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The Laplace Transform MultiQuadrics (LTMQ) for the Solution of the Groundwater Flow Equation

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MultiQuadrics (MQ) is a true scattered-data grid-free scheme for representing surfaces and bodies in an arbitrary number of dimensions by using approximations given by an expansion in terms of upper hyperboloids. It is continuously differentiable and integrable, and is capable of representing functions with steep gradients with very high accuracy. Hardy (1971) first derived MQ to approximate geographical surfaces and magnetic anomalies, but it was mostly ignored until Franke (1982) showed that MQ outperformed 29 other interpolation methods. Micchelli (1986) and Madych and Nelson (1988) provided the theoretical justification for the performance of MQ.

The extension of MQ to applications in the solution of Partial Differential Equations (PDE) in computational fluid dynamics is credited to Kansa (1990a,b), who employed MQ to solve the advection-diffusion equation, the von Neumann blast wave problem, and Poisson's equation. He showed that MQ (1) yields excellent results with a much coarser distribution of data points, (2) is an excellent estimator of partial derivatives, (3) does not need any special stabilizing treatment for instability and numerical dispersion, (4) is far more efficient and accurate than standard Finite Difference (FD) schemes, and (5) is considerably more flexible and robust than FD in the solution of the traditionally troublesome problem of steep moving fronts.

Laplace transforms are a powerful tool in the solution of PDEs, but their application was limited to simple one-dimensional problems with homogeneous properties. By combining traditional space discretization schemes with Laplace transforms, Moridis and Reddell (1990,1991a,b,c) developed a family of new numerical methods for the solution of parabolic and hyperbolic PDE's. These methods eliminate the need for time discretization of traditional numerical methods while maintaining their flexibility in the simulation of heterogeneous systems with irregular boundaries. The method of Laplace Transform MultiQuadrics (LTMQ) is based on the same concepts but uses MQ as the space approximation scheme.

THE LTMQ METHOD

The governing PDE of transient groundwater flow is

$$\nabla \cdot (K \nabla H) = S_0 \frac{\partial H}{\partial t} + Q \; , \tag{1}$$

where K is the hydraulic conductivity, H is the piezometric head, S_0 is the specific aquifer storativity, $Q = q\ \delta_c(x)\ \delta_c(y)\ \delta_c(z)$, q is the volumetric flow rate of a source or sink per unit volume, and δ_c is the Kronecker delta. The solution of Eq. (1) with the LTMQ method is accomplished in the four steps described in the following sections.

Step 1: The Laplace Transform of the PDE

For a homogeneous and anisotropic 2-D porous medium, the Laplace transform of Eq. (1) expanded in Cartesian coordinates yields

$$K_x \frac{\partial^2 \Psi}{\partial x^2} + K_y \frac{\partial^2 \Psi}{\partial y^2} = S_0 \lambda \Psi - S_0 H(0) + \frac{Q}{\lambda} \; , \tag{2}$$

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where λ is the Laplace space variable, $\Psi = L\{H\}$, and $L\{\}$ denotes the Laplace transform of the quantity in brackets. It should be noted that the analysis in cylindrical coordinates is entirely analogous.

Step 2: The MQ Scheme in the Laplace Space

Following Madych and Nelson (1986), we expand the continuous function Ψ in terms of MQ basis functions and an appended constant, i.e.,

$$\Psi(\mathbf{x}) = a_1 + \sum_{j=2}^{N} \hat{g}(\mathbf{x} - \mathbf{x}_j) a_j \ , \tag{3}$$

where

$$\hat{g}(\mathbf{x} - \mathbf{x}_j) = g(\mathbf{x} - \mathbf{x}_j) - g(\mathbf{x} - \mathbf{x}_1), \quad j = 2, \ldots, N \ , \tag{4}$$

$$g(\mathbf{x} - \mathbf{x}_j) = \left[(x - x_j)^2 + (y - y_j)^2 + r_j^2 \right]^{1/2} , \tag{5}$$

$$r_j^2 = r_{min}^2 \left(\frac{r_{max}^2}{r_{min}^2} \right)^{(j-1)/(N-1)} , \quad j = 1, \ldots, N \ , \tag{6}$$

N is the number of basis functions (i.e., data points in space), and r_{max}, r_{min} are input parameters (Kansa, 1990b). The set of linear equations relating the expansion coefficients a_j to the set of discretized values Ψ_i, $1 \le i \le N$ is

$$\Psi_i = \sum_{j=1}^{N} G_{ij} \, a_j \ , \tag{7}$$

where $G_{i1} = 1$ and $G_{ij} = \hat{g}(\mathbf{x}_i - \mathbf{x}_j)$ for $2 \le j \le N$. The terms G_{ij} represent the ith row of the coefficient matrix $\mathbf{G}$. The first and second partial derivatives of Ψ_i with respect to x are

