On a new preconditioning algorithm for iterative solution of generalized boundary element systems*

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Abstract: In this paper we introduce a new preconditioning algorithm for iterative solution of the generalized boundary element systems for partial differential equations. Sparse preconditioners are first considered for standard boundary element methods and then developed for the generalized boundary element methods (extended dual reciprocity methods). The use of discrete wavelet transforms to accelerate splitting based preconditioners is described. Attempts to compress radial basis matrices are made and new results using compactly supported radial basis functions are obtained. Some numerical results are reported.
Keywords: partial differential equations; generalized boundary element methods; discrete wavelet transforms; dense linear systems; preconditioned iterative methods.

1 Introduction

Various physical problems can be effectively modelled by systems of nonlinear partial differential equations (PDE's). The nonlinearities are usually treated by some kind of linearization methods. Thus numerical solution of linear PDE's is of importance, and remains one of the most active subjects in the mathematical sciences.

Popular numerical methods fall into two main categories, domain type and boundary type. The former includes the familiar methods of finite differences (FDM's), finite elements (FEM's) and finite volumes (FVM's). The latter usually refers to boundary element methods (BEM's). The BEM's, where applicable, have been more advantageous than the former type methods due to dimension reduction and exact representation of exterior boundaries.

However the latter type often cannot compete with the former for two reasons. Firstly, to apply BEM's, the fundamental solution of the underlying differential operator has to

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be available and this restricts the class of PDE's solvable by BEM's. The known solvable PDE's include the Laplace's, Helmholtz and bi-harmonic equations [1, 2]. Secondly, when applicable, the BEM's give rise to dense linear systems in contrast to sparse linear systems that are produced by domain type methods. Nevertheless, recent research advances have come closer to overcome these two problems.

In this paper, we address both of these problems with the emphasis on preconditioners for iterative methods. We shall first review the work on iterative methods with preconditioners to efficiently solve dense boundary element systems. Then we introduce the extended dual reciprocity methods (DRM) [3, 4], generalizing BEM's to solve PDE's previously not applicable. Some recent work on developing iterative methods for DRM solving these problems are presented.

2 Iterative methods for boundary element systems

Let $\Omega \in R^2$ denote a closed domain that may be interior and bounded, or exterior and unbounded, and $\Gamma = \partial\Omega$ be its (finite part) boundary that can be parameterized by $p = (x, y) = (x(s), y(s)), a \le s \le b$. The R^3 case can be studied similarly. Then a boundary integral equation that usually arises from reformulating an applicable PDE in Ω can be written as

$$U(p) - \int_\Gamma \bar{k}(p,q)U(q)dS_q = f(p), \qquad p \in \Gamma, \tag{1}$$

or
$$U(s) - \int_a^b k(s,t)U(t)dt = f(s), \qquad s \in [a,b], \tag{2}$$

or simply
$$(I - \mathcal{K})U = f. \tag{3}$$

Here, if the kernel function $k(s,t)$ is continuous or weakly singular, then operator $\mathcal{K}$ is compact; however, if $k(s,t)$ is strongly singular, $\mathcal{K}$ is no longer compact (see [5]).

To solve the above equation numerically, divide the boundary Γ (interval $[a,b]$) into m boundary elements (non-intersecting subintervals $E_i = [s_{i-1}, s_i]$). On each interval E_i, we may either approximate the unknown u by an interpolating polynomial of order η that leads to a collocation method, or apply a quadrature method (say the Gauss-Legendre rule) of η nodes and weights (w_i's) that gives rise to the Nyström method. Both discretization methods approximate equation (3) by

$$(I - \mathcal{K}_n)u_n = f, \tag{4}$$

where one can write

$$\mathcal{K}_n u = \mathcal{K}_n u_n = \sum_{j=1}^{m} \left[\sum_{i=1}^{\eta} w_i k(s, t_{ji}) u_{ji} \right], \quad u_n(t_{ji}) = U(t_{ji}) = u_{ji}, \quad \text{and} \quad n = m\eta.$$

Here for the collocation method, the weights w_i's come from integration of the basis functions and for simplicity we shall use a sized n vector $\underline{u}$ to denote u_{ji}'s at all nodes.

By collocating equation (4) at all nodes, one obtain a linear system of equations

$$(I - K)\underline{u} = f, \qquad \text{or} \qquad A\underline{u} = f, \tag{5}$$

where matrices K and A are dense and unsymmetric (in general). The conditioning of A depends on the smoothness of kernel function $k(s,t)$.

As far as the iterative solution is concerned, its success, not surprisingly, largely depends on the spectral properties of the integral operator or of the matrices of discrete linear systems. More precisely, if the underlying operator is smooth and compact, iterative methods can be very efficient without preconditioning; see [6] for the use of conjugate gradient normal methods (CGN), and [7, 8] for multigrid methods (MGM).

To state the class of problems, that may be represented by a smooth and compact operator equation and consequently solved by iterative methods, we note that boundary integral equations involve three layer operators: the single layer operator L_s, the double layer operator M_d and the hypersingular operator H_h. For the case of given smooth boundaries, all three operators have the known mapping properties in Sobolev spaces: $H^s(\Gamma) \longrightarrow H^{s+\alpha}(\Gamma)$; $\alpha = -1$ for L_s, $\alpha = 0$ for M_d and $\alpha = +1$ for H_h. Here s is an integer and α is called the index of an (pseudo-differential) operator. $\alpha \leq 0$ corresponds to a compact operator. See [5].

For the case of non-smooth boundaries, only the single layer L_s can be compact. Here preconditioning is required for iterative methods to converge. It have been found that the splitting techniques are effective for both CGN and MGM. See [9, 10, 11, 12].

For the case involving operator H_h, preconditioning is essential for iterative methods to converge. This is because a strong singularity (as $t \to s$) leads to non-compactness of operator $\mathcal{K}$. Some preconditioning techniques are discussed below.

