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Physics-based and data-driven surrogate models for pumping optimization of coastal aquifers

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Abstract: Data-driven surrogate models have been widely used in pumping optimization of coastal aquifers. However, their efficacy has not been previously compared to physics-based surrogate modelling techniques. In this work, we utilize a set of sharp interface models of different complexity to investigate the performance of a variable-fidelity optimization framework against a data-driven approach. In particular, the numerical solution of sharp interface flow represents the available high-fidelity seawater intrusion model. Furthermore, several analytical models represent lower-fidelity approximations for simulating seawater intrusion. To statistically assess the performance of the surrogate-based methods against the high-fidelity optimal solution, we utilized a total of 30 independent optimization runs for each approach. The results indicate that the analytical models which poorly approximate the numerical sharp interface model had also limited skills to approximate the high-fidelity optimal solution. On the other hand, the surrogate-based optimization frameworks that were developed by using either the most accurate analytical model or the data-driven surrogate model were in good agreement with the high-fidelity optimization results. It was also observed that the variable-fidelity optimization algorithm required fewer evaluations with the high-fidelity model in order to converge to the optimal solution. Moreover, the set of these seawater intrusion models could be conveniently used for further development and testing of variable-fidelity optimization frameworks in coastal aquifer management.

Key words: seawater intrusion; pumping optimization; surrogate modelling; variable-fidelity optimization

1. INTRODUCTION

A common optimization problem in water resources is the calculation of maximum groundwater abstraction from coastal aquifers, subject to constraints that control seawater intrusion (SWI) (Singh, 2014). The optimal search space is typically explored using evolutionary algorithms due to their ability to handle the non-convex nature of these problems (Ketabchi and Ataie-Ashtiani, 2015). However, evolutionary algorithms require a large number of function evaluations to converge and their combination with numerical models of SWI significantly increases the overall computational cost (Mantoglou and Papantoniou, 2008). In order to obtain optimal solutions within reasonable computational times, several studies in coastal aquifer management have applied surrogate modelling techniques (e.g. Kourakos and Mantoglou, 2009; Papadopoulou et al., 2010; Sreekanth and Datta, 2011; Christelis and Mantoglou, 2016a; Roy and Datta, 2017).

The majority of these studies have employed various data-driven surrogate models which are based on function approximation techniques and are built upon the input-output relations of the original computer models (Razavi et al., 2012b). Another competent approach for surrogate-based optimization (SBO) is the development of physics-based surrogate models and their use in the so-called variable-fidelity optimization framework (Robinson et al., 2006). Variable-fidelity SBO utilizes models which simulate the physical process at different fidelity levels and consequently at different computational complexity and cost (Forrester et al., 2008). The scope is to use the efficient low-fidelity (LF) models for most of the objective and/or constraint function evaluations and use the complex high-fidelity (HF) model only to correct or enhance the LF models towards the HF response. Physics-based surrogate models have been widely applied in other engineering fields (e.g. Bandler et al., 1994; Gano et al., 2004; Koziel et al., 2008; Koziel and Leifsson, 2016). However, their use is limited in water resources optimization (Asher et al., 2015). Sreekanth and Datta (2015), in their recent review paper, do not report any similar applications specifically developed for coastal aquifer management.

In the present work, we investigate the favourable and disadvantageous aspects of using physics-based surrogate modelling techniques for a single-objective pumping optimization problem of coastal aquifers. Several LF models are employed to approximate the HF model response for the calculation of optimal pumping rates. The variable-fidelity approach is embedded within the operations of an evolutionary algorithm. The results obtained from the variable-fidelity SBO are compared against the direct optimization with the HF model and a data-driven SBO method.

2. METHODS

2.1 The fidelity concept in SWI modelling

In general, two broad levels of fidelity can be defined in SWI modelling. First, the variable-density and solute transport numerical models which provide a realistic, HF representation of coastal aquifer processes at increased computational cost (Dokou and Karatzas, 2012; Werner et al., 2013). Second, the sharp interface assumption which represents a LF approximation of coastal aquifer flow since it neglects the mixing of freshwater with seawater (Cheng et al., 1999). However, a much wider taxonomy of fidelity levels can be realized either within the same model formulation (e.g. grid resolution, convergence criteria or dimensionality), or among the different mathematical formulations of the available SWI models. For example, several sharp interface models of varying accuracy have been developed in the literature to simulate SWI (e.g. Mantoglou, 2003; Pool and Carrera, 2011; Koussis et al. 2012; Koussis et al. 2015).

