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The Marching-Jury Backward Plate Equation for Contaminant Plume Spatial Distribution Recovery in Two-Dimensional Heterogeneous Media: Computational Issues

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Abstract

In this paper the *Marching-Jury Backward Plate Equation* (*MJBPE*) method to reconstruct conservative contaminant plume spatial distributions in two-dimensional (2D) heterogeneous media is presented. The *MJBPE*, based on its one-dimensional (1D) counterpart developed by Atmadja and Bagtzoglou (2001a), was used to recover contaminant spatial distributions in heterogeneous porous media for a variety of test cases with uniform and/or non-uniform transport velocity and dispersion coefficients. The computational complexity and associated cost of the 2D problem requires efficient solution of linear equations that involve very sparse, block-tridiagonal matrices. Various iterative approaches, of the conjugate gradient genre, are explored and tested. A comparison of the two most efficient approaches for various domain sizes concludes the paper.

1. INTRODUCTION

For the past fifteen years, several attempts have been made to tackle one of the most difficult problems of hydrologic inversion, namely to solve the Advection Dispersion Equation (ADE) backwards in time in order to identify pollution sources (Atmadja and Bagtzoglou, 2001b). In this paper we study the 2D advection-dispersion transport problem of a rectangular wave that is described by:

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial x}\left[D(x,y)\frac{\partial C}{\partial x}\right]+\frac{\partial}{\partial y}\left[D(x,y)\frac{\partial C}{\partial y}\right]-\frac{\partial}{\partial x}\left[u(x,y)C\right]-\frac{\partial}{\partial y}\left[v(x,y)C\right], \qquad (1)$$

in a coordinate system aligned to the principal axes, and subject to:

$$C(x,y,0)=0 \qquad \forall \;\; 0\le x<5.5 \text{ and } 6.5<x\le L \qquad (2)$$

$$\forall \;\; 0\le y\le 9$$

$$C(x,y,0)=C_1=1 \qquad \forall \;\; 5.5\le x\le 6.5 \qquad 0\le y\le 9 \qquad (3)$$

where C is the solute concentration, $D(x, y)$ is dispersion coefficient, and $u(x, y)$, and $v(x, y)$ are the transport velocity in the x and y directions, respectively.

2. *MJBPE* METHOD FOR HETEROGENEOUS MEDIA

The Backward Beam Equation (BBE) solves parabolic problems backwards in time and can be obtained by differentiating the governing equation of a parabolic equation with respect to time. This can be done because a solution of the parabolic equation, $f_t = f_{xx}$ also satisfies $f_{tt} = f_{xxxx}$. The 2D problem is described as follows:

$$\frac{\partial C}{\partial t} = -\mathbf{L}_o C \,, \qquad 0 < x < L_x \qquad 0 < y < L_y \,, \qquad t > 0 \tag{4}$$

subject to

$$C(x, y, 0) = f_1(x, y) \,, \qquad C(x, y, T_{ft}) = f_2(x, y) \,, \qquad 0 < x < L_x \qquad 0 < y < L_y \tag{5}$$

$$\begin{aligned} &C(0, y, t) = 0 \,, && C(12, y, t) = 0 \,, && 0 \le y \le 9 \quad t \ge 0 \\ &C(x, 0, t) = 0 \,, && C(x, 9, t) = 0 \,, && 0 \le x \le 12 \quad t \ge 0 \end{aligned} \tag{6}$$

where $\mathbf{L}_o$ is a differential operator in space and T_{ft} is the terminal time of the forward problem. In the case of a heterogeneous ADE wave transport problem, the space differential operator is

$$-\mathbf{L}_o \equiv \frac{\partial}{\partial x}\left[D(x, y) \frac{\partial}{\partial x} \right] + \frac{\partial}{\partial y}\left[D(x, y) \frac{\partial}{\partial y} \right] - \frac{\partial}{\partial x}\left[u\left(x, y\right) \right] - \frac{\partial}{\partial y}\left[v\left(x, y\right) \right] \tag{7}$$

and $f_1(x, y)$ and $f_2(x, y)$ are the initial and terminal data at times t=0 and T_{ft}, respectively. In the BBE method, instead of solving the ADE directly, we set

