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Iterative solution Techniques in the DRM-MD Approach

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Abstract
The purpose of this work is to analyse the performance of iterative methods for systems arising from the DRM-MD (Dual Reciprocity Method in Multi Domains). Particularly to check over the consistency and well established results yielded by this technique.
To check the results and relative speed the solutions obtained through the chosen iterative methods, are also contrasted against the solutions obtained applying some direct methods, as SVD, Golub's method and Cholesky decomposition. The numerical results are also compared with a benchmark analytical solution.

1 Introduction

Various research has been reported on the behaivour of the system of equations rising from Boundary Element techniques and its solution applying iterative methods.
The matrices of coefficients originated from standard single-zone BEM are, in general, unsymmetric, fully populated and very large. This fact represents a considerable disadvantage when comparing with the classical numerical methods since more computer operations are involved. The algebraic system of equations resulting from DRM in a single domain are large, fully populated and unsymmetric.
Bulgakov et al (1998), showed that the matrices of these systems have properties which allow the efficent use of Krylov iterative solvers like CGS and GMRES methods with Jacobi preconditioning. The

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GMRES method appeared to be more efficient than the CGS method. The same situation is usually observed when solving BEM problems. The multi-zone BEA techniques give rise to overall system matrices that have a blocked, sparse, and unsymmetric character.
Kane et al (1991), and Prassad et al (1994) report for multi-zone problems that they use considerably less storage that single-zone applications. Noting that the performance of the CGN approach was improved by multi-zone modelling, but it did not improve the performance of the GMRES approach. In all cases studied the converged solutions were as accurate as those derived using direct equation. They remarked that for both single-zone and multi-zone problems, the preconditioned iterative approaches were generally faster than the direct methods.
It is also known that matrices resulting from Dirichlet, Neumann or mixed (Robin) boundary conditions present appreciable distinctions, whatever the boundary element technique is applied.
Another boundary element technique, developed by Ramsak and Skerget (1999), based on mixed boundary elements and a subdomain technique yields a final discretised matrix system which is overdetermined and which they solve in a least square sense. Since the resulting system is sparse and block banded, they apply the iterative linear least squares solver by Paige and Saunders, accelerating the convergence through a diagonal preconditioning.

2 DRM-MD

The DRM approach using multi-domain decomposition carry on with the idea of Popov and Power (1999) of improving the DRM in such a way that the proposed numerical scheme will be equivalent to the Green element method, but without the need to resort to cell integration at each element. In the DRM-MD the contour of each subregion is defined in terms of straight lines and at each surface element a linear interpolation function is used in the approximation of the densities of the surface integrals. In this way the influence coefficients of the resulting matrices can be computed analytically.
Besides the quoted difference between the DRM-MD and the GEM, this technique permits the solution of the resulting over-determined system of algebraic equations for the complete set of nodal variables, namely the field variables and their derivatives, without the need of

additional interpolation..

We will introduce the basic concepts of the DRM-MD approach considering the linear convection-diffusion equation, where the transport of a substance with a concentration $c\left[kg\,m^{-3}\right]$ in a compressible or incompressible flow field with variable velocity $\overrightarrow{V}\left[m\,s^{-1}\right]$, with production term $P\left[kg\,m^{-3}\,s^{-1}\right]$, coefficient of diffusion $D\left[m^2\,s^{-1}\right]$ and reaction constant $k\left[s^{-1}\right]$, satisfies the equation

$$D\frac{\partial^2 c}{\partial x_l \partial x_l} - V_l\frac{\partial c}{\partial x_l} - c\frac{\partial V_l}{\partial x_l} + P - kc = 0 \tag{1}$$

In addition, in the case of incompressible flow, the continuity equation

$$\frac{\partial V_l}{\partial x_l} = 0 \tag{2}$$

also has to be satisfied.

To write equation 1 in terms of the Laplacian operator we will write the nonhomogeneous term b as

$$b = \frac{1}{D}\left(V_l\frac{\partial c}{\partial x_l} + c\frac{\partial V_l}{\partial x_l} - P + kc\right) \tag{3}$$

to obtain

$$\frac{\partial^2 c}{\partial x_l \partial x_l} = b \tag{4}$$

From the Green's integral representation formula, we found that the concentration at a point x of the i^{th} subregion bounded by the contour Γ_i that enclose the domain Ω_i, is given by

$$\lambda(x)\,c(x) + \int_{\Gamma_i} q^*(x,y)\,c(y)\,d\Gamma_y - \int_{\Gamma_i} c^*(x,y)\,q(y)\,d\Gamma_y = \int_{\Omega_i} c^*(x,y)\,b(y)\,d\Omega_y \tag{5}$$

for $i = 1, 2, ..., M$, where M is the total number of subregions.Here, $c^*(x,y)$ is the fundamental solution of the Laplace equation given by

$$c^*(x,y) = \frac{1}{2\pi}\ln\frac{1}{r} \tag{6}$$

where r is the distance from the point of application of the concentrated unit source to any other point under consideration, i.e.

