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THREE-DIMENSIONAL D4Z RENUMBERING FOR ITERATIVE SOLUTION OF GROUND-WATER FLOW AND TRANSPORT EQUATIONS

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D4 zigzag (D4Z), previously introduced in two space dimensions, is a renumbering scheme for incomplete LU preconditionings of conjugate-gradient-like iterative solvers for linear systems arising from five-point (seven-point in three dimensions) stencils. Compared to other orderings, it reduces sensitivity of convergence to the sequence of coordinate directions for renumbering in anisotropic media. This paper extends D4Z to three dimensions and demonstrates its insensitive behavior on two test problems.

INTRODUCTION

With increasing frequency, practical applications of models of ground-water flow and transport involve many thousands of discrete finite-difference or finite-element unknowns. In two and especially in three space dimensions, for reasons of computing time and storage, it is often infeasible to solve directly the systems of linear equations that determine these unknowns (or nonlinear iterates of them). Thus, robust, efficient iterative solvers are of considerable and increasing importance. In practice, where there may not be time or expertise to fine-tune algorithm parameters, a robust approach that behaves in an average manner, avoiding worst-case scenarios, is of significant interest.

Due to anisotropies in subsurface formations and to aspect ratios in grid cells, discrete flow coefficients commonly favor one coordinate direction over others. It is well-known that this affects the convergence efficiency of many iterative methods; for example, line successive overrelaxation is motivated by this. However, anisotropies and aspect ratios may be quite heterogeneous, causing methods based on the choice of a preferred direction to be unreliable. Historically, modelers of subsurface flows have found conjugate-gradient-like iterative solvers such as Orthomin, preconditioned by incomplete LU (ILU) decompositions (Meijerink and van der Vorst, 1977), to be more dependable. In this context, directional sensitivity arises more subtly in the preconditioner.

The idea of ILU preconditioning is to apply the conjugate-gradient-like algorithm to the system $\mathbf{MA}x = \mathbf{M}b$, where $\mathbf{A}x = b$ is the discrete system to be solved, $\mathbf{M} = (\mathbf{LU})^{-1} \approx \mathbf{A}^{-1}$, and $\mathbf{L}$ and $\mathbf{U}$ are approximate lower- and upper-triangular factors of $\mathbf{A}$. Since $\mathbf{MA}$ is in some sense close to the identity matrix, the preconditioned iteration should converge more rapidly than the original. Another useful device is a red-black reduction of the original 2-cyclic system, assuming a standard seven-point finite-difference stencil as in the HST3D code (Kipp, 1987) used in this study. This procedure assigns colors in a checkerboard fashion, then numbers all red nodes first, resulting in the block matrix

$$\mathbf{A} = \begin{bmatrix} \mathbf{D}_R & \mathbf{A}_{RB} \\ \mathbf{A}_{BR} & \mathbf{D}_B \end{bmatrix},$$

where $\mathbf{D}_R$ and $\mathbf{D}_B$ are diagonal matrices. Elimination yields the "black matrix"

$$\mathbf{R} = \mathbf{D}_B - \mathbf{A}_{BR}\mathbf{D}_R^{-1}\mathbf{A}_{RB},$$

a matrix with half as many unknowns and enhanced diagonal dominance. These features generally result in still faster preconditioned iterative convergence. This paper considers ILU preconditioning of $\mathbf{R}$ with no added fill, i.e., the nonzero diagonals of $\mathbf{L}$ and $\mathbf{U}$ are limited to those of $\mathbf{R}$, corresponding to ICCG(1,1) in the notation of Meijerink and van der Vorst (1977). The basic iterative procedure is Orthomin(s), in which Orthomin is restarted after every $s + 1$ iterations, i.e., a maximum of s search directions are saved.

ORDERINGS

Without preconditioning, the ordering of the unknowns of $\mathbf{R}$ would not affect the Orthomin iterates. Different orderings yield different ILU factors and hence different preconditioned algorithms. For the reduced matrix $\mathbf{R}$, the simplest ordering, which we denote by RB (red-black), numbers the black nodes in natural order. This was first considered for iterative subsurface-flow computations by Tan and Letkeman (1982). Natural ordering has a clear directional bias, so the alternate diagonal (D4) ordering of the black nodes was proposed as an alternative (Behie and Forsyth, 1984; Eisenstat *et al.*, 1988). In a previous paper (Kipp *et al.*, 1992), we have found that D4 exhibits the same sensitivity to direction as RB in two dimensions. That is, traversing the same D4 diagonal lines in the opposite direction has the same effect as exchanging the primary and secondary directions in the RB ordering.

