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Numerical Exploitation of Equivariance

Linear operators in equations describing physical problems on a symmetric domain often are also equivariant, which means that they commute with its symmetries, i.e., with the group of orthogonal transformations which leave the domain invariant. Under suitable discretizations the resulting system matrices are also equivariant with respect to a group of permutations. Methods for exploiting this equivariance in the numerical solution of linear systems of equations and eigenvalue problems via symmetry reduction *are described. A very significant reduction in computational expense can be obtained in this way. The basic ideas underlying this method and its analysis involve group representation theory. The symmetry reduction method is complicated somewhat by the presence of nodes or elements which remain fixed under some of the symmetries. Two methods (regularization and projection) for handling such situations are described. The former increases the number of unknowns in the symmetry reduced system, the latter does not but needs more overhead. Some examples are given to illustrate this situation. Our methods circumvent the explicit use of symmetry adapted bases, but our methods can also be used to automatically generate such bases if they are neede for some other purpose. A software package has been posted on the internet.*

Keywords: equivariant operator equations, symmetry groups, linear equation solvers, finite Fourier transform, representation theory, boundary element methods, collocation methods

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1 Introduction

Many problems in science and mathematics exhibit symmetry phenomena which may be exploited to analyze them, and also to effect a significant cost reduction in their numerical treatment. Usually the symmetry stems from the domain or body on which the problem is considered. The numerical treatment of problems such as partial differential equations and integral equations generally involves discretizations which ought (as far as possible) to incorporate or respect such symmetries. The present paper summarizes some of the recent work of the authors concerning systematic techniques for exploiting symmetry in the numerical treatment of systems of linear equations that arise from discretizing operator equations displaying symmetries. The unifying concept is a generalization of the Fourier transform for arbitrary finite groups. We study here the general case which incorporates non-abelian groups (i.e., having irreducible representations of dimension > 1) and the possibility that some nodes of the discretization remain fixed under some of the symmetries. This latter case is of considerable practical importance since it naturally occurs in the most frequently used finite element or boundary element discretizations, and since it considerably complicates the algorithmic approach.

Some of the material has been presented in various forms in [2, 4, 5, 16, 17, 18, 27, 29]. We give here a unified and simplified view. The regularization techniques discussed in Section 6 are new.

Although the algebraic tool employed here is the classical representation theory of groups, the systematic exploitation of these tools in numerical analysis has only recently begun, e.g., Stiefel and Fässler [14, 26]. They introduced symmetry adapted bases to analyze equivariant linear maps. This tool has been exploited in many papers on bifurcation theory under group actions in the spirit of [20, 21, 30] for numerical purposes, see, e.g., [11, 15, 22, 23, 24, 31]. Our approach can be easily used to *automatically* generate symmetry adapted bases of discretized problems which have often been used in the context of bifurcation and eigenvalue analysis. This is important for standard discretizations of operator equations which will typically contain nodes that are fixed under some of the symmetries, so that the generation of symmetry adapted bases is not very simple. Our reduction procedures actually sidestep the need to generate and make use of such symmetry adapted bases.

Let us note that our approach is limited to case that the discretization method generates an action of a permutation group. For example, the lattice dome discussed in [23] is not of this type.

In the context of partial differential equations under group actions, a different approach for exploiting the symmetry structure has been to effect a domain reduction. The same PDE has to be repeatedly solved over a reduced domain (symmetry cell) with varying boundary conditions on the new boundaries, see, e.g., [1, 7, 8, 9, 10, 12, 13]. We will not cover this topic in the present paper.

2 Group Theoretical Background

Let us briefly outline the group theoretical background and motivation of our reduction method. Underlying the symmetry reduction method is a decomposition of equivariant linear operators via projectors defined by means of group representations. Familiarity with these group concepts is not required for understanding the subsequent sections of the paper.

Let Γ be a finite group, H a finite dimensional complex vector space, $T : \Gamma \to L(H)$ a linear unitary representation (i.e., an action) of Γ on H, and $A \in L(H)$ a linear operator. We call A *equivariant* if A commutes with T, i.e., $AT(g) = T(g)A$ for all $g \in \Gamma$.

If A is equivariant, then it is well known that H splits into a canonical direct sum

$$H = \bigoplus_{\mathbf{r},\rho} H_{\mathbf{r},\rho} \quad \text{via the projectors} \quad P_{\mathbf{r},\rho} : H \to H_{\mathbf{r},\rho} \quad \text{defined by} \quad P_{\mathbf{r},\rho} = \tfrac{\dim \mathbf{r}}{|\Gamma|} \sum_{g\in\Gamma} \mathbf{r}_{\rho,\rho}(g^{-1})\, T(g) \tag{1}$$

where $\mathbf{r}$ runs through a complete list $\mathcal{R}$ of irreducible representations of Γ and $\rho = 1 : \dim \mathbf{r}$. See Section 4 for definitions of these notions.

It is well known that the equivariance of A leads to a splitting

$$A = \bigoplus_{\mathbf{r},\rho} A_{\mathbf{r},\rho} \quad \text{where} \quad A_{\mathbf{r},\rho} : H_{\mathbf{r},\rho} \to H_{\mathbf{r},\rho}\,. \tag{2}$$

This can be exploited to solve linear equations or eigenvalue problems involving A. Hence the linear equations or eigenvalue problems are solved over each of the subspaces $H_{\mathbf{r},\rho}$. We call this approach the *symmetry reduction method.*

In earlier literature, this splitting is performed by introducing a symmetry adapted basis, i.e., a collection of bases for each subspace $H_{\mathbf{r},\rho}$, see [14, 26]. For some applications such bases can be seen easily enough. However, for large scale discretizations of operator equations where typically some of the nodes are fixed under some symmetries, it is desirable to implement this approach more systematically. We are led to generating the symmetry adapted bases automatically or (our preferred point of view) to avoiding their explicit use by transforming directly to the new coordinates. This is the approach we now describe. The applications we have in mind are finite element discretizations of partial differential or integral equations which display some symmetry structure. We will see that the sum in (1) and variations thereof will remain (not surprisingly) a basic theme of the method. The splitting (2) is described in (24). It turns out that the $A_{\mathbf{r},\rho}$ for fixed $\mathbf{r}$ are all represented by the same submatrix $\mathcal{A}_{\mathbf{r}}$ in (24).

3 A Simple Example

Let us motivate our discussion with a very simple but already significant example which displays all essential difficulties that can be encountered. Consider Laplace's equation

$$\Delta u = 0 \text{ in } \Omega; \quad u = g \text{ on } \partial\Omega,$$

where $\Omega \subset \mathbb{R}^2$ is a bounded domain with smooth boundary $\partial\Omega$. Let us emphasize here that our actual research interest is in 3-dimensional bodies and various operator equations, not just Laplace's equation.

To be specific, let us use a domain Ω with the following boundary

$$\partial\Omega := \{\, P(t) \,:\, t \in [0\,, 2\pi) \,\} \quad \text{where} \quad P(t) := (1 - .3 \sin 3t) \begin{bmatrix} \cos t \\ \sin t \end{bmatrix}, \qquad \text{see Figure 1.}$$

It is easily seen that Ω has the symmetry of an equilateral triangle, i.e., it is invariant under the reflection F about the y-axis, and under a (say) clockwise rotation R by $2\pi/3$. Note that $FP(t) = P(\pi - t)$ and $RP(t) = P\left(t - \frac{2}{3}\pi\right)$. The group generated by these two orthogonal transformations is usually denoted by D_3 (a dihedral group). Its elements are:

$$\Gamma = \left\{ \mathrm{I},\ R,\ R^2,\ F,\ RF,\ R^2F \right\}$$

where I denotes the identity element.

