3-D SYMMETRY DETECTION USING THE PSEUDO-POLAR FOURIER TRANSFORM

Amit Bermanis

School of Mathematical Sciences,

Tel-Aviv University, Tel-Aviv 69978, Israel.

Email: amitberm@post.tau.ac.il

Amir Averbuch

School of Computer Science,

Tel-Aviv University, Tel-Aviv 69978, Israel.

Email: amir@math.tau.ac.il

Abstract. Symmetry detection in $3D$ images is an important task in many fields such as computer vision, pattern recognition to name a few. An algebraic based $3D$ symmetry detection algorithm is presented. The $3D$ volume is transformed to the Fourier domain by using the pseudo-polar Fourier transform. The pseudo-polar representation enables to analyze angular properties such as finite symmetric properties that stay invariant under the transform. The algorithm is based on analysis of the angular correspondence rate of the given volume and its rotated and rotated-inverted replicas in their pseudo-polar representations. Initially, the algorithm detects the rotations symmetry group of the given volume. This group enables to detect the rest of the symmetries. The complexity of the algorithm is $O\left(N^3log(N)\right)$, where $N \times N \times N$ is the volumetric size. The complexity of the proposed algorithm is independent of the number of detected symmetries. Different types of objects were tested. The results demonstrate that all the symmetries, including imperfect ones, are detected by the proposed algorithm.

Key words = {3D Symmetry, Pseudo-Polar, Symmetry Groups}.

AMS classification = {51N30, 58D19, 58J70}.

1. Introduction

Many objects around us exhibit some form of symmetry, i.e., repeated patterns. Much of our perception of the world is based on recognition of repeated structures, and so is our sense of aesthetics [1]. In addition, many man-made objects such as airplanes and houses, and natural objects such as insects and molecules (see Fig. 1) exhibit some form of symmetry. Hence, symmetry detection has become a fundamental task in computer vision.

Our paper presents a new algebraic based method to symmetries detection of a $3D$ volume using the

FIGURE 1. Symmetric objects

(a) (b) (c) (d)

(a) Airplane - reflective symmetry in respect to the horizontal plane. (b) House. (c) Insect - reflective symmetry in respect to the vertical plane. (d) H_2O molecule - reflective symmetries in respect to the $x - z$ and $y - z$ planes and rotational symmetry in respect to z-axis.

$3D$ Pseudo-Polar Fourier Transform (3DPPFT) [2] and the Angular Difference Function[1] (ADF), which measures the correspondence rate between two volumes along rays in the same direction. The algorithm detects both perfect and imperfect symmetries. The term ***volume*** refers to a $3D$ image, which formally is a function $V : C \rightarrow G$, where C is a $3D$ Cartesian grid, G is a set of real scalars representing gray levels, and the support of V is a bounded set. Our goal is to detect all the isometries $T : \mathbb{R}^3 \rightarrow \mathbb{R}^3$, s.t. V is invariant under their action, which will be defined in section 3. For example, the molecule in Fig. 1(d) stays unchanged by rotating it with $\pi\, radians$ around the z-axis and also by reflecting it in respect to the $x - z$ and $y - z$ planes. Therefore, in addition to the identity transformation, the described transformations constitute the symmetry group of the molecule. Since $3D$ symmetry is a polar property, the use of the pseudo-polar grid [2] becomes a natural option. The symmetry groups that we explore are finite and according to the boundness of the volumes, they do not include translations, but only isometries which have a fixed point. These isometries have two types [3]: Direct (rotations), which preserve orientation, and opposite (rotation-inversions), which do not preserve orientation. There are five different categories for finite, nontrivial, fixed point rotational symmetry groups. In section 3 we show the connections between the rotations group of a volume and its opposite symmetries. The algorithm is based on the analysis of the ADF of the given volume and its rotated and rotated-inverted replicas in their 3DPPFT representation. Initially, the algorithm detects the rotations symmetry group of the given volume. This group enables to detect the opposite symmetries. The complexity of the algorithm is $O\left(N^3 log(N)\right)$, where $N \times N \times N$ is the volumetric size.

The paper presents two major results: Theorem 4.8, which constitutes the algebraic basis for the algorithm and the algorithm itself (Algorithm 4.21). The complexity of the execution of the costly steps in Algorithm 4.21 is independent of the number of symmetries of the volume.

[1]The idea of using the ADF was first presented in [4].

The paper is organized as follows: Section 2 presents works that are related to $3D$ symmetry detection. Section 3 provides the mathematical formulation of symmetries as well as the angular properties of the Fourier domain and the ADF. Section 4 presents the $3D$ Symmetry Detection Algorithm ($3DSDA$). The experimental results, which are described in section 5, demonstrate the application of the algorithm on both perfect and imperfect symmetric models.

2. Related Works

Most of the works regarding $3D$ symmetry detection are based on recognition of features in the $3D$ object, which is usually represented as a set of points in $\mathbb{R}^3$ rather than a $3D$ volume. A continuous symmetry measure, which quantifies the symmetry of an object, is defined in [5]. A multi-resolution scheme for hierarchical analysis of patterns is presented in [6]. This method enables to detect inexact symmetries as a human face, for example. A method for detection both hierarchical and partial symmetry of models with components constructed from a few straight edges or polynomials is presented in [7]. The hierarchical approach is based on detection process that is applied recursively on partial objects. This method is computationally intensive. A model for general $3D$ objects with an algorithm to test congruence or symmetry in these objects is given in [8]. Since the model relies on a mapping between points in the object, it is topology dependent. In addition, the model can be implemented only on polyhedral connected objects. The Extended Gaussian Image method is presented in [9]. It identifies symmetries by looking at correlations in the Gaussian image and relies on the PCA to identify potential symmetry axes. It detects only rotational and reflectional symmetries, even though there are other types of symmetries. The generalized moment functions is used in [10]. It computes the spherical harmonics coefficients for these functions, which enable to recover the shapes symmetries. A computational geometric approach is described in [11]. It is based on projection of the body on a sphere, construction of a convex hull, and analysis of the resulting geometric model. A symmetry descriptor is used in [12]. It provides a continuous measure of rotational and reflective symmetries, using spherical harmonics analysis. It does not deal with other fixed point symmetries. An algorithm for reflective symmetries detection is described in [13]. It suggests to examine each plane, which passes through the center of mass of the given object. Statistical methods and local geometric features analysis are used in [14]. Our proposed method is different from these.

3. Mathematical Preliminaries

3.1. **Normal transformations.**

Definition 3.1. Let $T:\mathbb{R}^3\to\mathbb{R}^3$ be a linear transformation. ***The adjoint transformation of*** T, denoted by $T^\star$, is the linear transformation $T^\star:\mathbb{R}^3\to\mathbb{R}^3$, which satisfies for all $\vec{x},\vec{y}\in\mathbb{R}^3$

$$\langle T\vec{x},\vec{y}\rangle=\langle\vec{x},T^\star\vec{y}\rangle\,. \tag{1}$$

Lemma 3.2. *Let $T:\mathbb{R}^3\to\mathbb{R}^3$ be a linear transformation, then, $null\,(T^\star)=Im\,(T)^\perp$.*

Definition 3.3. Let $T:\mathbb{R}^3\to\mathbb{R}^3$ be a linear transformation. T is called ***normal*** if it commutes with its adjoint, i.e., $TT^\star=T^\star T$.

Lemma 3.4. *Let $T:\mathbb{R}^3\to\mathbb{R}^3$ be a normal transformation, then, $null\,(T)=null\,(T^\star)$.*

From Lemmas 3.2 and 3.4 we conclude:

Corollary 3.5. *If T is normal, then $Im\,(T)^\perp=null\,(T)$.*

3.2. **Isometries in $\mathbb{R}^3$.**

Definition 3.6. A linear transformation $O:\mathbb{R}^3\to\mathbb{R}^3$ is called ***isometry***, if for any vector $\vec{x}\in\mathbb{R}^3$, $\|O\vec{x}\|=\|\vec{x}\|$.

From $\langle\vec{x},\vec{y}\rangle=\frac{1}{4}\left[\langle\vec{x}+\vec{y},\vec{x}+\vec{y}\rangle-\langle\vec{x}-\vec{y},\vec{x}-\vec{y}\rangle\right]$, it follows that

$$\langle\vec{x},\vec{y}\rangle=\langle O\vec{x},O\vec{y}\rangle\,,\ \vec{x},\vec{y}\in\mathbb{R}^3 \tag{2}$$

for any isometry O. A trivial example of such transformation is the identity transformation E. Obviously, the composition of every two isometries is also an isometry. Any isometry O satisfies ([3])

$$det(O)\in\{\pm1\}. \tag{3}$$

Definition 3.7. ***The orthogonal group in*** $\mathbb{R}^3$, denoted by $\mathcal{O}(3)$, is the group of all isometries $O:\mathbb{R}^3\to\mathbb{R}^3$ whose operation is the standard transformations composition.

For any $O\in\mathcal{O}(3)$

$$O^{-1}=O^\star. \tag{4}$$

O is called ***rotation*** if $det(O)=1$, otherwise, O is called ***rotation-inversion***.

3.2.1. *Rotations.*

Definition 3.8. The ***special orthogonal group in*** $\mathbb{R}^3$, denoted by $\mathcal{SO}(3)$, is the subgroup of all the rotations in $\mathcal{O}(3)$.

Theorem 3.9. *([3])* Let $O \in \mathcal{SO}(3)$. Then, there is a vector $\vec{f} \in \mathbb{R}^3$, $\left\|\vec{f}\right\| = 1$, such that $O\vec{f} = \vec{f}$.

Theorem 3.9 also states that any rotation O has an eigenvalue 1. If $O \in \mathcal{SO}(3)$, $O \neq E$, then, the axis designated by $\pm\vec{f}$ is called the ***rotation axis of*** O and since $O^{-1}\vec{f} = \vec{f}$, it is also the rotation axis of O^{-1}. Any rotation $O \in \mathcal{SO}(3)$ can be identified by two parameters - the angle of rotation γ and the rotation axis $\vec{f} = (f_1\, f_2\, f_3)^t$, i.e., for each $\vec{x} \in \mathbb{R}^3$, s.t. $\vec{x} \perp \vec{f}$, we have $\sphericalangle(\vec{x}, O\vec{x}) = \gamma$. Two additional eigenvalues of O are $e^{i\gamma}$ and $e^{-i\gamma}$ ([15]). $\vec{f}$ can be identified by two spherical angles θ and ϕ, which satisfy $f_1 = sin\phi cos\theta$, $f_2 = sin\phi sin\theta$, $f_3 = cos\phi$, where $0 \leq \theta < 2\pi$ and $0 \leq \phi < \pi$. According to Euler's rotation theorem [15], the rotation matrix of O is

$$O = Ecos\gamma + (1 - cos\gamma)\begin{pmatrix} f_1^2 & f_1f_2 & f_1f_3 \\ f_1f_2 & f_2^2 & f_2f_3 \\ f_1f_3 & f_2f_3 & f_3^2 \end{pmatrix} + sin\gamma\begin{pmatrix} 0 & -f_3 & f_2 \\ f_3 & 0 & -f_1 \\ -f_2 & f_1 & 0 \end{pmatrix}, \tag{5}$$

where E is the 3×3 identity matrix.
If $\gamma = \frac{2\pi}{n}$, $n \in \mathbb{N}$, then, O is called a ***rotation of order* n**. Obviously, if O_1 and O_2 are two rotations sharing the same rotation axis $\vec{f}$, whose rotation angles are γ_1 and γ_2, respectively, then the rotation axis of O_2O_1 is $\vec{f}$ with the rotation angle $\gamma = \gamma_1 + \gamma_2$. Therefore, O is rotation of order n if and only if n is the smallest integer which satisfies $O^n = E$. Not all the rotations in $\mathcal{SO}(3)$ are of finite order: let O be a rotation with rotation angle $\gamma = 2radians$. In this case, there is no $n \in N$ s.t. $\gamma = \frac{2\pi}{n}$.