This can be intuitively understood by examining the (in two dimensions) nine-diagonal $\mathbf{R}$ under RB or D4 ordering, assuming significant anisotropy. Depending on directional choices, the largest off-diagonal elements will be far from the main diagonal (faster convergence) or close to it (slower convergence), in a similar manner for both methods. For details, see Kipp *et al.* (1992), where the two-dimensional alternating

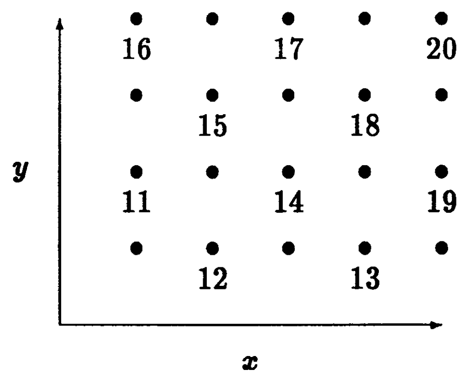

Figure 1: Two-dimensional D4Z ordering for black nodes of 5 × 4 grid.

diagonal zigzag (D4Z) scheme was proposed. This approach reverses direction from one diagonal to the next (see Figure 1), resulting in about the same proximity of large off-diagonal elements to the main diagonal irrespective of directional choices (one could reverse the direction of traverse of all diagonal lines and still have a zigzag pattern). For model problems, the expected insensitivity of D4Z was observed in iteration counts and in the condition numbers and eigenvalue distributions of preconditioned reduced matrices. D4Z iteration counts were near the average of those for different RB and D4 directional choices in cases with at least slight compressibility. D4Z was closer to the slower RB and D4 choices in an incompressible case.

D4Z IN THREE DIMENSIONS

If i, j, k denote coordinate indices, the black nodes in three dimensions are those for which $i + j + k$ is even; denote it by 2ℓ. Diagonal planes are obtained by a constant value $2, 3, 4, \ldots,$ of ℓ. Associated with each plane (value of ℓ) is one of the designations kji,jik,ikj in cyclic order. For example, kji for $\ell = 2$, jik for $\ell = 3$, ikj for $\ell = 4$, kji again for $\ell = 5$, and so on. It remains to describe how each plane is ordered; consider jik for $\ell = 3$ as an illustration. The first index, j, is primary, so the nodes of plane $i + j + k = 6$ are ordered in lines along which j is constant, starting at the maximum value, 4, of j and proceeding in descending order through $j = 3, 2, 1$. The next index, i, is secondary, so it is secondary in lines $j = 4$ and $j = 2$, tertiary in lines $j = 3$ and $j = 1$. Thus, in lines $j = 4$ and $j = 2$, i starts at its maximum and decreases, while in lines $j = 3$ and $j = 1$, k does the same. The resulting zigzag ordering of the nodes (i, j, k) in the plane is shown in Figure 2.

The preceding paragraph describes three possible D4Z orderings of the three-dimensional grid: zyx,yxz,xzy, in which the first plane $\ell = 2$ is designated kji,jik,ikj, respectively (thus we used zyx in the example). Three others (xyz,yzx,zxy) use the designations ijk,jki,kij in an analogous fashion. The same total of six permutations is reached for RB and D4 by choosing a primary, secondary, and tertiary direction in

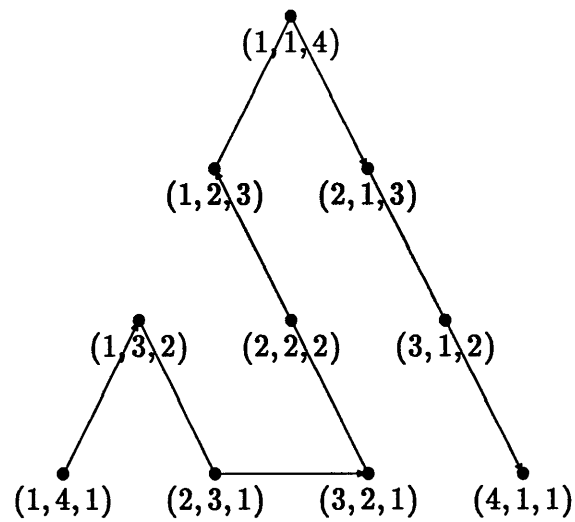

Figure 2: jik zigzag ordering of nodes in plane $i + j + k = 6$

all possible ways.