Using the ansatz that the solution u can be written in the form

$$u(Q) = \tfrac{1}{2\pi} \int_{\partial\Omega} \ln|Q - P|\, w(P)\, ds(P)\,,$$

where ds denotes the line element, then it is well-known that the unknown function w solves the integral equation of the first kind

$$\frac{1}{2\pi}\int_{\partial\Omega} \ln|Q-P|\, w(P)\, ds(P) = g(Q)\,, \qquad Q \in \partial\Omega\,. \tag{3}$$

For illustration, let us consider a simple collocation method with linear elements for solving this integral equation. We introduce n collocation points

$$P_k := (1-.3\sin 3t_k)\begin{bmatrix}\cos t_k\\ \sin t_k\end{bmatrix} \quad \text{where} \quad t_k = -\tfrac{\pi}{6} - \tfrac{2\pi}{n}(k-1) \;\; \text{for} \;\; k = 1:n.$$

Here n has to be divisible by 6. Next, we define the basis functions $\varphi_k : \partial\Omega \to \mathbb{R}$ for $k = 1:n$ by setting

$$\varphi_k(P(t)) = \begin{cases} \frac{n}{2\pi}(t-t_{k-1}) & t \in [t_{k-1}, t_k]\,, \\ 1-\frac{n}{2\pi}(t-t_k) & t\in[t_k,t_{k+1}]\,, \\ 0 & \text{else}\,. \end{cases}$$

Note that these basis functions are merely the standard hat functions mapped via the parametrization $P(t)$. For our example, we choose $n = 12$, see Figure 1.

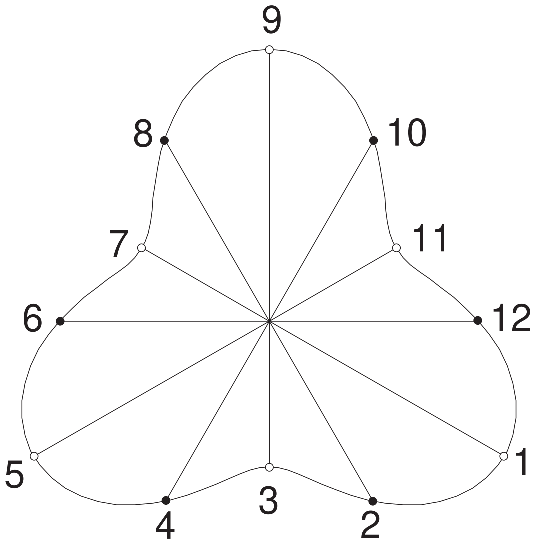

Figure 1: Domain with a D_3-symmetry

Note that this discretization respects the given symmetries: Namely,

$$FP_k = P_{4n/3+2-k}\,, \qquad RP_k = P_{k+n/3}\,,$$
$$\varphi_k \circ F^{-1} = \varphi_{4n/3+2-k}\,, \qquad \varphi_k \circ R^{-1} = \varphi_{k+n/3}\,,$$

where the index operations are understood to be performed modulo n. Hence, from the point of view of the discretization, we view the action of the symmetry group as a permutation group acting on the indices of the nodes $\{1,\ldots,n\}$:

$$\begin{aligned} \mathrm{I} &: k \longmapsto k \\ F &: k \longmapsto 4n/3+2-k \\ R &: k \longmapsto k+n/3 \end{aligned}$$

From the action of the generators we obtain immediately (by composition) the action of the other group elements of D_3:

$$\begin{aligned} RF &: k \longmapsto 5n/3+2-k \\ RR &: k \longmapsto k+2n/3 \\ RRF &: k \longmapsto n+2-k \end{aligned}$$

Let us remind the reader that the nodal indices are viewed modulo n.

Applying this simple collocation method to the integral equation (3) leads to

$$\sum_k \underbrace{\frac{1}{2\pi}\int_{\partial\Omega} \ln|P_i - P|\,\varphi_k(P)\,ds(P)}_{A[i,k]}\,x[k] = \underbrace{g(P_i)}_{b[i]}, \quad i,k = i:n \tag{4}$$

where we use the collocation approximation $w(P) \approx \sum_k x[k]\,\varphi_k(P)$. Hence we obtain a linear equation of the form $Ax = b$ which needs to be solved for x. From the above construction we have

Lemma 1. The system matrix A of (4) is *equivariant*, i.e., we have

$$\begin{array}{rrcll} & A[gi,k] & = & A[i,g^{-1}k], & g \in \Gamma,\ i,k = 1:n \\ \text{or equivalently} & A[gi,gk] & = & A[i,k], & g \in \Gamma,\ i,k = 1:n. \end{array} \tag{5}$$

4 Generalized Fourier Transform

Generally, when symmetry is present in scientific models, the need arises to solve linear systems of equations $Ax = b$ or eigenvalue problems $Ax = \lambda x$ where the system matrix A is equivariant. Let us now describe a systematic way to numerically exploit this structure for reducing the computational expense.

Assumption. Let us assume in the sequel that A is an equivariant square matrix of size n in the sense of equation 5 with respect to a group of permutations Γ acting on the indices $\{1,\ldots,n\}$.

By a *selection* $\mathbb{S}$ of indices we mean a minimal subset

$$\mathbb{S} \subset \{1,2,\ldots,n\} \text{ such that } \{gi : g\in\Gamma,\ i\in\mathbb{S}\} = \{1,2,\ldots,n\}.$$

For purposes of storing the matrix A, it is sufficient to know a selected number of its columns (or rows). This is immediately evident from (5).

A (unitary) *representation* of Γ is a group homomorphism $\mathbf{r} : \Gamma \to \mathcal{U}_d$, where $\mathcal{U}_d$ is the group of unitary matrices of size d, such that the identity permutation 1 is mapped onto the identity matrix $\mathbf{r}(1)$. The number $d_{\mathbf{r}} := d$ is called the *dimension* of $\mathbf{r}$. The representation is called *irreducible* if it has no proper invariant subspaces. Two representations are called *equivalent* if they differ only by a similarity transformation. A maximal number of non-equivalent irreducible representations is called a *complete list* $\mathcal{R}$ of representations for Γ.

For many of the groups which are important in applications (in particular groups of geometric symmetries) such a complete list is known and can be found in standard books such as [25]. The lists have been implemented in [19] for a number of groups.

The following result can be found in standard textbooks which discuss group representation theory:

Theorem 2. (Orthogonality Relation) Let $\mathcal{R}$ be a complete list of representations for a finite group Γ. For a fixed $\mathbf{r}\in\mathcal{R}$ and fixed indices $i,j = 1:d_{\mathbf{r}}$ we can view $g \mapsto \mathbf{r}_{i,j}(g)$ as a column in $\mathbb{C}^{|\Gamma|}$ where $|\Gamma|$ denotes the *order* of the group. Then

$$\left(\sqrt{\tfrac{d_{\mathbf{r}}}{|\Gamma|}}\,\mathbf{r}_{i,j}(g)\right)_{g\in\Gamma} \quad \text{for } \mathbf{r}\in\mathcal{R} \text{ and } i,j = 1:d_{\mathbf{r}}$$

is an orthonormal basis of $\mathbb{C}^{|\Gamma|}$.

