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COMPUTATIONALLY EFFICIENT INVERSION OF STEADY-STATE STOCHASTIC MOMENT EQUATIONS OF GROUNDWATER FLOW

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1 INTRODUCTION

The impact of various sources of uncertainty on predictions of groundwater flow is conveniently tackled by casting the governing equations in a stochastic framework. Different inverse stochastic approaches have been developed to condition hydrogeological models' predictions not only on direct measurements of parameters but also on information on state variables. Here, we focus on the inversion of stochastic moment equations of groundwater flow, as originally proposed by Hernandez et al.[1],[2]. In their approach, hydraulic conductivity is parameterized geostatistically based on measured values at discrete locations and unknown values at discrete pilot points. Prior estimates of pilot point values are obtained by generalized kriging. Posterior estimates at pilot points and (optionally) at measurement points are obtained by calibrating mean flow against measured values of head. The parameters are then projected onto a computational grid via kriging. Maximum likelihood calibration is employed to estimate not only hydraulic but also (optionally) unknown variogram parameters. The latter define the underlying geostatistical model. The approach yields covariance matrices for parameter estimation as well as head and flux prediction errors. The latter are obtained a posteriori by solving corresponding second-moment equations. Hernandez et al.[1],[2] implemented their inverse approach on a synthetic scenario, involving a general nonuniform flow condition in a bounded heterogeneous two-dimensional domain. Recently, Hendricks Franssen et al.[3] performed a comparative synthetic study assessing the relative performance of this moment equations-based inverse method and several types of Monte Carlo inverse methodologies. Results of that study showed that that observed differences between the performances of the tested methods were not very large. However, Monte Carlo inversion of

100 realizations needed considerably more CPU time than geostatistical inversion of moment equations did. Bianchi-Janetti et al.[4] applied the inverse moment-equations method to characterize the log-transmissivity distribution at a small scale field test site located in Montalto Uffugo (Italy). In their field application, information on hydraulic head is provided through self-potential signals recorded by a few surface electrodes during a pumping test, while only one transmissivity measurement was available.

Notwithstanding the theoretical and conceptual advantages of the method, the inversion of moment equations is still based on an optimization process which requires the numerical calculation of the derivatives of the objective function with respect to model parameters. These are in turn calculated from the derivatives of nodal heads (*i.e.*, the sensitivity matrix). This limits its applicability to situations where the number of parameters, *e.g.*, hydraulic conductivity values at pilot points, is not large because of the associated relevant computational cost. Here, we embed exact equations satisfied by the sensitivity matrix of the (ensemble) mean hydraulic head, up to its second-order of approximation, within the inverse modeling process. This renders the nonlinear inversion of stochastic moment equations feasible for a large number of unknown hydraulic parameters. We illustrate our algorithm and procedure with a synthetic example.