$$\left(\frac{\partial \Psi}{\partial x} \right) i = \sum_{j=2}^{N} \left(\frac{\partial \hat{g}_{ij}}{\partial x} \right) a_j = \sum_{j=2}^{N} \left(\frac{\partial g_{ij}}{\partial x} - \frac{\partial g_{i1}}{\partial x} \right) a_j \ , \tag{8}$$

$$\left(\frac{\partial^2 \Psi}{\partial x^2} \right) i = \sum_{j=2}^{N} \left(\frac{\partial^2 \hat{g}_{ij}}{\partial x^2} \right) a_j = \sum_{j=2}^{N} \left(\frac{\partial^2 g_{ij}}{\partial x^2} - \frac{\partial^2 g_{i1}}{\partial x^2} \right) a_j \ , \tag{9}$$

where

$$\frac{\partial^2 g_{ij}}{\partial x} = (x_i - x_j) \left[(x_i - x_j)^2 + (y_i - y_j)^2 + r_j^2 \right]^{-1/2} , \tag{10}$$

and

$$\frac{\partial^2 g_{ij}}{\partial x^2} = \left\{ 1 - \frac{(x_i - x_j)^2}{\left[(x_i - x_j)^2 + (y_i - y_j)^2 + r_j^2 \right]} \right\} \times \left[(x_i - x_j)^2 + (y_i - y_j)^2 + r_j^2 \right]^{-1/2} . \tag{11}$$

The partial derivatives with respect to y are obtained in exactly the same manner. Substitution in Eq. (2) leads to the matrix equation

$$\mathbf{W} \, \vec{a} = \vec{b} \ , \tag{12}$$

where the elements of the fully populated coefficient matrix $\mathbf{W}$ and the vector $\vec{b}$ are

$$W_{i1} = -S_0 \lambda \ ,$$

$$W_{ij} = K_x \frac{\partial^2 \hat{g}_{ij}}{\partial x^2} + K_y \frac{\partial^2 \hat{g}_{ij}}{\partial y^2} - S_0 \lambda \hat{g}_{ij}, \quad \text{for } 2 \le j \le N, \tag{13}$$

$$b_j = Q / \lambda - S_0 H(0)_{ij}, \quad \text{for } 1 \le j \le N \ .$$

Step 3: The Solution in the Laplace Space

The MQ approximation of the PDE in the Laplace space results in N simultaneous equations. Since the matrix $\mathbf{W}$ is nonsingular for distinct points, the vector of the MQ expansion coefficients $\vec{a}$ is given by

$$\vec{a} = \mathbf{W}^{-1} \vec{b} \ . \tag{14}$$

The computation of $\mathbf{W}$, $\mathbf{W}^{-1}$, and $\vec{b}$ necessitates values for the Laplace parameter λ. For a desired observation time t, λ is provided by the first part of the Stehfest (1970) algorithm as

$$\lambda_v = \frac{\ln 2}{t} v \ , \quad v = 1, \ldots, N_S \ , \tag{15}$$

where N_S is the number of summation terms in the algorithm and N_S is an even number between 6 and 20. Solution of Eq. (15) returns a set of N_S vectors of the transformed pressures $\vec{a}_v$

$$\vec{a}_v = \left[\mathbf{W}(\lambda_v)\right]^{-1} \vec{b}_v(\lambda_v), \qquad v = 1,\ldots,N_S . \tag{16}$$

To obtain a solution at a time t, all vectors $\vec{a}_v$, $v = 1,\ldots, N_S$ are needed, i.e., the system of simultaneous equations has to be solved N_S times.

Step 4: The Laplace Domain Predictions

Once the $\vec{a}_v$ vectors are known, the Laplace space solutions $\vec{\Psi}_v$ at the original $\mathbf{x}_j$, $j = 1,\ldots, N$ points are obtained from Eq. (7). Then the transformed dependent variable at any point $\mathbf{x}_K$ in the domain of interest is computed by direct substitution in the MQ Eq. (7).

Step 5: The Numerical Inversion of the Laplace Solution

The vector of the unknown heads $\vec{H}$ at any time t is obtained by using the Stehfest (1970) algorithm to numerically invert the Laplace solutions $\vec{\Psi}_v$, yielding

$$\vec{H}(t) = \frac{\ln 2}{t} \sum_{v=1}^{N_S} V_v \, \vec{\Psi}_v , \tag{17}$$

where the terms V_v are constants. The vector $\vec{\Psi}_v$ may include solutions at the original $\mathbf{x}_j$, $j = 1,\ldots, N$ points, predictions at another set of points $\mathbf{x}_K$, $k = 1,\ldots, K$, or both.

Inverting known functions, Stehfest (1970) determined the optimum $N_S = 18$ for double precision variables. However, Moridis and Reddell (1991a) determined that the performance of Laplace transform based numerical methods is practically insensitive to N_S for $6 \le N_S \le 20$.