A well-known consequence of this is

$$\sum_{\mathbf{r}\in\mathcal{R}} d_r^2 = |\Gamma|. \tag{6}$$

The main tool for our symmetry reduction method consists of the following Fourier transformation for general finite groups:

Definition 3. (Generalized Fourier Transform) Let Γ be a group of permutations acting on the indices $\{1,2,\ldots,n\}$. Let $\mathcal{R}$ be a complete list of representations of Γ. Then the generalized Fourier transform of a column $w \in \mathbb{C}^n$ is defined by

$$\hat{w}[\mathbf{r},k] := \sqrt{\tfrac{d_{\mathbf{r}}}{|\Gamma|}} \sum_{g\in\Gamma} w[gk]\ \mathbf{r}(g^{-1}) \quad \text{for } \mathbf{r}\in\mathcal{R} \text{ and } k = 1:n.$$

It is not difficult to see that this reduces to the standard definition of the finite Fourier transform for the special case that the group Γ is cyclic of order n, e.g., generated by the permutation

$$g : i \mapsto i + 1 \bmod n.$$

Note that each component $\hat{w}[\mathbf{r}, k]$ of the Fourier transform is a (small) square matrix of size $d_{\mathbf{r}}$.

Lemma 4. (Symmetry Relations) The following symmetry relation holds for the Fourier transform:

$$\hat{w}[\mathbf{r}, gk] = \mathbf{r}(g)\hat{w}[\mathbf{r}, k]. \tag{7}$$

Therefore, it is sufficient to describe $\hat{w}[\mathbf{r}, k]$ for indices k in a selection $\mathbb{S}$, since the other components are generated automatically by the above formula.

Proof:

$$\begin{aligned}\hat{w}[\mathbf{r}, gk] &= \sqrt{\tfrac{d_{\mathbf{r}}}{|\Gamma|}} \sum_{h\in\Gamma} w[hgk]\ \mathbf{r}(h^{-1}) = \sqrt{\tfrac{d_{\mathbf{r}}}{|\Gamma|}} \sum_{f\in\Gamma} w[fk]\ \mathbf{r}(gf^{-1}) \\ &= \sum_{f\in\Gamma} w[fk]\ \mathbf{r}(f^{-1}) = \mathbf{r}(g)\hat{w}[\mathbf{r}, k]\end{aligned}$$

□

The inverse Fourier transform is also important for numerical purposes:

Lemma 5. (Inverse Fourier Transform) For each irreducible representation $\mathbf{r} \in \mathcal{R}$ and each index $k = 1 : n$, let $f[\mathbf{r}, k]$ be a square matrix of size $d_{\mathbf{r}}$ such that the symmetry relations

$$f[\mathbf{r}, gk] = \mathbf{r}(g)f[\mathbf{r}, k] \tag{8}$$

hold. Then f is the Fourier transform of $w \in \mathbb{C}^n$ where

$$w[k] := \sum_{\mathbf{r}\in\mathcal{R}} \sqrt{\tfrac{d_{\mathbf{r}}}{|\Gamma|}}\, \mathrm{trace}\, f[\mathbf{r}, k]. \tag{9}$$

Furthermore, w is unique.

Proof: We exploit the symmetry relations:

$$\begin{aligned}\hat{w}[\mathbf{r}, k] :&= \sqrt{\tfrac{d_{\mathbf{r}}}{|\Gamma|}} \sum_{g\in\Gamma} w[gk]\ \mathbf{r}(g^{-1}) = \sqrt{\tfrac{d_{\mathbf{r}}}{|\Gamma|}} \sum_{g\in\Gamma}\sum_{\mathbf{s}\in\mathcal{R}} \sqrt{\tfrac{d_{\mathbf{s}}}{|\Gamma|}}\, \mathrm{trace}(f[\mathbf{s}, gk])\ \mathbf{r}(g^{-1}) \\ &= \sqrt{\tfrac{d_{\mathbf{r}}}{|\Gamma|}} \sum_{g\in\Gamma}\sum_{\mathbf{s}\in\mathcal{R}} \sqrt{\tfrac{d_{\mathbf{s}}}{|\Gamma|}}\, \mathrm{trace}(\mathbf{s}(g)f[\mathbf{s}, k])\ \mathbf{r}(g^{-1}).\end{aligned}$$

Hence, if we use subindices to denote the entries of all the square matrices, and if we exploit the orthogonality relations in Theorem 2, we obtain

$$\begin{aligned}\hat{w}_{p,q}[\mathbf{r}, k] &= \sqrt{\tfrac{d_{\mathbf{r}}}{|\Gamma|}} \sum_{g\in\Gamma}\sum_{\mathbf{s}\in\mathcal{R}} \sqrt{\tfrac{d_{\mathbf{s}}}{|\Gamma|}} \sum_{i,j=1}^{d_{\mathbf{s}}} \mathbf{s}_{i,j}(g) f_{j,i}[\mathbf{s}, k]\ \mathbf{r}_{p,q}(g^{-1}) \\ &= \sum_{\mathbf{s}\in\mathcal{R}} \sum_{i,j=1}^{d_{\mathbf{s}}} f_{j,i}[\mathbf{s}, k] \sum_{g\in\Gamma} \left(\sqrt{\tfrac{d_{\mathbf{s}}}{|\Gamma|}}\, \mathbf{s}_{i,j}(g)\right) \left(\sqrt{\tfrac{d_{\mathbf{r}}}{|\Gamma|}}\, \overline{\mathbf{r}_{q,p}(g)}\right) = \sum_{\mathbf{s}\in\mathcal{R}} \sum_{i,j=1}^{d_{\mathbf{s}}} f_{j,i}[\mathbf{s}, k] \delta^{\mathbf{s},i,j}_{\mathbf{r},q,p} = f_{p,q}[\mathbf{r}, k]\,.\end{aligned}$$

The uniqueness of w is shown by noting that the map $w \mapsto \hat{w}$ has a trivial kernel. In fact, if we fix k, then $\hat{w}_{i,j}[\mathbf{r}, k]$ is the scalar product of the function $g \mapsto w[gk]$ with members of the orthogonal basis described in Theorem 2. Hence, $\hat{w} = 0$ implies that all the functions $g \mapsto w[gk]$ vanish for all k. □

It turns out that indices which are fixed under some of the permutations $g \in \Gamma$ cause some complications. We therefore introduce the following

Definition 6. (Isotropy Subgroup) For $i = 1 : n$ we define the *isotropy subgroup* $\Gamma_i := \{g \in \Gamma : gi = i\}$. Obviously, i is not fixed under any (non-trivial) permutation $g \in \Gamma$ if and only if $|\Gamma_i| = 1$. We call the action of Γ on the indices $1, \ldots, n$ *fixed point free* if $|\Gamma_i| = 1$ holds for all $i = 1 : n$.

It is immediately seen that the action is fixed point free if and only if $|\Gamma| \cdot |\mathbb{S}| = n$. Here $|\mathbb{S}|$ denotes the cardinality of $\mathbb{S}$, i.e., the number of selected indices.

The following is easy to show and will be needed later:

Lemma 7. Let $(g,i),(h,k) \in \Gamma \times \mathbb{S}$. Then

$$gi = hk \iff \left[i = k \text{ and } g \in h\Gamma_k\right] \iff \left[i = k \text{ and } g\Gamma_i = h\Gamma_k\right].$$

The next lemma describes the basic step for obtaining a block diagonalization of the equation $Ax = b$ via the Fourier transform. Let us denote the columns of the equivariant matrix A by a_j, $j = 1:n$.