Remark 1 *We remark that for a general unsymmetric matrix, any ideal eigenvalue distribution alone is not sufficient for fast convergence of most iterative solvers; see [13]. Fortunately we found that this can be sufficient for Fredholm integral equations; see [14].*

3 Preconditioning methods for singular problems

Following above discussions of iterative methods, we assume that the underlying integral operator is singular and preconditioning is required. For such systems, there are some notable features e.g. the largest entry occurs at the diagonal and these features will used to construct preconditioners.

For equation (5) i.e. $A\underline{u} = f$, denote a preconditioner by M^{-1}. Then a (left) preconditioned system can be written as $M^{-1}A\underline{u} = M^{-1}f$. In general, two requirements are considered. Firstly a system $Mx = y$ for any vectors x, y should be efficiently solved in less than $O(n^2)$ operations or $O(n)$ operations if a more sophisticated method like the panel clustering is also used. This normally means that M or its inverse must be sparse and so it is natural to seek sparse preconditioners. Secondly the preconditioned matrix

$M^{-1}A$ should possess some better properties than A does, for example, eigenvalues are more clustered. Often we hope the condition number of $M^{-1}A$ will be smaller than that of A. In this sense, the best preconditioner M^{-1} should approach the inverse of A.

3.1 Direct sparse approximations

We review two such methods. The first method, due to [15], constructs M based on an approximation of $A = I - K$. Formally, let $n = \eta m$ with η, m integers. Then from matrix $K = (k_1, k_2, \cdots, k_n)$ of equation (5), construct column vectors by

$$k'_i = \begin{cases} k_i, & \text{if } \ i = \ell\eta, \quad 1 \le \ell \le m, \\ 0, & \text{otherwise,} \end{cases}$$

and define a new matrix by $K' = (k'_1, k'_2, \cdots, k'_n)$. Then use $M = A' = (I + \eta K')$ to define a preconditioner. It may be expected that A' is 'close' to $A = A_n$ because $A' \approx A_m$ which is the corresponding discrete matrix with m nodes. For example, with $n = 9, \eta = m = 3$,

$$M = \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix} = \begin{pmatrix} \times & & \times & & & \times & & & \times \\ & \times & \times & & & \times & & & \times \\ & & \boxed{\times} & & & \boxed{\times} & & & \boxed{\times} \\ & & \times & \times & & \times & & & \times \\ & & \times & & \times & \times & & & \times \\ & & \boxed{\times} & & & \boxed{\times} & & & \boxed{\times} \\ & & \times & & & \times & \times & & \times \\ & & \times & & & \times & & \times & \times \\ & & \boxed{\times} & & & \boxed{\times} & & & \boxed{\times} \end{pmatrix},$$

where each B_{ij} denotes a 3×3 block matrix. Note that $Mx = y$ for $x, y \in R^n$ can be solved in only $(n - m)m$ operations.

The second method, due to [16], constructs matrix M as an approximation of singularities rather than of A. Explicitly from A, $M_{ij} = A_{ij}$ for $|i - j| \le 1$ and $i = 1, \cdots, n$, $M_{1n} = A_{1n}$ and $M_{n1} = A_{n1}$. To illustrate, for $n = 5$, we have $M = LU$ as follows

$$\begin{pmatrix} \times & \times & & & \times \\ \times & \times & \times & & \\ & \times & \times & \times & \\ & & \times & \times & \times \\ \times & & & \times & \times \end{pmatrix} = \begin{pmatrix} P_{1,1} & & & & \\ P_{2,1} & P_{2,2} & & & \\ & P_{3,2} & P_{3,3} & & \\ & & P_{4,3} & P_{4,4} & \\ P_{5,1} & P_{5,2} & P_{5,3} & P_{5,4} & P_{5,5} \end{pmatrix} \begin{pmatrix} 1 & P_{1,2} & & & P_{1,5} \\ & 1 & P_{2,3} & & P_{2,5} \\ & & 1 & P_{3,4} & P_{3,5} \\ & & & 1 & P_{4,5} \\ & & & & 1 \end{pmatrix}.$$

Evidently, $Mx = y$ for $x, y \in R^n$ can be solved in only $O(n)$ operations.

3.2 Direct sparse inverse approximations

An alternative approach is to construct M^{-1} based on approximations to A^{-1} or singular parts of A^{-1}. Here assuming $M^{-1} = [m_1 \ m_2 \ \cdots \ m_n]$, we can solve for M^{-1} by a least

squares process

$$\min_{M^{-1}\in\mathcal{S}} \|AM^{-1} - I\|_F^2 = \sum_{j=1}^{n} \min_{m_j\in S_j} \|Am_j - e_j\|_2^2, \tag{6}$$

where $I = [e_1, \cdots, e_n]$, and $\mathcal{S} = [S_1\ S_2\ \cdots\ S_n]$ is a permissible matrix space. Here it is essential to specify the permissible matrix space as sparse e.g. all matrices which are quasi-tridiagonal. See [14, 17, 18, 19].

3.3 Discrete wavelets accelerations

It is impossible to exhaust all sparse patterns and experiment or analyse them as possible preconditioners. In [14], we recognized that for singular operator equations, most sparse preconditioners admit an operator splitting that determines the effectiveness of preconditioning and further proposed an even simpler and yet more efficient preconditioner.