2 POSITION OF THE PROBLEM AND COMPUTATIONAL DETAILS

We consider steady-state flow of groundwater in a randomly heterogeneous flow domain. The flux vector $\boldsymbol{q}(\mathbf{x})$ and the hydraulic head $h(\mathbf{x})$ obey the continuity equation and Darcy's Law subject to given forcing terms. Optimum unbiased predictions of $h(\mathbf{x})$ and $\boldsymbol{q}(\mathbf{x})$ can be rendered via their first ensemble (statistical) moments, $\langle h(\boldsymbol{x})\rangle$ and $\langle \boldsymbol{q}(\boldsymbol{x})\rangle$. Guadagnini and Neuman[5,6] showed how to solve the equations satisfied by the zero- and second-order components of mean hydraulic head by a Galerkin finite element scheme in a two-dimensional rectangular domain, in the presence of deterministic forcing terms. Here, the order of approximation (zero- or second-) of a quantity is given in terms of the standard deviation, σ_Y, of the natural logarithm of hydraulic conductivity, $Y = ln\ K$. The recursive finite element algorithm of Guadagnini and Neuman[6] is valid to second order in σ_Y. It assumes that one has at his/her disposal two functional parameters: a conditional unbiased estimate, $\langle Y(\boldsymbol{x})\rangle$, of the randomly varying Y field and the second conditional moment of associated estimation errors, $C_Y(\boldsymbol{x}, \boldsymbol{y})$. When conditioning is performed on the basis of existing measurements of Y at discrete points, $\langle Y(\boldsymbol{x})\rangle$ and $C_Y(\boldsymbol{x}, \boldsymbol{y})$ can be obtained (in principle) by means of geostatistical methods. We parameterize $\langle Y(\boldsymbol{x})\rangle$ as Hernandez et al.[1,2] did and express it as the weighted sum of precisely or imprecisely known values at discrete (N_M) measurement points and unknown values at discrete (N_p) pilot points. Both sets of values are treated (the first optionally) as unknown parameters to be estimated by inversion. Estimates of $\langle Y(\boldsymbol{x})\rangle$ and $C_Y(\boldsymbol{x}, \boldsymbol{y})$ based on log conductivity measurements (if available) are treated as prior information in the manner of Carrera and Neuman[7,8]. The weights of the sum are evaluated through universal kriging considering the variance of measurement errors at actual data points (assumed to be uncorrelated) and the covariance of estimation errors at pilot points (set equal to the inverse

Fisher information matrix of the most recent iterate). A Maximum Likelihood (ML) estimate of $\langle Y(\mathbf{x})\rangle$ is obtained by minimizing the negative log-likelihood criterion

$$NLL = \frac{F_h}{\sigma_{hE}^2} + \frac{F_Y}{\sigma_{YE}^2} + \ln\left|\mathbf{V}_Y\right| + \ln\left|\mathbf{V}_h\right| + N_h \ln\sigma_{hE}^2 + N_Y \ln\sigma_{YE}^2 + N_z \ln 2\pi \tag{1}$$

with respect to model parameters. Here, $N_Y = N_M + N_p$, N_h is the number of head measurements, $N_z = N_Y + N_h$, $\mathbf{V}_Y$ and $\mathbf{V}_h$ are the prior error covariance matrices of Y and h, defined as $\mathbf{C}_Y = \sigma_{YE}^2\mathbf{V}_Y$, $\mathbf{C}_h = \sigma_{YE}^2\mathbf{V}_h$. Following the work of Carrera and Neuman[7,8] we assume that the measurement errors of Y and h (a) lack correlation and (b) are multivariate Gaussian. It then follows that the matrix $\mathbf{V}_h$ is diagonal and $\mathbf{C}_Y$ is a matrix formed by the diagonal covariance matrix of Y measurements errors and the non-diagonal covariance matrix of Y estimation errors at pilot points. In (1), F_h and F_Y are the head residual criterion and the penalty parameter criterion, respectively

$$F_h = \left(\mathbf{h}^* - \left\langle \mathbf{h}^{[a]}\right\rangle\right)^T \mathbf{V}_h^{-1}\left(\mathbf{h}^* - \left\langle \mathbf{h}^{[a]}\right\rangle\right); \qquad F_Y = \left(\mathbf{Y}^* - \left\langle \mathbf{Y}\right\rangle\right)^T \mathbf{V}_Y^{-1}\left(\mathbf{Y}^* - \left\langle \mathbf{Y}\right\rangle\right) \tag{2}$$

where superscript T denotes transpose, $\mathbf{h}^*$ is the vector of head measurements, $\langle \mathbf{h}^{[a]}\rangle$ is a vector of a-order mean conditional hydraulic head values ($a = 0, 2$, depending on the order of approximation of $\langle \mathbf{h}\rangle$) calculated at head measurement locations; $\mathbf{Y}^*$ is the vector of Y measurements and Y prior estimates at pilot point locations, $\langle \mathbf{Y}\rangle$ is a vector of mean Y values evaluated during inversion (performed at order a) at Y measurement and pilot point locations.

