Interactive Multi-Objective Inverse Groundwater Modeling for the WIPP Site

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Abstract

This paper presents ongoing research on building an interactive and multi-objective framework to solve the groundwater inverse problem. Our research has shown that the inherent instability and non-uniqueness of this problem can be improved by incorporating expert knowledge about the hydro-geology of the site. The interactive multi-objective genetic algorithm (IMOGA) considers user preference (for different transmissivity fields) as an additional objective along with quantitative calibration measures, converging to a set of Pareto optimal solutions representing the best trade-off among all (qualitative as well as quantitative) objectives. An important part of groundwater inversion is assessing parameter uncertainty and its effect upon model predictions. To assess the uncertainty in prediction we a multi-level sampling approach is used that incorporates uncertainty in both large-scale trends and the small-scale stochastic variability. The large-scale uncertainty is modeled using a Bayesian approach where both calibration error and a prior transmissivity field (as specified by the expert through the interactive rankings of the IMOGA) are considered. A geostatistical approach is adopted for the small-scale uncertainty, which is considered to be unconditional and auto-correlated with a specified covariance structure. The prediction model is run using all simulated fields to get the distribution of predictions. This methodology is being applied to a field-scale case study based on the Waste Isolation Pilot Plant (WIPP) situated in Carlsbad, New Mexico. This work is still in progress and results will be presented at the EWRI conference.

Introduction

Groundwater inverse modeling is an essential step in developing meaningful models to better remediate and manage groundwater. In essence, inverse modeling consists of estimating a set of reasonable parameter values for mathematical models being used to represent physical systems (in this case groundwater flow and transport processes). The groundwater inverse problem of estimating hydraulic transmissivity values given hydraulic head measurements is typically 'ill-posed'(*Carrera and Neuman*, 1986; *Sun*,1995; and *McLaughlin and Townley*, 1997), i.e. there are multiple (in fact infinite) solutions possible and the solution itself is highly unstable with respect to small variations in the head observation data. Due to this non-uniqueness and instability of solutions it becomes a challenge to find reasonable parameter values for groundwater models given the scarce amount of field-data typically available for most real-world sites.

It is in this context that 'prior information' becomes of utmost importance to inverse modeling. Any kind of prior information can and should be used to assess the plausibility of the estimated parameters. Studies including *Hill* (1998)*, McLaughlin and Townley* (1997), *Doherty* (2003), and *Alcolea et al.* (2006) among many others have shown the importance of prior information for inverse modeling. Most automated calibration allow for quantitative prior information (in the form of field measurements of transmissivity or related aquifer parameters) to be included in the calibration process. However, at most real world sites there is a wealth of information that the site experts and field hydrologists have about the hydrogeology of the site that can be used to improve the plausibility of the parameter estimate. Expressing such subjective information is difficult in traditional calibration methodologies since these approaches require the expert to express essentially qualitative knowledge in purely quantitative terms. One of the problems is that the field-expert's knowledge about spatial characteristics can not be represented adequately in metrics or objectives that are used in traditional calibration. Such metrics suffer from what is known as the 'blindness of norms' – the loss of information when multi-dimensional information is represented by a low-dimensional statistic or norm (*Brill*, 1992). In additional, expert knowledge is dynamic and adaptive and can evolve as the expert is allowed to interact and learn from the model. Thus, there is a need for an adaptive environment that allows site experts to express qualitative (multi-dimensional) information during inverse modeling, while simultaneously evaluating and updating their own understanding.

Singh et al. (2005) have shown that the 'Interactive Multi-Objective Genetic Algorithm' (IMOGA) can adaptively incorporate qualitative expert knowledge in the groundwater inversion process to improve the estimate of transmissivity fields compared to non-interactive approaches. The IMOGA is an extension of interactive genetic algorithms (*Takagi*, 2001) – population-based evolutionary optimization algorithms that use interactive feedback from users to drive the search process. The IMOGA treats quantitative and qualitative criteria as multiple objectives within a Pareto optimization approach and generates multiple alternatives for the parameter field, each representing an optimal trade-off between different quantitative and qualitative criteria. To deal with the problem of user fatigue, *Singh et al*. (2006)

proposed a machine-learning and clustering-based methodology to reduce the number of solutions required to be evaluated by the user.