This work is then combined with discrete wavelets accelerations to perform new operator splittings; see [20]. Let $\mathbf{m}$ be the order of compactly supported wavelets, with $\mathbf{m}/2$ vanishing moments, $n = 2^L$, and τ an integer such that $2^\tau < m$ and $2^{\tau+1} \geq m$. Then a new algorithm accelerating an old splitting preconditioner based algorithm can be stated as follows

Algorithm 1

1. *Decide on a matrix splitting $A = D + C$;*
2. *From D, determine a band-width λ;*
3. *Apply a DWT to $A\underline{u} = f$ to obtain $\widetilde{A}x = z$, with $\widetilde{A} = WAW^T$;*
4. *Apply a permutation (matrix P) to $\widetilde{A}x = z$ to obtain $\widehat{A}x^* = z^*$, with $\widehat{A} = PWAW^TP^T$;*
5. *Select the preconditioner M^{-1} as the inverse of the band-width λ matrix of $\widehat{A}$ to solve $\widehat{A}x^* = z^*$ iteratively.*

Here $W = P_{\tau+1}W_{\tau+1}\cdots P_{L-1}W_{L-1}P_LW_L$ and $P = P_L^TP_{L-1}^T\cdots P_{\tau+2}^TP_{\tau+1}^T$, where each W_ν is a block diagonal and orthogonal matrix, and P_ν a permutation matrix. More precisely, $P_\nu = \begin{pmatrix} \bar{P}_\nu & \\ & I_\nu \end{pmatrix}$ with $\bar{P}_\nu$ a permutation matrix of size $2^\nu = 2^L - k_\nu$, that is, $\bar{P}_\nu = I(1, 3, \cdots, 2^\nu - 1, 2, 4, \cdots, 2^\nu)$, and $W_\nu = \begin{pmatrix} \bar{W}_\nu & \\ & I_\nu \end{pmatrix}$ with an orthogonal (sparse) matrix of size $2^\nu = 2^L - k_\nu$ and I_ν is a unit matrix of size k_ν, with $k_L = 0$ and $k_\mu = k_{\mu+1} + 2^\mu$ for $\mu = L-1, \cdots, \tau+1$.

For instance, with Daubechies' order $\mathbf{m} = 6$ wavelets with $\mathbf{m}/2 = 3$ vanishing moments, we have $W_\nu = \begin{pmatrix} \bar{W}_\nu & \\ & I_\nu \end{pmatrix}$ and

$$\bar{W}_\nu = \begin{pmatrix}
h_0 & h_1 & h_2 & h_3 & h_4 & h_5 & & & & & & \\
g_0 & g_1 & g_2 & g_3 & g_4 & g_5 & & & & & & \\
 & & h_0 & h_1 & h_2 & h_3 & h_4 & h_5 & & & & \\
 & & g_0 & g_1 & g_2 & g_3 & g_4 & g_5 & & & & \\
 & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & & \\
 & & & & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & & \\
 & & & & & & h_0 & h_1 & h_2 & h_3 & h_4 & h_5 \\
 & & & & & & g_0 & g_1 & g_2 & g_3 & g_4 & g_5 \\
h_4 & h_5 & & & & & & & h_0 & h_1 & h_2 & h_3 \\
g_4 & g_5 & & & & & & & g_0 & g_1 & g_2 & g_3 \\
h_2 & h_3 & h_4 & h_5 & & & & & & & h_0 & h_1 \\
g_2 & g_3 & g_4 & g_5 & & & & & & & g_0 & g_1
\end{pmatrix}$$

where the filtering coefficients $\{h_i, g_i\}$ are known to be

$$\begin{aligned}
h_0 &= \left(1 + \sqrt{10} + \sqrt{5 + 2\sqrt{10}}\right)/(16\sqrt{2}), \\
h_1 &= \left(5 + \sqrt{10} + 3\sqrt{5 + 2\sqrt{10}}\right)/(16\sqrt{2}), \\
h_2 &= \left(10 - 2\sqrt{10} + 2\sqrt{5 + 2\sqrt{10}}\right)/(16\sqrt{2}), \\
h_3 &= \left(10 - 2\sqrt{10} - 2\sqrt{5 + 2\sqrt{10}}\right)/(16\sqrt{2}), \\
h_4 &= \left(5 + \sqrt{10} - 3\sqrt{5 + 2\sqrt{10}}\right)/(16\sqrt{2}), \\
h_5 &= \left(1 + \sqrt{10} - \sqrt{5 + 2\sqrt{10}}\right)/(16\sqrt{2})
\end{aligned}$$

and $g_0 = h_5,\ g_1 = -h_4,\ g_2 = h_3,\ g_3 = -h_2,\ g_4 = h_1,\ g_5 = -h_0$. Refer to [21].

As we have used orthogonal wavelet transforms, eigenvalues are unchanged after preconditioning. This is because we can write the inverse of the preconditioner as $M = PW(D + C_1)W^T P^T$ where $A = D + C$ as in Algorithm 1 and matrix D is sparse. Therefore, the new preconditioned system $M^{-1}\widehat{A} = PW(D+C_1)^{-1}AW^T P^T = PW(D+C_1)^{-1}(D + C)W^T P^T = PW\left(I + (D + C_1)^{-1}C_2\right)W^T P^T$, with $C = C_1 + C_2$, spectrally equivalent to matrix $\left(I + (D + C_1)^{-1}C_2\right)$. The acceleration is thus due to making C_2 small and $(D + C_1)$ almost as dense as A. However, as this equivalence is implemented implicitly through the discrete wavelet transforms, our accelerated preconditioner $(D + C_1)^{-1}$ is inexpensive.

4 A class of generalized boundary element methods

Up to now our discussions have been about standard boundary element methods i.e. BEM's for solving a class of special PDE's. Here we shall first review some recent advances in generalizing BEM's to tackle more general PDE's and then discuss iterative solution methods.

4.1 The dual reciprocity method

Consider a linear and inhomogeneous PDE for the unknown $u = u(x, y)$

$$\nabla^2 u + a(x,y)\frac{\partial u}{\partial x} + b(x,y)\frac{\partial u}{\partial y} + c(x,y)u + d(x,y) = 0 \tag{7}$$

which is defined in a 2D domain Ω with the following mixed boundary conditions

$$\begin{cases} u = u_{b1}, & (x,y) \in \Gamma_1, \\ \frac{\partial u}{\partial \mathbf{n}} = q_{b2}, & (x,y) \in \Gamma_2, \end{cases} \tag{8}$$

where $\mathbf{n} = (n_1, n_2)$ is the unit normal pointing to the exterior domain (outward normal) and the boundary is consisted of non-overlapping parts Γ_1 and Γ_2 i.e. $\Gamma = \Gamma_1 + \Gamma_2 = \partial\Omega$.