3.2.2. *Rotation-inversions.*
Obviously, if R is a rotation-inversion, then, $O_R \triangleq -R$ is a rotation. Hence, any rotation-inversion R can be written as $R = -O_R$. As a consequence, we get that any rotation-inversion R has an eigenvalue -1 and two other eigenvalues $-e^{i\gamma}$ and $-e^{-i\gamma}$, where γ is the rotation angle of O. Two examples of rotation-inversions are reflection and inversion.

Definition 3.10. A rotation-inversion R is called ***reflection*** if it has two eigenvalues 1. The eigenspace, which corresponds to eigenvalue 1, is called the ***reflection plane of*** R, and the eigenvector, which corresponds to eigenvalue -1, is called the ***reflection axis of*** R.

Lemma 3.11. *Let R be a reflection, then, the reflection plane of R is perpendicular to the reflection axis of R.*

The reflection operator, whose axis is $\vec{f}$, is ([18])

$$R_{\vec{f}}\left(\vec{x}\right) = \bar{x} - 2\frac{\left\langle \vec{x}, \vec{f}\right\rangle}{\left\|\vec{f}\right\|^2}\vec{f}. \tag{6}$$

Obviously, $R_{\vec{f}} = R_{-\vec{f}}$.

Lemma 3.12. *Let R be a reflection, then $R^2 = E$.*

Proof. According to definition 3.10, R^2 has three eigenvalues 1, i.e. $R^2 = E$. ☐

From Lemma 3.12 and Eqs. 3 and 4 it follows that any reflection R satisfies

$$R = R^{-1},\ R = R^{\star}. \tag{7}$$

Lemma 3.13. *Given two normal vectors $\vec{a}, \vec{b} \in \mathbb{R}^3$, $\vec{a} \neq \vec{b}$, then, the only reflection R, that satisfies*

$$R\vec{a} = \vec{b} \tag{8}$$

is $R = R_{\vec{f}}$, where $\vec{f} = \frac{\vec{a}-\langle\vec{a},\vec{v}\rangle\vec{v}}{\|\vec{a}-\langle\vec{a},\vec{v}\rangle\vec{v}\|^2}$ and $\vec{v} = \frac{\vec{a}+\vec{b}}{\left\|\vec{a}+\vec{b}\right\|}$ is the normal angle bisector between $\vec{a}$ and $\vec{b}$. Moreover, if $\vec{p} \in span\left\{\vec{a}, \vec{b}\right\}^{\perp}$, then, $R_{\vec{f}}\left(\vec{p}\right) = \vec{p}$.

Definition 3.14. ***Inversion***, denoted by I, is the linear transformation $I\left(\vec{x}\right) = -\vec{x}$.

Obviously, I has three eigenvalues -1 and $I^2 = E$.

Lemma 3.15. *If R is rotation-inversion, which satisfies $R^2 = E$, then, R is either reflection or inversion.*

Proof. Since the eigenvalues of R are -1, $-e^{i\gamma}$ and $-e^{-i\gamma}$ and $R^2 = E$ it follows that $e^{2i\gamma} = 1$, i.e., $2i\gamma = 0$ or $2i\gamma = 2\pi$. The first option leads to $\gamma = 0$, which means that the eigenvalues of R are all -1, i.e., R is inversion. The second option leads to $\gamma = -i\pi$, which means that the eigenvalues of R are -1, 1 and 1, i.e., R is reflection. ☐

3.3. **Finite Symmetric Volumes.**

Symmetric volumes, whose rotations groups are finite and nontrivial, are classified into five different categories. In addition, the connection between the rotations group of a volume and the rest of its symmetry group is revealed.

Let $S \subset \mathbb{R}^3$ be a bounded set. A function $V : S \rightarrow \mathbb{R}$ is called a $3D$ volume, or, in a nutshell, *volume*.

Definition 3.16. Let V be a volume and let T be a non-singular linear transformation. The ***action of*** T ***on*** V, denoted by $\Lambda(T)V$, is the function

$$\Lambda(T)V(\vec{x}) \triangleq V\left(T^{-1}\vec{x}\right), \ \vec{x} \in \mathbb{R}^3, \tag{9}$$

and the composition rule for two actions is

$$\Lambda(T_2)\Lambda(T_1)V \triangleq \Lambda(T_2T_1)V \tag{10}$$

(T_2 operates after T_1), where T_1 and T_2 are two non-singular linear transformations.

Definition 3.17. Let V be a volume. $O \in \mathcal{O}(3)$ is called ***a symmetry of*** V if $\Lambda(O)V = V$.

The ***symmetry group of*** V, denoted by $\mathcal{G}_V$, is the group of all symmetries of V, whose operation is defined in definition 3.16. Since $E \in \mathcal{G}_V$ for any volume V, $\mathcal{G}_V \neq \emptyset$. The subgroup of $\mathcal{G}_V$, which contains only rotations, is called the ***rotations group of*** V, denoted by $\mathcal{K}_V$. We are interested only in volumes whose symmetry groups are finite, unlike a ball, for instance, whose symmetry group is $\mathcal{O}(3)$.
V is called ***symmetric volume*** if $\mathcal{G}_V \neq \{E\}$. A vector $\vec{f} \in \mathbb{R}^3$ is called ***a rotation axis of*** V if there is rotation $O \in \mathcal{K}_V$ whose rotation axis is $\vec{f}$. If $\vec{f}$ is a rotation axis of V, then, there is a rotation $O \in \mathcal{K}_V$ of maximal order $n \in \mathbb{N}$, whose axis is $\vec{f}$, i.e. there are n rotations in $\mathcal{K}_V$, which are associated with $\vec{f}$. The subgroup of these rotations is the ***cyclic group***, whose ***generator*** is O, i.e., $\langle O \rangle \triangleq \left\{O^k : k = 1, 2, ..., n-1\right\}$. In this case, $\vec{f}$ is called **n-*fold rotation axis of*** V. $\mathcal{P}$ is called ***reflection plane of*** V and $\vec{f}$ is called ***reflection axis of*** V if there is a reflection $R \in \mathcal{G}_V$, s.t., $\mathcal{P}$ and $\vec{f}$ are its reflection plane and reflection axis, respectively.

Lemma 3.18. *Let $\vec{f} \in \mathbb{R}^3$ be an n-fold rotation axis of V and let $S \in \mathcal{G}_V$. Then, $S\vec{f}$ is also an n-fold axis of V.*

Proof. Define $\tilde{O} \triangleq SOS^{-1}$, where O is the rotation of order n associated with $\vec{f}$. Obviously, $\tilde{O} \in \mathcal{K}_V$ and $\tilde{O}S\vec{f} = S\vec{f}$, i.e., $S\vec{f}$ is a rotation axis of V. In addition, $\tilde{O}^n = \left(SOS^{-1}\right)^n = SO^nS^{-1} = E$. Suppose that there is $k < n$, s.t. $\tilde{O}^k = E$, then, $SO^kS^{-1} = E$, i.e., $O^k = E$, which contradicts the fact that O is a rotation of order n. □

Lemma 3.19. *Let $\mathcal{G}$ be a subgroup of $\mathcal{O}(3)$ and let $\mathcal{K}$ be the rotations subgroup of $\mathcal{G}$, i.e., $\mathcal{K} \triangleq \mathcal{G} \cap \mathcal{SO}(3)$. Then, either $\mathcal{G} = \mathcal{K}$ or $\mathcal{G} = \mathcal{K} \cup R\mathcal{K}$, where R is any rotation-inversion in $\mathcal{G}$ and $R\mathcal{K} \triangleq \{RO : O \in \mathcal{K}\}$.*

Proof. If $\mathcal{G} \neq \mathcal{K}$ then there is a rotation-inversion $R \in \mathcal{G}$. Let $S \in \mathcal{G}$. If S is a rotation, then, $S \in \mathcal{K}$. Otherwise, S is a rotation-inversion and $R^{-1}S$ is a rotation in $\mathcal{G}$, i.e., there is a rotation $O \in \mathcal{K}$ such that $R^{-1}S = O$, hence, $S = RO \in R\mathcal{K}$. The opposite direction is straightforward. □

Corollary 3.20. *In order to fully characterize a finite symmetry group, it suffices to find its rotations subgroup and a single rotation-inversion, if there is any.*

Lemma 3.21. *(*[16]*)Any finite symmetry group $\mathcal{G}$ either consists of rotations only, i.e., $\mathcal{G} = \mathcal{K}$ or it contains a rotation-inversion of order two.*

From Lemmas 3.15 and 3.21 we conclude:

Corollary 3.22. *If $\mathcal{G}_V \neq \mathcal{K}_V$, then, $\mathcal{G}_V$ contains either inversion or reflection.*

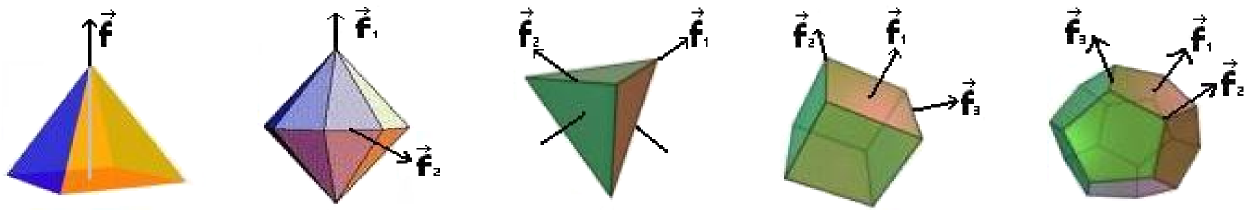
Theorem 3.23. *(*[3]*)Let V be a volume whose symmetry group $\mathcal{G}_V$ is finite. Let $\mathcal{K}_V \triangleq \mathcal{G}_V \cap \mathcal{SO}(3)$ be the rotations group of V and let $n \triangleq |\mathcal{K}_V|$. Then, unless $\mathcal{K}_V$ is trivial, it belongs to exactly one of the next five categories:*

(1) ***Cyclic:*** $\mathcal{K}_V$ is a cyclic group, i.e., there is $O \in \mathcal{SO}(3)$ of order n, such that $\mathcal{K} = \langle O \rangle \triangleq \{O^k,\, k = 0, 1, ..., n-1\}$. In this case, V has exactly one n-fold rotation axis, see Fig. 2(a).
(2) ***Dihedric:*** $n = 2m$, $m \geq 2$. In this case, V has one m-fold rotation axis, which is called the ***principle axis of*** V, and m twofold rotation axes, which are called the ***secondary rotation axes of*** V . The secondary rotation axes are all perpendicular to the principle axis. The angle between any two adjacent axes of these twofold axes is $\frac{\pi}{m}$, see Fig. 2(b).
(3) ***Tetrahedric:*** $n = 12$. V has four threefold rotation axes and three twofold rotation axes, see Fig. 2(c).
(4) ***Octahedric:*** $n = 24$. V has three fourfold rotation axes, four threefold rotation axes and six twofold rotation axes, see Fig. 2(d).
(5) ***Icosahedric:*** $n = 60$. V has six fivefold rotation axes, ten threefold rotation axes and fifteen twofold rotation axes, see Fig. 2(e).

