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A Computationally Efficient Metamodeling-Based Approach for the Automatic Calibration of Coupled Hydrodynamic and Water Quality Models

Kandris K.[1,*], Romas E.[1], Tzimas A.[1], Pechlivanidis I.[2], Giardino C.[3], Bresciani M.[3], Schenk K.[4], Bernert H.[4]

[1] Emvis Consultant Engineers SA, Paparrigopoulou 21, Ag. Paraskevi 153 43, Greece

[2] Swedish Meteorological and Hydrological Institute, Norrköping, Sweden

[3] CNR-IREA,Via Bassini 15, 20133 Milano, Italy

[4] EOMAP GmbH & Co.KG, Schlosshof 4, 82229-Seefeld, Germany

*corresponding author :e-mail: kkandris@emvis.gr

Abstract

Computational budget is a severe limitation on the automatic calibration of expensive hydrodynamic and water quality models. To tackle this limitation, the present work formulated a metamodeling-based approach for parameter estimation of such models and assessed the computational gains of this approach compared to a benchmark alternative (a derivative-free optimization method). A response surface proxy of the original model was designed to emulate the behavior of the underlying system, employing Latin hypercube sampling as a strategy for the design of computer experiments and kriging as the technique for the analysis of computer experiments. The response surface proxy of the original model was employed in the automatic fine-tuning of model parameters and, finally, the computational gain over the benchmark alternative was estimated. The metamodeling-based approach was tested in the calibration of the hydrodynamic and water quality models of two water reservoirs. The benchmark alternative analysis indicated that the metamodeling-based approach required 20% to 38% less function evaluations to reach a solution with the same quality compared to the benchmark alternative.

Keywords: Metamodeling; calibration; hydrodynamics; water quality modeling

1. Introduction

Model calibration is essential for the credible prediction of the hydrodynamic and ecological status of surface water reservoirs. Yet, automatic calibration algorithms are demanding, as the simulation of three-dimensional reservoir models is computationally expensive. Therefore, model calibration is typically performed through trial-and-error approaches which entail a high degree of expert opinion and, thus, subjectiveness.

In this work, a metamodeling-based approach for the calibration of hydrodynamic and water quality models of surface water reservoirs was devised. This approach created a response surface proxy of the original model to reduce the number of simulations required in the search of optimal parameter sets. We examined the extent to which the method represented an improvement over a derivative-free optimizer that was used as a benchmark. Both calibration methods were tested in two case studies, in Mulargia (Italy) and Aposelemis (Greece) reservoirs

2. Formulation Of The Model Calibration Problem

Model calibration was treated as a box-constrained minimization problem, described as follows:

$$min\ f(x) \tag{1}$$

subject to

$$x_{min} \le x_k \le x_{max}, k \in \{1,..,d\} \tag{2}$$

where, x is the d-dimensional vector of model parameters bound by x_{max} and x_{min}, and $f(x)$ is the Kling-Gupta Efficiency (Gupta et al., 2009):

$$KGE = 1 - \sqrt{(cc-1)^2 + (a-1)^2 + (b-1)^2} \tag{3}$$

where cc is the linear cross-correlation coefficient between observed and modeled values, a is equal to the standard deviation of modeled values over the standard deviation of the observed, and b is the mean of modeled over the mean of observed. For a perfect model, KGE is 1. KGE allows for a multi-objective perspective by focusing on separately minimizing the correlation (timing), variability, and bias of errors. Observed values contained EO-derived and in-situ observed water temperature, chlorophyll-a concentrations and turbidities.

Hydrodynamic and water quality forward simulations were performed in the Delft3D modeling. Conceptually, hydrodynamics was dictated by three external forcings: (1) river discharges (as modeled by the E-HYPE hydrological model) and water abstraction, (2) wind forcings, and (3) heat flux exchanges and heat forcings. The conceptual ecological models of the reservoirs described phytoplankton growth and mortality and the cycles of dissolved oxygen, carbon, nitrogen, and phosphorus. Thus, the active processes of the models comprised: sedimentation and resuspension of particulate matter, growth limitations of phytoplankton, light extinction, mineralization processes, nitrification, denitrification, adsorption kinetics, reaeration and sediment oxygen demand.