While Hernandez et al.[1,2] minimize (1) by adopting the finite differences method to calculate numerically the model sensitivity matrix, we develop novel equations satisfied by the derivatives of the second-order mean head with respect to model parameters. A finite element algorithm to solve these equations has been implemented in a new code, named INME (INverse Moment Equations). It extends the earlier code by Guadagnini and Neuman[6] to (i) handle irregular domain shapes, rectangular and triangular elements, and general boundary conditions (Dirichlet, Neuman and Cauchy type), and (ii) perform the inversion of the flow moment equations including the evaluation of the exact sensitivity matrix. The derivative of the second-order approximation of the mean conditional head, $\langle h^{[2]}\rangle$, with respect to the j-th hydraulic parameter Y_{H_j} ($j = 1,\ldots, N_Y$) is given by

$$\frac{\partial\left\langle h^{[2]}\right\rangle}{\partial Y_{H_j}} = \frac{\partial\left\langle h^{(0)}\right\rangle}{\partial Y_{H_j}} + \frac{\partial\left\langle h^{(2)}\right\rangle}{\partial Y_{H_j}} \tag{3}$$

$\langle h^{(0)}\rangle$ and $\langle h^{(2)}\rangle$ respectively being the zero- and second-order component of mean hydraulic heads. Details on the evaluation of the derivatives of $\langle h^{(0)}\rangle$ and $\langle h^{(2)}\rangle$ are presented by Riva et al.[9]. In essence, the equations satisfied by the derivatives included in (3) can be obtained on the basis of (i) the zero- and second- order equations for the mean hydraulic head, and (ii) the equations adopted to compute the kriging estimates (and associated covariance matrix) of Y. They only involve terms which are calculated during the forward solution of the equation satisfied either by $\langle h^{(0)}\rangle$ or $\langle h^{(2)}\rangle$ as well as the kriging weights and posterior kriging estimates (and covariance matrix) of the Y field.

3 ILLUSTRATIVE EXAMPLE

We consider a rectangular domain of length 18 and width 8 (all quantities hereinafter are given in consistent units), which is discretized into N_e = 3600 square elements of uniform size δ = 0.2. Figure 1a depicts a sketch of the flow domain, with the type of boundary conditions used. A well is located in the center of the domain and pumps continuously at a constant unit rate. Using a sequential Gaussian simulator [GCOSIM3D[10]] we generate a single unconditional realization of Y with zero mean, exponential isotropic variogram with given sill, σ_Y^2 = 4.0, and integral scale, I_Y = 1.0. We use a standard finite element algorithm to obtain the corresponding distribution of heads. These constitute our reference fields of hydraulic conductivity and heads. We sample the reference head field at 36 measurement locations (depicted by cross in Figure 1a) and the Y field at 16 points (indicated by triangles in Figure 1a). In our analysis we consider six different networks with 16, 32, 64, 103, 150 and 200 pilot points. Figure 1b reports the details on the number and location of pilot points for each of the scenarios investigated.