$r = |x - y|$, $q(y) = \frac{\partial c(y)}{\partial n}$ and $q^*(x,y) = \frac{\partial c^*(y)}{\partial n}$. It is important to observe that in equation 5 all the integrals are over the contour of the subregion i except for the one corresponding to the term $b(y)$, which represents the sum of the non-homogeneous terms in equation 4.
At each interface, the flux leaving one subregion has to be equal to the flux entering the other. Therefore, it is necessary that the following flux matching conditions hold at the m^{th} interface of the subregions i and $i+1$

$$\left(D\frac{\partial c^i}{\partial n} - c^i V_l^i n_l\right)\Bigg|_m = \left(D\frac{\partial c^{i+1}}{\partial n} - c^{i+1} V_l^{i+1} n_l\right)\Bigg|_m \tag{7}$$

Besides the above conditions, the concentration at each interface needs to be continuous, i.e.

$$c^i|_m = c^{i+1}|_m \tag{8}$$

Each of the local matrix systems, that is for each $i = 1, 2, ..., M$, has to be assembled with its neighbouring systems according to the concentration and flux matching conditions, resulting in this way in an over-determined banded global matrix system.Different schemes proposed in the literature intend to reduce the overdetermined system resulting from a domain decomposition to a closed system. The use of discontinuous elements completly avoids the problem at the expense of obtaining a very large system. For the sake of simplicity, we will consider in this work subregions made up of four linear continuous elements with one internal node each.

In this work we will be using the classical DRM radial funciont $f = 1 + r$.

3 Overview of Iterative Methods

3.1 Conjugate Gradient

The standard form of the conjugate gradient method was first developed in the late 1940s and early 1950s. However the method did not come into widespread use until the early 1970s.
The popularity of the method is due to many factors

(a) It has an optimality over the relevant solution space, which usually means convergence to an acceptable accuracy with far fewer

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steps than the number required for the finite termination property—i.e., it has a relatively high rate of convergence.

(b) The rate of convergence can be much improved with various preconditioning techniques.

(c) The method is parameter-free—i.e., the user is not required to estimate any method parameter.

(d) The short recurrence relation makes the execution time per iteration and the memory requirements acceptable.

(e) The roundoff error properties are acceptable.

By the late 1970s, an extensive search was under way for generalized CG methods that could be applied to nonsymmetric and/or indefinite problems and that possessed all, or most, of these appealing properties.

By the early 1980s new versions of generalized conjugate gradient methods were developed, however, none of the methods for general nonsymmetric problems worked in practice as well as the CG method did for symmetric positive definite problems. However, generalyzed conjugate gradient methods can still work very satisfactorily even for nonsymmetric problems if they are properly preconditioned.

A frequently used version of CG for non-symmetric matrices is CGN wich work with the normal equations and a Krylov subspace based on $[A]^T[A]$. The matrix product $[A]^T[A]$ is purely symbolic, since it is never performed (Kane et al,1991).

3.1.1 Minimization

To find a minimizer of f, we will use an iterative method where at each stage we construct a new *search direction* d^k (which will be conjugately orthogonal to the previous search directions). We compute the local minimizer along this search direction—i.e., given x^k, the approximation at stage k, we compute $\tau = \tau_k$ such that

$$f\left(x^k + \tau d^k\right), \quad -\infty < \tau < \infty$$

is minimized by τ_k and then let

$$x^{k+1} = x^k + \tau_k d^k$$

be the new approximation.

When the search directions are conjugately orthogonal, the residuals (or gradients) become orthogonal to the previous search directions.

This property implies that the method computes the best approximation $x^{k+1} = x^k + d$ of all vectors d in V_k.
The method whereby the search directions are computed is called the *conjugate gradient method.* There is a somewhat simpler, but less efficient, method of computing the minimizer of f, called the *steepest descent* method. In this one the search of a local minimum takes place along the current gradient vector. On the other hand, in teh conjugate gradient method we move along a plane spanned by the gradient at the most recent point and the most recent search direction.