Theorem 3.24. *(*[16]*) If $\mathcal{K}_V \neq \mathcal{G}_V$, $\mathcal{K}_V \neq \{E\}$ is finite and $I \notin \mathcal{G}_V$, then, $\mathcal{K}_V$ is either Cyclic, Dihedric or Tetrahedric.*

In the rest of this section, we will explore the finite subgroups of $\mathcal{O}(3)$ that contain not only rotations, whose rotations subgroups are either Cyclic or Dihedric or Tetrahedric. We will also assume that these subgroups do not include the inversion I. According to corollary 3.22, under these conditions, each of the above subgroups contains a reflection R.

FIGURE 2. Symmetric volumes with nontrivial rotations groups



(a) (b) (c) (d) (e)

(a) Cyclic rotations group. $\vec{f}$ is a single fourfold rotation axis. (b) Dihedric rotations group. $\vec{f_1}$ is the principle sixfold rotation axis and $\vec{f_2}$ is one of six twofold rotation axes. (c) Tetrahedric rotations group. $\vec{f_1}$ is one of four threefold axes and $\vec{f_2}$ is one of three twofold axes. (d) Octahedric rotations group. $\vec{f_1}$ is one of three fourfold axes, $\vec{f_2}$ is one of four threefold axes and $\vec{f_3}$ is one of six twofold axes. (e) Icosahedric rotations group. $\vec{f_1}$ is one of six fivefold axes, $\vec{f_2}$ is one of ten threefold axes and $\vec{f_3}$ is one of fifteen twofold axes.

Cyclic rotations subgroup:

Lemma 3.25. *Let $\mathcal{K}_V = \langle O \rangle$ be a Cyclic group of order n, $\mathcal{G}_V \neq \mathcal{K}_V$ and $I \notin \mathcal{G}_V$. Then, there is a reflection $R \in \mathcal{G}_V$, which either satisfies $R\vec{f} = \vec{f}$ or $R\vec{f} = -\vec{f}$, where $\vec{f}$ is the rotation axis of O (see Fig. 3 (c) and (d)). Moreover, if $R\vec{f} = \vec{f}$, then, RO^k, $k = 0, 1, ..., n-1$ are all reflections.*

Proof. From Corollary 3.22 it follows that there is a reflection $R \in \mathcal{G}_V$. Since $ROR \in \mathcal{K}_V$, there is $j \in \mathbb{N}$, s.t. $ROR = O^j$, hence, $ROR\vec{f} = \vec{f}$ and from Eq. 7 we get $OR\vec{f} = R\vec{f}$. Hence, $R\vec{f} = \vec{f}$ or $R\vec{f} = -\vec{f}$. If $R\vec{f} = \vec{f}$, then, $RO^k\vec{f} = \vec{f}$ i.e. RO^k is rotation-inversion with eigenvalue 1, hence, RO^k is a reflection for any $k = 0, 1, ..., n-1$. □

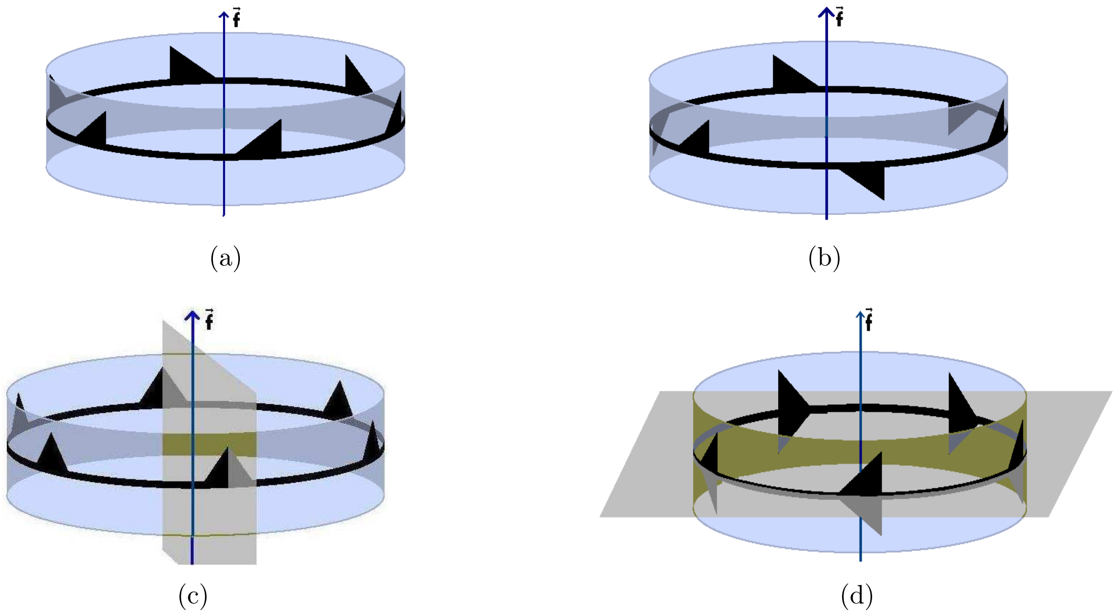
Corollary 3.26. *From Lemmas 3.19 and 3.25 it follows that if $R\vec{f} = \vec{f}$, then, $\left\{RO^k\right\}_{k=0}^{n-1}$ are all the rotation-inversions in $\mathcal{G}_V$ and they are all reflections.*

Dihedric rotations subgroup:

Lemma 3.27. *Let V be a Dihedron, $\mathcal{G}_V \neq \mathcal{K}_V$ and $I \notin \mathcal{K}_V$. Then, there is a reflection $\tilde{R} \in \mathcal{G}_V$, which satisfies $\tilde{R}\vec{f} = \vec{f}$, where $\vec{f}$ is the principle axis of V.*

Proof. From corollary 3.22 it follows that there is a reflection $R \in \mathcal{G}_V$. Let $O \in \mathcal{K}_V$ be the rotation associated with $\vec{f}$. Since $ROR \in \mathcal{K}_V$, there are two possibilities: Either $ROR = O^k$, $k \in \mathbb{Z}$, or $ROR = O_j$, where $O_j \in \mathcal{K}_V$ is a secondary rotation. Considering the first possibility, from Eq. 7 we get $OR\vec{f} = R\vec{f}$, i.e. either $R\vec{f} = \vec{f}$ or $R\vec{f} = -\vec{f}$. If $R\vec{f} = \vec{f}$, then, $\tilde{R} = R$. Otherwise, $R\vec{f} = -\vec{f}$. Let $O_j \in \mathcal{K}_V$ be a secondary rotation and let $\tilde{R} \triangleq O_jR$. Then, from Theorem 3.23 it follows that $\tilde{R} \in \mathcal{G}_V$ is a rotation-inversion, which satisfies

FIGURE 3. Cyclic rotations groups



(a) $\mathcal{G}_V = \mathcal{K}_V$ is cyclic of order six with a rotation axis $\vec{f}$. (b) $\mathcal{K}_V$ is cyclic of order three, $I \in \mathcal{G}_V$. (c) $\mathcal{K}_V$ is cyclic of order six, $R \in \mathcal{G}_V$ is a reflection, which satisfies $R\vec{f} = \vec{f}$. (d) $\mathcal{K}_V$ is cyclic of order five, $R \in \mathcal{G}_V$ is a reflection which satisfies $R\vec{f} = -\vec{f}$.

$\tilde{R}\vec{f} = \vec{f}$, i.e., $\tilde{R}$ is reflection, which satisfies the required. Considering the second possibility, we get $ROR\vec{f} = O_j\vec{f} = -\vec{f}$, or equivalently, from Eq. 7 $OR\vec{f} = -R\vec{f}$, i.e. O has eigenvalue -1, hence, O is of order two. Then, from Theorem 3.23, $\left\{\vec{f},\, \vec{f}_1,\, \vec{f}_2\right\}$ is an orthogonal set, where $\vec{f}_1$ and $\vec{f}_2$ are the two additional rotation axes of V. Without loss of generality, assume that $ROR = O_1$, where O_1 is the secondary rotation associated with $\vec{f}_1$. In this case, $OR\vec{f}_1 = R\vec{f}_1$, i.e. $R\vec{f}_1 = \pm\vec{f}$ and according to Lemma 3.13 $R\vec{f}_2 = \vec{f}_2$. If $ROR = O_1$ is assumed, we get $R\vec{f}_1 = \vec{f}_1$. $\square$

If $\vec{f}$ is a twofold rotation axis of V, then, each of the rotation axes can be considered as the principle axis.

Let $\vec{f}_0$ be one of the secondary rotation axes of a Dihedron. The rest of the secondary rotation axes can be enumerated according to the rule $\vec{f}_j \triangleq O^j\vec{f}_0$, $j = 1, ...m-1$. Obviously, $\sphericalangle\left(\vec{f}_l, \vec{f}_k\right) = \pi\frac{|l-k|}{m}$.

Lemma 3.28. *Let V be a Dihedron, whose principle axis is $\vec{f}$, $\mathcal{G}_V \neq \mathcal{K}_V$ and $I \notin \mathcal{K}_V$. Then, there is a reflection $R \in \mathcal{G}_V$, which satisfies $R\vec{f} = \vec{f}$ and $R\vec{v} = \vec{v}$, where $\vec{v} \in \mathbb{R}^3$ is an angle bisector between two adjacent secondary rotation axes of V.*

Proof. From corollary 3.22 and Lemma 3.27, it follows that there is a reflection $R \in \mathcal{G}_V$, which satisfies $Rf = f$. Let $\vec{v} \in \mathbb{R}^3$ be a vector, which satisfies $\vec{v} \perp \vec{f}$ and $R\vec{v} = \vec{v}$.

Then, according to Theorem 3.23, $\vec{v} \in span\left\{\vec{f}_j\right\}_{j=0}^{m-1}$, where $\left\{\vec{f}_j\right\}_{j=0}^{m-1}$ are the secondary rotation axes of V and m is the order of the principle rotation O. Assume that $\vec{v}$ is not one of the secondary rotation axes and let $\vec{f}_k$ be the secondary rotation axis, which satisfies $\sphericalangle\left(\vec{v}, \vec{f}_k\right) = \underset{j=0,\dots,m-1}{min} \sphericalangle\left(\vec{v}, \vec{f}_j\right)$. According to Lemma 3.18, $\vec{f}_l \triangleq R\vec{f}_k$ is also a secondary rotation axis, and according to Lemma 3.13 $\sphericalangle\left(\vec{v}, \vec{f}_k\right) = \sphericalangle\left(\vec{v}, \vec{f}_l\right)$. Obviously, if $\vec{f}_k$ and $\vec{f}_l$ are not adjacent axes, then, there is another secondary rotation axis $\vec{f}_i$ s.t.$\sphericalangle\left(\vec{v}, \vec{f}_i\right) < \sphericalangle\left(\vec{v}, \vec{f}_k\right)$, which is a contradiction to the way $\vec{f}_k$ was chosen. According to Theorem 3.23, if m is odd, then, any angle bisector of two adjacent secondary rotation axes is also a secondary rotation axis.