$$w = e^{kt} C \,, \qquad 0 \le t \le T_{ft} \tag{8}$$

where

$$k = \left(\frac{1}{T_{ft}} \right) \ln\left(\frac{M}{\delta} \right) \tag{9}$$

as given by Buzbee and Carasso (1973) where δ and M are bounds on the errors generated by this procedure. Let such a bound be

$$\left\| \, f\left(T_{ft}\right) - f_2 \, \right\|_2 \le \delta \tag{10}$$

for the initial data, where δ can be chosen to be the error between the measured and the exact values. Let the bound in the resulting errors in the terminal data be

$$\| \; f(0) - f_1 \; \|_2 \leq M \tag{11}$$

where M is the acceptance level for the errors in the predicted terminal values. Equation (9) is an exact approximation for the k parameter in the case of homogeneous media. For heterogeneous cases this approximation is no longer exact but can serve as a very good estimate or starting point for searching for k.

Taking first the derivative of equation (8) with respect to time and substituting equation (1), we obtain:

$$\frac{\partial w}{\partial t} = -\left(\frac{\partial}{\partial x}\left[D(x,y)\frac{\partial}{\partial x} \right] + \frac{\partial}{\partial y}\left[D(x,y)\frac{\partial}{\partial y} \right] - \frac{\partial}{\partial x}\left[u(x,y) \right] - \frac{\partial}{\partial y}\left[v(x,y) \right] - k \right) w \tag{12}$$

Taking the derivative of equation (12) with respect to time once more, we get the auxiliary problem of (1):

$$\frac{\partial^2 w}{\partial t^2} = \left(\frac{\partial}{\partial x}\left[D(x,y)\frac{\partial}{\partial x} \right] + \frac{\partial}{\partial y}\left[D(x,y)\frac{\partial}{\partial y} \right] - \frac{\partial}{\partial x}\left[u(x,y) \right] - \frac{\partial}{\partial y}\left[v(x,y) \right] - k \right)^2 w \tag{13}$$

For the purpose of solving a backward problem, we set $t=T_{ft} \equiv T_{bi}$ as our present day or initial time and $t=0=T_{fi} \equiv T_{bt}$ as our terminal time (i.e., the terminal condition of a forward solution, T_{ft}, will be equal to the initial condition of a backward solution, T_{bi}, and *vice versa*). The corresponding initial and terminal conditions for the auxiliary problem are:

$$w(x,y,T_{bi}) = e^{kT_{bi}} f_2 \quad , \qquad w(x,y,0) = e^{kT_{bi}} f_1 = 0 \tag{14}$$

Boundary conditions associated with (13) are:

$$w(0,y,t) = w(12,y,t) = 0\,, \qquad 0 \leq y \leq 9 \quad t \geq 0 \tag{15}$$

$$w(x,0,t) = w(x,9,t) = 0\,, \qquad 0 \leq x \leq 12 \quad t \geq 0$$

$$w_t(0,y,t) = w_t(12,y,t) = -\left[\frac{\partial}{\partial x}\left[D(x,y)\frac{\partial}{\partial x} \right] + \frac{\partial}{\partial y}\left[D(x,y)\frac{\partial}{\partial y} \right] - \frac{\partial}{\partial x}\left[u(x,y) \right] - \frac{\partial}{\partial y}\left[v(x,y) \right] - k \right] w = 0$$

$$0 \leq y \leq 9 \quad t \geq 0 \tag{16}$$

$$w_t(x,0,t) = w_t(x,9,t) = -\left[\frac{\partial}{\partial x}\left[D(x,y)\frac{\partial}{\partial x} \right] + \frac{\partial}{\partial y}\left[D(x,y)\frac{\partial}{\partial y} \right] - \frac{\partial}{\partial x}\left[u(x,y) \right] - \frac{\partial}{\partial y}\left[v(x,y) \right] - k \right] w = 0$$

$$0 \leq x \leq 12 \quad t \geq 0 \tag{17}$$

3. COMPUTATIONAL FORMULATION

Let $$\boldsymbol{P} = \left(\frac{\partial}{\partial x}\left[D(x,y)\frac{\partial}{\partial x} \right] + \frac{\partial}{\partial y}\left[D(x,y)\frac{\partial}{\partial y} \right] - \frac{\partial}{\partial x}\left[u(x,y) \right] - \frac{\partial}{\partial y}\left[v(x,y) \right] - k \right).$$