Theorem 8. If $Ax = b$, then

$$\sqrt{\tfrac{|\Gamma|}{d_{\mathbf{r}}}} \sum_{l \in \mathbb{S}} \tfrac{1}{|\Gamma_l|} \hat{a}_l[\mathbf{r},k]\, \hat{x}[\mathbf{r},l] = \hat{b}[\mathbf{r},k]\,. \tag{10}$$

Note that for each fixed irreducible representation $\mathbf{r} \in \mathcal{R}$, these are linear equations for the $d_{\mathbf{r}}^2 \cdot |\,\mathbb{S}\,|$ unknowns $\hat{x}[\mathbf{r},l]$, $l \in \mathbb{S}$, involving the matrix

$$\mathbf{A}_{\mathbf{r}}[k,l] := \sqrt{\tfrac{|\Gamma|}{d_{\mathbf{r}}}}\, \tfrac{1}{|\Gamma_l|} \hat{a}_l[\mathbf{r},k], \quad k,l \in \mathbb{S}\,. \tag{11}$$

Thus, the linear system $Ax = b$ is transformed into the block-diagonal form

$$\sum_{l \in \mathbb{S}} \mathbf{A}_{\mathbf{r}}[k,l] \hat{x}[\mathbf{r},l] = \hat{b}[\mathbf{r},k], \quad k,l \in \mathbb{S}, \quad \mathbf{r} \in \mathcal{R}, \tag{12}$$

where each square block $\mathbf{A}_{\mathbf{r}}$ has size $d_{\mathbf{r}} \cdot |\,\mathbb{S}\,|$ and appears $d_{\mathbf{r}}$ times.

Proof: We have

$$\begin{aligned}
\hat{b}[\mathbf{r},k] :&= \sqrt{\tfrac{d_{\mathbf{r}}}{|\Gamma|}} \sum_{g \in \Gamma} b[gk]\, \mathbf{r}(g^{-1}) = \sqrt{\tfrac{d_{\mathbf{r}}}{|\Gamma|}} \sum_{g \in \Gamma} \sum_{j=1}^{n} A[gk,j]\, x[j]\, \mathbf{r}(g^{-1}) = \sqrt{\tfrac{d_{\mathbf{r}}}{|\Gamma|}} \sum_{g \in \Gamma} \sum_{j=1}^{n} A[k,g^{-1}j]\, x[j]\, \mathbf{r}(g^{-1}) \\
&= \sqrt{\tfrac{d_{\mathbf{r}}}{|\Gamma|}} \sum_{g \in \Gamma} \sum_{i=1}^{n} A[k,i]\, x[gi]\, \mathbf{r}(g^{-1}) = \sum_{i=1}^{n} A[k,i]\, \hat{x}[\mathbf{r},i] = \sum_{l \in \mathbb{S}} \sum_{g \in \Gamma} \tfrac{1}{|\Gamma_l|} A[g^{-1}k,l]\, \mathbf{r}(g)\, \hat{x}[\mathbf{r},l] \\
&= \sum_{l \in \mathbb{S}} \sum_{g \in \Gamma} \tfrac{1}{|\Gamma_l|} A[gk,l]\, \mathbf{r}(g^{-1})\, \hat{x}[\mathbf{r},l] = \sqrt{\tfrac{|\Gamma|}{d_{\mathbf{r}}}} \sum_{l \in \mathbb{S}} \tfrac{1}{|\Gamma_l|} \hat{a}_l[\mathbf{r},k]\, \hat{x}[\mathbf{r},l]
\end{aligned}$$

□

For later use we also prove the converse of Theorem 8:

Lemma 9. Let $x, b \in \mathbb{C}^n$. If the symmetry reduced equations (12) hold, then $Ax = b$.

Proof: Let (12) hold. We define $c := Ax$. By Theorem 8 we have that

$$\sum_{l \in \mathbb{S}} \mathbf{A}_{\mathbf{r}}[k,l] \hat{x}[\mathbf{r},l] = \hat{c}[\mathbf{r},k], \quad k,l \in \mathbb{S}, \quad \mathbf{r} \in \mathcal{R}\,.$$

Hence, since also (12) holds, we have that $\hat{b} = \hat{c}$. By Lemma 5 it follows that $b = c$. □

5 Symmetry Reduction Method: Fixed Point Free Case

Lemma 10. Let the action of the permutation group Γ on the indices $1, \ldots, n$ be fixed point free. Then A is non-singular if and only if all blocks $\mathbf{A}_{\mathbf{r}}$ are non-singular.

Proof: The proof is in fact a simple argument from linear algebra (exploiting commutative diagrams). We give it here for the sake of completeness.

Assume that A is nonsingular. Assume further that

$$\sum_{l \in \mathbb{S}} \mathbf{A}_{\mathbf{r}}[k,l] f[\mathbf{r},l] = 0, \quad k,l \in \mathbb{S}, \quad \mathbf{r} \in \mathcal{R},$$

where $f[\mathbf{r},l]$ are square matrices of size $d_{\mathbf{r}}$. We extend f for all $k = 1:n$ via the symmetry relations

$$f[\mathbf{r},k] = \mathbf{r}(g) f[\mathbf{r},l]$$

where $g \in \Gamma$ and $l \in \mathbb{S}$ are uniquely defined by $k = gl$. This is possible since the action of Γ on the indices $\{1, \ldots, n\}$ is fixed point free. It is easy to see that f now satisfies the assumptions of Lemma 5, and hence $f = \hat{x}$ for some $x \in \mathbb{C}^n$. By Lemma 9 we have $Ax = 0$, and the non-singularity of A implies $x = 0$. Hence $f = \hat{x} = 0$.

Conversely, let all blocks $\mathbf{A_r}$ be non-singular. Assume $Ax = 0$. Then

$$\sum_{l \in \mathbb{S}} \mathbf{A_r}[k,l]\hat{x}[\mathbf{r},l] = 0, \quad k,l \in \mathbb{S}, \quad \mathbf{r} \in \mathcal{R},$$

and hence $\hat{x} = 0$. By the inverse Fourier transform (9) we have $x = 0$. □

Hence, the symmetry reduction method for this case can be summarized in the following steps.

1. Calculate the Fourier transform $\hat{b}$ of b.
2. Calculate the Fourier transform $\hat{a}_l$ of a selection of columns a_l to generate the submatrices $\mathbf{A_r}$ in (11).
3. Solve the reduced problems (12) for a complete list of irreducible representations $\mathbf{r} \in \mathcal{R}$.
4. Use the symmetry relations (7) to obtain $\hat{x}[\mathbf{r}, k]$ for $k = 1 : n$.
5. Use the inverse Fourier transform (9) to retrieve x from $\hat{x}$.

Let us note that the number of variables is the same for the equation $Ax = b$ and the symmetry reduced equations (12). This follows from (6) and $|\mathbb{S}||\Gamma| = n$ since the action of Γ on $\{1 : n\}$ is assumed to be fixed point free. Using the Fourier transform and its inverse, it is readily seen that A is non-singular if and only if all the block matrices $\mathbf{A_r}$ are non-singular.