Due to the exploratory nature of our study, we employ the SWI models presented in Mantoglou (2003), which are based on the sharp interface theory and the single-potential formulation of Strack (1976). They provide a convenient mathematical model that has been widely used in the development of simulation-optimization routines (e.g. Mantoglou et al., 2004; Mantoglou and Papantoniou, 2008; Christelis et al., 2012; Kourakos and Mantoglou, 2015; Karatzas and Dokou, 2015). Our analysis follows the comparisons performed by Mantoglou (2003) for sharp interface models of different fidelity, in the case of finite-size coastal aquifers.

2.2 SWI models

Consider the finite-sized, coastal aquifer of rectangular shape presented in Figure 1.

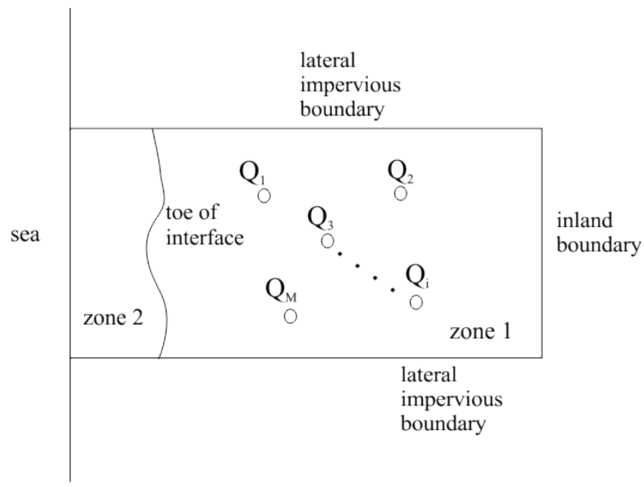

Figure 1. Plan view of a coastal aquifer of finite size pumped by M wells.

Besides the coastal fixed head boundary three other boundaries exist which affect flow. The two lateral no-flow boundaries and an inland constant flux boundary. Seawater is considered to be static and aquifer flow is horizontal and steady-state. In zone 1 unconfined flow is assumed and the aquifer is replenished by distributed groundwater recharge N while in zone 2 a freshwater lens floats above the static saltwater layer. The aquifer is pumped by M wells and a "toe" of the sharp interface between freshwater and saltwater is formed. As the groundwater abstraction from the pumping wells increases, the "toe" advances further inland. Based on the single-potential formulation of Strack (1976), the following differential equation governs the entire flow domain:

$$\frac{\partial}{\partial x}\left(K\frac{\partial \phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(K\frac{\partial \phi}{\partial y}\right)+N-Q(x,y)=0 \tag{1}$$

where ϕ is the flow potential (Strack, 1976) and K is the aquifer's hydraulic conductivity. The distributed pumping rate $Q(x,y)$ is expressed as: $Q(x,y)=\sum_{j=1}^{M} Q_j\ \delta\left(x-xw_j, y-yw_j\right)$ where (xw_j, yw_j) are the coordinates of a pumping well j with rate Q_j and $\delta\left(x-xw_j, y-yw_j\right)$ is the Dirac delta function.

Mantoglou (2003) developed fast analytical SWI models for solving equation (1), by using the method of images, in the case of finite-sized coastal aquifers with homogeneous hydraulic parameters. A general expression of the derived analytical model for unconfined coastal aquifer flow is presented below:

$$\begin{aligned}
\phi(x,y)=\ &\frac{q}{K}x+\frac{N}{K}x\left(L-\frac{x}{2}\right)+\\
&+\sum_{j=1}^{M}\frac{Q_j}{4\pi K}\ln\left[\frac{\left(x-x_j\right)^2+\left(y-y_j\right)^2}{\left(x+x_j\right)^2+\left(y-y_j\right)^2}\right]+\sum_{j=1}^{M}\frac{Q_j}{4\pi K}\ln\left[\frac{\left(x-x_j\right)^2+\left(y+y_j\right)^2}{\left(x+x_j\right)^2+\left(y+y_j\right)^2}\right]+\\
&+\sum_{j=1}^{M}\frac{Q_j}{4\pi K}\ln\left[\frac{\left(x-x_j\right)^2+\left[y-\left(2b-y_j\right)\right]^2}{\left(x+x_j\right)^2+\left[y-\left(2b-y_j\right)\right]^2}\right]+\sum_{j=1}^{M}\frac{Q_j}{4\pi K}\ln\left[\frac{\left(x-x_j\right)^2+\left[y+\left(2b-y_j\right)\right]^2}{\left(x+x_j\right)^2+\left[y+\left(2b-y_j\right)\right]^2}\right]+\\
&+\sum_{j=1}^{M}\frac{Q_j}{4\pi K}\ln\left[\frac{\left(x-x_j\right)^2+\left[y-\left(2b+y_j\right)\right]^2}{\left(x+x_j\right)^2+\left[y-\left(2b+y_j\right)\right]^2}\right]+\sum_{j=1}^{M}\frac{Q_j}{4\pi K}\ln\left[\frac{\left(x-x_j\right)^2+\left[y+\left(2b+y_j\right)\right]^2}{\left(x+x_j\right)^2+\left[y+\left(2b+y_j\right)\right]^2}\right]+\\
&+\sum_{j=1}^{M}\frac{Q_j}{4\pi K}\ln\left[\frac{\left(x-x_j\right)^2+\left[y-\left(4b-y_j\right)\right]^2}{\left(x+x_j\right)^2+\left[y-\left(4b-y_j\right)\right]^2}\right]+\sum_{j=1}^{M}\frac{Q_j}{4\pi K}\ln\left[\frac{\left(x-x_j\right)^2+\left[y+\left(4b-y_j\right)\right]^2}{\left(x+x_j\right)^2+\left[y+\left(4b-y_j\right)\right]^2}\right]+\\
&\sum_{j=1}^{M}\frac{Q_j}{4\pi K}\ln\left[\frac{\left(x-x_j\right)^2+\left[y-\left(4b+y_j\right)\right]^2}{\left(x+x_j\right)^2+\left[y-\left(4b+y_j\right)\right]^2}\right]+\sum_{j=1}^{M}\frac{Q_j}{4\pi K}\ln\left[\frac{\left(x-x_j\right)^2+\left[y+\left(4b+y_j\right)\right]^2}{\left(x+x_j\right)^2+\left[y+\left(4b+y_j\right)\right]^2}\right]+\\
&+\cdots
\end{aligned} \tag{2}$$

where the term $\frac{q}{K}x$ represents ambient flow and the term $\frac{N}{K}x\left(L-\frac{x}{2}\right)$ accounts for surface accretion for an aquifer of length L (Mantoglou, 2003). As the number of additive terms in equation (2) is increased, the analytical model better approximates the numerical solution of equation (1) (for details see Mantoglou, 2003). Based on the above and by following Mantoglou (2003), we define 5 models of different fidelity for simulating SWI:

- LF1: the analytical model considers only the coastal boundary assuming semi-infinite dimensions.
- LF2: the analytical model considers the coastal boundary and the two lateral no-flow boundaries.
- LF3: the analytical model considers the coastal boundary, the two lateral no-flow boundaries and the inland boundary.
- LF4: the analytical model is the same with LF3 in terms of boundary conditions, but, uses more reflections for the real pumping wells to increase the accuracy of the flow solution.
- HF: the numerical solution of equation (1), using a groundwater flow code, represents the available HF simulation.

Obviously, the computational times produced by the above models are not significant since the sharp interface approximation is considered. However, they represent a hierarchy of model fidelity and complexity for simulating SWI and are utilized as a paradigm for investigating physics-based surrogate modelling techniques in coastal aquifer management.

2.3 Pumping optimization frameworks

The following optimization problem is solved in order to control SWI and calculate maximum groundwater abstraction:

$$\begin{aligned} &\min -\sum_{i=1}^{M} Q_i \\ &s.t.\ x_i^{toe}\left(Q_1,Q_2,\ldots Q_M\right) < xw_i, \forall i = 1,2,\ldots M \\ &\quad Q_{\min} \le Q_i \le Q_{\max}, i = 1,2,\ldots M \end{aligned} \tag{3}$$