Using the central difference approximation for the $\frac{\partial^2}{\partial t^2}, \frac{\partial^2}{\partial x^2}, \frac{\partial^2}{\partial y^2}, \frac{\partial}{\partial x}$, and $\frac{\partial}{\partial y}$ terms and denoting by w^n a vector of w values at all discrete spatial locations at time step n, (13) becomes:

$$\frac{\left(w^{n+1} - 2w^n + w^{n-1} \right)}{\Delta t^2} - \boldsymbol{A} \quad w^n = 0, \qquad n=1,2,\ldots,N_t-1 \tag{18}$$

$$w^{N_t} = e^{kT_{bi}} f_2, \qquad w^0 = 0, \tag{19}$$

where N_t is the number of discrete temporal points used in a marching sequence, $\boldsymbol{A} = \boldsymbol{P}^2$ and P is approximated as:

$$\mathsf{P} = \frac{1}{\Delta x^2}\begin{bmatrix} D_{i+\frac{1}{2},j}+D_{i-\frac{1}{2},j} & -D_{i+\frac{1}{2},j} & & & \\ -D_{i-\frac{1}{2},j} & D_{i+\frac{1}{2},j}+D_{i-\frac{1}{2},j} & -D_{i+\frac{1}{2},j} & & \\ & \ddots & \ddots & \ddots & \\ & & -D_{i-\frac{1}{2},j} & D_{i+\frac{1}{2},j}+D_{i-\frac{1}{2},j} & -D_{i+\frac{1}{2},j} \\ & & & -D_{i-\frac{1}{2},j} & D_{i+\frac{1}{2},j}+D_{i-\frac{1}{2},j} \end{bmatrix} - \frac{1}{2\,\Delta x}\begin{bmatrix} 0 & -u_{i+1,j} & & & \\ u_{i-1,j} & 0 & -u_{i+1,j} & & \\ & \ddots & \ddots & \ddots & \\ & & u_{i-1,j} & 0 & -u_{i+1,j} \\ & & & u_{i-1,j} & 0 \end{bmatrix}$$

$$+ \frac{1}{\Delta y^2}\begin{bmatrix} D_{i,j+\frac{1}{2}}+D_{i,j-\frac{1}{2}} & \cdots & -D_{i,j+\frac{1}{2}} & & & \\ -D_{i,j-\frac{1}{2}} \cdots & D_{i,j+\frac{1}{2}}+D_{i,j-\frac{1}{2}} & \cdots & -D_{i,j+\frac{1}{2}} & & \\ & \ddots & & \ddots & \ddots & \\ & & -D_{i,j-\frac{1}{2}} \cdots & D_{i,j+\frac{1}{2}}+D_{i,j-\frac{1}{2}} & \cdots & -D_{i,j+\frac{1}{2}} \\ & & & -D_{i,j-\frac{1}{2}} \cdots & D_{i,j+\frac{1}{2}}+D_{i,j-\frac{1}{2}} & \end{bmatrix} \tag{20}$$

$$-\frac{1}{2\,\Delta y}\begin{bmatrix} 0 & \cdots & -u_{i,j+1} & & & & \\ u_{i,j-1} & \cdots & 0 & \cdots & -u_{i,j+1} & & \\ & & \ddots & & \ddots & & \ddots \\ & & & u_{i,j-1} & \cdots & 0 & \cdots & -u_{i,j+1} \\ & & & & u_{i,j-1} & \cdots & 0 \end{bmatrix} - k\left[I\right]$$