It can be seen that the overhead of this method (i.e., counting everything but the solving of the reduced system in step 3) is asymptotically n^2 flops for full matrices. The savings in computational expense are significant. If we consider using a direct solver for both the unreduced problem $Ax = b$ and the symmetry reduced subproblems, respectively, then asymptotically we have $f_1 := Cn^3 = C|\Gamma|^3|\mathbb{S}|^3$ flops against $f_2 := C\sum_{\mathbf{r}\in\mathcal{R}} |S|^3 d_{\mathbf{r}}^3$ and hence the quotient which asymptotically describes the reduction factor in the number of flops is

$$\frac{f_2}{f_1} = \frac{\sum_{\mathbf{r}\in\mathcal{R}} d_{\mathbf{r}}^3}{|\Gamma|^3}.$$

For example, if Γ is the symmetry group of the three dimensional cube, then $\frac{f_2}{f_1} = 128/48^2 \approx 0.00116$. We recall that the system matrices arising in boundary element methods and other discretized integral equations are in fact full matrices.

6 Handling Fixed Points via Regularization

Let us now consider the general case in which some of the indices are fixed under some of the permutations $g \in \Gamma$. This is a very typical case for discretization methods. For example, in the discretization of Section 3 for n=12, see Figure 1, the even numbered collocation points are fixed point free, whereas the isotropy groups for the remaining points are $\Gamma_1 = \Gamma_7 = \{\mathrm{I}, R^2F\}$, $\Gamma_3 = \Gamma_9 = \{\mathrm{I}, F\}$, and $\Gamma_5 = \Gamma_{11} = \{\mathrm{I}, RF\}$.

Generally, if some indices are fixed under some of the permutations $g \in \Gamma$, then the symmetry reduced equations (12) are still valid, however the matrices $\mathbf{A_r}$ are singular. The solution is still unique if we take into account that $\hat{x}[\mathbf{r}, l]$ satisfies the symmetry conditions (7). We will discuss two ways to overcome the difficulty that the equations (12) are singular:

1. Implementing a regularization of (12). This method will be discussed in the present section.
2. Further reducing (12) via projectors related to the isotropy groups. This method will be discussed in the next section.

For $\mathbf{r} \in \mathcal{R}$ and $i = 1 : n$ we introduce the projectors

$$\mathrm{P}_{\mathbf{r},i} := \frac{1}{|\Gamma_i|}\sum_{g\in\Gamma_i} \mathbf{r}(g) \quad \text{which have rank} \quad m_{\mathbf{r},i} := \operatorname{rank} \mathrm{P}_{\mathbf{r},i} = \operatorname{trace} \mathrm{P}_{\mathbf{r},i}\,. \tag{13}$$

It is easily seen that the $\mathrm{P}_{\mathbf{r},i}$ are orthogonal projectors.

Note that in practice, many of the $\mathrm{P}_{\mathbf{r},i}$ will be identical, and this can be numerically exploited.

From the symmetry relations (7) we obtain immediately

Lemma 11. Let $w \in \mathbb{C}^n$. Then for each $\mathbf{r} \in \mathcal{R}$ and each $k = 1 : n$ we have $\mathrm{P}_{\mathbf{r},i}\, \hat{w}[\mathbf{r}, i] = \hat{w}[\mathbf{r}, i]$.

Lemma 12. For each irreducible representation $\mathbf{r} \in \mathcal{R}$ and each index $i \in \mathbb{S}$, let $f[\mathbf{r}, i]$ be a square matrix of size $d_{\mathbf{r}}$ such that

$$f[\mathbf{r}, i] = \mathrm{P}_{\mathbf{r},i}\, f[\mathbf{r}, i]$$

holds. For $j = 1 : n$, define $f[\mathbf{r}, j] := \mathbf{r}(g) f[\mathbf{r}, i]$ for $g \in \Gamma$, $i \in \mathbb{S}$ such that $j = gi$. Then the definition has no ambiguity, and f satisfies the symmetry relations (8). Hence it is a Fourier transform.

Proof: Let us first show that $gi = hk$ for $g, h \in \Gamma$ and $i, k \in \mathbb{S}$ implies that $\mathbf{r}(g) f_{\mathbf{r},i} = \mathbf{r}(h) f_{\mathbf{r},k}$. By Lemma 7, we know that $i = k$ and hence $h^{-1}g \in \Gamma_i$. From definition (13) it follows immediately that $\mathbf{r}(h^{-1}g)\, \mathrm{P}_{\mathbf{r},i} = \mathrm{P}_{\mathbf{r},i}$. Therefore,

$$f_{\mathbf{r},i} = \mathrm{P}_{\mathbf{r},i}\, f_{\mathbf{r},i} = \mathbf{r}(h^{-1}g)\, \mathrm{P}_{\mathbf{r},i}\, f_{\mathbf{r},i} = \mathbf{r}(h^{-1}g) f_{\mathbf{r},i} = \mathbf{r}(h)^{-1}\, \mathbf{r}(g) f_{\mathbf{r},i}$$

and hence

$$\mathbf{r}(h) f_{\mathbf{r},i} = \mathbf{r}(g) f_{\mathbf{r},i} = \mathbf{r}(g) f_{\mathbf{r},k}.$$

Hence the definition has no ambiguity.

Let us next show that the extended f satisfies the symmetry relations (8). Let $j \in \{1, \ldots, n\}$ and $h \in \Gamma$. We want to show that $f[\mathbf{r}, hj] = \mathbf{r}(h) f[\mathbf{r}, j]$. Let $g \in \Gamma$ and $i \in \mathbb{S}$ be such that $j = gi$. Then

$$f[\mathbf{r}, hj] = f[\mathbf{r}, hgi] = \mathbf{r}(hg) f[\mathbf{r}, i] = \mathbf{r}(h)\, \mathbf{r}(g) f[\mathbf{r}, i] = \mathbf{r}(h) f[\mathbf{r}, j].$$

The rest of the assertion now follows from Lemma 5. □

Theorem 13. (Regularized Symmetry Reduced Equations) Let $Ax = b$, and let $\alpha > 0$. Then the linear equations

$$\sum_{l \in \mathbb{S}} \left(\mathbf{A}_{\mathbf{r}}[k, l] + \alpha \delta_k^l \left(\mathrm{I} - \mathrm{P}_{\mathbf{r},l} \right) \right) \hat{x}[\mathbf{r}, l] = \hat{b}[\mathbf{r}, k], \quad k, l \in \mathbb{S} \tag{14}$$

hold.

Proof: By Lemma 11 we have $(\mathrm{I} - \mathrm{P}_{\mathbf{r},l})\, \hat{x}[\mathbf{r}, l] = 0$, and hence the validity of (14) is an immediate consequence of (12). □

Note that for each fixed irreducible representation $\mathbf{r} \in \mathcal{R}$, these are linear equations for the $d_{\mathbf{r}}^2 \cdot |\,\mathbb{S}\,|$ unknowns $\hat{x}[\mathbf{r}, l]$, $l \in \mathbb{S}$, involving the matrix

$$\mathbb{A}_{\mathbf{r}}[k, l] := \left(\mathbf{A}_{\mathbf{r}}[k, l] + \alpha \delta_k^l \left(\mathrm{I} - \mathrm{P}_{\mathbf{r},l} \right) \right), \quad k, l \in \mathbb{S}. \tag{15}$$

Note that the regularization term shifts the eigenvalues 0 into α. The linear system $Ax = b$ is transformed into the block-diagonal form

$$\sum_{l \in \mathbb{S}} \mathbb{A}_{\mathbf{r}}[k, l] \hat{x}[\mathbf{r}, l] = \hat{b}[\mathbf{r}, k], \quad k, l \in \mathbb{S}, \quad \mathbf{r} \in \mathcal{R}, \tag{16}$$

where each square block $\mathbb{A}_{\mathbf{r}}$ has size $d_{\mathbf{r}} \cdot |\,\mathbb{S}\,|$ and appears $d_{\mathbf{r}}$ times.