Rewrite equation (7) as

$$\nabla^2 u = R \tag{9}$$

where the right hand side of (9) is

$$R(u) = -a\frac{\partial u}{\partial x} - b\frac{\partial u}{\partial y} - cu - d. \tag{10}$$

Recall that the function $G^* = G^*(p) = \frac{1}{2\pi}\ln\frac{1}{r}$ is the fundamental solution to the Laplacian operator i.e. $\nabla^2 G^* = -\delta(p - p_0)$ with $p = (x, y)$, $p_0 = (x_0, y_0)$, $r = \|p - p_0\|_2$. Multiplying (9) by G^* and applying Green's second theorem

$$\int_\Omega G^* \nabla^2 u d\Omega = \int_\Omega u \nabla^2 G^* d\Omega + \int_\Gamma \left(G^* \frac{\partial u}{\partial n} - u\frac{\partial G^*}{\partial n} \right) d\Gamma,$$

we obtain (for $p \in \Gamma$)

$$\gamma u(p) + \int_\Gamma (q^* u - G^* q)\, d\Gamma = \int_\Omega R G^* d\Omega \tag{11}$$

where, with θ the interior angle at point p,

$$\gamma = \begin{cases} \frac{\theta}{2\pi}, & p \in \Gamma \quad \text{(Note: } \theta = \pi \text{ at all smooth points)} \\ 1, & p \in \Omega, \end{cases} \tag{12}$$

and $q^* = \frac{\partial G^*}{\partial \mathbf{n}} = \frac{\partial G^*}{\partial r}\frac{\partial r}{\partial \mathbf{n}} = \frac{\partial G^*}{\partial r}(n_1\frac{\partial r}{\partial x} + n_2\frac{\partial r}{\partial y})$.

The central idea of the DRM is to convert the domain integral on the right hand side of (11) into boundary integrals by seeking an approximation

$$R(u) \approx \widehat{R}(u) \equiv \sum_{j=1}^{N} \alpha_j \nabla^2 \widehat{u}_j \tag{13}$$

where functions $\widehat{u}_j(p)$ are analytically known and the coefficient vector $\underline{\alpha} = (\alpha_1,\ \alpha_2,\ \cdots\ \alpha_N)^T$ is determined by

$$R(u_i) = \widehat{R}(u_i), \qquad i = 1, \cdots, N \tag{14}$$

or in matrix-vector notation after defining $f_j(p) = \nabla^2 \widehat{u}_j(p)$, $F_{ij} = f_j(p_i)$, $(\underline{R})_j = R(u_j)$

$$F\underline{\alpha} = \underline{R}. \tag{15}$$

In the above interpolation, a total number of $N = N_b + N_i$ points are selected, with N_b nodes denoted by $p_1, p_2, \cdots, p_{N_b}$ on Γ (in particular the first N_{b1} points are assumed in Γ_1) and N_i internal points $p_{N_b+1}, \cdots, p_{N_b+N_i}$ in Ω. Denote $N_{b2} = N_b - N_{b1}$.

On substituting R by $\widehat{R}$ in (11), a boundary integral equation (BIE) is obtained

$$\gamma u(p) + \int_\Gamma (q^* u - G^* q)\, d\Gamma = \sum_{j=1}^{N} \alpha_j \left[\gamma \widehat{u}_j(p) + \int_\Gamma (q^* \widehat{u}_j - G^* q_j)\, d\Gamma \right] \tag{16}$$

where $q_j = \frac{\partial u_j}{\partial \mathbf{n}}$. Note that $\underline{\alpha}$ is related to the unknown vector $\underline{u} = (u_1,\ u_2,\ \cdots,\ u_N)^T$ through $\underline{R}$.

The BIE (16) can now be discretized by the usual boundary element technique [22], yielding the linear system

$$\mathcal{K}\underline{u} + \mathcal{G}\underline{q} = \mathcal{H}\underline{\alpha} \tag{17}$$

where $\mathcal{K}$ and $\mathcal{H}$ are $N \times N$ matrices, $\mathcal{G}$ is an $N \times N_b$ matrix and $\mathcal{H}$ is known. Note that due to boundary integration, both $\mathcal{K}$ and $\mathcal{G}$ only have N_b nonzero columns (apart from diagonals of $\mathcal{K}$ in the remaining columns).

To impose the boundary conditions, we need to partition the matrices $\mathcal{K}$, $\mathcal{G}$ into block submatrices in long columns and partition the vectors into short vectors, according to the location of interpolation points

$$\mathcal{K} = [\ \mathcal{K}_1 \mid \mathcal{K}_2 \mid \mathcal{M}_3\ ] \qquad \underline{u} = \left(\underline{u}_{b1}^T,\ \underline{u}_{b2}^T,\ \underline{u}_i^T\right)^T$$

$$\mathcal{G} = [\ \mathcal{G}_1 \mid \mathcal{G}_2\ ] \qquad \underline{q} = \left(\underline{q}_{b1}^T,\ \underline{q}_{b2}^T,\ \underline{u}_i^T\right)^T$$

where $\mathcal{K}_1, \mathcal{G}_1$ are of $N \times N_{b1}$, $\mathcal{K}_2$ and $\mathcal{G}_2$ of $N \times N_{b2}$, $\mathcal{M}_3$ of $N \times N_i$, and $\underline{u}_{b1}$ and $\underline{q}_{b1}$ are column vectors of size N_{b1}, $\underline{u}_{b2}$ and $\underline{q}_{b2}$ of N_{b2}, and $\underline{u}_i$ of N_i as before. Note that the first N_b rows of $\mathcal{M}_3$ are zero and the remaining N_i rows form an identity matrix.