The IMOGA finds solutions corresponding to large-scale trends for transmissivity that best match field measurements as well as the experts' understanding of the site. One important use of these transmissivity fields is for predictions to support environmental management decisions. The task of predictive uncertainty analysis is to characterize the uncertainty in predictions and relate it to uncertainty in parameters. This paper presents work to extend the IMOGA by including predictive uncertainty analysis for the modeled site. It also presents a field-scale case-study based on the Waste Isolation Pilot Plant (WIPP) site situated near Carlsbad in New Mexico. The IMOGA is being applied to this case-study and results will be presented for this at the conference.

This paper is organized into four parts. The first part gives a broad overview of the IMOGA framework. The second part discusses the predictive uncertainty analysis to be carried out with the IMOGA solutions. Next, the WIPP case-study is presented and work on implementing the IMOGA on this case-study is discussed. The final section gives a summary and discusses future directions for research.

IMOGA Framework

The IMOGA framework is shown in Figure 1. The first step in the interactive framework is to solve the problem without any user interaction. For this we use the elitist non-dominated sorting genetic algorithm (NSGA-II) (*Deb et al, 2000*), which has been shown to be a reliable and efficient algorithm for solving multi-objective problems. Since this step does not require interaction, much larger population sizes and number of generations can be used to ensure that the quantitative objectives are sufficiently optimized. Solutions are then selected from the trade-off front of the non-interactive run and used to seed the IMOGA. *Babbar et al.* (2006) have shown that this is an efficient approach for minimizing user evaluation of early solutions that may be of poor quality, while still maintaining good solution quality. The initial generation of the IMOGA also has a random component that ensures diversity in the search space for the IMOGA. The IMOGA itself is based on the NSGA-II. As with all genetic algorithms, the IMOGA performs the usual operations of selection, crossover, and mutation (*Goldberg*, 1989). However, unlike typical GAs the population size and number of generations is kept small (typically 20-50 individuals in each population, and 20-30 generations) to reduce the number of evaluations required from the user.

For each solution in the GA population the quantitative objectives are first calculated. Next, the transmissivity and predicted head fields are shown to the user through a graphical user interface. The user then gives them a rank from 1 (best) to 5 (worst). Since the user can not be expected to evaluate every solution in the GA population (even for small population sizes the user fatigue can still be significant) representative solutions are chosen from the population to be ranked by the user. Since the transmissivity fields are essentially two-dimensional 'images,' we use an efficient 'image-clustering' algorithm – N-cuts clustering (*Ng et al.,* 2002) – to find the best clusters based on each transmissivity field's spatial information. Candidate solutions are then selected from each cluster for user ranking.

Once the user has ranked these solutions the unranked solutions also need to be given an objective that reflects user preference. This requires a model to be built of user preference. This is accomplished by archiving past solutions ranked by the user and using them as training data to build a 'surrogate' machine-learning model to evaluate the unranked solutions. Once all solutions in the population have been given ranks based on human preference (directly by the expert or indirectly by the surrogate model), the IMOGA continues until the solutions converge to a stable Pareto front or the expert stops the GA iterations.

The IMOGA has been applied and tested on a hypothetical test case and results indicate that it can effectively search for solutions that improve on purely-quantitative calibration results by including expert knowledge and preferences (*Singh et al*, 2005). Results also show that the image clustering and machine-learning approach leads to significant reduction in the number of user evaluations without deteriorating solution quality (*Singh et al*, 2006).