Theorem 14. A is non-singular if and only if all $\mathbb{A}_{\mathbf{r}}$ are non-singular. Hence the equations (16) can be considered to be a regularization of (12).

Proof: Assume that A is non-singular. We only need to show that the homogeneous equations

$$\sum_{l \in \mathbb{S}} \left(\mathbf{A}_{\mathbf{r}}[k, l] + \alpha \delta_k^l \left(\mathrm{I} - \mathrm{P}_{\mathbf{r},l} \right) \right) f[\mathbf{r}, l] = 0, \quad k, l \in \mathbb{S} \tag{17}$$

have only the trivial solution. Here the $f[\mathbf{r}, l]$ are assumed to be square matrices of size $d_{\mathbf{r}}$ for each $\mathbf{r} \in \mathcal{R}$ and $l \in \mathbb{S}$. Hence we have to show that (17) implies that $f[\mathbf{r}, l] = 0$. If we multiply (17) from the left with $\mathrm{I} - \mathrm{P}_{\mathbf{r},k}$, then Lemma 11 and equation (11) imply that

$$(\mathrm{I} - \mathrm{P}_{\mathbf{r},k})\, f[\mathbf{r}, k] = 0, \quad k \in \mathbb{S}$$

and hence

$$\sum_{l\in\mathbb{S}} \mathbf{A}_{\mathbf{r}}[k,l] f[\mathbf{r},l] = 0, \quad k,l \in \mathbb{S}\,.$$

Note that f satisfies the assumptions of Lemma 12, and hence $f = \hat{w}$ for some $w \in \mathbb{C}^n$. Now Lemma 9 implies that $Aw = 0$. By the non-singularity of A we have $w = 0$ and hence $f = \hat{w} = 0$.

Conversely, let all $\mathbb{A}_{\mathbf{r}}$ be non-singular. We show that the homogeneous equation $Ax = 0$ has only the trivial solution. However, from Theorem 13 it follows that $\hat{x}$ is a solution of (17). Hence $\hat{x} = 0$ by assumption. Now the inverse Fourier transform (9) shows that $x = 0$. ☐

Recall that the regularization term shifts the 0 eigenvalues into α. Hence for small α we would still have a large condition numbers $\mathrm{cond}(\mathbb{A}_{\mathbf{r}})$. For practical purposes we therefore choose $\alpha = \mathcal{O}(||A||)$.

Let us summarize the symmetry reduction method of solving $Ax = b$ for the case that fixed points are handled via regularization:

1. Calculate the Fourier transform $\hat{b}$ of b.
2. Calculate the Fourier transform $\hat{a}_l$ of a selection of columns a_l to generate the submatrices $\mathbf{A}_{\mathbf{r}}$ in (11).
3. Solve the regularized reduced problems (14) for a complete list of irreducible representations $\mathbf{r} \in \mathcal{R}$.
4. Use the symmetry relations (7) to obtain $\hat{x}[\mathbf{r},k]$ for all $k = 1:n$.
5. Use the inverse Fourier transform (9) to retrieve x from $\hat{x}$.

The efficiency discussion at the end of Section 5 remains largely valid. Note, however, that the equations (14) have $|\,\mathbb{S}\,| \cdot |\Gamma| > n$ variables. We take into account an increased amount of variables to handle fixed points. For typical discretization methods, the fixed indices refer to nodes that are in the invariant subspaces of some reflections contained in the symmetry group Γ. Hence, especially for finer discretizations, most nodes are fixed point free. More precisely, we have $n/(|\,\mathbb{S}\,| \cdot |\Gamma|) \to 1$ as the discretization becomes finer, and hence the increase $|\,\mathbb{S}\,| \cdot |\Gamma| - n$ in variables is not significant.

7 Handling Fixed Points via Projections

Let us now describe an alternative way of handling fixed points without increasing the number of variables.

For each $\mathbf{r} \in \mathcal{R}$ and $i \in \mathbb{S}$ we introduce a matrix $u_{\mathbf{r},i}$ of size $(d_{\mathbf{r}}\,,\, m_{\mathbf{r},i})$ whose columns are an orthonormal basis of the range of the projectors $\mathrm{P}_{\mathbf{r},i}$. Hence

$$u_{\mathbf{r},i} u_{\mathbf{r},i}^* = \mathrm{P}_{\mathbf{r},i} \quad \text{and} \quad u_{\mathbf{r},i}^* u_{\mathbf{r},i} = \mathrm{I}\,. \tag{18}$$

Note that for the symmetry groups corresponding to discretizations of three dimensional problems, $d_{\mathbf{r}}$ is very small and typically has values in $\{1,2,3\}$. For a given column $w \in \mathbb{C}^n$ we introduce a *modified Fourier transform*

$$\tilde{w}[\mathbf{r},i] := u_{\mathbf{r},i}^* \hat{w}[\mathbf{r},i]. \tag{19}$$

Note that Lemma 11 and (18) imply

$$\hat{w}[\mathbf{r},i] = u_{\mathbf{r},i} \tilde{w}[\mathbf{r},i]. \tag{20}$$

Lemma 15. If $Ax = b$, then

$$\sqrt{\tfrac{|\Gamma|}{d_{\mathbf{r}}}} \sum_{l\in\mathbb{S}} \tfrac{1}{|\Gamma_l|} \tilde{a}_l[\mathbf{r},k] u_{\mathbf{r},l}\, \tilde{x}[\mathbf{r},l] = \tilde{b}[\mathbf{r},k], \quad \mathbf{r} \in \mathcal{R},\ k \in \mathbb{S}\,. \tag{21}$$

Note that for each fixed irreducible representation $\mathbf{r} \in \mathcal{R}$, these are linear equations for the $\sum_{l\in\mathbb{S}} m_{\mathbf{r},l} \cdot d_{\mathbf{r}}$ unknowns $\tilde{x}[\mathbf{r},l]$, $l \in \mathbb{S}$, involving the matrix

$$\mathcal{A}_{\mathbf{r}}[k,l] := \sqrt{\tfrac{|\Gamma|}{d_{\mathbf{r}}}}\, \tfrac{1}{|\Gamma_l|} \tilde{a}_l[\mathbf{r},k] u_{\mathbf{r},l}, \quad k,l \in \mathbb{S}\,. \tag{22}$$

Note that (22) implies

$$\mathcal{A}_{\mathbf{r}}[k,l] = u_{\mathbf{r},k}^* \mathbf{A}_{\mathbf{r}}[k,l] u_{\mathbf{r},l}\,, \quad \mathbf{r} \in \mathcal{R},\ k,l \in \mathbb{S}\,. \tag{23}$$

Thus, the linear system $Ax = b$ is transformed into the block-diagonal form

$$\sum_{l\in\mathbb{S}} \mathcal{A}_{\mathbf{r}}[k,l]\, \tilde{x}[\mathbf{r},l] = \tilde{b}[\mathbf{r},k], \quad k,l\in\mathbb{S}, \quad \mathbf{r}\in\mathcal{R}, \tag{24}$$

where each square block $\mathcal{A}_{\mathbf{r}}$ has size $\sum_{l\in\mathbb{S}} m_{\mathbf{r},l}$ and appears $d_{\mathbf{r}}$ times. We note again that (24) represents the splitting discussed in (2).

