Exploiting Symmetry in 3D Boundary Element Methods

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Abstract

Many linear operator equations are defined on regions which are invariant under a group Γ of symmetry transformations. If in addition, the linear operator is equivariant with respect to Γ and if a discretization is made which respects the equivariance, the original discretized problem can be decomposed into a collection of much smaller problems, and a significant reduction of computational cost can be effected. Since these ideas are not yet commonplace in the literature of numerical analysis, we give an accessible introduction and illustrate the efficacy of the ideas in the case of a boundary element method corresponding to a three-dimensional exterior Neumann problem the discretization of which has the same symmetry as a cube.

1 Introduction

In many cases, operator equations exhibit symmetries which can be described by the action of a certain group Γ. Under appropriate discretizions of such equations, these symmetries can be exploited to considerably reduce the computational cost of solving them. We illustrate this reduction for the case of a typical boundary integral equation of the second kind. The approach obviously generalizes to many other cases.

The first approaches along these lines have been given by Stiefel and Fässler [11, 7] and Bossavit [4]. More recently, other authors have begun to use group representations as a tool to reduce the computational cost of solving discretizations of operator equations, see [1, 6, 8, 9]. The present paper follows general ideas outlined in [8] where the optimal reduction in computational cost was described. With the aim of

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making these ideas more accessible to the numerical community, we first give a simple description of the symmetry reduction method, using only as much group theory as is absolutely necessary. We then put these ideas into application in the case of an integral equation which exhibits a high degree of symmetry.

2 A Case Study

Let us consider a boundary integral equation

$$u(x) - \int_{\mathcal{B}} K(x,y)u(y)\,\mu(dy) = f(x) \tag{1}$$

in $L^2(\mathcal{B})$, where μ is the standard measure (surface element) on the piecewise smooth surface $\mathcal{B}$ which is the boundary of a bounded domain in $\mathbf{R}^3$. This example is typical for boundary element methods where the kernel K is usually weakly singular.

Frequently the surface $\mathcal{B}$ has a certain symmetry with respect to a finite group Γ of orthogonal transformations in $\mathbf{R}^3$, i.e., $\mathcal{B} = \gamma\mathcal{B}$ for $\gamma \in \Gamma$. In order to exploit this symmetry, we also need a corresponding invariance property for the kernel: we call K *equivariant* with respect to Γ if

$$K(\gamma x, y) = K(x, \gamma^{-1} y) \tag{2}$$

holds for $\gamma \in \Gamma$ and $x, y \in \mathcal{B}$. Many kernels arising in the applications of classical physics have this property, e.g., the single and double layer potential kernels related to Poisson's equation, see [1].

Ordinarily, integral equations of the above type are solved numerically via a discretization method. The above invariance properties can be exploited if the discretization respects this structure. We display the symmetry reduction method for one of the simplest cases, namely a collocation method with constant elements.

Let us assume that $\mathcal{B}_i$ is a subdivision of the surface $\mathcal{B}$ and that $p_i \in \mathcal{B}_i$ are collocation points, $i = 1, \ldots, n$, such that the group Γ induces a group $\bar{\Gamma}$ of permutations on the indices, i.e.,

$$\gamma\mathcal{B}_i = \mathcal{B}_{\bar{\gamma}i}, \quad \gamma p_i = p_{\bar{\gamma}i}, \tag{3}$$

where $\gamma \in \Gamma \mapsto \bar{\gamma} \in \bar{\Gamma}$ is a group isomorphism. Since there will be no confusion between these two groups, we will drop the distinction.

The collocation equation associated with (1) is

$$u_i - \sum_{j=1}^{n} K_{i,j} u_j = f_i\,,$$

where $u_i = u(p_i)$, $f_i = f(p_i)$, and $K_{i,j} = \int_{\mathcal{B}_j} K(p_i, y)\,\mu(dy)$. By using the invariance of the suface element μ with respect to orthogonal transformations, the equivariance of the kernel K and the equations (3), we obtain

$$\begin{aligned} K_{\gamma i,j} &= \int_{\mathcal{B}_j} K(\gamma p_i, y)\,\mu(dy) = \int_{\mathcal{B}_j} K(p_i, \gamma^{-1} y)\,\mu(dy) \\ &= \int_{\gamma^{-1}\mathcal{B}_j} K(p_i, z)\,\mu(dz) = K_{i,\gamma^{-1}j} \end{aligned}$$

for all $\gamma \in \Gamma$, i.e., the system matrix with elements $K_{i,j}$ is equivariant with respect to the permutation group Γ. Of course, the matrix corresponding to the operator $\mathrm{Id} - K$ is also equivariant.

