g. water flow and plant growth), human decision-making processes (cropping plan and crop management, water releases from dams, water use restriction) and socio-economic dynamics (e.g. demography and land cover changes).
Sensitivity analysis aims at increasing our knowledge of models through the study of the influence of parameters on outputs. It allows to distinguish influential parameters and to quantify their influences, in order to point which require a calibration step. Some authors (e.g. Sorooshian and Gupta, 1995) consider that the parameter specification steps (i.e. the choice of parameters) is one of the most important step of the calibration process. For hydrological models, calibration is a difficult problem, due to the complex structure of models and the high number of parameters to consider. Moreover, running those models is usually time consuming, which induces high constrains on the calibration process (Tang et al., 2006). In addition to the hand-calibration (also called "trial-and-error") which needs a lot of expertise and is time-consuming, a large set of algorithms and criteria exists (e.g. Bekele and Nicklow, 2007; Zhang et al., 2009). In the hydrological model domains, local search algorithms (such as gradient descent) have been replaced by genetic algorithm to avoid convergence problem (Bekele and Nicklow, 2007). Calibration of platforms simulating interactions between agents decision-making and ecological processes, of which hydrological ones, like MAELIA, remains a great scientific challenge.

This paper presents methods developed to calibrate the MAELIA multi-agent simulation platform (Figure 1). The second section gives a brief description of the MAELIA model which reveals to be time consuming (about 6 hours for 10 years simulations) and memory demanding (up to 5 Go of RAM needed), so that the number of simulations that can be run is strongly reduced. The third and the fourth section detail respectively the sensitivity analysis method (step 2 of Figure 1) and the calibration process (step 3 and 4). The need for an efficient sensitivity analysis method leads to chose the Morris method (Morris, 1991), but to be able to distinguish all parameter’s effects, we applied a multiple sensitivity analysis. For the same reason, the optimisation method is based on the Design and Analysis of Simulation Experiment (DACE) (Kleijnen, 2008). For calibration itself, we used the Multi-point Approximation Method (MAM) (e.g. Polykin and Toropov, 2012). The principle of this method is to replace the original optimization problem by a succession of simpler and time-negligible problems. This approximation is achieved thanks to metamodels on a limited part of the parameter space. Once a local optimum is found, we start from this point for the next step. In section five, we analysis and discuss the results. The concluding section identifies key results and explores future research needs.

2. THE MAELIA MODEL

The Maelia model is implemented with GAMA (Taillard et al., 2012), an open-source generic agent-based modeling and simulation platform. The model represents interactions between ecological and socio-economic processes and human activities. The water flows representation is based on the SWAT model (Soil and Water Assessment Tool; Arnold et al., 1998). A description of the agricultural processes can be found in (Murgue et al., 2014, this conference) and a more complete description of the whole Maelia model in (Therond et al., this conference). The Maelia model uses a lot of data coming from different sources. Most of them require pre-processing to solve heterogeneity, compatibility and consistency issues and to be put at the required temporal and spatial resolutions (i.e. form days to yearly resolution, and plot to region scale). Input data relate to environmental (climate, soil properties, topography, Å) and socio-economical (e.g. land use and land cover changes, domestic and industrial water use, water norms, Å) characteristics of a water basin. The model is applied in the Adour-Garonne Basin (AGB, South-West France), were water scarcity is a serious problem with an annual deficit between demands and resources of 250 million m³. In this river basin, irrigated agriculture is the main consumer of water (about 80%) during the low-water period. The model is modular in the way that the user can activate or not some module (e.g. farmers modules with prescribed land-use or farmers with decision-making of land-use). This aspect is important, as it helps reproducing different type of situations.

3. SENSITIVITY ANALYSIS

Sensitivity analysis aims to provide significant information on the model behaviour. This is the key first step of model validation process. It allows:
- to check model stability (failure frequency or model divergence);
- to verify whether parameters are influential at an expected level on the right processes (e.g., whether some parameters are influential whereas they should not, or at the opposite if they are not whereas they should be);
- to check the interactions between processes by quantifying the influence of parameters characteristic of one process on other processes.

3.1. The Morris method

The Elementary Effects screening method initially developed by Morris (1991) and extended by Campolongo et al. (2007) allows identifying the important parameters of a model, including those involved in interactions. It is based on a "One-factor-At-a-Time" (OAT) design of experiments, and is generally used when the number of model parameters is large enough to require computationally expensive simulations. For each parameter, two sensitivity estimates are obtained, both based on the calculation of incremental ratios at various points in the input space of parameters. We improved the exploration of the parameter space by the use of a Latin Hypercube Sampling (LHS, McKay et al., 1979), as already applied, for example, in Van Griensven et al. (2002). Around each point of the LHS of dimension t, an OAT is achieved, so the total number of model evaluations needed is t(n+1), where n is the number of parameter. In order to improve the quality of the design we used an LHS maximised by the ‘maximin’ criterion (Johnson et al., 1990), which maximizes the minimum distance between two points of the design.