$D_{i\pm\frac{1}{2},j}$ and $D_{i,j\pm\frac{1}{2}}$ are the interfacial values of D, obtained by using harmonic averaging. $\boldsymbol{P}$ is a $N_g \times N_g$ matrix, where N_g is the number of grid points and $[I]$ is the identity matrix $N_g \times N_g$. In matrix form, equation (18) becomes:

$$\Lambda w = 0 \tag{21}$$

where

$$\Lambda = \begin{bmatrix} -\left(2+\boldsymbol{A}\quad\Delta t^2\right) & I & & & & \\ I & -\left(2+\boldsymbol{A}\quad\Delta t^2\right) & I & & & \\ & & \ddots & \ddots & & \\ & \ddots & & & & \\ & & I & -\left(2+\boldsymbol{A}\quad\Delta t^2\right) & I \\ & & & I & -\left(2+\boldsymbol{A}\quad\Delta t^2\right) \end{bmatrix} \tag{22}$$

is a $N_t\ N_g \times N_t\ N_g$ matrix. It is clear that for 2D problems of moderate size (e.g., $N_g = 20\times20 = 400$) and temporal resolution ($N_t = 10$) the matrices involved are formidable (4000×4000). Once we solved the auxiliary problem and obtained $w(x, y, t)$, to get the solutions sought, we apply

$$C(x,y,t) = e^{-kt}w(x,y,t) \tag{23}$$

4. NUMERICAL CODE TESTING

The 2D *MJBPE* formulation was tested by comparing the backward results obtained to: (i) 2D forward simulation, (ii) 1D backward simulation, and (iii) 1D forward simulation results. The problem solved entails a domain of 12×9 length units in the x and y direction, respectively. The instantaneous concentration release is as described in Equations (2) and (3). There exists also a deterministic heterogeneity in the dispersion coefficient as follows. A vertical strip of 2 length units in width, with a D=0.75 is placed exactly in the middle of the domain and is surrounded by an area, which has a D=0.25. The transport velocity is kept constant at u=0.4 and v=0. The spatial domain is discretized in N_g=108 cells of Δx=Δy=1 length units while the temporal domain is discretized using a Δt=0.02 in 10 successive marches of N_t=5. The forward ADE simulation is run up to time t=T_{ft}=2.0 and this result is assumed as our present day configuration. We also saved the forward results at different snapshots in time and treated these as our exact plume distribution for comparison purposes. 1D simulations are also conducted at the middle transect, that is y=4.5 for testing. Using the *MJBPE*, the concentration configuration at t=T_{ft}=T_{bi} is taken as $f_2(x, y)$. Since in the *MJBBE* method one needs to assume the spatial distribution at t=0 to be equal to zero, the spatial distribution at that time will be impossible to recover. Therefore, in our synthetic examples, we assumed our terminal time to be t=T_{bt}=1 (i.e., the furthest back we can hope to recover is t=1) and there is no recoverable concentration distribution for t<1. In this case, our total time of simulation becomes T_{sim}=T_{bi}-T_{bt}=1. We want to recover the spatial distribution from t=2.0 to t=1.1, which is approximately half of the duration of the forward simulation. Figure 1 depicts these comparisons at t=1.4, that is 60% backwards time, at the middle transect, that is y=4.5 and, despite the minor undershoot of the 2D results at x=4, are considered satisfactory.