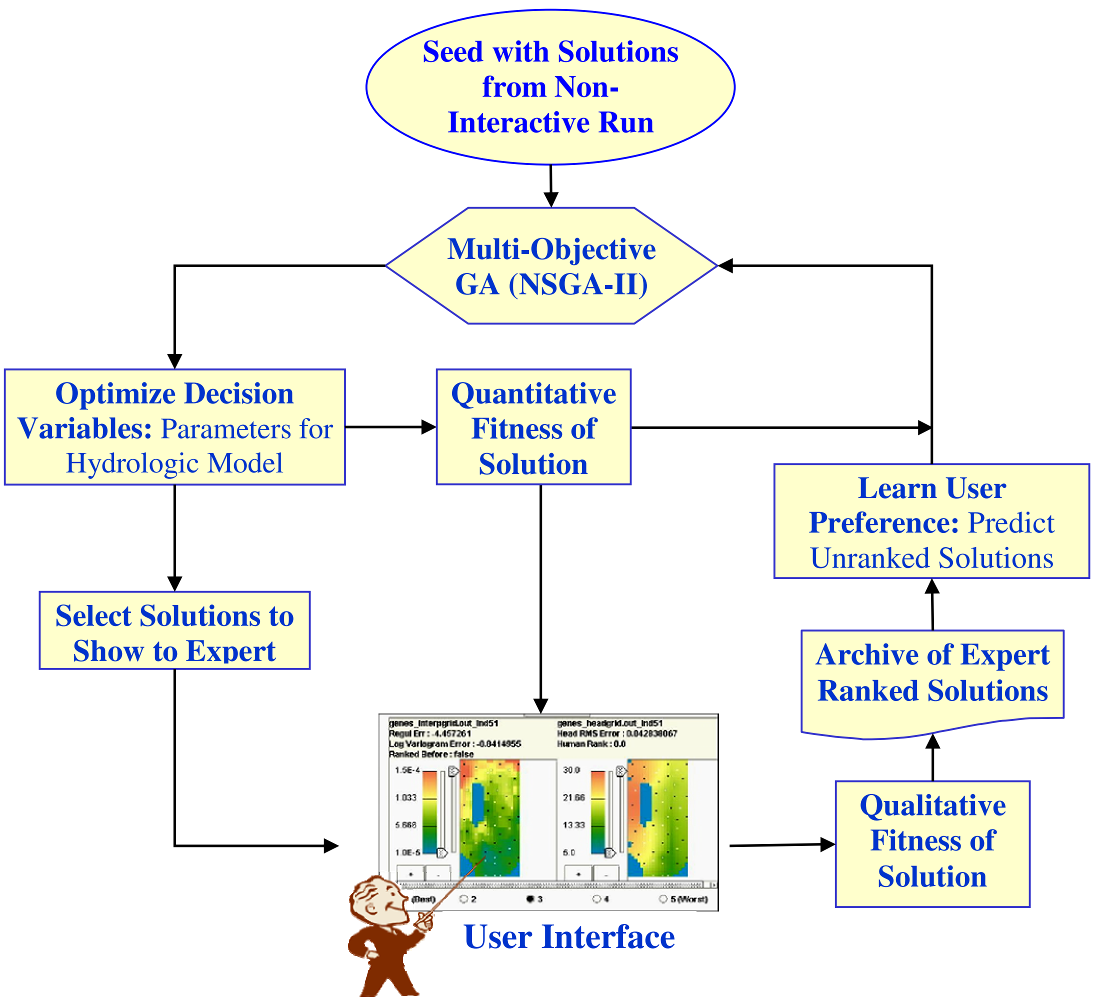

Figure 1. IMOGA Framework

Predictive Uncertainty analysis for IMOGA

The IMOGA converges to a Pareto front that represents the best trade-off between calibration error, spatial heterogeneity, and expert preferences for certain geospatial patterns. These solutions on the Pareto front correspond to large-scale transmissivity trends that fit both the hydraulic head measurements and the experts' understanding of the site.

Most researchers [*Mclaughlin and Townley*, 1996; *Alcolea et al*, 2005] assume that the transmissivity field $T(x)$ can be decomposed into a large-scale trend $T_L(x)$ and small-scale variability $T_S(x)$ (see Figure 2):

$$T(x) = T_L(x) + T_S(x) \rightarrow T_S(x) \in N(0, C_V) \qquad (1)$$

where $N(0,C_v)$ is the multi-Gaussian distribution with 0 mean and covariance given by C_v. In practice, $T_L(x)$ is whatever trend we can estimate based on the data we have, while $T_s(x)$ are the unidentifiable small-scale fluctuations from this large-scale trend. Using this framework we can address prediction uncertainty with respect to the transmissivity field. The predictions for the groundwater model can either be related directly to the head field or to contaminant transport processes. If the predictions relate directly to the head field then the large-scale transmissivity fields generated by the IMOGA can be used directly for predictive uncertainty analysis. However, if the predictions are for contaminant transport then they will also depend on small-scale variability.