3.2. Implementation

As our aim is at the same time to screen influential parameters for calibration and to check the model consistency, we choose an approach based on multiple sensitivity analysis. This step-by-step sensitivity analyses enabled to disentangle the different influences and interactions.

In our case, the sensitivity analyses were performed respectively over 30, 7 or 37 parameters (all belonging respectively to the hydrologic sub-model, to the farmers sub-model with forced cropping plan or farmer choice, or to the full model). The chosen size of the LHS is twelve, and the elementary increment of the OAT corresponds to a shift of 1/12 probability over his Uniform distribution. The resulting number of simulations (372, for 12 local OAT of 31 simulations; 96 for 12 local OAT of 8 simulations; 456 for 12 local OAT of 38 simulations) is in accordance with literature which suggest at least five OAT for robustness (Confalonieri et al., 2010), and the same number of levels and trajectories (e.g. Saltelli et al., 2004). As we do not have enough information to chose a distribution, we used the Uniform one as in the SWAT literature (e.g. Moreau et al., 2013) where authors also recognize that they do not have enough information to determine a distribution curve. The use of Uniform distribution is highly common when the main objective is to get knowledge about the model behaviour (Monod et al., 2006). Simulations were performed over ten years (2000-2009), but the two first years were considered as spin-up period and ignored when looking at the hydrologic sensitivity.

Table 1. List of output considered in the sensitivity analyses

<table>
<thead>
<tr>
<th>Description</th>
<th>Unit</th>
<th>Total irrigation volume</th>
<th>m³</th>
</tr>
</thead>
<tbody>
<tr>
<td>Real Evapotranspiration</td>
<td>mm</td>
<td>Water flow over 22 locations</td>
<td>m³</td>
</tr>
<tr>
<td>Soil water content</td>
<td>mm</td>
<td>(hydrographic points)</td>
<td>s⁻¹</td>
</tr>
<tr>
<td>Percolation</td>
<td>mm</td>
<td>Daily Farmers work</td>
<td>h</td>
</tr>
<tr>
<td>Water input in aquifers</td>
<td>mm</td>
<td>Number of working dates</td>
<td>-</td>
</tr>
<tr>
<td>Deep water aquifers input</td>
<td>mm</td>
<td>Working dates</td>
<td>Doy</td>
</tr>
<tr>
<td>Capillary rise water amount</td>
<td>mm</td>
<td>First Irrigation date of each farmer</td>
<td>Doy</td>
</tr>
<tr>
<td>Shallow water aquifers content</td>
<td>mm</td>
<td>Last Irrigation date of each farmer</td>
<td>Doy</td>
</tr>
<tr>
<td>Runoff</td>
<td>mm</td>
<td>Crop yields</td>
<td>t ha⁻¹</td>
</tr>
<tr>
<td>Lateral flow</td>
<td>mm</td>
<td>Surfaces per type of crops</td>
<td>ha</td>
</tr>
<tr>
<td>Deep water flow</td>
<td>mm</td>
<td>Number of parcels per type of crops</td>
<td>-</td>
</tr>
</tbody>
</table>
Simulations were partly distributed on a local computer (Quad-Core Intel Xeon: 8 threads with 32 Go RAM) and on the VO biomed European grid. Then sensitivity indices were calculated thanks to the 'sensitivity' R package (http://rss.acs.unt.edu/Rdoc/library/sensitivity/html/sensitivity-package.html).

Sensitivity of 14 types of outputs (Table 1) was calculated, by considering scaled parameters (i.e. a [0; 1] parameter range values). The sensitivity was considered either over the full year or during the low water period (1st of May-30th September). For each output, sensitivity of the average or the standard deviation, were studied, excepted for dates were the coefficient of variation was used as a proxy of uniformity measure. The hydrologic sensitivity was also check over spatial pattern (e.g. upstream and downstream area).