Summarizing, the collocation method leads to a linear system of equations

$$Au = f,$$

where the (dense) matrix A is equivariant with respect to a certain permutation group Γ, i.e.,

$$A(\gamma i, j) = A(i, \gamma^{-1} j) \quad \text{or} \quad A(\gamma i, \gamma j) = A(i, j) \tag{4}$$

holds for $i, j = 1, \ldots, n$ and $\gamma \in \Gamma$.

Often the calculation of the entries of a system matrix A involves costly calculations such as the numerical quadratures arising in a boundary element method. If however, A is equivariant with respect to a group Γ, then it is only necessary to calculate a fraction of the entries: The rest of the matrix can be obtained by means of the equivariance property (4). For example, if an (n, n) matrix is equivariant with respect to a group of order k, then it is only necessary to compute n/k rows or columns of A.

3 The Symmetry Reduction Method

The purpose of this paper is to show how the equivariance of A can be exploited to design a very efficient direct solver for the linear equation $Au = f$. The preceding section discussed a case where equivariant matrices arise. Many other problems can also lead to equivariant matrices. Let us emphasize that the reduction technique to be discussed below applies whenever A is equivariant in the sense of (4). Hence, hereafter the source of this equivariance is irrelevant.

For example, one of the standard structures occurring in matrix analysis is that of block circulant matrices, see, e.g., [5]. A matrix A of size $(mk, mk) = (n, n)$ which is block circulant with blocks of size (k, k) has the property

$$A[i + k (\operatorname{mod} n), j + k (\operatorname{mod} n)] = A[i, j]$$

for $i, j = 1 \ldots n$. This property is merely equivariance with respect to the cyclic group Γ of order m, generated by the cyclic shift $\gamma(i) = i + k (\operatorname{mod} n)$. The cyclic shift equivariance usually arises from geometric invariance with respect to a group of rotations. If further invariances hold with respect to reflections, they may be overlooked in the structure of A, and we suspect, are usually not exploited in the solution of the system $Au = f$.

In order to keep the exposition as simple as possible, we make one additional assumption on A:

Assumption 5 *The permutation group* Γ *is fixed point free, i.e., if* $\gamma \in \Gamma$, $i \in \{1, \dots, n\}$ *and if* $\gamma i = i$, *then* γ *is the identity element of* Γ.

This assumption is quite natural for certain types of discretization methods, but not so natural for others. In any case, Georg and Miranda have recently obtained preliminary results for handling the case of groups having fixed points. The results of their investigation will be published elsewhere.

Let $|\Gamma|$ denote the order of the group. An immediate consequence of the above assumption is that all *orbits* $\{\gamma i : \gamma \in \Gamma\}$ have $|\Gamma|$ elements and form a partition of the index set $\{1, \dots, n\}$. This implies that n must be divisible by $|\Gamma|$. Furthermore, we will later consider a *selection* of indices $\mathcal{S} \subset \{1, \dots, n\}$ such that $\{\gamma i : \gamma \in \Gamma\}_{i \in \mathcal{S}}$ is a partition of $\{1, \dots, n\}$. Clearly, $\mathcal{S}$ contains $n/|\Gamma|$ indices.

The symmetry reduction method is conveniently described by using a tensor product notation. We denote by $\mathcal{M}(k, m)$ the space of (k, m)-matrices over the complex numbers. If d is a positive integer (later it will be a dimension), we view the (dk, dm)-matrices as block (k, m)-matrices, where the blocks consist of (d, d)-matrices. In tensor notation: $\mathcal{M}(dk, dm) = \mathcal{M}(d, d) \bigotimes \mathcal{M}(k, m)$. Furthermore, if R is a (d, d)-matrix and B a (k, m)-matrix, then $R \otimes B$ denotes the usual tensor product, i.e., the block (k, m)-matrix in which the (i, j)-block consists of $B(i, j)R$. In particular, we will use this block structure for the two cases: (1) where $k = m = n$, i.e., (n, n)-square matrices; (2) where $k = n$ and $m = 1$, i.e., n-columns.