For our mixed boundary conditions (8), vectors $\underline{u}_{b1}$ and $\underline{q}_{b2}$ are known. In equation (17), the only unknown quantity regarding the solution is

$$\underline{P} = (\underline{q}_{b1}^T,\ \underline{u}_{b2}^T,\ \underline{u}_i^T)^T$$

after incorporating boundary conditions. Now define the known vector $\underline{g}_m = \mathcal{K}_1 \underline{u}_{b1} + \mathcal{G}_2 \underline{g}_{b2}$ and a new matrix

$$\mathcal{M} = [\ \mathcal{G}_1 \mid \mathcal{K}_2 \mid \mathcal{M}_3\ ],$$

where 'm' in $\underline{g}_m$ indicates that the mixed boundary conditions have been imposed. Then the collocation equation is

$$\mathcal{M}\underline{P} = \mathcal{H}\underline{\alpha} + \underline{g}_m. \tag{18}$$

To relate $\underline{\alpha}$ to $\underline{P}$, we need to specify $\widehat{u}_j$'s in (13). In the original work of [4], the following is suggested

$$\widehat{u}_j = \frac{r_j^{k+2}}{(k+2)^2} \qquad \text{for } k \geq 0,$$

and in particular a simple choice is recommended

$$\widehat{u}_j = \frac{r_j^2}{4} + \frac{r_j^3}{9}.$$

As function R from (13) is approximated by basis functions $\{f_1(p),\ f_2(p),\ \cdots,\ f_N(p)\}$, we now consider an approximation of individual terms in R by this basis in order to relate $\underline{\alpha}$ to $\underline{P}$. Firstly consider

$$u \approx \widehat{u} = \sum_{j=1}^{N} \beta_j f_j(p) \qquad \text{with } F\underline{\beta} = \underline{u},$$

where $(\underline{\beta})_j = \beta_j$. Secondly consider related approximations

$$\begin{array}{lll} \frac{\partial u}{\partial x} \approx \frac{\partial \widehat{u}}{\partial x} = \sum_{j=1}^{N} \beta_j \frac{\partial f_j(p)}{\partial x} & \text{with} & \frac{\partial F}{\partial x}\underline{\beta} = \frac{\partial \underline{u}}{\partial x}, \\ \frac{\partial u}{\partial y} \approx \frac{\partial \widehat{u}}{\partial y} = \sum_{j=1}^{N} \beta_j \frac{\partial f_j(p)}{\partial y} & \text{with} & \frac{\partial F}{\partial y}\underline{\beta} = \frac{\partial \underline{u}}{\partial y}, \end{array}$$

where $(\frac{\partial F}{\partial x})_{ij} = \frac{\partial f_j(p_i)}{\partial x}$ and $(\frac{\partial \underline{u}}{\partial x})_j = \frac{\partial u}{\partial x}(p_j)$ and so on.

Combining the above relations and noting $\underline{R} = F\underline{\alpha}$, we can obtain

$$F\underline{\alpha} = -\left(A\frac{\partial F}{\partial x} + B\frac{\partial F}{\partial y}\right)\underline{\beta} - C\underline{u} - \underline{d} \tag{19}$$

or

$$\underline{\alpha} = -F^{-1}\left(A\frac{\partial F}{\partial x} + B\frac{\partial F}{\partial y}\right)F^{-1}\underline{u} - F^{-1}C\underline{u} - F^{-1}\underline{d}, \tag{20}$$

where $\underline{d}$ is a column vector of size N and A, B, C are all $N \times N$ diagonal matrices with $\underline{d}_i = d(p_i)$ and $A_{ii} = a(p_i)$ etc.

We now consider the relation between $\underline{u}$ and $\underline{P}$, before relating $\underline{\alpha}$ to $\underline{P}$. From the decomposition

$$\underline{u} = \begin{pmatrix} \underline{u}_{b1} \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ \underline{u}_{b2} \\ \underline{u}_i \end{pmatrix}, \qquad \text{and} \qquad \underline{P} = \begin{pmatrix} \underline{q}_{b1} \\ \underline{u}_{b2} \\ \underline{u}_i \end{pmatrix},$$

we can write

$$\underline{u} = \begin{pmatrix} \underline{u}_{b1} \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 & \\ & I_{i*} \end{pmatrix} \underline{P}, \tag{21}$$

where the first term is known and I_{i*} is the identity matrix of size $i^* = N_{b2} + N_i$. To isolate the unknown in $\underline{\alpha}$ from (20), we need the partition

$$C = \begin{pmatrix} C_{b1} & \\ & C_{i*} \end{pmatrix},$$

where C_{b1} is the first block diagonal of matrix C sized N_{b1} and C_{i*} the second diagonal of C sized N_{i*}. Thus we are in a position to rewrite (19)-(20) respectively as

$$F\underline{\alpha} + \left(A\frac{\partial F}{\partial x} + B\frac{\partial F}{\partial y}\right)\underline{\beta} + \begin{pmatrix} 0 & \\ & C_{i^*} \end{pmatrix}\underline{P} = -\begin{pmatrix} C_{b1}\underline{u}_{b1} \\ 0 \end{pmatrix} - \underline{d} \tag{22}$$

and

$$\underline{\alpha} = -F^{-1}\left(A\frac{\partial F}{\partial x} + B\frac{\partial F}{\partial y}\right)F^{-1}\begin{pmatrix} 0 & \\ & I_{i^*} \end{pmatrix}\underline{P} - F^{-1}\begin{pmatrix} 0 & \\ & C_{i^*} \end{pmatrix}\underline{P} + \widetilde{\underline{d}}, \tag{23}$$

where vector $\widetilde{\underline{d}}$ contains only known quantities

$$\widetilde{\underline{d}} = -F^{-1}\left(A\frac{\partial F}{\partial x} + B\frac{\partial F}{\partial y}\right)F^{-1}\begin{pmatrix} \underline{u}_{b1} \\ 0 \end{pmatrix} - F^{-1}\begin{pmatrix} C_{b1}\underline{u}_{b1} \\ 0 \end{pmatrix} - F^{-1}\underline{d}.$$