4. CALIBRATION

Once influential parameters are ranked (step 2), we can start the calibration step (step 3 and 4, on Figure 1) on parameters that have not been discard as non (or not enough) influential parameters at the sensitivity analysis step. However, as our model is time consuming, sequential approaches (e.g. classical Bayesian calibration) would not be possible. We need a distributed optimisation method and the use of high performance computing to achieve it. But still with the use of the European grid, the number of simulations must remain low, as the number of available computing nodes is limited by the length of the simulation (about 6 hours) and the RAM (about 6 Go) used by each simulation. This is why we used the Design and Analysis of Simulation Experiment (DACE) (Kleijnen, 2008) domain. Indeed, the use of a proper design of experiments allows to reduce the number of simulations and by the way the needed computing time. On top of that, we think that the use of metamodels is necessary to achieve our calibration. A response surface, also called metamodel, is a model or approximation of this implicit Input/Output (I/O) function that characterizes the relationships between inputs and outputs in much simpler terms than the full simulation (Kleijnen et al., 2005).

Figure 1 Description of the calibration process

Another aspect of our calibration problem is that we want to perform a multi-objective calibration. To solve such inverse problem, different types of optimisation methods exist. Two main strategies can be used. In the first one, we rank criteria and optimize them in this order or combine criteria into a single objective function. While the second strategy consists in searching for a set of parameters values on the Pareto front. Keeping a set of parameters allows building the parameter distribution and so easily performing an uncertainty analysis at the end of our process. In order to reduce the size of the calibration problem, we will first calibrate the hydrological parameters (step 3) on the first data set. Then, a second step (step 4, on Figure 1) will consist in calibrating other influential parameters (i.e.
non hydrologic parameters, e.g. the number of working hours per day per labor unit) and adjusting previously calibrated parameters (e.g. no change of value higher than 15 %) if needed.

To perform our calibration, we used the Multi-point Approximation Method (MAM) (e.g. Polynkin and Toropov, 2012), which is a multi-objective calibration method, based on the DACE domain. The principle of this method is to replace the original optimization problem by a succession of simpler and negligible in time problems. This approximation is achieved thanks to metamodels on a limited part of the parameter space. Once a local optimum is found, we start from this point for the next step. A new parameter space is defined and optimization is repeated until convergence. Metamodels are regressed on simulation from a local experimental plan. The MAM is known to be able to deal with a high number of parameters (Polynkin and Toropov, 2012).

4.1. Comparison data

To perform our calibration, we have access to two sets of (semi) observed data. The first one consists of water flow data on which irrigation effects have been removed (data provided by the SMEAG, a public institute in charge of water management), named hereafter unaffected data. They cover the low water period (1st June to 31st October) from 1979 to 2008 on three locations (hydrographic points). This data set was used in the first calibration step (step 3, in Figure 1). Indeed, by using the model with forced land use, we get a model mainly sensitive to hydrologic parameters and that reproduce the comparison data set. The second data set contains observed data at 22 locations over the whole case study area from 2000 to 2010 (data provided by the regional State service for environment). It will be used in the second calibration step (step 4, in Figure 1).

4.2. Comparison criteria

As our aim is to calibrate the model in order to well reproduce water flow (values and dynamics) and more precisely during the low water period, we used four different criteria. The first one aims at reproducing values and dynamic of flow during the low water period while the three others focus on dates and length of this period. Our first criterion (C1) of comparison is based on the L2 norm with the variance-covariance matrix estimated on unaffected data. Some weights are added to give more influence to low water period than to the rest of the year, and to reduce influence of hydrological flow peaks. The three other criteria correspond to the squared error of the length, the starting date and the ending date of the low water periods. Each criterion was calculated on the three hydrographic points of the unaffected data set. Then, in order to reduce our number of criteria (twelve, i.e. four per location), we summed the sites, leading to only four numerical criteria to optimize.

4.3. Implementation

We only present preliminary results of calibration to illustrate this approach. After selection of most influential parameters (step 2), we started the calibration process with an LHS (step 3.1 and 3.2), optimized by the maximin criterion, which contains 160 points. We regressed three different kriging metamodels (depending on covariance assumption) (step 3.3). For each metamodel, we used 600 chains of the first descent heuristic (French, 1982) (a local search metheuristic) to search for the optimal parameter sets (step 3.4). Based on these optimal points, we searched for those located on the Pareto front. To define the new trusted area (step 3.5) for next step of the calibration, we merged the intervals [5 – 95 %] of each metamodels, and then run again the whole procedure.

5. RESULTS AND DISCUSSION

Thanks to the sensitivity analysis, we got a list of influential parameters (Table 2). But it was also useful to check (and to correct) the model consistency and to disentangle the different effects (for example, to understand how some hydrologic parameter may appear as the most influential on the irrigation process). In addition of bug detection, the sensitivity analysis led us to question the precision
of some forcing data. Indeed, getting some process (runoff and snow processes) more influential than expected has incited us to refine the number of slope and altitude classes in input (data not shown).