For the large-scale trends, there is uncertainty due to the non-uniqueness of the solution and the uncertainty in the expert's knowledge of the site. This is addressed by using multiple transmissivity fields that all honor the data as well as the expert's understanding of the site. Unlike Bayesian inversion, the IMOGA does not give us the probability distribution for the large-scale trend. It does, however, give us many possible alternative hypotheses for the large-scale trends that fit the data and the expert's knowledge to different degrees. We use the image-clustering technique mentioned previously to group the final solutions into clusters of similar large-scale patterns. Representative samples from the clusters represent the salient trends that are applicable for the site. To use these fields within a probabilistic framework it is necessary to 'weight' each field based on how likely it is. This weight should correspond to the 'belief', 'likelihood' or 'probability' for that transmissivity field. Using Bayesian statistics, the probability of a particular transmissivity field is inversely proportional to its calibration error and increasing departures from the 'prior' field, as given by Equation 2:

$$p(T \mid d, \overline{T}) \propto \exp\left\{-\frac{1}{2}\left[d - f(T)\right]^T C_H^{-1}\left[d - f(T)\right] - \frac{1}{2}\left[\overline{T} - T\right]^T C_T^{-1}\left[\overline{T} - T\right]\right\} \qquad (2)$$

where $p(T \mid d, \overline{T})$ is the a posteriori probability for transmissivity field T given the data d and the prior transmissivity field $(\overline{T})$, d is the observation vector, $f(T)$ is the forward prediction model (using transmissivity field T), C_H is the covariance for the errors between model predictions and data, and C_T is the covariance for the errors between the prior transmissivity field $(\overline{T})$ and a given T field. With the IMOGA, the fields that best fit the user's 'prior' knowledge are the fields that have been ranked most highly by the expert. The representative samples from the clusters with rank 1 transmissivity fields can then be used as $\overline{T}$. The calibration error for each field has already been calculated for each of the fields in evaluating the quantitative objectives. In this way, the large-scale transmissivity fields are weighted based on both the calibration error and expert's knowledge. These weights are then used when sampling over the range of large-scale fields.

With respect to the small-scale variability, this variability can not be estimated from the inverse process; the only way to characterize it is to treat it as a spatial random variable that has some specified (or measured) covariance structure, given by C_v (see equation 1). Given this covariance structure, multiple unconditional, correlated transmissivity fields with small-scale heterogeneity are simulated. This small-scale variability is then added to the large-scale transmissivity to give the combined transmissivity field. The prediction model can now be run using all simulated fields to get the distribution of predictions.

This approach is now being implemented and will be applied to the WIPP site.

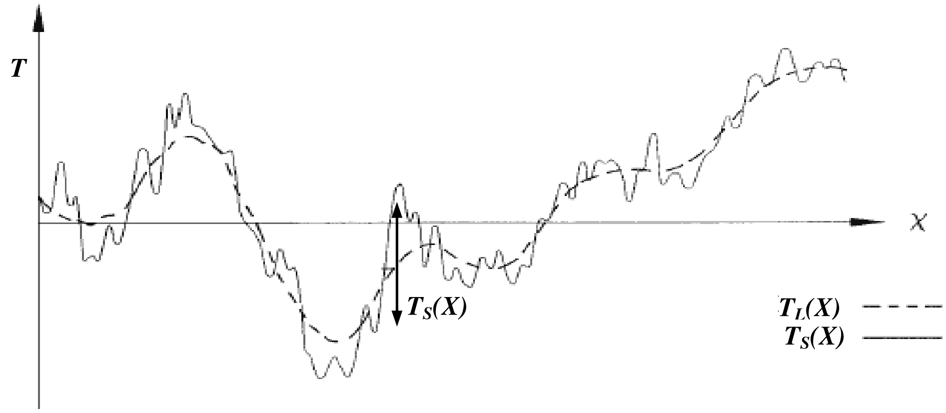

Figure 2. Decomposition of transmissivity field into large – $T_L(x)$ – and small-scale components – $T_S(x)$ (Figure adapted from *Mclaughlin and Townley*, 1996).