Finally, combining (23) and (18), we obtain a linear system for unknown $\underline{P}$

$$\widehat{\mathcal{M}}\underline{P} = \widehat{\underline{d}} \tag{24}$$

where $\widehat{\mathcal{M}} = \mathcal{M} + \mathcal{S}_m$, $\widehat{\underline{d}} = \underline{g}_m + \mathcal{H}\widetilde{\underline{d}}$, and

$$\mathcal{S}_m = \mathcal{H}F^{-1}\left[(A\frac{\partial F}{\partial x} + B\frac{\partial F}{\partial y})F^{-1}\begin{pmatrix} 0 & \\ & I_{i^*} \end{pmatrix} + \begin{pmatrix} 0 & \\ & C_{i^*} \end{pmatrix}\right].$$

Remark 2 *Matrix $\mathcal{S}_m$ from the present DRM contains the explicit inverse of matrix F, which is of the size $N \times N$ as large as the underlying problem. Thus direct solution can be expensive for large N and furthermore direct application of iterative methods for (24) is difficult.*

4.2 The extended method

The functions $\widehat{u}_j$ introduced above involve the distance functions with distinct points p_j with $j = 1, \cdots, N$. These belong to a large class of functions often called the *radial basis functions* (RBF's); see [23]. Recently this fact has been recognized and several

papers have used other RBF's to extend the DRM. One example is the so-called thin plate splines function with

$$\widehat{u}_j = 2[(k+1)\log(r_j) - 1]\frac{r_j^{2k+2}}{(2k+2)^3}.$$

See [2, 24] for more examples.

4.3 Some convergence results

Despite a number of successes in applying the DRM and its variants to solve various PDE's, a complete convergence analysis of the method is still missing. Recently, we have done an analysis of the DRM for the Poisson's equation [25]. Our main result states that for thin plate splines (with $\rho_d = 2$), the DRM error satisfies

$$\|u - u_h\|_{L^2(\Omega)} \leq C_d h_d^{\rho_d} + C_b h_b^{\rho_b}$$

where C_d, C_b are generic constants, h_d and h_b are respectively domain and boundary step lengths, and ρ_b is the order of boundary elements (say 2 for quadratic elements). For the linear RBF as in [4], $\rho_d = 3/2$ and so linear elements are adequate ($\rho_b = 1$).

4.4 Test examples

We select two linear PDE's as test problems

Problem 1: $\Omega_1 = [0,1] \times [0,1]$ — a unit square

$$\nabla^2 u - v\frac{\partial u}{\partial x} + \alpha^2\left(1 - e^{(x-1)v}\right)\sin(\alpha y) = 0,\ p = (x,y) \in \Omega_1;$$

Problem 2: Ω_2 — an ellipse of axis length 2×1

$$\nabla^2 u + v_2^2\frac{\partial u}{\partial x} - v_1^2\frac{\partial u}{\partial y} + k^2 u - kv_1v_2\left(v_2\cos(kx) + v_1\sin(ky)\right) = 0,\ p = (x,y) \in \Omega_2,$$

where we take $v = 15, \alpha = 1.5\pi,\ v_1 = 1,\ v_2 = 0.5,\ k = 0.25$. To test the accuracy of the DRM, we shall compare to the exact solutions $u = (1 - e^{(x-1)v})\sin(ky)$ (Problem 1) and $u = v_1\sin(kx) + v_2\cos(ky)$ (Problem 2).

For both the internal nodes (N_i) and boundary nodes (N_b), we choose an uniform distribution. For the boundary elements, we use the piecewise linears for approximating both u and q. As this preliminary work is to establish trends of iterative methods, we only take a relatively large tolerance $TOL = 10^{-3}$ for all of our experiments.

To compare the influence of RBF's on the convergence of the DRM, we have considered the following (referred as **RBF1**, **RBF2**, **RBF3**, **RBF4** respectively)

1. **Linear RBF**. $\widehat{u}_j = \frac{r_j^2}{4} + \frac{r_j^3}{9}$ and $f_j = 1 + r_j$.

Table 1: Convergence results for the standard DRM (**RBF4**)

Problem	Method	N	N_b	N_i	Steps	Er
1	CGN	32	16	16	20	1E-2
		128	64	64	33	9E-3
		256	112	144	65	3E-3
	GMRES(5)	32	16	16	9	1E-3
		128	64	64	*	*
		256	112	144	*	*
2	CGN	32	20	12	9	8E-3
		128	68	60	10	7E-4
		256	132	124	10	4E-3
	GMRES(5)	32	20	12	9	8E-3
		128	68	60	3	4E-4
		256	132	124	3	2E-4

2. **Thin-plate spines RBF**. $\widehat{u}_j = [2\log(r_j) - 1]\frac{r_j^4}{32}$ and $f_j = r_j^2\log(r_j)$.
3. **Inverse multi-quadric RBF**. $\widehat{u}_j = \sqrt{c_o^2 + r^2} + c_o * \left(\ln(2c_o/(c_o + \sqrt{c_o^2 + r^2})) - 1\right)$ and $f_j = 1/\sqrt{c_o^2 + r^2}$.
4. **Compactly supported RBF of Wendlend [26]**. $f_j = (1 - r_j/\delta_o)_+^4(4r_j/\delta_o + 1)$ and $\widehat{u}_j = r_j^2\,(1/4 - 5/8(r_j/\delta_o)^2 + 4/5(r_j/\delta_o)^3 - 5/12(r_j/\delta_o)^4 + 4/49(r_j/\delta_o)^5)$.

Here the constants are specified as $c_o = 100$ and $\delta_o = 0.1$.

4.5 Iterative methods

One can observe that the matrix $\widehat{M}$ in the above DRM method (24) is consisted of an usual contribution from boundary integral operators plus that from low order differential operators. As we have remarked, the formulation is not suitable to apply iterative methods because one inversion is already needed.

However to gain some insights of the behaviour of the coefficient matrix $\widehat{M}$, we now consider the use of two iterative solvers: CGN and the generalized minimal residual method GMRES(k); see [13].

As the present work is our first attempt of using iterative methods and no other work has been reported as far as we are aware of, we shall take a relatively small tolerance $TOL = 10^{-3}$ for testing residuals. Our first observation is that both iterative methods (CGN and GMRES(5)) do not converge for tests using **RBF1–3**. However, convergence has been achieved with using **RBF4**. For this case, in Table 1, the number of iteration steps ('Steps') and the residual error ('Er') are presented for the two test problems in §4.4 respectively. Here '*' denotes no convergence.