TEST PROBLEMS

Problem 1 discretizes a 2 m $\times$ 0.2 m $\times$ 2 m region (vertical slab) with a uniform $11 \times 3 \times 11$ point-centered grid (Figure 3 shows boundary conditions). The porosity is 10%, with directional permeabilities 10^{-8}, 10^{-8}, and 10^{-10} m^2. At time zero, with initial hydrostatic equilibrium of fresh water, a pressure increase of 5386 Pa is imposed at the short horizontal column $x = z = 0$, while atmospheric pressure is maintained at $x = z = 2$ m, causing inflow of saline water (density 10% greater than that of the resident fresh water) at $x = z = 0$ and outflow at $x = z = 2$. As time progresses, a plume of dense saline water invades the region. Incompressible and compressible (water compressibility 5×10^{-10} Pa^{-1}, matrix 10^{-8} Pa^{-1}) versions were run. The difference discretizations were centered in both space and time, covering one second in five equal time steps comprising ten linear solutions (two outer Picard iterations per step). The (nonsymmetric) flow and transport equations were solved sequentially; only flow results (totals over the ten linear solutions) are presented because the transport solution was always obtained in one or two Orthomin iterations. The solver was Orthomin(4), with convergence upon reduction of the L^2 norm of the residual by a factor of 10^{-7}.

Problem 2 is a field-scale simulation (see Huyakorn *et al.*, 1987, for further details). The region is 14400 ft $\times$ 9600 ft $\times$ 200 ft with a uniform $62 \times 19 \times 11$ point-centered grid (12,958 nodes). Porosity is 20%; horizontal and vertical hydraulic conductivities are 2000 ft/day and 200 ft/day, respectively. The problem calculates the steady-state response of the aquifer to two pumping wells, respectively screened in the upper and