Proof: From (10) and Lemma 11 we obtain

$$\sqrt{\tfrac{|\Gamma|}{d_{\mathbf{r}}}} \sum_{l\in\mathbb{S}} \tfrac{1}{|\Gamma_l|} u^*_{\mathbf{r},k} \hat{a}_l[\mathbf{r},k]\ \mathrm{P}_{\mathbf{r},l}\ \hat{x}[\mathbf{r},l] = u^*_{\mathbf{r},k}\hat{b}[\mathbf{r},k] = \sqrt{\tfrac{|\Gamma|}{d_{\mathbf{r}}}} \sum_{l\in\mathbb{S}} \tfrac{1}{|\Gamma_l|} u^*_{\mathbf{r},k} \hat{a}_l[\mathbf{r},k] u_{\mathbf{r},l}\ u^*_{\mathbf{r},l}\hat{x}[\mathbf{r},l]$$

which shows (21). □

Lemma 16. A is non-singular if and only if all the block matrices $\mathcal{A}_{\mathbf{r}}$ are non-singular.

Proof: Let A be non-singular. We show that the homogeneous equations

$$\sum_{l\in\mathbb{S}} \mathcal{A}_{\mathbf{r}}[k,l] f[\mathbf{r},l] = 0, \quad k,l\in\mathbb{S}, \quad \mathbf{r}\in\mathcal{R}, \tag{25}$$

where $f[\mathbf{r},l]$ is of size $(m_{\mathbf{r},l}\,,\, d_{\mathbf{r}})$, have only the trivial solution. In fact, given (25), we obtain from (23) that

$$\sum_{l\in\mathbb{S}} u_{\mathbf{r},k}\mathcal{A}_{\mathbf{r}}[k,l] f[\mathbf{r},l] = \sum_{l\in\mathbb{S}} \mathbf{A}_{\mathbf{r}}[k,l] u_{\mathbf{r},l} f[\mathbf{r},l] = 0.$$

Hence $(\mathrm{I}-\mathrm{P}_{\mathbf{r},l})\, u_{\mathbf{r},l} f[\mathbf{r},l] = 0$ implies

$$\sum_{l\in\mathbb{S}} \left(\mathbf{A}_{\mathbf{r}}[k,l] + \alpha\delta_k^l\, (\mathrm{I}-\mathrm{P}_{\mathbf{r},l})\right) u_{\mathbf{r},l} f[\mathbf{r},l] = 0.$$

From Theorem 13 it now follows that all $u_{\mathbf{r},k} f[\mathbf{r},l] = 0$ and hence all $f[\mathbf{r},l] = 0$.

Conversely, assume that all the block matrices $\mathcal{A}_{\mathbf{r}}$ are non-singular. We show that $Ax = 0$ implies $x = 0$. By Lemma 15 we have that $\tilde{x}$ satisfies the homogeneous equations (25). Therefore $\tilde{x} = 0$. From (20) it follows that $\hat{x} = 0$. Now the inverse Fourier transform (9) shows that $x = 0$. □

By steps similar to those above we can also show:

Lemma 17. Let $\tilde{F}^n$ be the space of coordinates $f[\mathbf{r},l]$, $\mathbf{r}\in\mathcal{R}$, $l\in\mathbb{S}$ where each block $f[\mathbf{r},l]$ is of size $(m_{\mathbf{r},l}\,,\, d_{\mathbf{r}})$. Then the modified Fourier transform is an isomorphism from $\mathbb{C}^n$ onto $\tilde{F}^n$.

Corollary 18. The above dimensions satisfy the equation

$$\sum_{\mathbf{r}\in\mathcal{R}} \sum_{l\in\mathbb{S}} m_{\mathbf{r},l}\ d_{\mathbf{r}} = n.$$

Hence, symmetry reduction by projections does not increase the number of unknowns and yields a non-singular block diagonal system of equations.

Comparing with the symmetry adapted basis method, if the action of Γ on $\mathbb{R}^n$ is split into irreducible representations, then each $\mathbf{r}\in\mathcal{R}$ occurs with a certain multiplicity $c_{\mathbf{r}}$. It can be easily seen that we have

$$c_{\mathbf{r}} = \sum_{l\in\mathbb{S}} m_{\mathbf{r},l}\,.$$

Let us summarize the method of solving $Ax = b$ for the case that fixed points are handled via projections:

1. Calculate the modified Fourier transform $\tilde{b}$ of b.
2. Calculate the modified Fourier transform $\tilde{a}_l$ of a selection of columns a_l to generate the submatrices $\mathcal{A}_{\mathbf{r}}$ in (22).
3. Solve the reduced problems (24) for a complete list of irreducible representations $\mathbf{r}\in\mathcal{R}$.
4. Calculate $\hat{x}[\mathbf{r},k] = u_{\mathbf{r},k}\tilde{x}[\mathbf{r},k]$ for $\mathbf{r}\in\mathcal{R}$ and $k\in\mathbb{S}$, see (20).
5. Use the symmetry relations (7) to obtain $\hat{x}[\mathbf{r},k]$ for all $k = 1:n$.
6. Use the inverse Fourier transform (9) to retrieve x from $\hat{x}$.

8 Examples

Let us now return to our simple example of Figure 1, a complete list of irreducible representations for the dihedral group D_3 is given in Table 1. The symmetry reduction method via regularization and via projections is now described in Tables 2-3, respectively. For increasing n, the number of additional unknowns in the method using regularization obviously is of decreasing significance.

	I	R	R^2	F	RF	R^2F
$\mathbf{r}_1$	1	1	1	1	1	1
$\mathbf{r}_2$	1	1	1	-1	-1	-1
$\mathbf{r}_3$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$	$\begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$	$\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$	$\begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$

Table 1: Irreducible Representations of D_3

Total number of original unknowns: $n = 12$
Total number of transformed unknowns: $n + 6 = 18$
Irreducible representations and size of transformed unknowns in the resulting subsystems:
$\mathbf{r}_1, \mathbf{r}_2$: $(\, n/6+1\,,\,1\,) = (\,3\,,\,1\,)$ $\mathbf{r}_3$: $(\, n/3+2\,,\,2\,) = (\,6\,,\,2\,)$

Table 2: Symmetry Reduction for Figure 1 via Regularization

Total number of original unknowns: $n = 12$
Total number of transformed unknowns: $n = 12$
Irreducible representations and size of transformed unknowns in the resulting subsystems:
$\mathbf{r}_1$: $(\, n/6+1\,,\,1\,) = (\,3\,,\,1\,)$ $\mathbf{r}_2$: $(\, n/6-1\,,\,1\,) = (\,1\,,\,1\,)$
$\mathbf{r}_3$: $(\, n/3\,,\,2\,) = (\,4\,,\,2\,)$

Table 3: Symmetry Reduction for Figure 1 via Projection

The symmetry reduction method has been studied in some detail for the case that the domain under consideration displays the symmetry of the three dimensional cube, e.g., boundary element methods for an exterior boundary value problem, see [3, 18, 19, 28, 29]. Let us mention one example of a discretization of the surface of the cube via boundary element methods, namely collocation with quadratic elements. The numerical codes in [6] can be used to obtain the entries of the system matrix and right hand side.