Assume that $\vec{v}$ is a secondary rotation axis of V, i.e., $\vec{v} = \vec{f}_j$ for some $0 \leq j < m$. If m is even, then, according to Theorem 3.23 and Lemma 3.18, $\vec{f}_k \triangleq O^{\frac{m}{2}}\vec{v}$ is a secondary rotation axis and $\vec{f}_k \perp \vec{v}$. In addition, $\mathcal{B} \triangleq \left\{\vec{f}, \vec{v}, \vec{f}_k\right\}$ is an orthogonal basis for $\mathbb{R}^3$. Define $\tilde{R} \triangleq RO_k$, where $O_k \in \mathcal{K}_V$ is the secondary rotation associated with $\vec{f}_k$. By applying $\tilde{R}$ on the elements of $\mathcal{B}$, it follows that $\tilde{R}\vec{f} = RO_k\vec{f} = -R\vec{f} = -\vec{f}$, $\tilde{R}\vec{v} = RO_k\vec{v} = -R\vec{v} = -\vec{v}$ and $\tilde{R}\vec{f}_k = RO_k\vec{f}_k = R\vec{f}_k = -\vec{f}_k$, i.e. $\tilde{R} = I$, which contradicts to the assumption. $\square$

Lemma 3.29. *Under the conditions of Lemma 3.28, each vector $\vec{w}$, which bisects the angle between two adjacent secondary rotation axes of V, has a reflection $\tilde{R} \in \mathcal{G}_V$ that satisfies $\tilde{R}\vec{f} = \vec{f}$ and $\tilde{R}\vec{w} = \vec{w}$.*

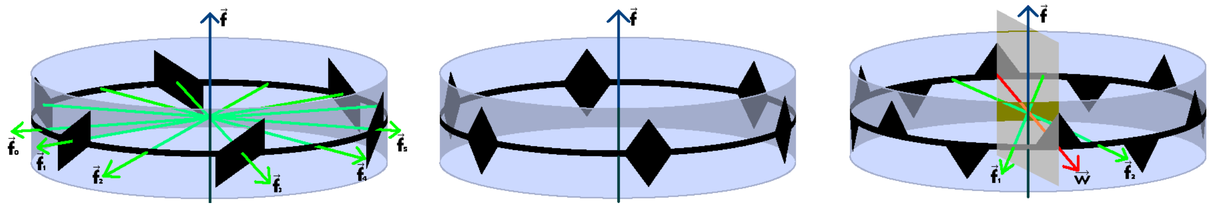
Proof. From Lemma 3.28 there is a reflection $R \in \mathcal{G}_V$, which satisfies $R\vec{f} = \vec{f}$ and $R\vec{v} = \vec{v}$, where $\vec{v}$ is an angle bisector between two adjacent secondary rotation axes of V. Let $R_k \triangleq O^kR$, $k = 1, ..., m-1$, where m is the order of O, which is the principle rotation of V. Then, $R_k \in \mathcal{G}_V$ is a rotation-inversion that satisfies $R_k\vec{f} = \vec{f}$, i.e., R_k has eigenvalue 1, hence, R_k is a reflection. Using the same arguments as in the proof of Lemma 3.28, we get that there is a vector $\vec{v}_k$, which bisects the angle between two adjacent secondary rotation axes of V that satisfies $R_k\vec{v}_k = \vec{v}_k$. Obviously, $\vec{v}_j = \vec{v_k}$ if and only if $j = k$, i.e., each one of the m angle bisector vectors between two adjacent secondary rotation axes of V has a reflection, which satisfies the lemma. $\square$

Tetrahedric rotations subgroup:

Lemma 3.30. *([17]) Let V be a Tetrahedron. If $\mathcal{G}_V \neq \mathcal{K}_V$ and $I \notin \mathcal{G}_V$, then, any twofold axis spans a reflection plane of V with any three-fold axis.*

For illustration of Lemma 3.30, see Fig. 5.

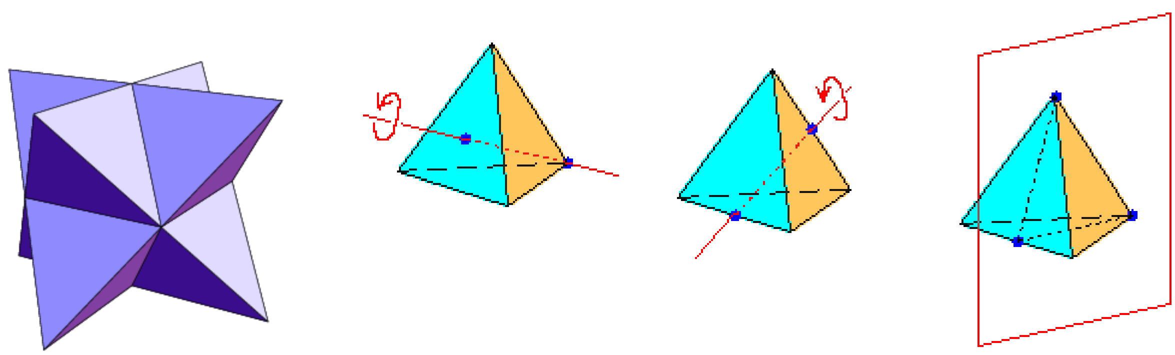
FIGURE 4. Dihedric rotations groups



(a) (b) (c)

(a) $\mathcal{G}_V = \mathcal{K}_V$ is Dihedric, $m = 6$. $\vec{f}$ is the principle $m-$fold axis. $\left\{\vec{f}_j\right\}_{j=0}^{m-1}$ are the secondary rotation axes. The angle between adjacent secondary rotation axes is $\frac{\pi}{m}$. (b) $\mathcal{K}_V$ is Dihedric, $\mathcal{G}_V \neq \mathcal{K}_V$ and $I \in \mathcal{G}_V$. The rotation axes are the same as the rotation axes in (a). (c) $\mathcal{K}_V$ is Dihedric, $\mathcal{G}_V \neq \mathcal{K}_V$ and $I \notin \mathcal{G}_V$. The rotation axes are the same as the rotation axes in (a). Any angle bisector between two adjacent secondary rotation axes spans a reflection plane with the principle axis.

FIGURE 5. Tetrahedric rotations groups, $\mathcal{G}_V \neq \mathcal{K}_V$



(a) (b)

(a) $\mathcal{G}_V$ is Tetrahedric, $I \in \mathcal{G}_V$. (b) $\mathcal{G}_V$ is Tetrahedric, $\mathcal{G}_V \neq \mathcal{K}_V$, $I \notin \mathcal{G}_V$. Left: a threefold rotation axis. Middle: a twofold rotation axis. Right: The reflection plane is spanned by the indicated axes.

3.4. **Properties of the Fourier transform.**

The Fourier transform is the main tool in deriving and analyzing the proposed algorithm. In this section, we present its properties that are required for the derivation of the main algorithm for detection of $3D$ symmetries.

Let $f : \mathbb{R}^3 \to \mathbb{R}$ be a function whose modulus is square integrable on $\mathbb{R}^3$. The $3D$ Fourier transform of f, denoted by $\hat{f}(\vec{w})$, $\vec{w} \in \mathbb{R}^3$, is given by $\hat{f}(\vec{w}) \triangleq \iiint_{\mathbb{R}^3} f(\vec{x})\, e^{-i\langle \vec{w},\vec{x}\rangle} d\vec{x}$, $\vec{x} \in \mathbb{R}^3$. The inverse Fourier transform is given by $f(\vec{x}) \triangleq \iiint_{\mathbb{R}^3} \hat{f}(\vec{w})\, e^{i\langle \vec{x},\vec{w}\rangle} d\vec{w}$.

Lemma 3.31. *Let $f : \mathbb{R}^3 \to \mathbb{R}$ and let $O \in \mathcal{O}(3)$. Then, $\widehat{\Lambda(O)f}(\vec{w}) = \Lambda(O)\hat{f}(\vec{w})$, $\vec{w} \in \mathbb{R}^3$.*

Proof. $\widehat{\Lambda(O)f}(\vec{w}) = \iiint_{\mathbb{R}^3} \Lambda(O) f(\vec{x})\, e^{-i\langle \vec{x},\vec{w}\rangle} d\vec{x} = \iiint_{\mathbb{R}^3} f(O^{-1}\vec{x})\, e^{-i\langle \vec{x},\vec{w}\rangle} d\vec{x}$. Substitute $\vec{z} = O^{-1}\vec{x}$, then, the last integral becomes $\iiint_{\mathbb{R}^3} f(\vec{z})\, e^{-i\langle O\vec{z},\vec{w}\rangle} J d\vec{z}$, where J is the Jacobian, i.e. $J = \left|\frac{\partial \vec{x}}{\partial \vec{z}}\right| =$

$|det\left(O^{-1}\right)|$. Since $O \in \mathcal{O}(3)$, then, Eq. 3 holds. Therefore, $J = 1$ and $\langle O\vec{z}, \vec{w}\rangle = \langle \vec{z}, O^{-1}\vec{w}\rangle$. As a consequence, we get $\widehat{\Lambda(O) f}(\vec{w}) = \iiint_{\mathbb{R}^3} f(\vec{z})\, e^{\left\langle \vec{z}, O^{-1}\vec{w}\right\rangle} d\vec{z} = \Lambda(O)\hat{f}(\vec{w})\ \ \forall \vec{w} \in \mathbb{R}^3$. ☐

Lemma 3.32. $\mathcal{G}_f = \mathcal{G}_{\hat{f}}$.

Proof. Let $O \in \mathcal{G}_f$, then, $\Lambda(O)\hat{f} = \widehat{\Lambda(O) f} = \hat{f}$. The first equality is derived from Lemma 3.31. The second is derived from the fact that $O \in \mathcal{G}_f$. If $O \in \mathcal{G}_{\hat{f}}$, then $\widehat{\Lambda(O) f} = \Lambda(O)\hat{f} = \hat{f}$, and by the fact that Fourier transform is bijective we conclude $\Lambda(O) f = f$, i.e. $O \in \mathcal{G}_f$. ☐

3.5. **The 3D pseudo-polar FFT.**

Given a volume V of size $N \times N \times N$, its $3D$ discrete Fourier transform, denoted $\hat{V}(\omega_x, \omega_y, \omega_z)$ (or by $\mathcal{F}_{3D}(V)$), is given by

$$\hat{V}(\omega_x, \omega_y, \omega_z) \equiv \mathcal{F}_{3D}(V)(\omega_x, \omega_y, \omega_z) \triangleq \sum_{u,v,w=-N/2}^{N/2-1} V(u, v, w)\, e^{-\frac{2\pi i}{M}(u\omega_x + v\omega_y + w\omega_z)}, \tag{11}$$

where $\omega_x, \omega_y, \omega_z \in R$. For simplicity, we assume that V has equal dimensions in the x, y and z directions and that N is even. For ω_x, ω_y and ω_z, which are sampled on the Cartesian grid $(\omega_x, \omega_y, \omega_z) = (m, k, l)$, $m, k, l = -\frac{M}{2}, \ldots\ldots, \frac{M}{2} - 1$, the discrete Fourier transform in Eq. 11 becomes

$$\hat{V}_{Cart}(m, k, l) \triangleq \hat{V}(m, k, l) = \sum_{u,v,w=-N/2}^{N/2-1} V(u, v, w)\, e^{-\frac{2\pi i}{M}(um + vk + wl)}, \tag{12}$$

where $m, k, l = -\frac{M}{2}, \ldots., \frac{M}{2} - 1$, which is usually referred to as $3D$ DFT of the volume V. M $(M \geq N)$ is the frequency resolution of the DFT. The DFT of V, given by Eq. 12, can be computed in $O\left(N^3 logN\right)$ operations.