A crucial definition we need is that of an irreducible representation. This is one of the basic tools for characterizing groups. We denote by $\mathcal{U}(d)$ the group of (complex) unitary (d, d)-matrices. A group homomorphism $R : \Gamma \to \mathcal{U}(d)$ is called an *irreducible representation* of Γ if for all non-trivial orthogonal projections $P \in \mathcal{M}(d, d)$ there is a $\gamma \in \Gamma$ such that $PR_\gamma(I_d - P) \neq 0$. Here I_d denotes the (d, d)-identity matrix. In this case, we call $d(R) := d$ the dimension of R.

Two irreducible representations $R, R' : \Gamma \to \mathcal{U}(d)$ are called *equivalent* if there is an invertible (d, d)-matrix T such that $TR_\gamma = R'_\gamma T$ holds for all $\gamma \in \Gamma$. For purposes of characterizing groups, equivalent irreducible representations are identified. Many finite groups of practical interest are classified by a complete table of irreducible representations. Such tables can be found in standard reference books, see, e.g., [10].

Let R be an irreducible representation of Γ with dimension d. Then we introduce the projector

$$P_R := \frac{1}{|\Gamma|} \sum_{\gamma \in \Gamma} R_\gamma \otimes \Pi_\gamma \in \mathcal{M}(dn, dn)$$

where Π_γ is the (n, n)-permutation matrix induced by the permutation $\gamma \in \Gamma$. More precisely, $(\Pi_\gamma u)(i) = u(\gamma^{-1} i)$. It can be shown, see [8, 9], that P_R is an orthogonal projection. Furthermore, a block column $w \in \mathcal{M}(dn, d)$ is in the range of P_R if and only if the symmetry condition

$$R_\gamma w(i) = w(\gamma i) \tag{6}$$

holds for all $i \in \{1, \ldots, n\}$ and all $\gamma \in \Gamma$. Here $w(i)$ denotes the i-th block of w. Note that it follows that any w in this range is characterized by the values of its blocks $w(i)$ for a selection of indices i.

We will use these projectors to form an orthogonal splitting. If I_d denotes the (d, d)-identity matrix, then the equation (in n variables) $Au = f$ can be *inflated* into the equivalent equation (in dn variables)

$$(I_d \otimes A)(I_d \otimes u) = (I_d \otimes f).$$

From the equivariance of A it can be seen that the orthogonal projector P_R and the inflated matrix $(I_d \otimes A)$ commute, and hence we obtain the reduced equation

$$(I_d \otimes A) \underbrace{P_R(I_d \otimes u)}_{=:\, u_R} = \underbrace{P_R(I_d \otimes f)}_{=:\, f_R}.$$

The numerical method for solving $Au = f$ is based on the following two observations:

First, it is possible to calculate the solution of the equation $(I_d \otimes A)u_R = f_R$ efficiently in the following way. For a selection of indices i and j, we introduce the *reduced matrix*:

$$A_R(i, j) = \sum_{\gamma \in \Gamma} A(i, \gamma j) R_\gamma \,.$$

It can be seen, see [8, 9], that the following *reduced equation* holds:

$$\sum_j A_R(i, j) u_R(j) = f_R(i)\,. \tag{7}$$

This equation is used to calculate the blocks $u_R(j)$ for a selection of indices j. The remaining blocks can be obtained via the symmetry condition (6). Note that the system matrix of the reduced equation (7) has the size $dn/|\Gamma|$.

Second, we note that the solution u of the equation $Au = f$ can be constructed once the block columns u_R are known for a complete list of irreducible representations R. Namely,

$$u(j) = \sum_R d(R) \operatorname{trace} u_R(j) \tag{8}$$

for $j \in \{1, \ldots, n\}$. The last equation has been shown in [8, 9]. It is based on the well-known fact that the characters of a group lead to a decomposition of the space on which the group acts.

If the dense linear system $Au = f$ is solved with a direct solver, then Cn^3 arithmetic operations are needed. If instead, symmetry reduction is applied as outlined above, then the same solver requires ρCn^3 arithmetic operations, where

$$\rho = \frac{1}{|\Gamma|^3} \sum_R d^3(R).$$

Since it is well-known that $\sum_R d^2(R) = |\Gamma|$ holds, the *reduction factor* ρ is small, e.g., for the full symmetry group of the 3-cube we have

$$\rho = 128/48^3 \approx 0.00116, \tag{9}$$

see [8, 9]. Let us also note that the symmetry reduced systems (7) are well suited for parallel computation.