The WIPP Site

The Waste Isolate Pilot Plant site situated near Carlsbad in New Mexico is the world's first underground repository used to dispose of transuranic radioactive waste from the research and production of nuclear weapons. WIPP began operations in 1999 after almost 20 years of extensive scientific studies, public input, and regulatory struggles. What makes the WIPP site an ideal test bed for this study is that it is perhaps the most extensively studied site for stochastic inverse modeling [*LaVenue and Pickens*, 1992; *RamaRao et al*, 1995; *LaVenue et al*, 1995; *Capilla et al*, 1998; *Zimmerman et al*, 1998]. The Sandia National Laboratory has been responsible for the characterization and modeling of the site. The concern at the WIPP site has been if the radioactive wastes stored in the repository might leak and contaminate the Culebra dolomite aquifer, which is a highly permeable formation about 1000 feet above the repository. Thus, most inverse modeling techniques have focused on characterizing the Culebra aquifer, which could prove to be an important pathway for contaminants in the case of a leak.

For this study we consider the steady state model used by *McKenna and Hart* (2003). Figure 3 shows the modeled domain. The model corresponds to the confined

Culebra dolomite in the 'Rustler formation' at the WIPP site. The model domain is 30.5 x 20.5 km^2 consisting of a total of 274,011 cells (447 east-west by 613 north-south), each being 50 x 50 m^2. The land-withdrawal boundary (also known as the WIPP site) is 6.4 x 6.4 km^2 and situated roughly in the center of the model domain. There is a no-flow boundary (shown by the purple line) that runs from north to south along the center of a geological feature at the site called the Nash draw (this no-flow boundary is imposed because Karst topology is thought to exist west of the Nash draw). A total of 62,118 cells lie in the no-flow region. Steady state head measurements are available from the years 1980, 1990, 1996, and 2000 (Beauheim, 2002) with 16, 28, 34, and 37 head measurements from each year, respectively. Transmissivity (T) measurements are available at 43 locations (shown by the pink squares in Figure 3). The Culebra transmissivities are thought to exist in three geological zones. The highest transmissivities are on the western edge of the site (these correspond to the outer boundary of the Nash draw) and are shown in Figure 3 with the brown line. The lowest transmissivities are on the eastern edge of the site and are shown by the dark blue line.

McKenna and Hart (2003) used non-linear inversion based on the concept of 'pilot-points' (*Doherty*, 2003). Pilot points are spatial control points spread across the modeling domain where the parameters of interest need to be estimated. The values at the pilot points are then interpolated to give the continuous field of interest. For this problem the pilot points represent point values of transmissivities that are interpolated (using kriging) to give a particular transmissivity field. The values of the pilot points were fixed at the T measurement locations to ensure that the calibrated field matches the field measurements at these locations. A total of 115 variable pilot point locations (shown by the dark blue diamonds in Figure 3) were used for this study. The objective of the IMOGA (or any other calibration methodology) is to find the best values for the pilot points to minimize calibration error between field head measurements and model predictions. With such a large number of pilot-points it is also necessary to constrain the complexity of the resulting transmissivity field by minimizing an additional 'regularization' term (*Moore and Doherty*, 2006), making the problem multi-objective.