Since a symmetry of $3D$ volume is a polar property, it is desirable to compute the Fourier transform of V in spherical coordinates. The $3D$ pseudo-polar Fourier transform (3DPPFT) ([2]) evaluates accurately the $3D$ Fourier transform of a volume on the $3D$ pseudo-polar grid. Formally, the $3D$ pseudo-polar grid is given by the set of samples

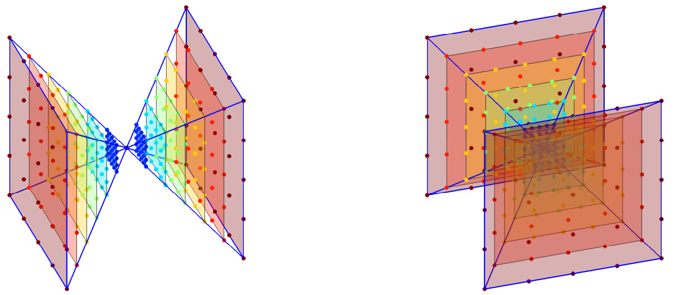
$$P \triangleq P_1 \cup P_2 \cup P_3, \tag{13}$$

where

(14)
$$P_1 \triangleq \left\{\left(m, -\frac{2k}{N}m, -\frac{2l}{N}m\right)\right\},\ P_2 \triangleq \left\{\left(-\frac{2k}{N}m, m, -\frac{2l}{N}m\right)\right\},\ P_3 \triangleq \left\{\left(-\frac{2k}{N}m, -\frac{2l}{N}m, m\right)\right\},$$

and $k, l = -\frac{N}{2}, \ldots, \frac{N}{2}$, $m = -\frac{3N}{2}, \ldots, \frac{3N}{2}$, N even. See Fig. 6 for an illustration of the sets P_1, P_2 and P_3. We define the $3D$ pseudo-polar Fourier transform of V as the samples of the Fourier transform

FIGURE 6. The pseudo-polar grid



(a) (b) (c)

(a) Sector P_1. (b) Sector P_2. (c) Sector P_3.

$\hat{V}$, given by Eq. 11, on the $3D$ pseudo-polar grid P, given by Eqs. 13 and 14. Formally, the $3D$ pseudo-polar Fourier-transform, denoted by $\hat{V}^s_{PP}\,(s=1,2,3)$, is a linear transformation, which defined for $m=-\frac{3N}{2},...,\frac{3N}{2}$ and $k,l=-\frac{N}{2},...,\frac{N}{2}$,

$$\hat{V}^1_{PP}\,(m,k,l) \triangleq \hat{V}\left(m,-\frac{2k}{N}m,-\frac{2l}{N}m\right) = \sum_{u,v,w=-N/2}^{N/2-1} V\,(u,v,w)\,e^{-\frac{2\pi i}{M}\left(mu-\frac{2k}{N}mv-\frac{2l}{N}mw\right)},$$

$$\hat{V}^2_{PP}\,(m,k,l) \triangleq \hat{V}\left(-\frac{2k}{N}m,m,-\frac{2l}{N}m\right) = \sum_{u,v,w=-N/2}^{N/2-1} V\,(u,v,w)\,e^{-\frac{2\pi i}{M}\left(-\frac{2k}{N}mu+mv-\frac{2l}{N}mw\right)},$$

$$\hat{V}^3_{PP}\,(m,k,l) \triangleq \hat{V}\left(-\frac{2k}{N}m,-\frac{2l}{N}m,m\right) = \sum_{u,v,w=-N/2}^{N/2-1} V\,(u,v,w)\,e^{-\frac{2\pi i}{M}\left(-\frac{2k}{N}mu-\frac{2l}{N}mv+mw\right)},$$

where $\hat{V}$ is given by Eq. 11. The set P, given by Eq. 13, can be written in pseudo-polar coordinates as

$$P=\left\{(r_i cos\theta_j sin\phi_k,\ r_i sin\theta_j sin\phi_k,\ r_i cos\phi_k)\mid(r_i,\theta_j,\phi_k)\in\Gamma\right\},$$

where the set Γ contains all triplets that correspond to points on the pseudo-polar grid P. A full description of the 3DPPFT algorithm is given in [2].

3.6. The Angular Difference Function.

Let V_1 and V_2 be two volumes, given in pseudo-polar coordinates, i.e., $V_1=V_1\left(r_i,\theta_j,\phi_k\right),\ V_2=V_2\left(r_i,\theta_j,\phi_k\right),\ \left(r_i,\theta_j,\phi_k\right)\in\Gamma$. The ***Angular Difference Function (ADF)*** of V_1 and V_2 on the interval $[0,\ r_0]$ is

$$\Delta_{V_1,V_2}\left(\theta_j,\phi_k\right)\triangleq\sum_{0\le r_i\le r_0}\left|V_1\left(r_i,\theta_j,\phi_k\right)-V_2\left(r_i,\theta_j,\phi_k\right)\right|. \tag{15}$$

Obviously, $\Delta_{V_1,V_2}(\theta_j,\phi_k) \geq 0$, and the equality is obtained if and only if $V_1(\cdot,\theta_j,\phi_k) = V_2(\cdot,\theta_j,\phi_k)$. Whenever the notation $\Delta_{V_1,V_2}\left(\vec{f}\right)$ is used, it represents $\Delta_{V_1,V_2}(\theta_j,\phi_k)$, where θ_j and ϕ_k are the pseudo-polar angular coordinates of $\vec{f}$.

4. The 3D Symmetry Detection Algorithm

In this section, we introduce the $3D$ Symmetry Detection Algorithm (3DSDA). According to corollary 3.20, we will first find $\mathcal{K}_V$. Then, in order to detect the full symmetries group $\mathcal{G}_V$, we will find a single rotation-inversion. The algorithm is based on the analysis of the ADF of the given volume V and rotated and rotated-inverted replicas of V.

4.1. Detection of a single rotation axis.

Let V be a given volume and let $\tilde{V} \triangleq \Lambda\left(\tilde{O}\right)V$, $\tilde{O} \in \mathcal{SO}(3)$, $\tilde{O} \notin \mathcal{K}_V$, where $\vec{f_0}$ is the rotation axis and δ the the rotation angle of $\tilde{O}$. First, we present the method for the detection of a single rotation axis by computing the ADF of V and $\tilde{V}$.

Lemma 4.1. *Let $O \in \mathcal{K}_V$. If $\vec{f}$ is the rotation axis of $\tilde{O}O$, then, $\Delta_{V,\tilde{V}}\left(\vec{f}\right) = 0$.*

Proof. Since $\vec{f}$ is the rotation axis of $\tilde{O}O$, the equality $\tilde{O}O\vec{f} = \vec{f}$ holds. In addition, from Eqs. 9 and 10 we get $\tilde{V}\left(\vec{f}\right) = \Lambda\left(\tilde{O}\right)V\left(\vec{f}\right) = \Lambda\left(\tilde{O}\right)\Lambda(O)V\left(\vec{f}\right) = \Lambda\left(\tilde{O}O\right)V\left(\vec{f}\right) = V\left(\left(\tilde{O}O\right)^{-1}\vec{f}\right) = V\left(\vec{f}\right)$, hence, $\Delta_{V,\tilde{V}}\left(\vec{f}\right) = 0$. □

Lemma 4.2. *If for any $O \in \mathcal{K}_V$ the rotation axis of $\tilde{O}O$ is not one of the rotation axes of V, then, any rotation of the form $\tilde{O}O$, $O \in \mathcal{K}_V$ has a unique rotation axis.*

Proof. Let $O_1, O_2 \in \mathcal{K}_V$ and assume that $\vec{f}$ is a common rotation axis of $\tilde{O}O_1$ and $\tilde{O}O_2$, i.e., $\tilde{O}O_1\vec{f} = \vec{f}$ and $\tilde{O}O_2\vec{f} = \vec{f}$, then, $O_1^{-1}O_2\vec{f} = \vec{f}$, i.e., $\vec{f}$ is a rotation axis of V, which contradicts the assumption. □

Since the number of symmetry axes of V is finite, the probability that lemma 4.2 is violated tends to zero.

From Lemma 4.1 and under the assumption of Lemma 4.2, it follows that all the eigenvectors of $\tilde{O}O$ can be detected from $\Delta_{V,\tilde{V}}$ and they are all different. Let $\vec{f}$ be an n-fold axis of V and let O be the rotation of order n associated with $\vec{f}$, i.e.,

$$O\vec{f} = \vec{f}. \tag{16}$$

The rotation angle is $\gamma = \frac{2\pi}{n}$. Define the linear transformations

$$T_k \triangleq O^k - E,\ k = 1, 2, .., n-1, \tag{17}$$

then, obviously,

$$null\,(T_k) = span\{\vec{f}\}. \tag{18}$$

Lemma 4.3. T_k, $k = 1, 2, ..., n-1$, *is a normal operator.*

From Corollary 3.5, Eq. 18 and Lemma 4.3 we conclude:

Corollary 4.4. $Im\,(T_k) = span\left\{\vec{f}\right\}^{\perp}$, $k = 1, 2, ..., n-1$.

We denote by $\vec{f}_k$ the rotation axis of $\tilde{O}O^k$, $k = 0, 1, ..., n-1$, i.e.,

$$\tilde{O}O^k \vec{f}_k = \vec{f}_k. \tag{19}$$

Lemma 4.5. $\vec{f}_0 \perp T_k \vec{f}_k$, $k = 1, 2, ..., n-1$.

Proof. From Eqs. 2, 4, 17 and 19, we get $\left\langle \vec{f}_0, T_k \vec{f}_k \right\rangle = \left\langle \vec{f}_0, \left(O^k - E\right) \vec{f}_k \right\rangle =$
$\left\langle \tilde{O}\vec{f}_0, \tilde{O}\left(O^k - E\right) \vec{f}_k \right\rangle = \left\langle \vec{f}_0, \tilde{O}O^k \vec{f}_k - \tilde{O}\vec{f}_k \right\rangle = \left\langle \vec{f}_0, \vec{f}_k - \tilde{O}\vec{f}_k \right\rangle = \left\langle \vec{f}_0, \left(E - \tilde{O}\right) \vec{f}_k \right\rangle =$
$\left\langle \left(E - \tilde{O}\right)^{\star} \vec{f}_0, \vec{f}_k \right\rangle = \left\langle \left(E - \tilde{O}^{-1}\right) \vec{f}_0, \vec{f}_k \right\rangle = \left\langle \vec{f}_0 - \tilde{O}^{-1}\vec{f}_0, \vec{f}_k \right\rangle = \left\langle \vec{0}, \vec{f}_k \right\rangle = 0.$ □

From Corollary 4.4 and Lemma 4.5 we conclude that $T_k \vec{f}_k \in span\left\{\vec{f}, \vec{f}_0\right\}^{\perp}$, $k = 1, 2, ..., n-1$. Under the assumption of Lemma 4.2, $\vec{f}$ and $\vec{f}_0$ are linearly independent and $T_k \vec{f}_k \neq \vec{0}$, $k = 1, 2, ..., n-1$. As a consequence, we conclude that $dim\left\{span\left\{T_k \vec{f}_k\right\}_{k=1}^{n-1}\right\} = 1$ and the next corollary holds:

Corollary 4.6. *There is a vector* $\vec{\omega} \in \mathbb{R}^3$, $\vec{\omega} \neq \vec{0}$ *and scalars* $a_k \in \mathbb{R}$, $a_k \neq 0$ *s.t.* $T_k \vec{f}_k = a_k \vec{\omega}$, $k = 1, 2, .., n-1$.

Lemma 4.7. *Under the assumption of Lemma 4.2, each pair of vectors from* $\left\{\vec{f}_j\right\}_{j=0}^{n-1}$ *is linearly independent.*

Proof. Assume that $\vec{f}_j = a\vec{f}_k$, $a \in \mathbb{R}$, $j < k$, then, from Eq. 19 we get $\tilde{O}O^j \vec{f}_j = a\tilde{O}O^k \vec{f}_k$. As a consequence, $\vec{f}_j = aO^{k-j}\vec{f}_k = O^{k-j}\vec{f}_j$, i.e., $\vec{f}_j$ is the rotation axis of O, which contradicts the assumption of Lemma 4.2. □

Theorem 4.8. $\vec{f}_j \in span\left\{\vec{f}_0, \vec{f}_1\right\}$, $j = 2, ..., n-1$.