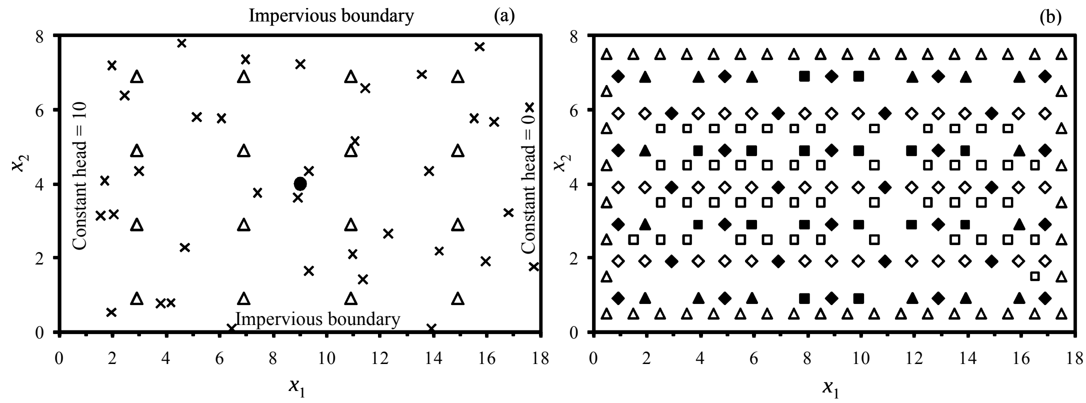

Figure 1: (a) Geometry of the test problem, location of the pumping well (●), Y (△) and h (×) measurement points; (b) pilot point locations: N_p = 16 (■), N_p = 32 (■ and ▲), N_p = 64 (■, ▲ and ◆), N_p = 103 (■, ▲, ◆ and ◇), N_p = 150 (■, ▲, ◆, ◇ and △), N_p = 200 (■, ▲, ◆, ◇, △ and □)

We superimpose a white Gaussian measurement error with unit variance on both sets of measurements ($\sigma_{YE}^2 = \sigma_{hE}^2 = 1.0$) and estimate Y at pilot points by prior ordinary kriging of the noisy Y "measurements". Figure 2a reports the perturbed values of Y, $Y_{perturbed}$, versus their true counterparts, Y_{true}, together with the associated percentage measurement errors. The corresponding depiction for hydraulic heads, h, showing perturbed values of h, $h_{perturbed}$, versus their true counterparts, h_{true}, is reported in Figure 2b. The percentage measurement errors associated with hydraulic head increases from 10% (close to the left boundary) to more than 100% (in the proximity of the right boundary, where h is close to zero) with an average value of about 50%. The average percentage error associated with the conductivity measurements is about 100%. These large uncertainties are not uncommon in practical situations where only the order of magnitude of hydraulic conductivity is often known, *e.g.*, on the basis of interpretation of particle-size distributions, and hydraulic head information are affected by the accuracy of the instruments, operational errors and external factors (*e.g.*, electrical interference and variations in atmospheric pressure).

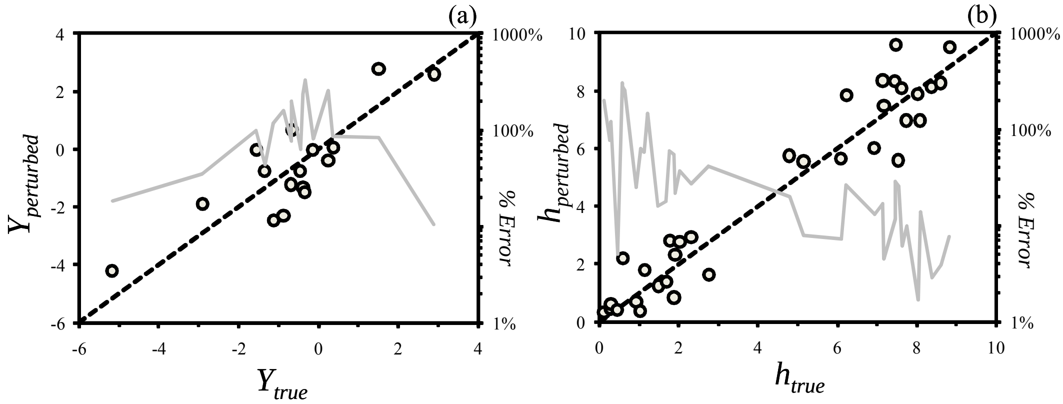

Figure 2: (a) $Y_{perturbed}$ versus Y_{true} at measurements Y locations; (b) $h_{perturbed}$ versus h_{true} at measurements h locations. Percentage measurement errors are also reported (grey lines)