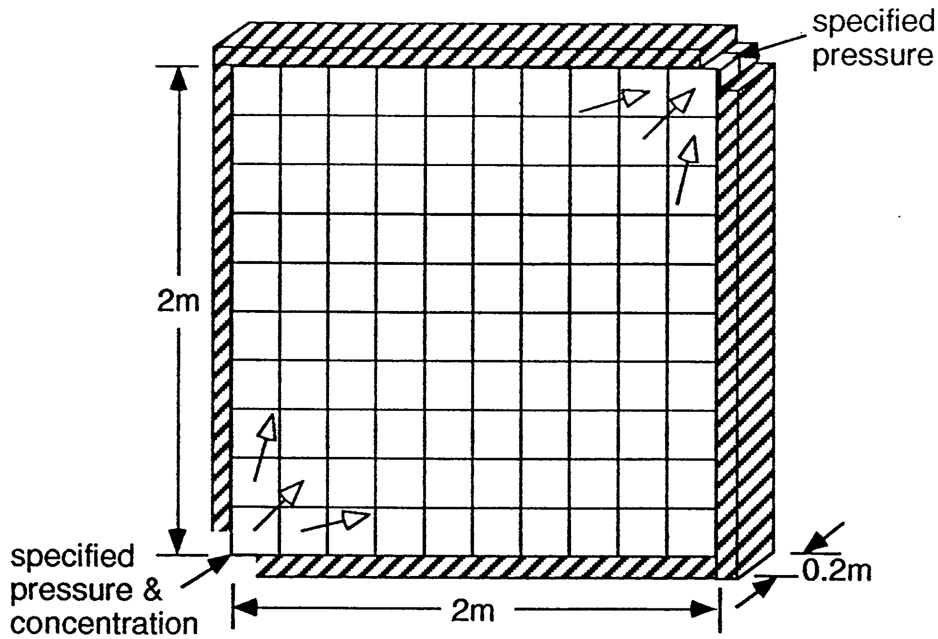

Figure 3: Region and boundary conditions for Problem 1

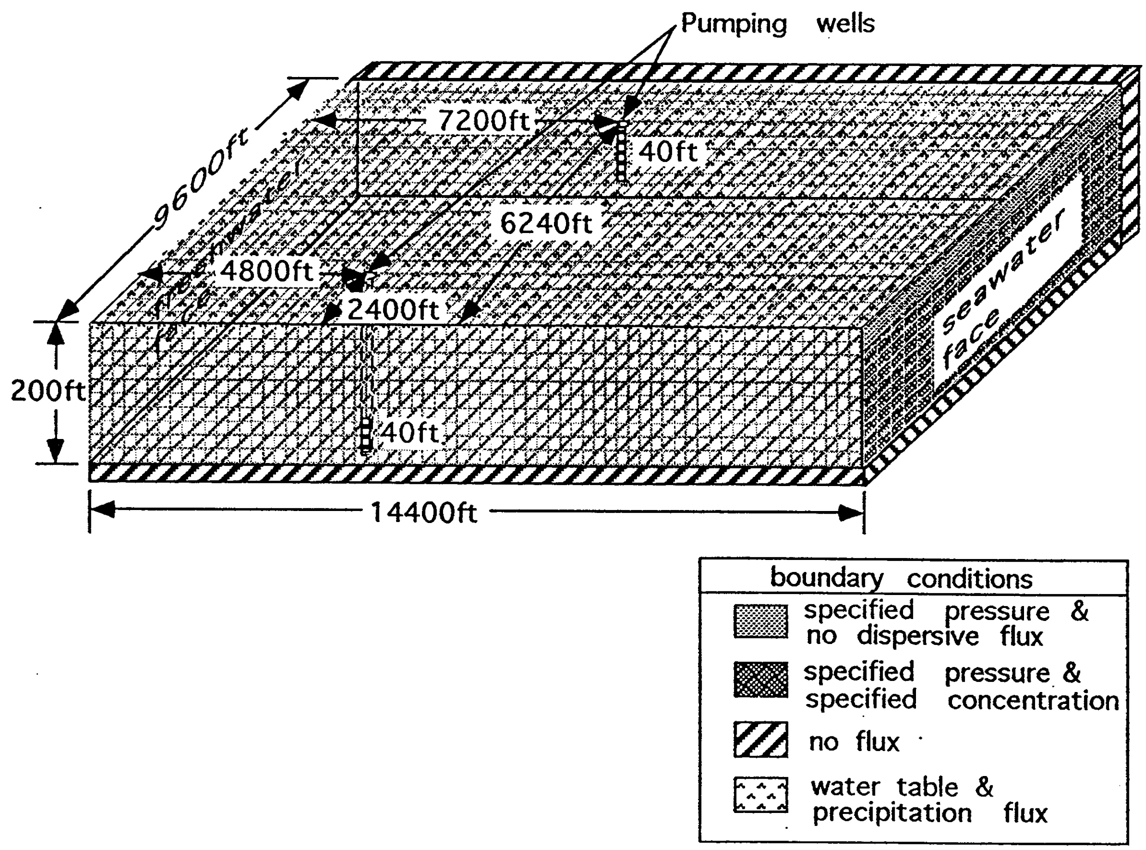

Figure 4: Region and boundary conditions for Problem 2

lower 40 ft and withdrawing water at 0.5×10^6 and 1.0×10^6 ft^3/day. The bottom, north, and south boundaries are impermeable; the west boundary is fresh water with horizontally linear pressure; the east is seawater on the lower 180 ft with no dispersive flux on the upper 20 ft; the top is uniformly recharged at 1 ft/year (see Figure 4). Initial conditions are hydrostatic pressure (uniform horizontally) and fresh water. Again incompressible and compressible (water 3.5×10^{-6} psi^{-1}, matrix 7×10^{-6} psi^{-1}) versions were run. Differencing was upstream in space and backward in time over 25,000 days in 31 time steps (62 outer Picard iterations). Again Orthomin(4) was used, this time with tolerance 10^{-6}.

RESULTS AND DISCUSSION

Results are presented graphically in Figures 5 and 6 for Problems 1 and 2, respectively. In both problems, modified ILU (MILU) preconditioning of the flow equation, where discarded fill-in terms were added to the main diagonal, was tried in the incompressible and compressible versions and was much more efficient than ILU, by factors of 2 to 5. This agrees with earlier experience (Behie and Forsyth, 1984; Eisenstat *et al.*, 1988). The figures present total iteration counts, over all Picard iterations for all time steps, for the incompressible (MILU only, with all three numbering methods) and compressible (MILU only, with RB and D4Z) versions of both problems (MILU was not run with D4 in the compressible case because these results could be expected to duplicate RB based on the incompressible data). In each case, counts for the six ordering permutations determine the representations in the figures. The maximum, minimum, mean, and standard deviation range of the six numbers are depicted. ILU data are not shown, as this would alter the vertical scale. For Problem 1 with ILU, the maximum, minimum, mean, and standard deviation for each method were: RB — 1764, 641, 1182, 561; D4 — 1764, 641, 1182, 561; D4Z — 1380, 1134, 1273, 103. For Problem 2: RB — 5928, 2893, 4370, 1449; D4 — 5928, 2893, 4370, 1449; D4Z — 3784, 3751, 3769, 11. These ILU results are for the incompressible cases only.