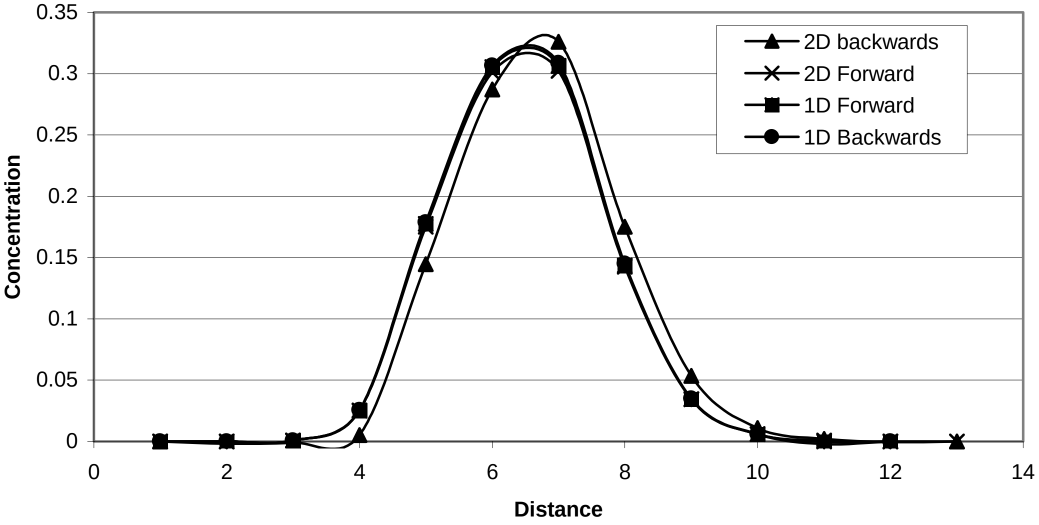

Figure 1. Comparisons of 2D backward, forward, and 1D backward and forward results at t=1.4, that is 60% backwards time.

5. COMPUTATIONAL ISSUES

The two iterative approaches that appear to be most efficient for this type of problem are the Conjugate Gradient Squared (CGS) and Generalized Minimal Residual (GMRES) algorithms (Barrett *et al.*, 1994). Figure 2 presents this comparison in terms of CPU (seconds) and memory (MB) requirements for a variety of problem sizes ranging from N_g=100 and N_t=5 (slightly smaller than the benchmark case presented above) to N_g=625 and N_t=25. All runs have been conducted using a dual processor 700 MHz PC, taking advantage of MATLAB sparse allocation capabilities, where possible. It should be noted that the CPU requirements reported here are for a single matrix equation solution only, which corresponds to one marching sequence of the *MJBPE*. Based on these results it appears that CGS is the favorite not only because of its attractive memory requirements (approximately an order of magnitude less) compared to GMRES, but also its speed (5 times less). However, a closer look at the trend appearing for the very large problems seems to indicate that, provided that memory requirements are of no concern, the GMRES may be an attractive alternative to CGS.