The dimension of the model parameter vector, *d*, was indicated by a preliminary sensitivity analysis of the models; insensitive model parameters were omitted form the parameter vector *x*. As a result, *d* was equal to 4 for hydrodynamic models and equal to 12 for the water quality models. Parameter boundaries, i.e. x_{max} and x_{min}, were set by the range of reported values from Bowie et al. (1985) and Mao et al. (2015).

3. Alternative Algorithms For Model Calibration

3.1 Alternative 1: Derivative-free optimizer

The benchmark alternative of the metamodeling-based approach is a derivative-free, generating set search (GSS) method, which evaluates the objective function at a mesh of candidate points, which form a stencil around each iterate. If a candidate point has a lower function value, it is considered as the new iterate, the center of the stencil is shifted to this new point and the size of the stencil becomes four-fold greater. Otherwise, the algorithm does not change the current point and the size of the stencil becomes four-fold smaller in search of a new iterate. The algorithm stops when: (a) the mesh size is less than the mesh tolerance, (b) the number of iterations reaches the maximum-allowed iterations, (c) after a successful poll, the distance between the point found in the previous two iterations and the mesh size are both less than the user-defined tolerance, (d) after a successful poll, the change in the objective function in the previous two iterations is less than the user-supplied function tolerance and the mesh size is less than a user-defined parameter tolerance.

3.2 Alternative 2: A metamodeling-enabled optimizer

The metamodeling-based optimization algorithm is realized in seven steps: (1) generate an initial design of experiments to portray the behavior of the underlying system using the Latin-hypercube sampling method, (2) evaluate the original model at the 2(*d*+1) design sites generated, (3) fit a kriging-based metamodel to the data produced by the two previous steps, (4) use the metamodel to predict the objective function values at unsampled points and decide at which point should the original model be evaluated, (5) evaluate the original model indicated by the previous step, (6) update the metamodel, (7) check if (a) the maximum number of allowed function evaluations has been reached (it was set equal to ten times the number of the explanatory variables of the problem) or (b) the maximum number of failed improvement efforts (heuristically, this number was set equal to ten efforts) – if not, re-iterate steps 4 to 6.

4. Computational Saving From The Metamodeling-Based Approach

The computational saving, C_s, was estimated as follows:

$$C_s = 100\% \frac{t-ts}{t} \qquad (4)$$

where *t* are the function evaluations required to reach a solution through the GSS method, and t_s are the function evaluations that the metamodeling-enabled algorithm requires to reach a solution with the same quality.

The two calibration algorithms converged to nearly coinciding KGE values but after different function evaluations. For the hydrodynamic models (Figures 1a and 1c), C_S from the metamodeling-based approach was 38% and 20% for the Mulargia and Aposelemis case studies, respectively. For the water quality models (Figures 1b and 1d), C_S was 38% and 32% for the two case studies.

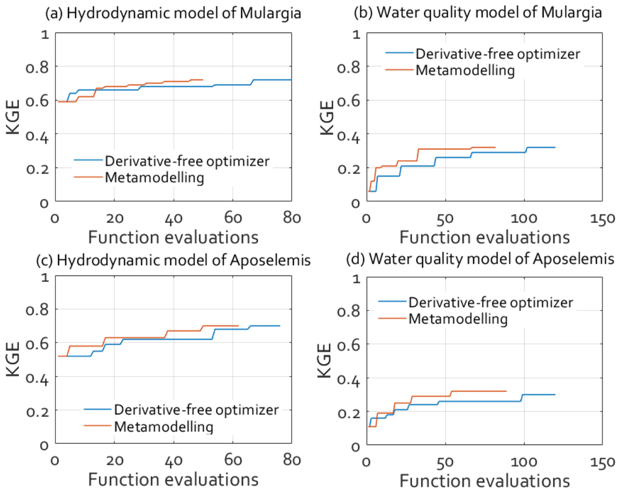

Figure 1. Comparative evaluation of KGE values versus function evaluations for the hydrodynamic and water quality models of Mulargia and Aposelemis.

5. Conclusions

Despite the sizeable growth of computational power over the years, computational limitations pose a sever obstacle in the calibration of process-based simulation models. Metamodeling is an advance in the automatic calibration of complex mathematical models. Herein, a metamodeling-based approach was formulated and utilized in the automatic calibration of the hydrodynamic and water quality models of two reservoirs. The metamodeling-based approach was benchmarked against a derivative-free optimizer. Benchmarking indicated that the metamodeling-based approach is a promising technique for the efficient parameter fine-tuning of expensive process-based models.

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