4 RESULTS AND DISCUSSION

Here, we explore the benefit of basing the inversion of moment equations on the direct (and exact) calculation of the derivatives. We analyze the impact of a complete second-order solution by performing the inversion in two different ways: (*i*) approximating the mean hydraulic head in (2) by its zero-order component (a = 0; we denote this scenario as zero-order inversion), and (*ii*) computing the complete second-order solution for the mean hydraulic head (a = 2 in (2); we denote this scenario as second-order inversion). For comparison purposes, we perform our calculations (*i*) with the procedure of Hernandez et al.[1],[2], who couple the solution of the flow problem with the public domain code PEST[11], and (*ii*) with our code INME, which makes full use of the expressions satisfied by the derivatives of mean hydraulic heads with respect to the hydraulic parameters of the model. For illustration purposes, we assume that one has at his/her disposal a data-base allowing to infer reliable estimates of σ_Y^2 and I_Y (which we set equal to the reference values adopted during the generation procedure), and that $\sigma_{hE}^2 / \sigma_{YE}^2$ is known. On this basis, minimizing (1) corresponds to the minimization of

$$J = F_h + \frac{\sigma_{hE}^2}{\sigma_{YE}^2} F_Y \tag{4}$$

Figure 3 shows how J evaluated with INME and with the procedure of Hernandez et al.[1],[2] converges as the number of iterations increases for zero- and second order inversion with N_p = 16 and N_p =103. Similar results have been obtained for all the pilot points networks analyzed. The inversion perform with INME requires less iterations and reaches a lower minimum of J

than the one performed with the procedure of Hernandez et al.[1],[2]. Table 1 lists the minimum values of J, J_{min}, attained at the end of the inversion together with the CPU time (in hours) needed. All the numerical computations have been performed on a CILEA supercomputer, cluster Xeon - Exadron of 128 2-ways nodes with Intel Xeon 3.06GHz CPU. The zero-order inversion performed with INME requires less than one minute for all the cases (corresponding CPU times are not reported here). The difference in terms of CPU time requested by the two methodologies increases as N_p increases, rendering the inverse solution of Moment Equations practically unfeasible for large values of N_p without the direct evaluation of (3). The CPU time required by INME increases (approximately) linearly with N_p, while it exhibits a quadratic dependence on N_p when the procedure of Hernandez et al.[1],[2] is adopted.

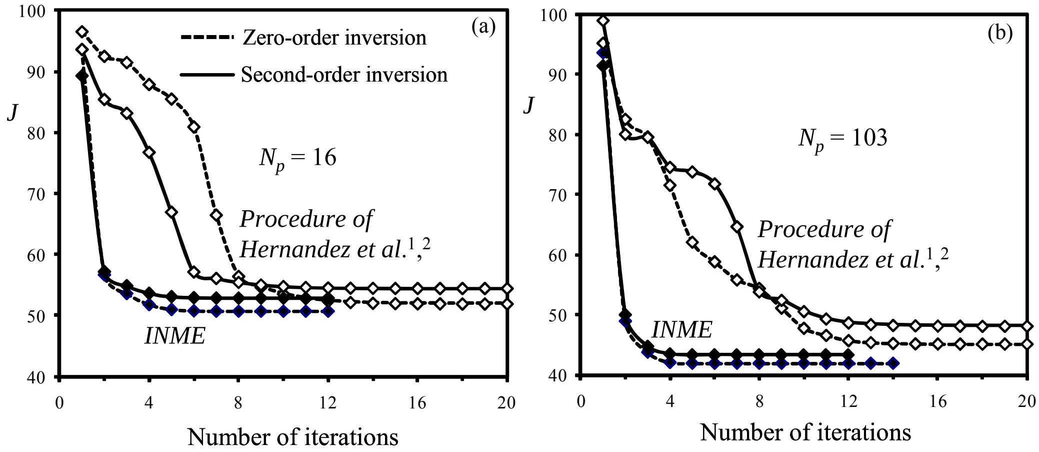

Figure 3: Dependence of J on the number of iterations for zero- and second order inversions performed with INME (♦) and with the procedure of Hernandez et al.[1],[2] (◊) with (a) N_p = 16 and N_p = 103