4 A Simple Example

Let us illustrate the symmetry reduction method by a very simple example: a $(6,6)$-matrix which is equivariant with respect to the symmetry group Γ of an equilateral triangle. This group has 6 elements and is one of the simplest possible non-abelian groups. We view Γ as a permutation group on the indices $\{1, \ldots, 6\}$, see Figure 1.

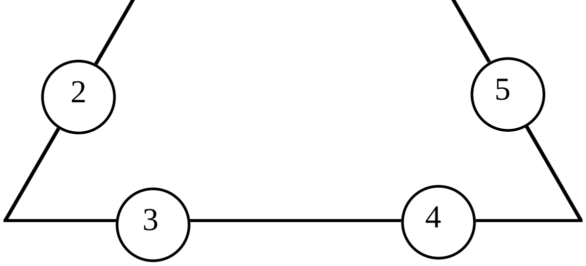

Figure 1: The Symmetry Group of an Equilateral Triangle

The elements of Γ are written as functions of i (modulo 6). Table 1 gives a complete list of irreducible representations for Γ.

	i	$i+2$	$i+4$	$7-i$	$5-i$	$3-i$
R_1	1	1	1	1	1	1
R_2	1	1	1	-1	-1	-1
R_3	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$

Table 1: The Symmetry Group of an Equilateral Triangle: Irreducible Representations

The following is a linear system in which the coefficient matrix is equivariant with respect to this group.

$$\underbrace{\begin{pmatrix} 1 & 5 & 6 & 2 & 3 & 4 \\ 5 & 1 & 4 & 3 & 2 & 6 \\ 3 & 4 & 1 & 5 & 6 & 2 \\ 2 & 6 & 5 & 1 & 4 & 3 \\ 6 & 2 & 3 & 4 & 1 & 5 \\ 4 & 3 & 2 & 6 & 5 & 1 \end{pmatrix}}_{=:\,A} \underbrace{\begin{pmatrix} 1 \\ 2 \\ -3 \\ -1 \\ 2 \\ 3 \end{pmatrix}}_{=:\,u} = \underbrace{\begin{pmatrix} 9 \\ 14 \\ 21 \\ 15 \\ 14 \\ 11 \end{pmatrix}}_{=:\,f}$$

Let us now illustrate how the solution u can be generated by using the symmetry reduction method. Note that we have a very trivial selection $\{1\}$ of indices. The respective reduced systems (using this selection) are:

$$\underbrace{(21)}_{A_{R_1}(1,1)} \; \underbrace{(0.6667)}_{u_{R_1}(1)} = \underbrace{(14)}_{f_{R_1}(1)}$$

$$\underbrace{(-1)}_{A_{R_2}(1,1)} \; \underbrace{(-0.6667)}_{u_{R_2}(1)} = \underbrace{(0.6667)}_{f_{R_2}(1)}$$

$$\underbrace{\begin{pmatrix} -4 & -5.1962 \\ 0 & -3 \end{pmatrix}}_{A_{R_3}(1,1)} \underbrace{\begin{pmatrix} -0.1667 & -1.1547 \\ 0.2887 & 0.6667 \end{pmatrix}}_{u_{R_3}(1)} = \underbrace{\begin{pmatrix} -0.8333 & 1.1547 \\ -0.866 & -2 \end{pmatrix}}_{f_{R_2}(1)}$$

By using the symmetry condidtion (6), these solutions can be easily extended for all indices $\{1, \ldots, 6\}$:

$$u_{R_1} = \begin{pmatrix} 0.6667 \\ 0.6667 \\ 0.6667 \\ 0.6667 \\ 0.6667 \\ 0.6667 \end{pmatrix}; \quad u_{R_2} = \begin{pmatrix} -0.6667 \\ 0.6667 \\ -0.6667 \\ 0.6667 \\ -0.6667 \\ 0.6667 \end{pmatrix}; \quad u_{R_3} = \begin{pmatrix} \begin{pmatrix} -0.1667 & -1.1547 \\ 0.2887 & 0.6667 \end{pmatrix} \\ \begin{pmatrix} -0.3333 & -1.1547 \\ 0.0000 & 0.6667 \end{pmatrix} \\ \begin{pmatrix} -0.1667 & 0.0000 \\ -0.2887 & -1.3333 \end{pmatrix} \\ \begin{pmatrix} 0.1667 & -0.0000 \\ -0.2887 & -1.3333 \end{pmatrix} \\ \begin{pmatrix} 0.3333 & 1.1547 \\ 0.0000 & 0.6667 \end{pmatrix} \\ \begin{pmatrix} 0.1667 & 1.1547 \\ 0.2887 & 0.6667 \end{pmatrix} \end{pmatrix}.$$

