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Groundwater modelling: Towards an estimation of the acceleration factors of iterative methods via an analysis of the transmissivity spatial variability

Modèles de nappes: vers une amélioration des solveurs numériques itératifs via une analyse de la variabilité spatiale des transmissivités

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ABSTRACT

When running a groundwater flow model, a recurrent and seemingly subsidiary question arises at the starting step of computations: what value of acceleration parameter do we need to optimize the numerical solver? A method is proposed to provide a practical estimate of the optimal acceleration parameter via a geostatistical analysis of the spatial variability of the logarithm of the transmissivity field *Y*. The background of the approach is illustrated on the successive over-relaxation method (SOR) used, either as a stand-alone solver, or as a symmetric preconditioner (SSOR) to the gradient conjugate method, or as a smoother in multigrid methods. It shows that this optimum acceleration factor is a function of the standard deviation and the correlation length of *Y*. This provides an easy-to-use heuristic procedure to estimate the acceleration factors, which could even be incorporated in the software package. A case study illustrates the steps needed to perform this estimation.

RÉSUMÉ

Lors de l'exécution des modèles de nappes, l'utilisateur est invité à faire le choix d'un solveur numérique dont le fonctionnement optimal requiert, lui-même, le choix d'un préconditionneur. Une méthode est proposée pour que ce choix soit réalisé à partir d'une analyse géostatistique de la variabilité spatiale du champ des transmissivités du système aquifère. Le principe de la méthode est illustré sur la méthode itérative de la surrelaxation (SOR) et de sa variante la méthode SSOR utilisées, soit comme méthodes de résolution, soit comme auxiliaires de la méthode du gradient préconditionné ou de celle des méthodes multigrilles. Les simulations réalisées mettent en évidence une variation du coefficient de surrelaxation optimal ω_{opt} avec les paramètres caractéristiques de l'hétérogénéité du logarithme des transmissivités. Un catalogue de courbes caractéristiques de ω_{opt} est proposé pour que ce choix soit réalisé moyennant la donnée de l'écart-type et de la longueur de corrélation du logarithme des transmissivités. Une illustration en est donnée sur un exemple.

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1. Introduction

The development of computer science has greatly enhanced the use of numerical methods to provide solutions of the flow equation of natural groundwater systems. Recent trends on groundwater models dealing with heterogeneity (Marsily et al., 2005) underline this fact. Unfortunately, increasing grid resolution increases the size of the corresponding matrix equations.

To face this problem, earlier flow solvers used the method of successive over-relaxation to accelerate the convergence of Southwell's original relaxation matrix (1946). Nevertheless, a quick analysis shows that a meaningful representation of the variability of the logarithmic transmissivity implies a computational requirement which involves a number of finite difference blocks N on the order 10^4 for a two-dimensional flow and of 10^6 for a three-dimensional one (Ababou et al., 1985).

That is to say that, respectively 10^6 and 10^9 iterations are needed to reach this numerical accuracy with SOR whose convergence grows as $N^{3/2}$, whereas the convergence of multigrid methods grows as $N \log N$ and involves 4×10^4 and 6×10^6 iterations.

Consequently, standard numerical methods are unpractical in terms of time and storage to tract such matrix sizes, which is why most groundwater modelling software is now using preconditioned conjugate gradient methods (Hill, 1990) and multigrid methods (Mehl and Hill, 2001; Stüben and Klees, 2005) which can give a new use to SOR as a preconditioner.

However, it is a matter to regret that these new solvers are less users-friendly despite the increasing conviviality of the current software packages and the potentialities of the new graphical user interfaces. Currently, the context-sensitive help given in these packages to users unfamiliar with groundwater modelling refers still to textbooks such as Chiang et al. (1998).

An easy-to-use governing criterion for the selection of a preconditioner to the flow solvers remains a sensitive question for the users.

This article attempts at giving a preliminary response to some of these perceived weaknesses. A qualitative geological concept is linked to a mathematical one in order to provide an understanding of the numerical solver in a manner that will enable users of groundwater models to make these choices based on their original background, i.e. geology.

We will use SOR to support the illustration of this task for four reasons:

- its simplicity allows us to give a straightforward idea on the relationship between statistical hydrogeological parameters and convergence issues;
- SOR is still an efficient iterative stand-alone solver for small-size problems, as was very well shown by Ehrlich (1981);
- SOR is an effective preconditioner for Preconditioned Gradient (PCG) methods handling symmetric successive over-relaxation (SSOR);
- contrary to existing belief, SOR may be a suitable smoother (Popa, 2008) in the strategy of multigrid dealing with moderate anisotropy (Yavneh, 1996) or for solving 2-D Poisson equations (Zhang, 1996).

Investigating the efficiency of SOR as a stand-alone solver, as a preconditioner and as a smoother for heterogeneous fields is the subject of this article. The smoothing property is only formally examined herein. It will be experimented in further work. In the following, Monte Carlo simulations are performed to compute the spectral radii of flow matrices arising in groundwater flow modelling through multiple replications of a non-homogeneous aquifer. These are considered as different equiprobable realizations of a random function. Inspection of the optimal relaxation factor of the SOR method is pursued following an analytical determination in the homogeneous case and through the Young formula in the heterogeneous case. Then, variations of the optimum relaxation factor are expressed as a function of the standard deviation of the logarithm of the transmissivity field Y and parameterized on the correlation lengths of this field.

2. On the flow model

In steady state conditions, the groundwater flow is described by Poisson's equation (Bear, 1972):

$$\mathrm{div}(T \ \mathrm{grad} \ h) = q \tag{1}$$

with appropriate boundary conditions reflecting the prevailing hydrogeological context.

In Eq. (1) h is the dependant variable, the hydraulic head, and T is a distributed parameter called transmissivity, whereas q is a source term. The equivalent finite difference form of Eq. (1), derived with the centred difference scheme, can be compacted, and expressed in matrix notation (Golub and Van Loan, 1996) as:

$$\mathbf{Bh} = \mathbf{q} \tag{2}$$

where $\mathbf{B}$ is a square matrix called the flow matrix, $\mathbf{h}$ a column matrix of unknown heads h_{ij}, and $\mathbf{q}$ a column matrix involving source terms and boundary conditions.

A quick inspection of $\mathbf{B}$ shows that it is a real irreducibly diagonally dominant symmetric matrix with negative diagonal entries and non-negative off-diagonal entries.

3. Preliminary numerical considerations

3.1. On the numerical solver

When a numerical solver of Eq. (1) is selected, it needs to be efficient for solving the set of linear algebraic Eq. (2). Although SOR performs well for small-size problems, it cannot efficiently solve large ones. However, it is useful to evaluate its efficiency either as a convergence accelerator in PCG or as an error smoother in multigrid algorithms.

3.2. Optimized relaxation

SOR may be defined from the regular splitting of the flow matrix $\mathbf{B}$:

$$\mathbf{B} = \mathbf{D} - (\mathbf{E} + \mathbf{E}^{\mathbf{t}}) \tag{3}$$