3.2 GMRES

The GMRES iterative method is a projection method based on taking $\mathcal{K} = \mathcal{K}_m$ and $\mathcal{L} = A\mathcal{K}_m$, in which $\mathcal{K}_m$ is the m-th Krylov subspace. Such a technique minimizes the residual norm over all vectors in $x_0 + \mathcal{K}_m$. The implementation of an algorithm based on this approach is similar to that of the full orthogonalization method.
In general the behaviour of GMRES cannot be determined from eigenvalues alone. We do not have simple estimates based on the ratio of largest to smallest eigenvalue to describe the convergence of this method, but a good distribution in the complex plane still applies. Eigenvalues tightly clustered about a single point (away from the origin) are good. Eigenvalues all around the origin are bad (because of the maximum principle) it is impossible to have a polynomial that is 1 at the origin and less than 1 everywhere on some closed curve around the origin.
A difficulty with GMRES is that the number of vectors that needs to be stored increases with the number of steps, and the number of multiplications to be performed is proportional to the square of the number of iterations. A way to amend this drawback is to restart the algorithm every k steps, where k is some fixed integer parameter. Thus, however the new solution vector is calculated only once after k iterations, the residual is being obtained and checked at every iteration. If the residual falls below a certain tolerance, there is no need to continue until the k iterations are performed, and the iteration process is terminated.
When k is set to such a number that convergence occurs before the iteration count reaches this value k, the resulting method is called non-restarting GMRES.

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3.3 LSQR

LSQR is an iterative method for computing a solution x to either unsymmetric equations $Ax = b$ or linear least squares $\min \|Ax - b\|_2$. Developed by Paige and Saunders in 1982, it is based on the bidiagonalization procedure of Golub and Kahan. It is analitically equivalent to the standard method of conjugate gradients, but posseses more favourable numerical properties.
A is a real matrix with m rows and n columns and b is a real vector. It will usually be true that $m \geq n$ and $\text{rank}(A) = n$, but these conditions are not essential.LSQR is similar in style to CG as applied to the least-squares problem. The matrix A is used only to compute products of the form Av and $A^T u$ for various vectors v and u. Hence A will normally be large and sparse or will be expressible as a product of matices that are sparse of have special structure. CG-like methods are most useful when A is well conditioned and has many nearly equal singular values.
LSQR generates a sequence of approximations $\{x_k\}$ such that the residual norm $\|r_k\|_2$ decreases monotonically, where $r_k = b - Ax_k$.
The stopping criteria is set in terms of three dimensionless quantities, which the user is required to specify. These rules are based on allowable perturbations in the data, and in an attempt to regularize ill-conditioned systems.
After having performed various numerical comparisons, the autohrs of LSQR recommend to apply the symmetric CG to the normal equations $A^T Ax = A^T b$ only if it would produce a satisfactory estimate of x in very few iterations. For matrices ill-conditioned, LSQR should be more reliable than least squares adaption of symmetric CG, at the expense of more storage and work per iteration.

3.4 Preconditioning

The use of preconditioners can increase the rate of convergence of iterative solution methods considerably. If C is s.p.d. (in practice an approximation to A), we can let the inner product be defined by C, that is,

$$(x, y) = x^T Cy$$

A preconditioned algorithm minimizes the same functional, $r^T A^{-1} r$, where $r = Ax - b$ as for the unpreconditioned method but on the

Krylov subspace $\left\{r^0, AC^{-1}r^0, ..., \left(AC^{-1}\right)^k r^0\right\}$. With an appropriate preconditioner, this Krylov subspace can generate vectors to minimize $f(x)$ much faster than for the unpreconditioned subspace.
Because of the features of matrices arising from DRM-MD to apply some preconditioners we had to perform some previous partial pivoting to get rid of the zero entries in the main diagonal of the matrix. Even though these permutations often destroy any useful sparsity structure A may have.