Proof. According to Corollary 4.6 and Eq. 17, there is a scalar $b \neq 0$ s.t. $\tilde{O}T_j \vec{f}_j = \tilde{O}bT_1\vec{f}_1 = b\left[\tilde{O}O\vec{f}_1 - \tilde{O}\vec{f}_1\right] = b\vec{f}_1 - b\tilde{O}\vec{f}_1$. On the other hand, we have $\tilde{O}T_j\vec{f}_j = \tilde{O}O^j\vec{f}_j - \tilde{O}\vec{f}_j = \vec{f}_j - \tilde{O}\vec{f}_j$. Finally, we get $\tilde{O}\left(b\vec{f}_1 - \vec{f}_j\right) = b\vec{f}_1 - \vec{f}_j$, i.e., $b\vec{f}_1 - \vec{f}_j$ is either $\vec{0}$ or proportional to $\vec{f}_0$. According to Lemma 4.7, the first option is invalid, i.e., $b\vec{f}_1 - \vec{f}_j = c\vec{f}_0$, or, in other words, $\vec{f}_j \in span\left\{\vec{f}_0, \vec{f}_1\right\}$, $j = 2, ..., n-1$. □

Theorem 4.8 actually states that the rotation axes of $\tilde{O}O^k$, $k = 0, 1, .., n-1$, belong to a single plane in $\mathbb{R}^3$, i.e., to $span\left\{\vec{f}_0, \vec{f}_1\right\}$. We call this plane the ***characteristic plane (CP) of*** O ***in respect to*** $\tilde{O}$.

Next, we reveal the geometric relations between $\vec{f}$, which is the rotation axis of O, and the CP of O, which is denoted by $\mathcal{S}$ (see Fig. 7). By Grahm-Schmidt procedure, we find an orthonormal basis for $\mathcal{S}$. Assume that $\vec{f}_0$ is normal, i.e., $\left\|\vec{f}_0\right\| = 1$. Let

$$\vec{b} \triangleq \vec{f}_1 - \left\langle \vec{f}_1, \vec{f}_0 \right\rangle \vec{f}_0 \ \ and \ \ \vec{a} \triangleq \frac{\vec{b}}{\left\|\vec{b}\right\|}. \tag{20}$$

Then, $\left\{\vec{f}_0, \vec{a}\right\}$ is an orthonormal basis for $\mathcal{S}$. Define

$$\vec{x} \triangleq \vec{f} - \left\langle \vec{f}, \vec{f}_0 \right\rangle \vec{f}_0 \ \ and \ \ \vec{y} \triangleq \tilde{O}\vec{f} - \left\langle \tilde{O}\vec{f}, \vec{f}_0 \right\rangle \vec{f}_0 \tag{21}$$

to be the orthogonal projections of $\vec{f}$ and $\tilde{O}\vec{f}$, respectively, on the plane perpendicular to $\vec{f}_0$, denoted by $\mathcal{P}$, then $\vec{x}, \vec{y}$ and $\vec{a}$ belong to $\mathcal{P}$.

Lemma 4.9. $\left\langle \vec{f}, \vec{f}_0 \right\rangle = \left\langle \tilde{O}\vec{f}, \vec{f}_0 \right\rangle$ *and* $\left\langle \vec{f}, \vec{f}_1 \right\rangle = \left\langle \tilde{O}\vec{f}, \vec{f}_1 \right\rangle$.

Lemma 4.10. $\sphericalangle(\vec{a}, \vec{x}) = \sphericalangle(\vec{a}, \vec{y})$.

From Eq. 19 we get

$$\tilde{O}\vec{x} = \tilde{O}\vec{f} - \left\langle \vec{f}, \vec{f}_0 \right\rangle \tilde{O}\vec{f}_0 = \tilde{O}\vec{f} - \left\langle \tilde{O}\vec{f}, \vec{f}_0 \right\rangle \vec{f}_0 = \vec{y}. \tag{22}$$

From Lemma 4.10 and Eq. 22 we conclude that

$$\tilde{O}^{-\frac{1}{2}}\vec{a} = \frac{\vec{x}}{\|\vec{x}\|}, \tag{23}$$

where $\tilde{O}^{-\frac{1}{2}}$ denotes the rotation by angle $-\frac{\delta}{2}$ around $\vec{f}_0$. Define

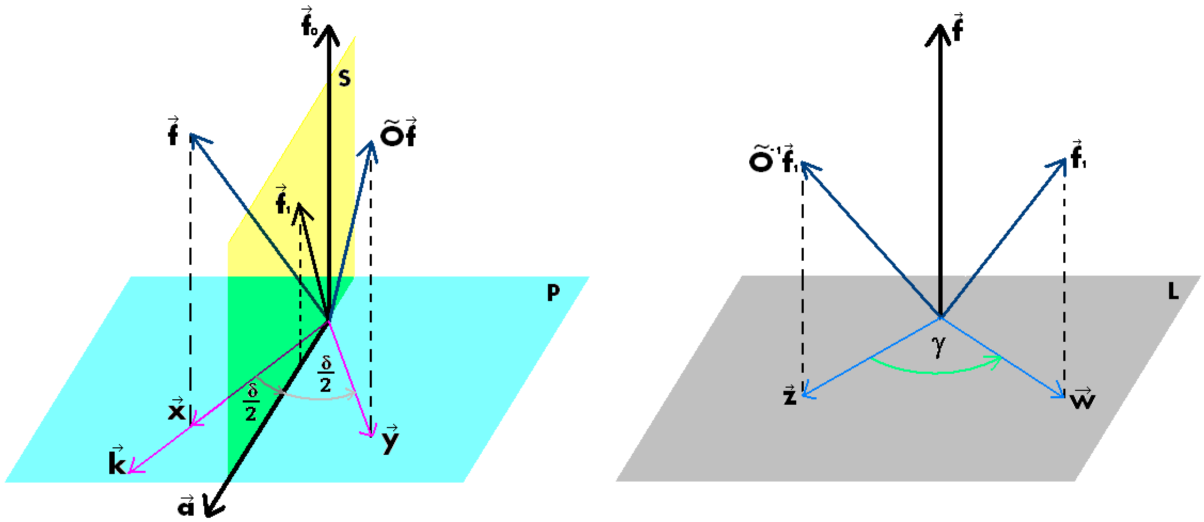
$$\vec{k} \triangleq \tilde{O}^{-\frac{1}{2}}\vec{a}. \tag{24}$$

From Eqs. 21, 23 and 24 we conclude:

Corollary 4.11. $\vec{f} \in span\left\{\vec{k}, \vec{f}_0\right\}$, *i.e.* $\vec{f} = b\vec{f}_0 + c\vec{k}$ (See Fig. 7(a)).

At this point, γ, which is the rotation angle of O, is already known since $\gamma = \frac{2\pi}{n}$, where n is the number of detected vectors, i.e., the vectors which satisfy $\Delta_{V,\tilde{V}}\left(\vec{f}\right) = 0$. Our next goal is to find b

FIGURE 7. The geometric relations between $\vec{f}$ and $\mathcal{S}$



(a) (b)

(a) $\vec{f_0}$ and δ are the rotation axis and the rotation angle of $\tilde{O}$, respectively. $\vec{f_0}$ and $\vec{f_1}$ belong to $\mathcal{S}$, which is the CP of O in respect to $\tilde{O}$. $\mathcal{P}$ is the perpendicular plane to $\vec{f_0}$. $\vec{x}$ and $\vec{y}$ are the orthogonal projections of $\vec{f}$ and $\tilde{O}\vec{f}$ on $\mathcal{P}$, respectively. $\vec{a}$ is the normalized orthogonal projection of $\vec{f_1}$ on $\mathcal{P}$. $\vec{k} = \tilde{O}^{-\frac{1}{2}}\vec{a}$. (b) $\vec{f}$ and γ are the rotation axis and the rotation angle of O, respectively. $\mathcal{L}$ is the perpendicular plane to $\vec{f}$. $\vec{w}$ and $\vec{z}$ are the orthogonal projections of $\vec{f_1}$ and $\tilde{O}^{-1}\vec{f_1}$, respectively.

and c, s.t. Corollary 4.11 holds. Define

$$\vec{\omega} \triangleq \vec{f_1} - \left\langle \vec{f_1}, \vec{f} \right\rangle \vec{f} \text{ and } \vec{z} \triangleq \tilde{O}^{-1}\vec{f_1} - \left\langle \tilde{O}^{-1}\vec{f_1}, \vec{f} \right\rangle \vec{f} \tag{25}$$

to be the orthogonal projections of $\vec{f_1}$ and $\tilde{O}^{-1}\vec{f_1}$, respectively, on the plane that is perpendicular to $\vec{f}$, denoted by $\mathcal{L}$ (see Fig. 7(b)).

Lemma 4.12. $\sphericalangle(\vec{\omega}, \vec{z}) = \gamma$.

Proof. Since $\bar{\omega}$ and $\bar{z}$ are both belong to the plane that is perpendicular to $\bar{f}$, it suffices to prove that

$$O\vec{\omega} = \vec{z}. \tag{26}$$

From Eqs. 4,16,19 and 25 and Lemma 4.9, we get $O\vec{\omega} = O\vec{f_1} - \left\langle \vec{f_1}, \vec{f} \right\rangle O\vec{f} = \tilde{O}^{-1}\vec{f_1} - \left\langle \vec{f_1}, \vec{f} \right\rangle \vec{f} = \tilde{O}^{-1}\vec{f_1} - \left\langle \tilde{O}^{-1}\vec{f_1}, \vec{f} \right\rangle \vec{f} = \vec{z}$. $\square$

Figure 7 (b) illustrates the above.

Lemma 4.13. $\left\langle \vec{f_1}, \vec{k} \right\rangle = \left\langle \vec{f_1}, \tilde{O}\vec{k} \right\rangle$.

According to Lemma 4.12, remains to find b and c s.t.

$$\frac{\langle\vec{w},\vec{z}\rangle}{\|\vec{w}\|\,\|\vec{z}\|}=cos\left(\gamma\right) \tag{27}$$

holds. The next calculations enable to reformulate Eq. 27 with b and c. From Eqs. 4, 19, 25, the normalization of $\vec{f}$, Corollary 4.11 and Lemma 4.13, it follows that $\langle\vec{\omega},\vec{z}\rangle=\left\langle\tilde{O}\vec{f_1},\,\vec{f_1}\right\rangle-\left(b\left\langle\vec{f_1},\vec{f_0}\right\rangle+c\left\langle\vec{f_1},\vec{k}\right\rangle\right)^2$. In addition, if $\vec{f_1}$ is normal, we get $\|\vec{\omega}\|^2=1-\left[b\left\langle\vec{f_1},\vec{f_0}\right\rangle+c\left\langle\vec{f_1},\vec{k}\right\rangle\right]^2$. From Eqs. 2 and 26, we get $\|\vec{\omega}\|=\|\vec{z}\|$. Hence, by substituting $g=\left\langle\tilde{O}\vec{f_1},\,\vec{f_1}\right\rangle$, $h=\left\langle\vec{f_1},\vec{f_0}\right\rangle$ and $j=\left\langle\vec{f_1},\vec{k}\right\rangle$, Eq. 27 becomes

$$\frac{g-\left(bh+cj\right)^2}{1-\left(bh+cj\right)^2}=cos\left(\gamma\right). \tag{28}$$

An additional equation is obtained from the normalization of $\vec{f}$, i.e.,

$$b^2+c^2=1. \tag{29}$$

The solution to Eqs. 28 and 29 is $c_{1,2}=\frac{\pm Gj+h\sqrt{h^2+j^2-G^2}}{j^2+h^2}$, where $G=\sqrt{\frac{g-cos(\gamma)}{1-cos(\gamma)}}$. $b_{1,2}$ can be found in respect to $c_{1,2}$. Only one pair of solutions $\left(b_j,c_j\right)$, $j=1,2,$ satisfies Eq. 28.
Algorithm 4.14 detects a single rotation in the symmetry group of a volume B.