The list of influential parameters is consistent with the SWAT literature. However some difference may be noticed. For example, the initial water content of shallow aquifers is influential in our model whereas most papers ignore it. This implies that a spin-up run step should be added to the model. Moreover, one can see a spatial pattern on influential parameter, which may imply that it will be necessary to calibrate more than one set of parameters. For example, we could calibrate one set for the lowland and one for the upland part, or one set per sub-watershed.

Our sensitivity analysis is robust relatively to the size of the design of experiment. Indeed, the list of influential parameters and their ranking has already converged whether we use eight instead of twelve chains (data not shown). Moreover previous studies have shown that the Morris method is relevant for screening parameters of environmental models (e.g. Drouet et al., 2011) and that the ranking of parameters is consistent with more accurate (and more expensive) methods.

Each step of the calibration procedure allows for a reduction of the Pareto-optimal distribution (Figure 2) and a more accurate parameter set. In order to improve the efficiency of the calibration, we could make new iterations. This will allow us to get a more optimal parameter set, and above all a more precise parameter set distribution and therefore a more accurate uncertainty evaluation (step 6, in Figure 1). It is interesting to note that if some default parameter value (i.e. the one from literature) are well situated in the Pareto-optimal set, some other shows high difference, which might be due to the specificity of the AGB basin or to the SWAT integration into MAELIA.

Table 2. List of parameter considered as influential on water flow in the MAELIA platform. For each parameter, we consider whether the mean or standard deviation of the elementary effect of the parameter is higher than 10% of the maximum value.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Frequency of occurrence of the parameter above the threshold</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface runoff lag time</td>
<td>100%</td>
</tr>
<tr>
<td>SCS curve number for forest</td>
<td>100%</td>
</tr>
<tr>
<td>Threshold water level in shallow aquifer for revap process</td>
<td>83%</td>
</tr>
<tr>
<td>Grassland leaf Area</td>
<td>83%</td>
</tr>
<tr>
<td>Deep groundwater revap coefficient</td>
<td>75%</td>
</tr>
<tr>
<td>SCS curve number for grassland</td>
<td>75%</td>
</tr>
<tr>
<td>Shallow aquifer initialisation</td>
<td>75%</td>
</tr>
<tr>
<td>Groundwater revap coefficient</td>
<td>67%</td>
</tr>
<tr>
<td>Manning coefficient for tributary channel</td>
<td>58%</td>
</tr>
<tr>
<td>Precipitations change with altitude</td>
<td>58%</td>
</tr>
<tr>
<td>Groundwater delay</td>
<td>50%</td>
</tr>
<tr>
<td>Threshold water level in shallow aquifer for baseflow process</td>
<td>50%</td>
</tr>
<tr>
<td>Temperature change with altitude</td>
<td>50%</td>
</tr>
<tr>
<td>Minimum snowmelt rate</td>
<td>50%</td>
</tr>
<tr>
<td>Snow fall min temperature</td>
<td>42%</td>
</tr>
<tr>
<td>SCS curve number for water</td>
<td>25%</td>
</tr>
<tr>
<td>Maximum snowmelt rate</td>
<td>17%</td>
</tr>
</tbody>
</table>
Figure 2 Boxplots of Pareto-optimal distribution obtained after the second step of the multi-point approximation method, for 6 parameters that have already converged. The values are scaled by the parameter range from the literature. The black bold line correspond to the median, the box represent the 0.25 to 0.75 quantile range. The whiskers extend to the 1.5 of the interquartile range from the box, and the red line corresponds to the default parameter value.

6. CONCLUSION

This paper presents a still going calibration process, that illustrates well the issues of calibrating a complex multi-agent model including an important number of interweaved heterogeneous processes. Indeed, the most common calibration methods would be inefficient due especially to the interactions between formalisms, which have different forms (from classical differential equations to agent behaviour algorithms) and spatiotemporal resolutions. In order to get an overview of the model behaviour and to screen influential parameters, multiple sensitivity analyses were performed, while considering some sub-sets of processes or not. This step-by-step sensitivity analyses enabled to disentangle the different influences and interactions, and was a preliminary step to the calibration process. In our case, the calibration, which is a multi-objective (e.g. reproducing water flows and anthropic dynamics, traduced by different numerical criteria such as joint use of L2-norm with variance-covariance matrix and indices of squared errors on water crisis temporality) optimization problem, was achieved thanks to the Multi-Point Approximation method. This latter consists in a succession of optimisation on metamodels thanks to a metaheuristic. The approximation models were regressed on an appropriate succession of models. This calibration approach gives us an ensemble of parameters set (all of them placed on the Pareto front). Based on that, the evaluation of the model will be completed by an uncertainty analysis.

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