Clearly it can be seen that both iterative methods only work well in certain cases. This suggests that preconditioning is in general needed.

5 An inversion free variant of the DRM

Guided by previous experiments, we hope to construct some suitable preconditioners. However, as mentioned in Remark 2, equation (24) containing explicit inverse of F is not appropriate for iterative methods. Here we first consider a reformulation of (24) and then discuss possible preconditioners.

5.1 Reformulation of the DRM

Below we propose a new inversion free variant of the method, which is more efficient and opens up the possibility of developing suitable iterative methods.

To avoid the presence of F^{-1}, we must treat $\underline{\alpha}$ and $\underline{\beta}$ as direct unknowns in addition to $\underline{P}$. For this purpose, we define a new augmented unknown vector as

$$\widehat{\widehat{P}} = \begin{pmatrix} \underline{P} \\ \underline{\alpha} \\ \underline{\beta} \end{pmatrix}.$$

Then we propose to solve the main DRM equation (18), together with (22) and the following (from (21))

$$F\underline{\alpha} - \begin{pmatrix} 0 & \\ & I_{i*} \end{pmatrix} \underline{P} = \begin{pmatrix} \underline{u}_{b1} \\ 0 \\ 0 \end{pmatrix}.$$

The combined equations can be written in a compact form

$$\widehat{\widehat{\mathcal{M}}}\widehat{\widehat{P}} = \widehat{\widehat{d}}, \tag{25}$$

where

$$\widehat{\widehat{\mathcal{M}}} = \begin{pmatrix} \mathcal{M} & -\mathcal{H} & 0 \\ \begin{pmatrix} 0 & \\ & C_{i^*} \end{pmatrix} & F & A\frac{\partial F}{\partial x} + B\frac{\partial F}{\partial y} \\ \begin{pmatrix} 0 & \\ & -I_{i^*} \end{pmatrix} & 0 & F \end{pmatrix} \quad \text{and} \quad \widehat{\widehat{d}} = \begin{pmatrix} \underline{g}_m \\ -\underline{d} - \begin{pmatrix} C_{b1}\underline{u}_{b1} \\ 0 \end{pmatrix} \\ \begin{pmatrix} \underline{u}_{b1} \\ 0 \end{pmatrix} \end{pmatrix}.$$

Here the new coefficient matrix is of size $3N$.

Remark 3 *For many commonly used RBF's, it is known that $det(F) \neq 0$; see [23]. The usual sufficient conditions are that all N nodes are distinct and not on the same line (or plane in 3D). From this fact, we can immediately show that*

$$det(\widehat{\widehat{\mathcal{M}}}) = \ det(F)^2 \ det\left(\widehat{\mathcal{M}}\right).$$

The proof follows from the following property: for a block 2×2 *matrix* X *(refer to [27, p164]), whenever* $det(X_{22}) \neq 0$,

$$det \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} = det(X_{22}) det(X_{11} - X_{12} X_{22}^{-1} X_{21}).$$

5.2 Direct solver for the reformulated equation

By a simple inspection of (25), we can claim that its direct solution would cost less than that of (24). This is because the zero matrix blocks in (25) can be avoided.

More precisely, we introduce the block permutation matrix (with identity matrix $I_{N \times N}$)

$$Q = \begin{pmatrix} & & I \\ & I & \\ I & & \end{pmatrix}. \tag{26}$$

Then apply it to (25) giving

$$Q \widehat{\widehat{\mathcal{M}}} Q^T (Q \hat{\hat{P}}) = Q \hat{\hat{d}}, \tag{27}$$

where

$$Q \widehat{\widehat{\mathcal{M}}} Q^T = \begin{pmatrix} F & 0 & \begin{pmatrix} 0 & \\ & -I_{i^*} \end{pmatrix} \\ A \frac{\partial F}{\partial x} + B \frac{\partial F}{\partial y} & F & \begin{pmatrix} 0 & \\ & C_{i^*} \end{pmatrix} \\ 0 & -\mathcal{H} & \mathcal{M} \end{pmatrix}.$$

As known, the inverse of a full $N \times N$ matrix requires at least $2N^3$ operations and a direct elimination method (based on LU factorization) requires $2N^3/3$ operations. To work out $\mathcal{S}_m$ in the standard DRM (24), 3 full matrix to matrix multiplications are needed. Therefore the cost of the standard DRM by the direct method is approximately $2N^3 + 3N^3 + 2/3N^3 = 6N^3$.

The inversion free form (25) of the DRM only requires about $3 \cdot 2N^3/3 = 2N^3$ operations for a direct solution and therefore the reformulated system only costs about $1/3$ as much as the standard version; this saving has been confirmed by experiments. Obviously the primary aim of our new formulation (25) is to assist the development of fast iterative methods — this is the topic of next section.

Remark 4 *For the eigenvalue problem with a Helmholtz equation, a related inversion free method of the DRM can be found in [28], although some inversion is still needed for the case of mixed boundary conditions.*

5.3 Iterative methods for the reformulated equation

We have used both iterative methods CGN and GMRES(k) for solving problems in §4.4. Consistent with observations of §4.5, no convergence was obtained when RBF's $1-3$ were

Table 2: Convergence results for the new DRM (**RBF4**)

Problem	Method	N	N_b	N_i	Steps	Er
2	CGN	32	20	12	9	8E-3
		128	68	60	14	1E-4
		256	132	124	10	4E-4
	GMRES(5)	32	20	12	12	1E-2
		128	68	60	4	8E-4
		256	132	124	3	4E-4

used. Different from §4.5, no convergence was observed for problem 1 for both iterative methods.

However, for problem 2 with RBF 4, some convergent results are obtained as shown in Table 2. Overall, the experiments suggest that preconditioning is needed in general.

5.4 Preconditioning for the reformulated equation

As the coefficient matrix from the reformulated equation (25) is not entirely related to integral operators, a simple splitting (to construct preconditioners) is no longer meaningful. So we consider the use of discrete wavelet transforms (DWT's) for designing preconditioners.