The collocation points are indicated in Figure 2 where only a selection of collocation points is shown, i.e., the remaining points are obtained by applying the 48 symmetries of the cube. Note that only one selected point, namely the one numbered 7, is not fixed under any symmetry transformation, i.e., has a trivial isotropy group.

In Table 4 the symmetry reduction via projections is portrayed. If regularization is used, then the number of unknowns changes drastically, see Table 5. However, let us note that the discretization as indicated here for the surface of the cube is extremely coarse. The same effect as in Table 2 takes place: if the discretization is refined, then the number of additional unknowns becomes insignificant vis-à-vis the overall number of unknowns, in particular when regarding the reduced equations.

9 Further Remarks

In applications it is often the case that an operator equation under investigation only displays approximate symmetries which may be flawed by either less important terms in the equation and/or imperfections in the geometrical shape, see, e.g., Figure 3.

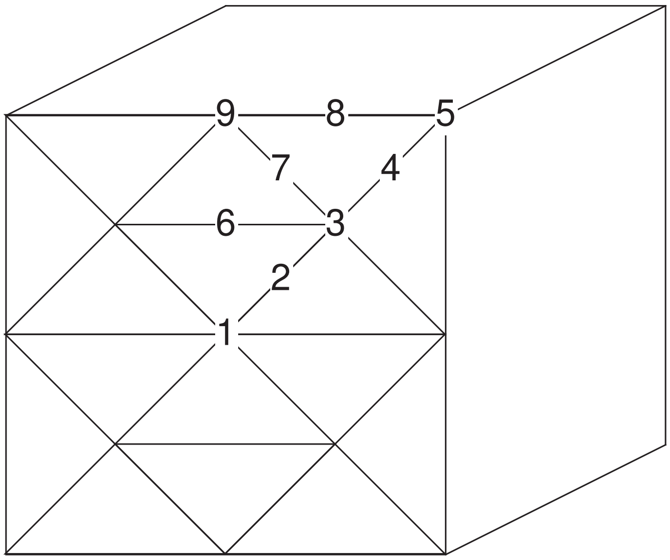

Figure 2: Cubical Surface with Collocation Points

Total number of original unknowns:	194						
Total number of transformed unknowns:	194						
Irreducible representations and size of transformed unknowns in the resulting subsystems:							
$\mathbf{r}_1$:	(9 , 1)	$\mathbf{r}_2$:	(1 , 1)	$\mathbf{r}_3$:	(2 , 1)	$\mathbf{r}_4$:	(6 , 1)
$\mathbf{r}_5$:	(10 , 2)	$\mathbf{r}_6$:	(6 , 2)	$\mathbf{r}_7$:	(16 , 3)	$\mathbf{r}_8$:	(8 , 3)
$\mathbf{r}_9$:	(10 , 3)	$\mathbf{r}_{10}$:	(14 , 3)				

Table 4: Symmetry Reduction for Figure 2 via Projection

In this case, it has been shown in the PhD thesis [28, 29] that an equivariant preconditioner for iterative solvers can be constructed which is efficient and improves convergence drastically, in particular for equations with bad conditioning (such as integral equations of the first kind).

Here, the action of a permutation group is evident from the discretization, however the equivariance conditions (5) are not quite satisfied by the system matrix A. In such situations the *equivariant part* of A

$$A_\Gamma[i,k] := \frac{1}{|\Gamma|} \sum_{g\in\Gamma} A[gi, gk]$$

is a very good preconditioner. In fact, it is easily seen that A_Γ is the equivariant matrix nearest to A in the Frobenius norm. Our symmetry reduction method asserts that the action A_Γ^{-1} can be implemented at a low computational expense.

If an eigenvalue problem of the type $Ax = \lambda x$ with an equivariant matrix A has to be solved, we can use our symmetry reduction method via projection analogously to (24) in order to generate eigenvalue subproblems

$$\sum_{l\in\mathbb{S}} \mathcal{A}_{\mathbf{r}}[k,l]\,\tilde{x}[\mathbf{r},l] = \lambda\tilde{x}[\mathbf{r},k], \quad k,l \in \mathbb{S}, \quad \mathbf{r}\in\mathcal{R}\,. \tag{26}$$

The symmetry reduction method (16) via extension is usually less suited here because an additional artificial eigenvalue α is generated ($\alpha = 0$ works in this case).

Since the subproblems (26) can be viewed as a block diagonalization of the original problem with respect to a suitable basis transformation (symmetry adapted basis), the eigenvalues of the original matrix A are distributed among the various blocks $\mathcal{A}_{\mathbf{r}}$. Multiplicities of eigenvalues generated by the symmetries disappear. Eigenvectors are also easily obtained from the subproblems.

In general, if A is a sparse matrix, the symmetry reduced submatrices $\mathbf{A}_{\mathbf{r}}$, $\mathcal{A}_{\mathbf{r}}$, or $\mathbb{A}_{\mathbf{r}}$ are still sparse. In general, we can only estimate how the sparseness structure of the block matrices looks, because this depends on the distribution of the non-zero entries in a column with respect to the orbits $\{\,gi\,:\,g\in\Gamma\,\}$, $i\in\mathbb{S}$ of the selected indices. Let us assume that each column of A contains maximally q non-zero entries. Then the worst case is that a submatrix has maximally $q\cdot d_{\mathbf{r}}$ non-zero entries per column, and the best case is that a submatrix has maximally $\mathrm{ceil}\,(q/|\Gamma|)\cdot d_{\mathbf{r}}$ non-zero entries per column, where $\mathrm{ceil}(a)$ rounds a to the nearest integer towards ∞.

Total number of original unknowns:	194
Total number of transformed unknowns:	432
Irreducible representations and size of transformed unknowns in the resulting subsystems:	
$\mathbf{r}_1,\ldots,\mathbf{r}_4$: (9 , 1) $\mathbf{r}_5,\mathbf{r}_6$: (18 , 2) $\mathbf{r}_7,\ldots,\mathbf{r}_{10}$: (27 , 3)	

Table 5: Symmetry Reduction for Figure 2 via Regularization

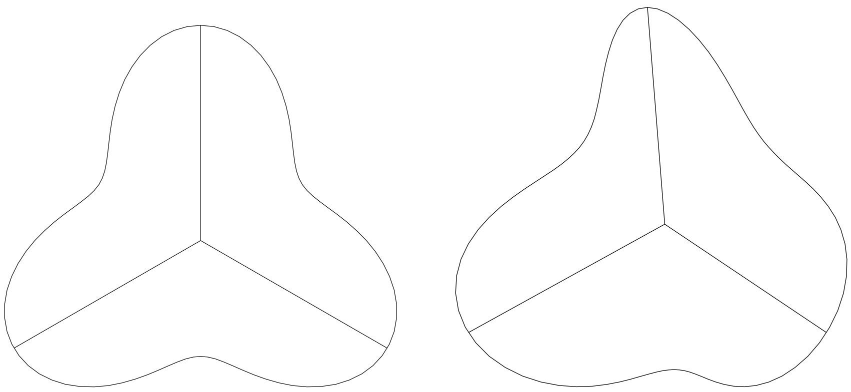

Figure 3: D_3-Symmetric and Nearly D_3-Symmetric Domain

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