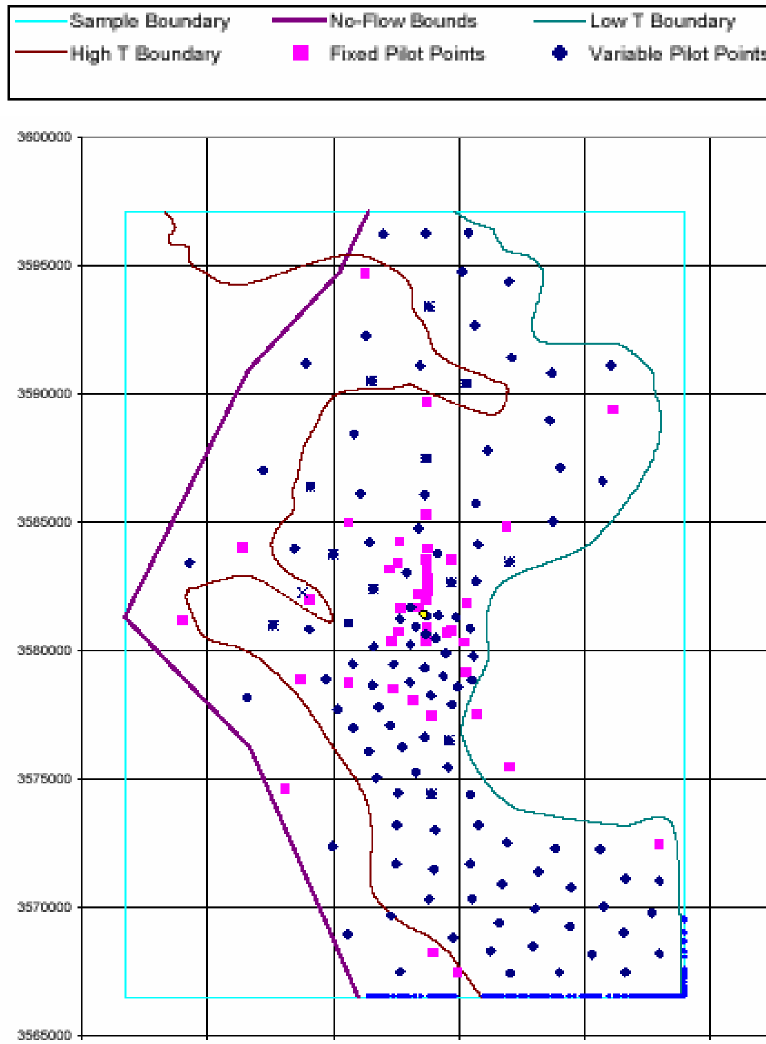

Figure 3. Modeled domain for WIPP site (taken from *McKenna and Hart*, 2003).

The predictive scenario for this case consists of tracking a single particle (assuming a constant advective porosity) released in the center of the WIPP repository until it exits the model boundary. The path and the travel time for this particle are of interest to the modelers as the particle is meant to simulate a possible leak in the WIPP repository. *McKenna and Hart* (2003) used MODFLOW (*McDonald and Harbaugh*, 1988) to simulate the groundwater flow of the model and the streamline particle-tracking code DTRKMF (*Rudeen*, 2003). The same predictive scenario is used for the transmissivity fields identified by the IMOGA and compared with results from *McKenna and Hart* (2003) and other non-interactive approaches to analyze the significance of expert knowledge for the model.

Summary

The IMOGA combines the search and optimization powers of a conventional genetic algorithm with the expertise and subjective judgment of groundwater modelers. The IMOGA is unique in that it allows model inversion to be solved as a multi-objective problem to assess the trade-off between different types of information (quantitative and qualitative). It is noteworthy that this process is interactive as well as adaptive – on one hand the solution space evolves with the user's preferences, and on the other hand the user's own understanding and conception of the model's requirements grow as they assess more potential solutions. To reduce user fatigue for the IMOGA, image-based clustering is used to select solutions to be shown to the expert and machine-learning based models are built to predict the ranks of the unevaluated solutions.

The IMOGA is currently being applied to a field-scale case-study based on the WIPP site - one of the most extensively studied sites for groundwater inverse modeling. The WIPP site is challenging in that it requires the prediction of contaminant fate and transport that depends on small-scale variability in conductivity values. This paper proposes a methodology to incorporate uncertainty in large-scale trends using a Bayesian framework. The small-scale variability is modeled as equally-likely, spatially correlated, unconditional simulations that can be added to the large-scale trends. These simulations are then used to assess the uncertainty in predictions (contaminant travel time and travel path for the WIPP site) with respect to the parameter of interest. This methodology is being tested and its results will be presented at the conference.

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