For the same reason, the DWT's may not compress the full matrix of size $3N$; in fact our other experiments have confirmed this. Therefore we have turned to block DWT's of the following form

$$B = \begin{pmatrix} W & & \\ & W & \\ & & W \end{pmatrix}, \tag{28}$$

where W is the usual DWT matrix of size N as in §3.3. By studying the sparsity of the DWT compressed matrix, we observed that the first leading submatrix block of size N was well compressed while the other blocks (mainly diagonal blocks F) did not compress well.

Thus we have considered the isolated problem of compressing matrix F alone. Extensive experiments have shown that F cannot be compressed well unless the underlying RBF basis is compactly supported. This may be due to the fact that F, though nonsingular, is ill-conditioned and its columns / rows do not show obvious periodic behaviour. This set of experiments on the compression of F may have explained the reason why convergence of the standard iterative methods was only observed with the use of RBF 4 – the compactly supported RBF. In what follows we shall restrict our attention to the case of RBF 4 which was due to [26].

Our strategy is to use block DWT's (28) to compress matrix $\widehat{\widehat{\mathcal{M}}}$ and then construct a preconditioner based on a block band form of the compressed matrix. The semi-band

Table 3: Convergence results of Algorithm 2

Problem	LEV	N	N_b	N_i	Steps	Er
1	3	32	16	16	3	8E-5
		128	64	64	2	9E-7
		256	112	144	3	1E-9
2	3	32	20	12	3	8E-4
		128	68	60	3	4E-5
		256	132	124	3	1E-4

width of each block is taken as $b_s = N/4$ to mimic the efficiency of a two grid method. This approach can be summaried as follows

Algorithm 2

1. *Apply a block DWT (28) to equation (25) with a fixed wavelet level (depth) LEV;*
2. *Extract the band matrix* $\mathbf{M}$ *from the compressed matrix* $B\widehat{\widehat{\mathcal{M}}}B^T$ *with semi-band width* $b_s = N/4$*;*
3. *Apply GMRES(k) to the preconditioned equation* $\mathbf{M}^{-1}\left(B\widehat{\widehat{\mathcal{M}}}B^T\right)\ \widehat{\widehat{P}} = \mathbf{M}^{-1}B\widehat{\widehat{d}}.$

Experimental results using Algorithm 2 are presented in Table 3, where the GMRES(5) and Daubechies' order 4 wavelets are used.

The results in Table 3 have clearly improved those of Tables 1-2. These results appear to be the first success in an efficient solution of the DRM by iterative methods. More theoretical questions need still be addressed and tests carried out.

6 Conclusions

The boundary element method, applicable to a restricted class of partial differential equations, gives rise to dense linear systems. In this paper we have surveyed some recent developments in preconditioned iterative methods for such systems.

A generalized boundary element method based on the DRM, applicable to a wide class of partial differential equations, is described and the algebraic structures of the method are detailed for a general mixed boundary condition. An inversion free variant of the DRM is proposed here for the first time, which allows for faster solutions by either direct or iterative methods. For the new inversion free variant, we have proposed a block preconditioner based on block discrete wavelet transforms which efficiently solves the dense linear system.

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Nomenclature

A	coefficient matrix of size n or N
$\underline{\alpha}$	unknown vector of size N, relating to R
$\underline{\beta}$	unknown vector of size N, relating to u
$\underline{\widehat{d}}$	Right hand side vector of the standard DRM
f_j	radial basis function (known) for u, relating to $\widehat{u}_j$
F	interpolation matrix of radial basis functions of size N
$\Gamma,\ \Gamma_1,\ \Gamma_2$	boundary of Ω, part 1 and 2 of boundary Γ
G^*	fundamental solution of the Laplace operator
$H^s(\Gamma)$	Sobolev spaces of integer order s, for functions defined on the boundary Γ
$I,\ I_\nu$	identity matrix of size N or size k_ν
i^*	integer $N_{b2}+N_i$, part of $\underline{P}$ relating u
$L^2(\Omega)$	L^2 space for functions defined in Ω
M^{-1}	preconditioner of size n or N
$\mathbf{M}^{-1}$	preconditioner of size $3N$
$\mathcal{M}$	matrix from discretizing the Laplace operator
$\widehat{M}$	denotes $\mathcal{M}+\mathcal{S}_m$, coefficient matrix $(N\times N)$ of the standard DRM
$\widehat{\widehat{M}}$	coefficient matrix $(3N\times 3N)$ of the new DRM variant
n	size of matrix A
$\mathbf{n}$	exterior normal vector
N	size of matrix $\widehat{M}$ and preconditioner M^{-1}
N_b	Number of nodes on boundary Γ
N_{b1}	Number of nodes on boundary Γ_1
N_{b2}	Number of nodes on boundary Γ_2
N_i	Number of nodes in domain Ω
Ω	given domain for the PDE
$p,\ p_j$	points $(x,y),\ (x_j,y_j)\in\Omega+\Gamma$
$P,\ P_j$	permutation matrix of size N (or n)
$\underline{P}$	unknown vector of size N for the standard DRM
$\underline{\widehat{\widehat{P}}}$	unknown vector of size $3N$ of the new DRM variant
q	normal function $q(x,y)$ of u on Γ
$\underline{q}_{b1}$	vector of unknown q values on boundary Γ_1
$\underline{q}_{b2}$	vector of known q values on boundary Γ_2
r_j	radial distance function $\|p-p_j\|_2$
R	residual function (unknown) for the PDE
u	unknown function $u(x,y)$ for the PDE
$\underline{u}$	vector of approximations to $u(x,y)$ at nodes
$\widehat{u}_j$	known RBF function for R, relating to f_j
$\underline{u}_{b1}$	vector of known u values on boundary Γ_1
$\underline{u}_{b2}$	vector of unknown u values on boundary Γ_2
W	discrete wavelet transform (DWT) matrix
W_i	one step of DWT matrix (quasi-band)