4 Matrix Structure in DRM-MD

The governing equation for the case we are presenting in this paper, a one-dimensional convection-diffusion problem with a variable velocity field, is

$$D\frac{d^2c}{dx^2} - \frac{d(V_x c)}{dx} = 0 \tag{9}$$

satisfying the boundary conditions $c(0) = C_0$ and $c(1) = C_1$. The convective velocioty field is

$$V_x = \ln\frac{C_1}{C_0} + k\left(x - \frac{1}{2}\right);\ V_y = 0 \tag{10}$$

corresponding to the flow of a hypotethical compressible fluid with a density variation inversely proportional to the velocity field. The analytical solution of the boundary valued problem for $D = 1\mathrm{m}^2\mathrm{s}^{-1}$ is given by

$$c = C_0 \exp\left\{\frac{k}{2}x^2 + \left(\ln\frac{C_1}{C_0} - \frac{k}{2}\right)x\right\} \tag{11}$$

For the numerical analysis this one-dimensional problem will be considered as two-dimensional in a rectangular domain with dimensions 1×0.7m, with $0 \leq x \leq 1$ and $-0.35 \leq y \leq 0.35$, subject to the following boundary conditions:

$$c(0, y) = C_0 = 300;\ c(1, y) = C_1 = 10 \tag{12}$$

$$\frac{\partial c}{\partial n}|_{y=-0.35} = 0;\ \frac{\partial c}{\partial n}|_{y=0.35} = 0 \tag{13}$$

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As we have stated in section 2 the system we obtain after applying DRM-MD is sparse, banded and overdetermined.

In this numerical implementation we use 80 subdomains, each made of four linear continuous elements with one internal point. The value of the parameter $k = 40$.
The resulting matrix $A\,(400, 343)$ has the following patern:

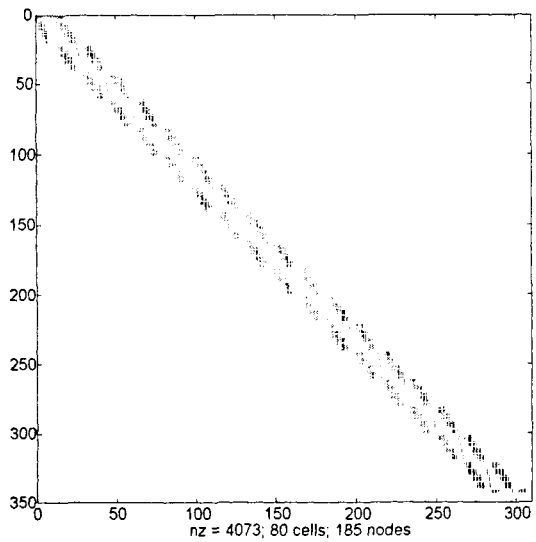


Figure 1: Matrix $A(400, 343)$

with *condition number* =573.77. This matrix was the input for LSQR, CGN, SVD and for Golub's method.
The normal equation $(A^T A)$ was introduced as input for CG, GMRES and Cholesky decomposition.

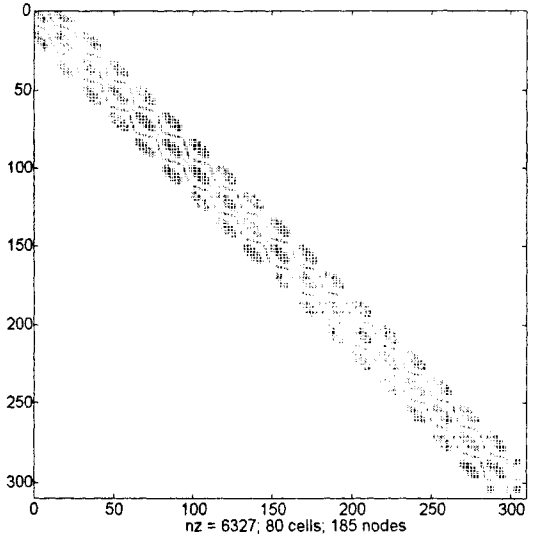


Figure 2: Matrix $A^TA(343, 343)$

with *condition number* =3.29E+05.
It is also presented the distribution of the Singular Values of the rectangular matrix A, and the eigenvalue distribution of A^TA.

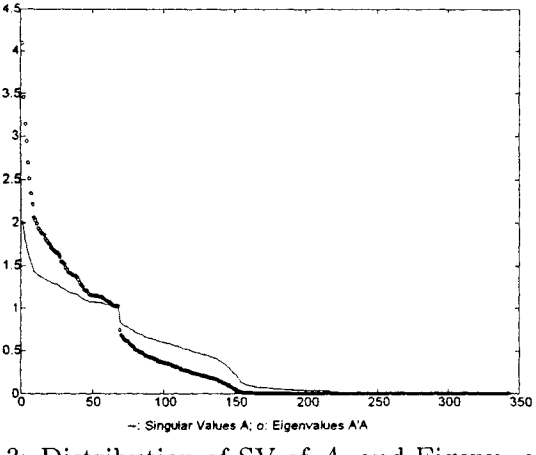


Figure 3: Distribution of SV of A, and Eigenv. of A^TA

And the distribution of the eigenvalues of A^TA with ILU preconditioning.