The solution in the Laplace space removes the need for time discretization and eliminates the stability and accuracy problems caused by the treatment of the time derivative. An unlimited time step size is thus possible without any loss of accuracy. Owing to the absence of a time truncation error, LTMQ offers a stable, nonincreasing roundoff error irrespective of the time of observation t_{obs}, because a single solution (involving N_S matrix inversions) is required, with a $\Delta t = t_{obs}$. On the other hand, in a standard MQ method or any other traditional numerical method, solutions must be obtained at all the intermediate times of the discretized time domain, requiring longer execution times and continuously accumulating roundoff error in the process.

VERIFICATION AND EVALUATION

The performance of the LTMQ method was evaluated in the solution of the problem of transient flow into a homogeneous and anisotropic aquifer with a fully penetrating well and constant discharge conditions. The LTMQ solution was verified through comparison with the analytical solution (Papadopulos, 1965), as well as the solution obtained from a standard implicit FD simulator. The origin of this 2-D, infinite-acting system is placed at the well. Assuming that the axes of the Cartesian system coincide with the principal axes of the permeability tensor, the piezometric head distribution at $t = 20$ days is predicted along the $x = y$ axis, i.e., at an angle of 45° from the x axis. Only one-quarter of the infinite domain (i.e., x in $[0,\infty)$, y in $[0,\infty)$) needs to be simulated in LTMQ and FD. For the LTMQ solution, $N = 35$ and $N_S = 8$. A total of 625 gridblocks was used in the FD simulation. Figure 1 presents (1) the analytical solution, (2) the LTMQ solution, (3) the FD solutions, as well as (4) relevant information on the parameters used in this simulation. It is obvious that the LTMQ method produces an accurate solution, a fact indicated by its virtual coincidence with the analytical solution and the FD solution for a large number of small Δt's.

SUMMARY AND DISCUSSION

A new numerical method, the Laplace Transform MultiQuadrics (LTMQ) method, has been developed for the solution of the diffusion-type parabolic Partial Differential Equation (PDE) of groundwater flow through porous media. LTMQ combines a MultiQuadrics (MQ) approximation scheme for the solution of the PDE with a Laplace transform formulation for the elimination of the need for time discretization. The use of MQ in the spatial approximations allows the accurate description of problems in complex porous media with a very limited number of gridded or scattered nodes. The Laplace transform formulation eliminates the time dependency of the problem and consequently the need for time discretization. An unlimited time step size is thus possible without any loss of accuracy. In a 2-D test problem for which an analytical solution exists, an excellent agreement between the LTMQ, the FD and analytical solutions was observed. Owing to its formulation, the LTMQ method requires solution of the simultaneous equations N_S times and a linear combination of the resulting N_S solutions. Compared with a standard FD method, LTMQ requires drastically fewer (at least one order of magnitude) gridded or scattered nodes for the same level of accuracy but produces fully populated matrices (as opposed to sparse banded matrices in FD). Execution times may be reduced by orders of magnitude because solutions in the LTMQ scheme are necessary only at the desired observation times, whereas in standard numerical and MQ schemes solutions are needed at all the intermediate times of the discretized time domain.

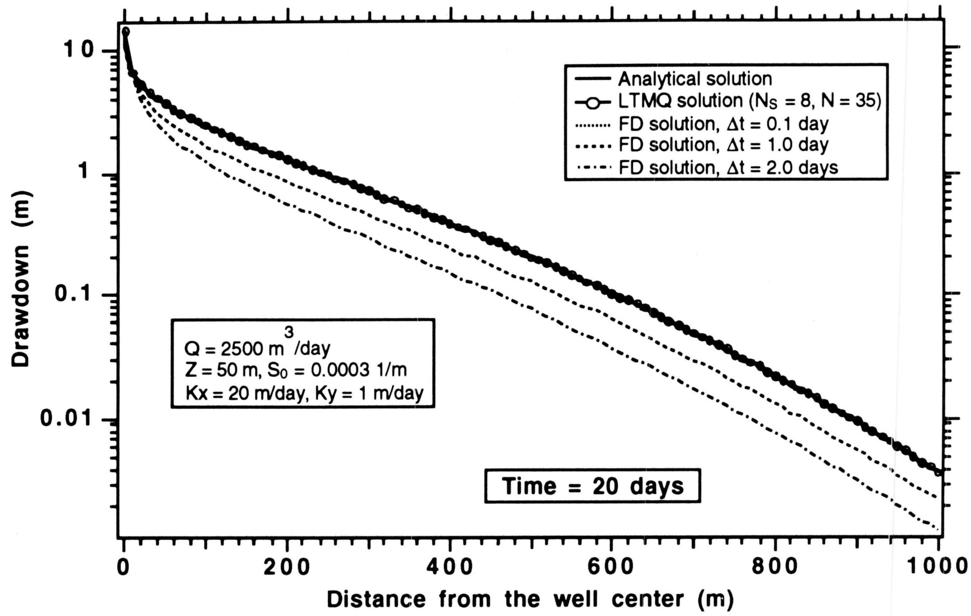

Figure 1. Comparison of the LTMQ solution to the analytical and the FD solutions along the $x = y$ axis in the test problem. [XBL 935-786]

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