	Zero-order inversion			**Second-order inversion**			
	INME	**Procedure of Hernandez et al.[1],[2]**		***INME***		**Procedure of Hernandez et al.[1],[2]**	
N_p	J_{min}	J_{min}	**CPU time[h]**	J_{min}	**CPU time[h]**	J_{min}	**CPU time[h]**
16	50.6	52.0	2.6	52.9	10.1	54.4	8.5
32	46.3	49.5	6.6	48.8	15.9	52.3	15.8
64	42.9	46.1	15.8	45.1	20.7	49.6	36.5
103	41.9	45.2	35.6	43.3	42.2	48.1	58.4
150	40.1	44.2	88.6	41.8	46.2	47.4	129.4
200	40.0	44.1	165.8	41.3	78.4	47.1	267.6

Table 1: Minimum values of J, J_{min}, and CPU time

A global quantitative analysis about the quality of the reconstructed Y field is carried out by evaluating mean absolute and root-mean square error ($\overline{e}_Y$ and $RMSE_Y$, respectively) of Y

$$\overline{e}_Y = \frac{1}{N_e}\sum_{i=1}^{N_e}\left|\left\langle Y(\mathbf{x}_i^e)\right\rangle^{[a]} - Y_{ref}(\mathbf{x}_i^e)\right|; \qquad RMSE_Y = \sqrt{\frac{1}{N_e}\sum_{i=1}^{N_e}\left[\left\langle Y(\mathbf{x}_i^e)\right\rangle^{[a]} - Y_{ref}(\mathbf{x}_i^e)\right]^2} \tag{5}$$

Here, $\left\langle Y(\mathbf{x}_i^e)\right\rangle^{[a]}$ (a = 0 or 2) is the mean Y field estimated during the a-order inversion at the N_e elements' centroids, $\mathbf{x}_i^e$; $Y_{ref}(\mathbf{x}_i^e)$ are error-free reference values of $\boldsymbol{Y}$, evaluated at $\mathbf{x}_i^e$. Figure 4 depicts the calculated $\overline{e}_Y$ (Figure 4a) and $RMSE_Y$ (Figure 4b) as a function of the number of pilot points and order of inversion. The results obtained with INME (continuous lines) are here contrasted with those computed approximating the sensitivity matrix by the incremental ratio calculated on the basis of PEST (dashed lines), according to Hernandez et al.[1],[2]. It is clear that the use of the exact sensitivity matrix results in a more accurate reconstruction of Y field, especially when a second order inversion is performed. As expected, $\overline{e}_Y$ and $RMSE_Y$ decrease as the number of pilot points increases. We note that they both display a steep rate of decrease when N_p increases from 16 to 64. Further increments of N_p only result in marginal additional reductions of $\overline{e}_Y$ and $RMSE_Y$. We note that $\overline{e}_Y$ and $RMSE_Y$ are slightly smaller for the second- than for the zero-order inversion.

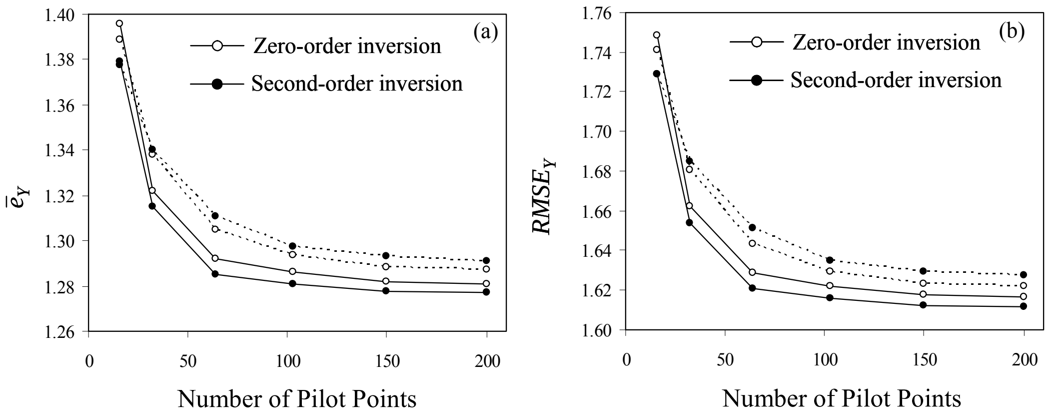

Figure 4: (a) Mean absolute error, $\overline{e}_Y$, and (b) root-mean square error, $RMSE_Y$, of Y versus the number of pilot points calculated with zero- and second-order inversion