The reader can easily check that the decomposition (8) holds, which in this case simplifies to

$$u(i) = u_{R_1}(i) + u_{R_2}(i) + 2\,\mathrm{trace}\,(u_{R_3}(i))\,.$$

5 A Numerical Example

Let us consider the problem of approximating the solution of the following exterior problem in $\mathbf{R^3}$ with Neumann boundary conditions:

$$\begin{array}{rcll} \Delta u & = & 0 & \text{in} \quad \mathcal{D}, \\ \frac{\partial u}{\partial \nu} & = & g & \text{on} \quad \mathcal{B}, \end{array}$$

where $\mathcal{D}$ is the region exterior to the unit sphere centered at the origin, $\mathcal{B} = \partial\mathcal{D}$ and $\nu(y)$ indicates the outer normal of $\partial\mathcal{D}$ at y $\in \partial\mathcal{D}$.

It it well-known, see, e.g., Atkinson [2, 3] that u satisfies the following Fredholm integral equation of the second kind:

$$2\pi u(x) + \int_{\mathcal{B}} K(x,y)u(y)\mu(dy) = \int_{\mathcal{B}} g(y)\frac{1}{|x-y|}\mu(dy),$$

where μ is the standard surface measure (surface element) of integration and

$$K(x,y) = \frac{\partial}{\partial\nu(y)}\left(\frac{1}{|x-y|}\right)$$

is the kernel of the so-called double-layer potential. It is routine to verify that $K(x,y)$ is equivariant in the sense of (2) with respect to *any* isometry group $\Gamma \in O(3)$, see [1].

Hence we can employ the collocation method for boundary integral equations with constant elements as described in Section 2.

The full symmetry group Γ of the 3-cube will be imposed on the sphere. We view Γ as a group of orthogonal (3,3)-matrices. A subdivison of the sphere is obtained by first subdividing the cube, then projecting the cube onto the sphere. To illustrate, let $\mathcal{C}$ be the surface of the cube and $E : \mathcal{C} \to \mathcal{B}$ be the radial projection of $\mathcal{C}$ onto $\mathcal{B}$. The surface of the cube is subdivided into 48 congruent triangles. If T is one of these triangles, then $\{\gamma T\}_{\gamma\in\Gamma}$ is a triangulation of the surface $\mathcal{C}$ and $\{\gamma(ET)\}_{\gamma\in\Gamma}$ is a subdivision of the sphere $\mathcal{B}$. Further subdivisions of T lead to refined subdivisions of $\mathcal{B}$ into n pieces.

Γ has 48 elements and 8 irreducible representations. Of the 8 representations, four are of dimension 1, two of dimension 2, and four of dimension 3. A preliminary C-code has been developed for handling the symmetry reduction method for a user specified symmetry group, see Walker [14]. This was used to generate the data for the present example.

In our numerical example we chose the data

$$g(x, y, z) = x + y + e^y z$$

on the boundary.

Table 2 lists the time (in seconds) for solving the full system and the time for solving via the reduction method for various values of n. The same direct solver (an F2C conversion of LINPACK codes from the NETLIB) on an IBM 6000/550 workstation was used in both cases.

Table 2:

n	symm	w/o symm	reduction factor
768	2.8	63.0	.044
1536	9.8	495.8	.0198
3072	37.65	3910.3	.0095
6144	165.34	**	.0052*
12288	822.63	**	.0032*

*Note: * indicates an extrapolated factor, ** ran out of memory.*

As can be seen, the theoretical reduction factor calculated in (9) is only gradually approached for large n. This is due to the significant role of the overhead which was neglected in (9).

For large n, greater efficiency can be achieved via a two-grid approach where a coarser grid serves to provide a preconditioner, see, e.g., Atkinson [2]. This was implemented in the above context by Walker [14]. Convergence theorems may be found in Atkinson [2] and Vainikko [12, 13].

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