The first line of the constraint functions formulate a nonlinear optimization problem (Mantoglou et al., 2004) while $Q_{\min}$ and $Q_{\max}$ define the lower and upper limits of pumping rates, respectively. The variable x^{toe} is the horizontal distance of the toe from the coast as a function of the pumping rates Q_i and xw is the horizontal distance of the wells from the coast. In order to honour the constraints, the "toe" of the interface is not allowed to reach the pumping wells. The above constrained optimization problem is transformed to an unconstrained formulation where the nonlinear constraints are embedded in the objective function using penalty terms as follows:

$$\min f\left(\mathbf{Q}\right) = \begin{cases} -\sum_{i=1}^{M} Q_i, \ if\ \forall i = 1,2\ldots M; x_i^{toe}\left(Q_1,Q_2,..Q_M\right) < xw_i \\ M_v \sum_{i=1}^{Mv}\left[\max\left(\left(x_i^{toe} - xw_i\right),0\right)\right]^2, if\ \exists i = 1,2\ldots M;\ x_i^{toe}\left(Q_1,Q_2,..Q_M\right) \ge xw_i \end{cases} \tag{4}$$

Here, the evolutionary annealing-simplex (EAS) algorithm (Efstratiadis and Koutsoyiannis, 2002; Rozos et al., 2004; Tsoukalas et al., 2016) was employed to solve the optimization problem defined in equation (4). One of the advantages of EAS algorithm is that rather few parameters must be previously set. These are the initial population length m, two annealing schedule controlling parameters λ and ψ, a mutation probability p_m and a convergence criterion ε. The global exploration of the optimal search space is ensured for initial populations in the order of $m = 8*D$, where D denotes the dimensionality of the decision variable vector (Kourakos and Mantoglou 2009). The other EAS parameters were set to $\lambda = 0.95$, $\psi = 2$, $p_m = 0.1$ and $\varepsilon = 10^{-4}$. All calculations, pre- and post-processing of the data were implemented in MATLAB environment.

Three different optimization frameworks are proposed in order to calculate the optimal solution for a problem with $M = 10$ pumping wells. The first, denoted as EAS-HF, is to combine the HF model with the EAS algorithm and solve a direct optimization problem without the use of surrogate models. This corresponds to the HF approach where the most complex and computationally expensive model is used. The second, demoted as EAS-VF, is the variable-fidelity approach that we develop in this paper.

Let the vectors $\mathbf{G}_{HF}(\mathbf{Q})$ and $\mathbf{G}_{LF}(\mathbf{Q})$ represent the x^{toe} calculations for the M pumping wells, of the HF and the LF model respectively. Where $\mathbf{Q}$, is a decision variable vector of pumping rates proposed by EAS-VF algorithm. The LF models approximate the location of the interface "toe" with errors comparative to the HF model (see Mantoglou, 2003). However, the LF models offer a faster, less complex approach in order to calculate the optimal pumping rates. Since the LF and the HF models share the shame physics, we apply a variable-fidelity SBO framework similar to the concept of implicit space mapping (ISM) developed by Bandler et al. (2004). In general, the ISM method proposes an optimization scheme where fixed parameters of the HF model are iteratively adjusted in the LF model in order to minimize the differences between the HF and LF models. A similar optimization scheme was developed by Christelis and Mantoglou (2016b) which corrects the density ratio of a LF sharp interface model and adjusts its response towards that of a variable-density and salt transport model. Although not explicitly formulated in their work, that approach has also some similarities with the ISM technique.

In this case, we select the hydraulic conductivity K fixed for the HF model, but, it is utilized as a black-box parameter subject to calibration in the LF models. Thus, an unconstrained optimization sub-problem is also defined where an optimal value K is calculated based on the following minimization:

$$\min_{K} g(K) = \sqrt{\frac{\left(\mathbf{G}_{HF}(\mathbf{Q}) - \mathbf{G}_{LF}(\mathbf{Q}, K)\right)^2}{M}} \tag{5}$$

Note that problem (5) is based on function evaluations with the LF model. Thus, if the latter is not significantly faster than the HF model, then it will add considerable cost to the primary optimization problem (equation 4). In order to further enhance the alignment between the HF and the LF models a relation is also established between the vector $\mathbf{Q}$ and the optimal value K, by using a data-driven model. In this study, we employ a cubic radial basis function (RBF) model which predicts an optimal value $\widehat{K}$, given a proposed vector $\mathbf{Q}$ from the EAS-VF algorithm. Thus, the x^{toe} calculation from the enhanced LF model is given by:

$$\widehat{\mathbf{G}}_{HF} = \mathbf{G}_{LF}\left(\mathbf{Q}, \widehat{K}\right) \tag{6}$$

In summary, the EAS-VF algorithm steps are the following:

1. Define the initial population of the EAS algorithm and other required parameters.
2. Create a sampling design of points $\mathbf{Q}$ and of size n and evaluate the HF model.
3. Find the best objective function value from step 2 and add the related vector $\mathbf{Q}$ to the initial population.
4. For each evaluated point from step 2, solve problem (5) and create an archive for the optimal K values and the related points $\mathbf{Q}$.
5. Train the RBF model on the archived multidimensional inputs $\mathbf{Q}$ and optimal values K.
6. Run EAS algorithm using the physics-based surrogate model (equation 6).
7. If a better current optimum is found with the physics-based surrogate model, evaluate the related $\mathbf{Q}$ with the HF model. Solve problem (5) and store $\mathbf{Q}$ and optimal K to the archive.
8. Are the EAS convergence criteria met? If yes provide optimal solution, else go to step 5.

For step 2 of EAS-VF we use a Latin Hypercube Sampling technique (Mckay et al., 2000) in the order of $2*D+1$. The third optimization approach, denoted as EAS-RBF, is a data-driven SBO approach which utilizes cubic RBF models for replacing the HF model and it is also embedded in the EAS algorithm (Christelis and Mantoglou, 2016a).

3. RESULTS AND CONCLUSIONS

The above optimization frameworks were tested for 30 independent trials due to the stochastic nature of EAS algorithm. The distribution of optimal solutions for all methods is demonstrated in Figure 2.

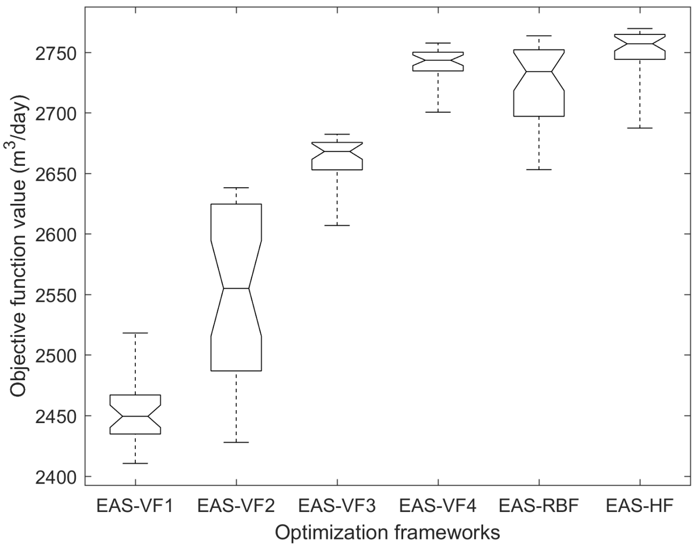

Figure 2. Boxplots of the distribution of best optimal values among the different optimization frameworks .

Results indicate that among the variable-fidelity optimization frameworks EAS-VF1, EAS-VF2, EAS-VF3 and EAS-VF4, only the one developed with the most accurate model LF4 provides a good agreement with the EAS-HF solutions. Thus, the differences between the HF and the other LF models could not be adequately reduced using the EAS-VF framework. The EAS-RBF results are also in good agreement with the HF-based optimization. EAS-RBF found a better maximum solution compared to the EAS-VF4, however, it has a less symmetrical distribution of optimal values and a lower median than EAS-VF4. Furthermore, none of the box plot notches of the SBO methods appear to overlap with those of the EAS-HF approach. This is an indication that the optimal SBO results may have a different “true” median from the EAS-HF algorithm. Note that despite the simplicity of the flow equation (1), the response of the constraint functions is markedly non-smooth and non-linear close to the region of optimal solutions (see Mantoglou, 2003). That is, the objective function receives increased penalty values even with small perturbations around the optimal solutions. As a result, the particular HF-based optimization problem is not an easy task for SBO strategies.

In terms of computational gains, it is worth mentioning the median of the number of HF evaluations required for EAS algorithm to converge. The EAS-HF has a median of 7322 HF runs, the EAS-VF4 has a median of 153 HF runs and the EAS-RBF has a median of 271 HF runs. Interestingly, the variable-fidelity SBO framework EAS-VF4 used almost half of the HF runs to converge among the 30 trials comparative to the data-driven approach EAS-RBF.

The results indicate that the developed variable-fidelity SBO method required a LF model which is in good agreement with the HF model in order to approximate the HF-based optimization results. Further research is underway on different correction and enhancement methods for the development of variable-fidelity SBO strategies in coastal aquifer management.

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