Algorithm 4.14. *Input: An $N\times N\times N$ volume B given by a Cartesian representation. Output: A single rotation $O\in\mathcal{K}_B$.*

(1) $\tilde{B}\triangleq\Lambda\left(\tilde{O}\right)B$, where $\tilde{O}$ is an arbitrary rotation whose axis is $\vec{f_0}$ and its rotation angle is δ (see Eqs. 5 and 9).
(2) $V\triangleq\mathcal{F}_{PP}\left(B\right)$ and $\tilde{V}\triangleq\mathcal{F}_{PP}\left(\tilde{B}\right)$, where $\mathcal{F}_{PP}$ is the 3DPPFT.
(3) For each pair of spherical angles $\left(\theta_j,\phi_k\right)$ in the pseudo-polar grid, compute $\Delta_{V,\tilde{V}}\left(\theta_j,\phi_k\right)$ (see Eq. 15).
(4) Find all the vectors $\vec{f}$, s.t., $\mathcal{A}\triangleq\left\{\vec{f}\in\mathbb{R}^3\,:\,\Delta_{V,\tilde{V}}\left(\vec{f}\right)=0\right\}$, $n\triangleq\left|\mathcal{A}\right|$.
(5) If $n=1$, i.e. $\mathcal{A}=\left\{\vec{f_0}\right\}$, stop - then the output is $\mathcal{K}_B=\{E\}$.
(6) Choose $\vec{f_1}\in\mathcal{A}$, $\vec{f_1}\neq\vec{f_0}$. Compute $\vec{k}\triangleq\tilde{O}^{-\frac{1}{2}}\left(\frac{\vec{f_1}-\left\langle\vec{f_1},\vec{f_0}\right\rangle\vec{f_0}}{\left\|\vec{f_1}-\left\langle\vec{f_1},\vec{f_0}\right\rangle\vec{f_0}\right\|}\right)$, where $\tilde{O}^{-\frac{1}{2}}$ is the rotation whose rotation axis and rotation angle are $\vec{f_0}$ and $-\frac{\delta}{2}$, respectively (see Eq. 5).
(7) Solve Eqs. 28 and 29 for b and c.
(8) Compute the rotation matrix O, whose rotation axis and angle are $\vec{f}\triangleq b\vec{f_0}+c\vec{k}$ and $\gamma\triangleq\frac{2\pi}{n}$, respectively (see Eq. 5).

We assume that $\tilde{O}$, which is arbitrarily chosen in step 1, satisfies the assumption in Lemma 4.2.
Complexity: Step 1 costs $O\left(N^3\right)$ operations. Step 2 costs $O\left(N^3 log\left(N\right)\right)$ operations ([2]). Step 3 takes $O\left(N^3\right)$ operations, since the size of the 3DPP grid is $3 \times (3N+1) \times (N+1) \times (N+1)$. Since the angular size of the 3DPP grid is $6\left(N+1\right)^2$, step 4 costs no more than $O\left(N^2\right)$ operations. Steps 6, 7 and 8 cost $O(1)$ operations each. Hence, the total complexity of Algorithm 4.14 is $O\left(N^3 log\left(N\right)\right)$.

4.2. **Detection of all the rotations axes.**
Let $\vec{v}_1$ and $\vec{v}_2$ be two rotation axes of V of orders n_1 and n_2, associated with rotations O_1 and O_2, respectively. Let $\left\{\vec{f}_j\right\}_{j=0}^{n_1-1}$ and $\{\vec{g_k}\}_{k=0}^{n_2-1}$ be the rotation axes of $\tilde{O}O_1^j$ and $\tilde{O}O_2^k$, respectively, i.e., $\tilde{O}O_1^j\vec{f}_j = \vec{f}_j$, $j = 0, 1, ..., n_1-1$, and $\tilde{O}O_2^k\vec{g_k} = \vec{g_k}$, $k = 0, 1, ..., n_2-1$. Obviously, $\vec{f}_0 = \vec{g_0}$. Let $\mathcal{S}_1$ and $\mathcal{S}_2$ be the CPs of O_1 and O_2, respectively. Our goal is to distinguish between $\mathcal{S}_1$ and $\mathcal{S}_2$ in order to distinguish between O_1 and O_2.

Lemma 4.15. *If $\vec{f}_0$ does not belong to $span\left\{\vec{v}_1, \vec{v}_2\right\}$, then $\mathcal{S}_1 \neq \mathcal{S}_2$.*

Proof. Assume that $\mathcal{S}_1 = \mathcal{S}_2$. Since $\mathcal{S}_1 = span\left\{\vec{f}_0, \vec{v}_1\right\}$ and $\mathcal{S}_2 = span\left\{\vec{f}_0, \vec{v}_2\right\}$, it follows that $\vec{v}_1$, $\vec{v}_2$ and $\vec{f}_0$ are linearly dependent. Since $\vec{v}_1$ and $\vec{v}_2$ are linearly independent, it follows that $\vec{f}_0 \in span\left\{\vec{v}_1, \vec{v}_2\right\}$, which contradicts the assumption. □

According to Lemma 4.15, if $\vec{f}_0$ does not belong to any plane, which is spanned by rotation axes of V, then, each $O \in \mathcal{K}_V$ has a unique CP.
$\mathcal{S}_1$ can be identified by a unique perpendicular vector, denoted by $\vec{F}_{O_1}$, i.e., $\vec{F}_{O_1} = \vec{f}_i \times \vec{f}_j$, $i \neq j$. Similarly, $\mathcal{S}_2$ can be identified by $\vec{F}_{O_2} = \vec{g_i} \times \vec{g_j}$, $i \neq j$. From the assumption of Lemma 4.15 it follows that $\vec{F}_{O_1} \neq \vec{F}_{O_2}$.
Algorithm 4.16 is an expanded version of Algorithm 4.14. It detects the full rotations subgroup of a given volume B.

Algorithm 4.16. *Input: An $N \times N \times N$ volume B given by a Cartesian representation.*
Output: $\mathcal{K}_B$.

(1) $\tilde{B} \triangleq \Lambda\left(\tilde{O}\right)B$, where $\tilde{O}$ is an arbitrary rotation whose axis is $\vec{f}_0$ and its rotation angle is δ (see Eqs. 5 and 9).
(2) $V \triangleq \mathcal{F}_{PP}\left(B\right)$ and $\tilde{V} \triangleq \mathcal{F}_{PP}\left(\tilde{B}\right)$, where $\mathcal{F}_{PP}$ is the 3DPPFT.
(3) For each pair of spherical angles (θ_j, ϕ_k) in the pseudo-polar grid compute $\Delta_{V,\tilde{V}}\left(\theta_j, \phi_k\right)$ (see Eq. 15).
(4) List all the vectors $\vec{g}$, which satisfy $\Delta_{V,\tilde{V}}\left(\vec{g}\right) = 0$. If the only detected vector is $\vec{f}_0$, stop - then $\mathcal{K}_V = \left\{E\right\}$.

(5) Divide the vectors from step 4 to CPs, where each CP $\mathcal{S}_O$ is characterized by a single vector $\vec{F_O}$, s.t., $\mathcal{S}_O \triangleq \left\{\vec{g} : \vec{g} \times \vec{f_0} = \vec{F_O}\right\} \cup \left\{\vec{f_0}\right\}$.

(6) For each CP $\mathcal{S}_O$, apply steps 6-8 from algorithm 4.14, where $\mathcal{A} = \mathcal{S}_O$.

We assume that $\tilde{O}$, which is arbitrarily chosen in step 1, satisfies the assumptions of Lemmas 4.2 and 4.15.

Since the complexity of Algorithm 4.14 is $O\left(N^3 log\left(N\right)\right)$, it follows that the complexity of Algorithm 4.16 is also $O\left(N^3 log\left(N\right)\right)$.

4.3. **Detection of a single rotation-inversion.**

In this section, we describe an algorithm, which detects a single rotation-inversion of a given volume V, while its rotations subgroup $\mathcal{K}_V$ is already known. From Corollary 3.20 it follows that this completes the whole process of symmetry group detection. According to Theorem 3.24, if $\mathcal{G}_V \neq \mathcal{K}_V$ and $I \notin \mathcal{G}_V$, then, $\mathcal{K}_V$ is either the trivial group $\{E\}$ or Cyclic or Dihedric or Tetrahedric. If $\mathcal{K}_V$ is Dihedric or Tetrahedric, then, from Lemmas 3.29 and 3.30, the geometric relation between the reflection planes and the rotation axes are well known. Hence, remains to establish a method for detection of a single reflection $R \in \mathcal{G}_V$, where $\mathcal{K}_V$ is either trivial or Cyclic. Define

$$\tilde{V} \triangleq \Lambda\left(\tilde{R}\right) V, \tag{30}$$

where $\tilde{R}$ is rotation-inversion.

Lemma 4.17. *Let $S \in \mathcal{G}_V$ be a rotation-inversion. If $\vec{f}$ is the rotation axis of $\tilde{R}S$, then $\Delta_{V,\tilde{V}}\left(\vec{f}\right) = 0$.*

Proof. Since $\vec{f}$ is the rotation axis of $\tilde{R}S$, the equality $\left(\tilde{R}S\right)^{-1}\vec{f} = \vec{f}$ holds. In addition, from Eqs. 9, 10 and 30, we get

$$\tilde{V}\left(\vec{f}\right) = \Lambda\left(\tilde{R}\right) V\left(\vec{f}\right) = \Lambda\left(\tilde{R}\right)\Lambda\left(S\right) V\left(\vec{f}\right) = \Lambda\left(\tilde{R}S\right) V\left(\vec{f}\right) = V\left(\left(\tilde{R}S\right)^{-1}\vec{f}\right) = V\left(\vec{f}\right),$$

hence, $\Delta_{V,\tilde{V}}\left(\vec{f}\right) = 0$. ☐

Lemma 4.18. *For any rotation-inversion $S \in \mathcal{G}_V$, if the rotation axis of $\tilde{R}S$ is not one of the rotation axes of V, then, any rotation of the form $\tilde{R}S$, $S \in \mathcal{G}_V$ has a unique rotation axis.*

Proof. Let $S_1, S_2 \in \mathcal{G}_V$ be two rotation-inversions. Assume that $\vec{f}$ is a common rotation axis of $\tilde{R}S_1$ and $\tilde{R}S_2$, i.e., $\tilde{R}S_1\vec{f} = \vec{f}$ and $\tilde{R}S_2\vec{f} = \vec{f}$, then, $S_1^{-1}S_2\vec{f} = \vec{f}$, i.e., $\vec{f}$ is a rotation axis of V. ☐

From Lemma 4.17 and under the assumption of Lemma 4.18, it follows that all the eigenvectors of $\tilde{R}S$ can be detected from $\Delta_{V,\tilde{V}}$ and they are all different.