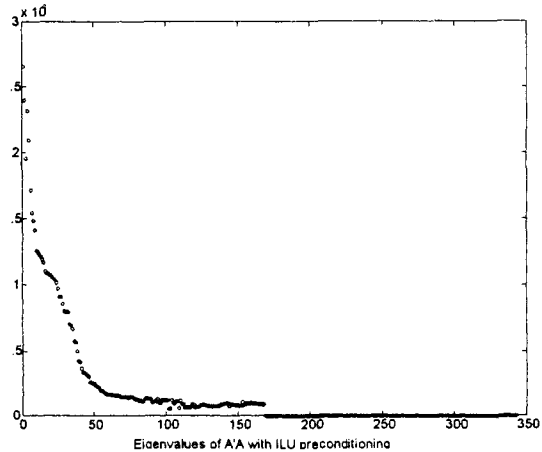


Figure 4: Eigenvalues of A^TA with ILU preconditioning

5 Numerical Results

In order to compare the efficiency of the solutions we present the following tables with the different methods and corresponding preconditioners employed, the number of iterations and the CPU time on a Pentium 120MHz.

Various direct methods have been tested to analyze their performance against the iterative methods described above. We used for that purpose Singular Value Decomposition (SVD) with backsubstitution, Cholesky decomposition and Golub's method (which using Householder transformations works directly with the matrix A and has the advantage that it is considerably more accurate than methods with invert A^TA). Only the results obtained from Golub's method are shown due to the high consuming time of SVD and Cholesky.

When implementing LSQR, was founded that the most efficient results were obtained by scaling the matrix, so that all the columns have the same euclidean norm; instead of using any preconditioner. Consequently we applied the same scaling to the methods whose input was the rectangular matrix, to make the results comparable.

For the CG and GMRES both, diagonal and ILU preconditioning where considered.

Matrix	CPU Time*(sec)*
A	**1.3670E+01**
A-Scale	1.42200E+01
A-Pivot	1.37200E+01
A-Pivot-DiagPrec.	1.39600E+01
A-Pivot-Scale-DiagPrec.	1.44300E+01

Table 1: *Golub's Method.* $CN(A)$=573.7714

Matrix	CPU Time*(sec)*	N_{iter}
A	2.74300E+01	194
A-Pivot	2.73700E+01	193
A-Pivot-DiagPrec.	5.05500E+01	361
A-Scale	**7.97000E+00**	**53**

Table 2: *CGN.* $CN(A)$=573.7714

Matrix	CPU Time*(sec)*	N_{iter}
A^TA	3.550000E+00	824
A^TA-DiagPrec.	1.392000E+01	3082
A^TA-ILUPrecond.	**2.73000E+00**	**343**

Table 3: *Conjugate Gradient Method.* $CN(A^TA)$=3.29E+05

Matrix	CPU Time*(sec)*	N_{iter}
A	1.0490E+01	1162
A-Pivot	1.05100E+01	1159
A-Pivot-Precond(Jac)	5.460000E+00	624
A-Scale	**9.500000E-01**	**100**

Table 4: *LSQR* $CN(A)$=573.7714

Matrix	CPU Time*(sec)*	N_{iter}
A^TA	7.920000E+00	232
A^TA-Diagonal Precond.	1.5000000E+00	76
A^TA-ILU Precond.	**2.30000E-01**	**12**

Table 5: *GMRES Method.* $CN(A^TA)$=3.29E+05

6 Conclusions

Several preconditioned iterative techniques have been presented for solving the linear systems rising from DRM-MD.
The GMRES approach outperformed the various iterative and direct methods applied.

The poor performance of CG and CGN reflects the bad behaviour of these methods when the condition number is big and the eigenvalues are clustered around zero.
LSQR has given accurate results in a few itarations if the matrix is scaled instead of preconditioned.
GMRES was the best performer among the methods studied in both senses, accuracy and efficiency. After ILU preconditioning all the real part of the eigenvalues were positive and well clustered. For the restarted version of GMRES, it was found that the total number of iterations was considerably increased as k was reduced. Better results were obtained when k was set as big as the order of the matrix.

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