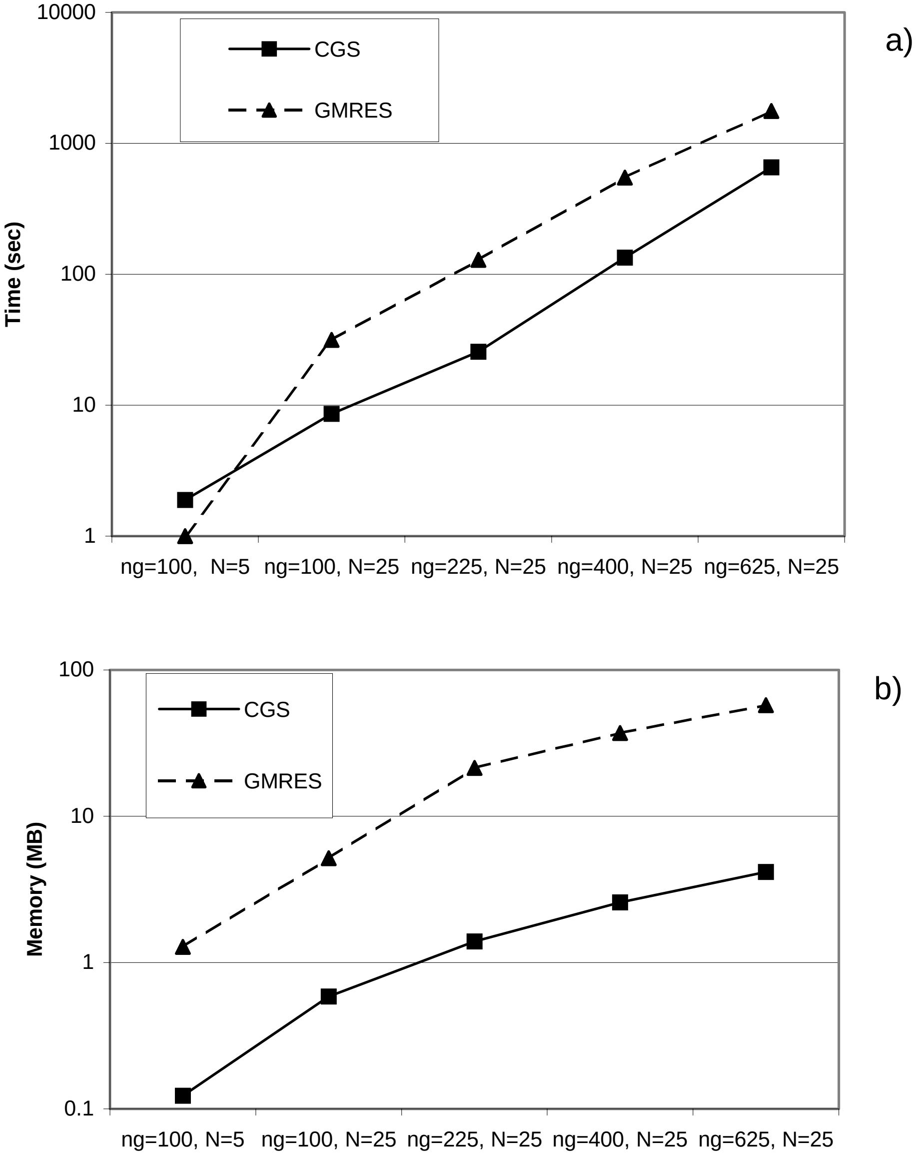

Figure 2. Comparison between GMRES and CGS algorithms in association with the *MJBPE* implementation in terms of a) CPU (seconds) and b) memory (MB) requirements for a variety of problem sizes.

Finally, Figure 3 depicts the convergence residual as a function of the iteration count (N_{it}) for both algorithms for the largest of the problems tested (N_g=625 and N_t=25). Couple of observations can be made. First, GMRES attains the desired convergence criterion (10^{-7}), approaching it at a rate of $(N_{it})^{-0.014}$, which is approximately 2.5 times faster than the corresponding $(N_{it})^{-0.006}$ of CGS. Second, and most importantly, GMRES exhibits a much more stable fluctuation of the residual than CGS. This is particularly important in the problem at hand, for which is almost impossible to estimate the optimal algorithmic parameters *a priori*. This implies that if during the plume recovery process the iteration count threshold were to be exceeded, the *MJBPE* method would possibly proceed to the next time marching period with totally erroneous initial conditions.

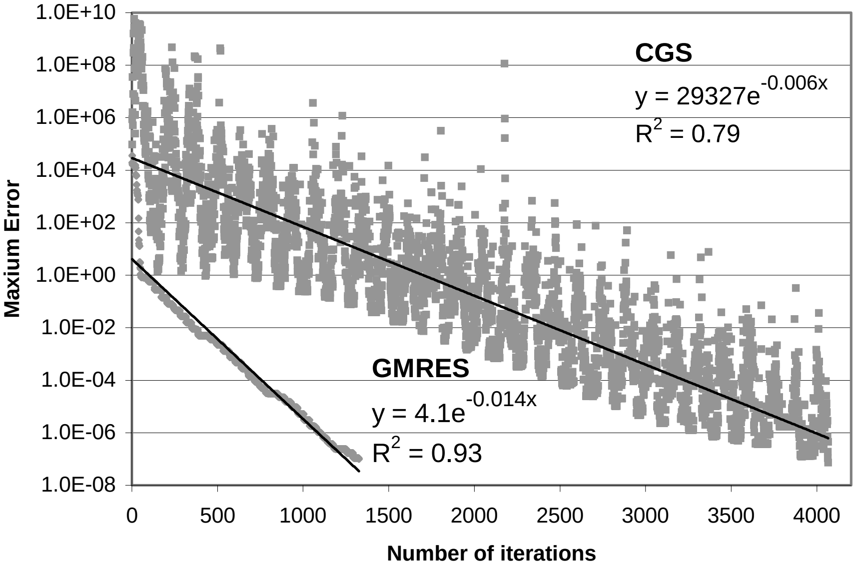

Figure 3. Comparison between GMRES and CGS algorithms in association with the *MJBPE* implementation in terms of the rate with which the iteration residual approaches the convergence criterion.

6. REFERENCES

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