5 CONCLUSIONS

We embed the equations satisfied by the sensitivity matrix of the (ensemble) mean hydraulic head in a geostatistical inverse procedure to condition zero- and second-order approximations of stochastic moment equations of flow on information on hydraulic conductivity and hydraulic head. During inversion, we directly solve the system of equations satisfied by the derivatives of the (ensemble mean) hydraulic heads with respect to model parameters. An advantage of this methodology is that the system matrices are identical for all the parameters and coincide with those used to solve the state equations. Relying on this approach allows considerable improvement of the methodology originally proposed by Hernandez et al.[1],[2] not only in terms of accuracy of the solution, but also in terms of the CPU time required for the calculations. This renders the nonlinear inversion of stochastic moment equations feasible for a large number of unknown hydraulic parameters.

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REFERENCES

[1] A.F. Hernandez, S.P. Neuman, A. Guadagnini and J. Carrera, "Conditioning mean steady state flow on hydraulic head and conductivity through geostatistical inversion", *Stoch Environ Res Risk Asses*, **17**, 329-338 (2003).

[2] A.F. Hernandez, S.P. Neuman, A. Guadagnini and J. Carrera, "Inverse stochastic moment analysis of steady state flow in randomly heterogeneous media", *Water Resour. Res.*, **42**, W05425 (2006).

[3] H.J. Hendricks Franssen, A. Alcolea, M. Riva, M. Bakr, N. van der Wiel, F. Stauffer, and A. Guadagnini, "A comparison of seven methods for the inverse modeling of groundwater flow. Application to the characterisation of well catchments", *Advances in Water Resources*, **32**(6), 851-872 (2009).

[4] E. Bianchi-Janetti, M. Riva, S. Straface and A. Guadagnini, "Stochastic characterization of the Montaldo Uffugo reasearch site (Italy) by geostatistical inversion of moment equations of groundwater flow", *J. Hydrol*, **381**, 42 – 51 (2010).

[5] A. Guadagnini and S.P. Neuman, "Nonlocal and localized analyses of conditional mean steady state flow in bounded, randomly nonuniform domains: 1. Theory and computational approach", *Water Resour. Res.*, **35**(10), 2999-3018 (1999).

[6] A. Guadagnini and S.P. Neuman, "Nonlocal and localized analyses of conditional mean steady state flow in bounded, randomly nonuniform domains: 2. Computational examples, *Water Resour. Res.*", **35**(10), 3019-3039 (1999).

[7] J. Carrera and S.P. Neuman, "Estimation of aquifer parameters under transient and steady state conditions: 1. Maximum likelihood method incorporating prior information", *Water Resour. Res.*, **22**(2), 199-210 (1986)

[8] J. Carrera and S.P. Neuman, "Estimation of aquifer parameters under transient and steady state conditions: 2. Uniqueness, stability, and solution algorithms", *Water Resour. Res.*, **22**(2), 211-227 (1986).

[9] M. Riva, A. Guadagnini, F. De Gaspari and A. Alcolea, "Exact sensitivity matrix and influence of the number of pilot points in the geostatistical inversion of moment equations of groundwater flow", *Water Resour. Res.,* submitted (2010).

[10] J.J. Gómez-Hernández, A. Sahuquillo and J.E. Capilla, "Stochastic simulation of transmissivity fields conditional to both transmissivity and piezometric data – 1. Theory", *J. Hydrol*, **203**(1 – 4), 162 – 174 (1997).

[11] J. Doherty, *PEST: Model Independent Parameter Estimation*, User Manual, 4th ed., Watermark Numer. Comput., Corinda, Queensland, Australia, (2002).