It is clear that D4Z is always less sensitive to directional change than RB or D4. The raw numbers show that there is an almost (in some cases, precisely) exact correspondence between iteration counts for RB and D4. As further examples, in incompressible Problem 2 with MILU, both RB and D4 yielded a total of 1110, 1415, 1692, 1880, 1919, and 2050 Orthomin iterations for the six permutations; in incompressible Problem 1 the numbers differed by no more than 2. For the model problem 1, especially with MILU, D4Z is at some disadvantage relative to the average efficiency of the others, though compressibility mitigates this to some extent as observed previously in two dimensions. This makes it very interesting that the disadvantage does not appear in the more practical field problem 2, where D4Z performs in a reliable average manner as intended, and better than average in one case (ILU), even without compressibility. Further study is needed to understand the reasons for this, but it appears that the somewhat pessimistic behavior observed in some model examples may not be relevant in practical cases. The present serial implementation may be parallelizable by incorporating zigzag ordering in recently developed parallel

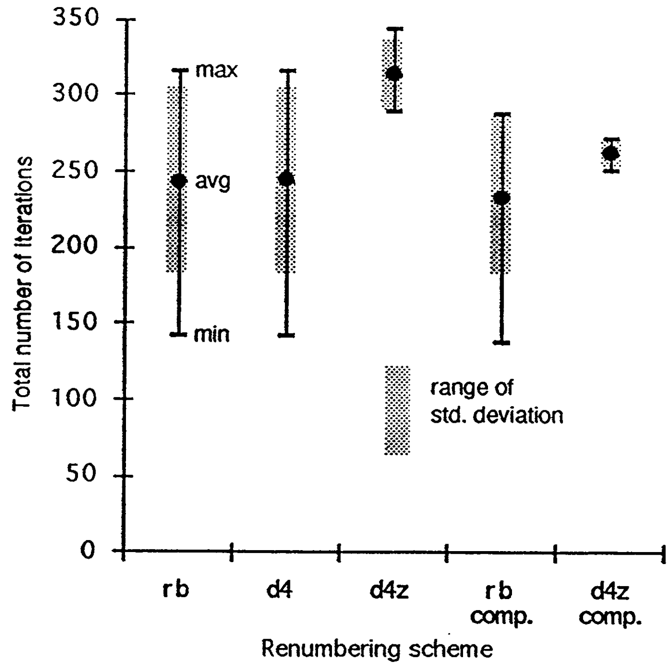

Figure 5: Distribution of iteration counts for directional permutations (Problem 1)

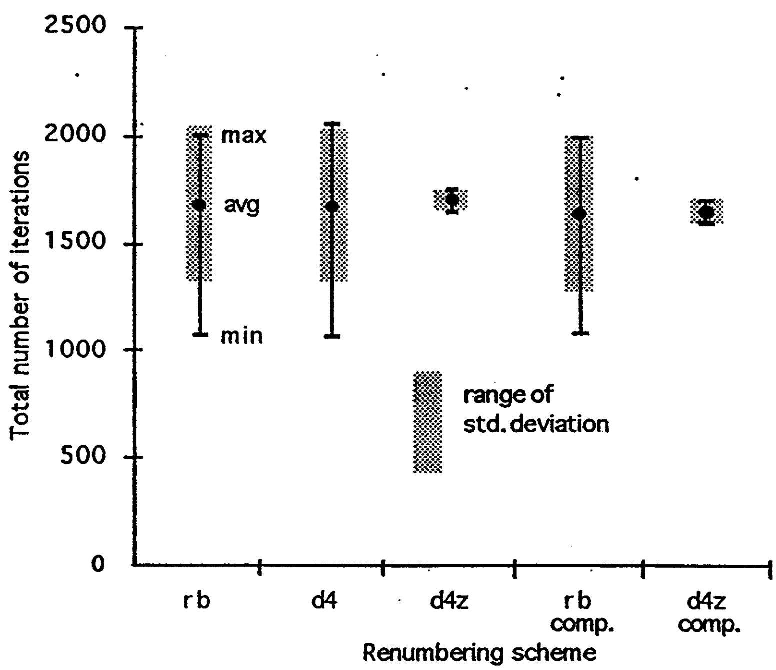

Figure 6: Distribution of iteration counts for directional permutations (Problem 2)

ILU frameworks (Elman and Golub, 1992).

CONCLUSIONS

D4Z has been extended to three-dimensional systems and applied to model and field problems. This renumbering scheme for ILU preconditioners is demonstrably insensitive to directional bias in anisotropic media. This enhances robustness in the sense that worst-case behavior of other approaches is avoided without user intervention or trial runs. The previously observed tendency for D4Z to be slower than the average of other methods in incompressible model problems was not observed in the field cases, where its insensitive performance was average or better. For flow equations, MILU preconditioning was distinctly preferable to ILU.

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