Lemma 4.19. *Let $O \in \mathcal{K}_V$ and let $\tilde{R}O$ be a reflection. Then, for any vector $\vec{f}$, which belongs to the reflection plane,* $\Delta_{V,\tilde{V}}\left(\vec{f}\right) = 0$.

Proof. Since $\vec{f}$ belongs to the reflection plane of $\tilde{R}O$, the equality $\left(\tilde{R}O\right)^{-1}\vec{f} = \vec{f}$ holds. In addition, from Eqs. 9, 10 and 30 we get

$$\tilde{V}\left(\vec{f}\right) = \Lambda\left(\tilde{R}\right)V\left(\vec{f}\right) = \Lambda\left(\tilde{R}\right)\Lambda\left(O\right)V\left(\vec{f}\right) = \Lambda\left(\tilde{R}O\right)V\left(\vec{f}\right) = V\left(\left(\tilde{R}O\right)^{-1}\vec{f}\right) = V\left(\vec{f}\right),$$

hence, $\Delta_{V,\tilde{V}}\left(\vec{f}\right) = 0$. □

In the following, the method for detection of a single rotation-inversion in $\mathcal{G}_V$ is described.

$\mathcal{K}_V$ **is trivial:**

Assume that $\mathcal{K}_V = \{E\}$. If $\mathcal{G}_V \neq \mathcal{K}_V$ and $I \notin \mathcal{G}_V$, then, from Corollary 3.22 we get $\mathcal{G}_V = \{E, R\}$, where R is a reflection. Let $\tilde{R}$ be a rotation-inversion and let $\tilde{V} \triangleq \Lambda\left(\tilde{R}\right)V$. Then, from Lemma 4.17, the vector $\vec{f}$, which satisfies $\Delta_{V,\tilde{V}}\left(\vec{f}\right) = 0$, is the rotation axis of $\tilde{R}R$, i.e.,

$$R\vec{f} = \tilde{R}^{-1}\vec{f}. \tag{31}$$

Unless $\tilde{R}$ is a reflection, then according to Lemma 3.13, there is a unique solution for R.

$\mathcal{K}_V$ **is Cyclic:**

Assume that $\mathcal{K}_V = \langle O \rangle$ is a cyclic group of order n, $\mathcal{G}_V \neq \mathcal{K}_V$ and $I \notin \mathcal{G}_V$. Suppose that the reflection $R_{\vec{f}} \notin \mathcal{G}_V$, where $\vec{f}$ is the rotation axis of O. Let $\vec{w}$ be a vector, which satisfies $\Delta_{V,\tilde{V}}\left(\vec{w}\right) = 0$. Then, according to Lemma 3.25, Corollary 3.26 and Lemma 4.17, there is a reflection $S \in \mathcal{G}_V$ s.t.

$$S\vec{w} = \tilde{R}^{-1}\vec{w}. \tag{32}$$

Unless $\tilde{R}$ is a reflection, then according to Lemma 3.13, there is a unique solution for S.

The next algorithm detects a single rotation-inversion R of a given volume B, whose rotations subgroup $\mathcal{K}_B$ is already known:

Algorithm 4.20. *Input: An $N \times N \times N$ volume B given by a Cartesian representation and its rotations subgroup $\mathcal{K}_B$.*
Output: A single rotation-inversion $R \in \mathcal{G}_B$.

(1) $\tilde{B} \triangleq \Lambda\left(I\right)B$, where I is the inversion transformation (see Eq. 9).
(2) Compute $\Delta B \triangleq \tilde{B} - B$. If $\Delta B \equiv 0$, stop - then, $R = I$, $R \in \mathcal{G}_B$.

(3) If $\mathcal{K}_B$ is Tetrahedric or Icosahedric, stop - then, $\mathcal{K}_B = \mathcal{G}_B$.

(4) $\tilde{B} \triangleq \Lambda\left(\tilde{R}\right) B$ (see Eq. 9), where $\tilde{R}$ is an arbitrary rotation-inversion.

(5) $V \triangleq \mathcal{F}_{PP}(B)$ and $\tilde{V} \triangleq \mathcal{F}_{PP}\left(\tilde{B}\right)$, where $\mathcal{F}_{PP}$ is the 3DPPFT.

(6) For each pair of spherical angles (θ_j, ϕ_k) in the pseudo-polar grid compute $\Delta_{V,\tilde{V}}(\theta_j, \phi_k)$ (see Eq. 15). If there is no vector $\vec{w}$, s.t. $\Delta_{V,\tilde{V}}(\vec{w}) = 0$, stop - then, $\mathcal{K}_B = \mathcal{G}_B$.

(7) If $\mathcal{K}_B = \{E\}$, choose the single vector $\vec{f}$, which satisfies $\Delta_{V,\tilde{V}}\left(\vec{f}\right) = 0$. Solve Eq. 31 for the reflection R. Stop - then, $R \in \mathcal{G}_B$.

(8) If $\mathcal{K}_B$ is Cyclic, let $\vec{f}$ be its rotation axis.
   (a) $\tilde{B}_1 \triangleq \Lambda\left(R_{\vec{f}}\right) B$, where $R_{\vec{f}}$ is the reflection whose axis is $\vec{f}$ (see Eqs. 6 and 9).
   (b) $\Delta B \triangleq \tilde{B} - B$. If $\Delta B \equiv 0$, stop - then $R = R_{\vec{f}}$, $R \in \mathcal{G}_B$.
   (c) Choose a vector $\vec{w}$, which satisfies $\Delta_{V,\tilde{V}}(\vec{w}) = 0$. Solve Eq. 32 for the reflection S. Stop - then, $R = S$, $R \in \mathcal{G}_B$.

(9) If $\mathcal{K}_B$ is Octahedric, let $\vec{v_1}$ and $\vec{v_2}$ be a twofold and threefold rotation axes of V, respectively. Compute $\vec{w} = \vec{v_1} \times \vec{v_2}$, stop - then $R = R_{\vec{w}}$, $R \in \mathcal{G}_B$ (see Eq. 6).

(10) $\mathcal{K}_B$ is Dihedric of order $2m$. If $m > 2$ go to step 10a. Otherwise, go to step 10b.
   (a) Define $\vec{v} \triangleq \vec{f_j} + \vec{f_k}$, where $\vec{f_j}$ and $\vec{f_k}$ are two adjacent secondary rotation axes of V and let $\vec{f}$ be the principle rotation axis of V. Compute $\vec{w} = \vec{v} \times \vec{f}$, stop - then, $R = R_{\vec{w}}$, $R \in \mathcal{G}_B$ (see Eq. 6).
   (b) Let $\left\{\vec{f_1}, \vec{f_2}, \vec{f_3}\right\}$ be the rotation axes of V. For each pair $j, k \in \{1,2,3\}$, define $\vec{v} \triangleq \vec{f_j} + \vec{f_k}$. Compute $\vec{w} = \vec{v} \times \vec{f_l}$, $l \neq \{j,k\}$, $R = R_{\vec{w}}$. If $B - \Lambda(R) B \equiv 0$, stop - then, $R \in \mathcal{G}_B$.

According to Lemmas 4.19 and 4.18, we assume that by an arbitrary choice of rotation-inversion $\tilde{R}$, neither $\tilde{R}O$ is a reflection nor the rotation axis of $\tilde{R}S$ is one of the rotation axes of V for any $O \in \mathcal{K}_V$ and any rotation-inversion $\mathcal{S} \in \mathcal{G}_V$.

Complexity: Step 1 costs $O\left(N^3 log(N)\right)$ operations. Step 2 costs $O\left(N^3\right)$ operations, since the size of the 3DPP grid is $3 \times (3N+1) \times (N+1) \times (N+1)$. Step 4 costs $O\left(N^3 log(N)\right)$ operations. Step 5 costs $O\left(N^3\right)$ operations. Steps 6 costs $O(1)$ operations. Step 7 costs $O\left(N^3 log(N)\right)$. Steps 8 and 10 cost $O(1)$ operations each. Hence, the total complexity of Algorithm 4.14 is $O\left(N^3 log(N)\right)$.

4.4. **The complete 3DSDA.**

Algorithm 4.21 describes the complete 3DSDA, which is based on Algorithms 4.16 and 4.20:

Algorithm 4.21. *Input: An $N \times N \times N$ volume B given by a Cartesian representation.*
Output: $\mathcal{G}_B$.

(1) $\tilde{B} \triangleq \Lambda\left(\tilde{O}\right) B$, where $\tilde{O}$ is an arbitrary rotation whose axis is $\vec{f_0}$ and its rotation angle is δ (see Eqs. 5 and 9).

(2) $V \triangleq \mathcal{F}_{PP}(B)$ and $\tilde{V} \triangleq \mathcal{F}_{PP}\left(\tilde{B}\right)$, where $\mathcal{F}_{PP}$ is the 3DPPFT.

(3) For each pair of spherical angles (θ_j, ϕ_k) in the pseudo-polar grid, compute $\Delta_{V,\tilde{V}}(\theta_j, \phi_k)$ (see Eq. 15).

(4) List all the vectors $\vec{a}$ that satisfy $\Delta_{V,\tilde{V}}(\vec{a}) = 0$. If the only detected vector is $\vec{f_0}$, then, $\mathcal{K}_B = \{E\}$. In this case, go to step 7, otherwise, continue to step 5.

(5) Divide the vectors from step 4 to CPs, where each CP $\mathcal{S}_O$ is characterized by a single vector $\vec{F_O}$, s.t., $\mathcal{S}_O \triangleq \left\{\vec{a} : \vec{a} \times \vec{f_0} = \vec{F_O}\right\} \cup \left\{\vec{f_0}\right\}$.

(6) Define $\mathcal{K}_B \triangleq \{E\}$ and $\tilde{O}^{-\frac{1}{2}}$ to be the rotation whose rotation axis and rotation angle are $\vec{f_0}$ and $\frac{-\delta}{2}$, respectively (see Eq. 5). For each CP $\mathcal{S}_O$, apply the following steps:
   (a) Choose $\vec{a_1} \in \mathcal{S}_O$, $\vec{a_1} \neq \vec{f_0}$. Compute $\vec{k} \triangleq \tilde{O}^{-\frac{1}{2}}\left(\frac{\vec{a_1} - \langle \vec{a_1}, \vec{f_0}\rangle \vec{f_0}}{\left\|\vec{a_1} - \langle \vec{a_1}, \vec{f_0}\rangle \vec{f_0}\right\|}\right)$.
   (b) Solve Eqs. 28 and 29 for b and c, where $n = |\mathcal{S}_O|$ and $\gamma = \frac{2\pi}{n}$.
   (c) Use Eq. 5 to compute the representing matrix of O whose rotation axis is $\vec{f} \triangleq b\vec{f_0} + c\vec{k}$ and its rotation angle is γ.
   (d) $\mathcal{K}_B = \mathcal{K}_B \cup \{O\}$.

(7) $\tilde{B} \triangleq \Lambda(I) B$, where I is the inversion transformation (see Eq. 9).

(8) Compute $\Delta B \triangleq \tilde{B} - B$. If $\Delta B \equiv 0$, then, $R = I$, $R \in \mathcal{G}_B$. In this case, go to step 19, otherwise, continue to step 9.

(9) If $\mathcal{K}_B$ is Cyclic, continue to step 9a. Otherwise, go to step 10.
   (a) Let $\vec{f}$ be the rotation axis, that was calculated in step 6c. $\tilde{B} \triangleq \Lambda\left(R_{\vec{f}}\right) B$, where $R_{\vec{f}}$ is the reflection whose axis is $\vec{f}$ (see Eqs. 6 and 9) .
   (b) Compute $\Delta B \triangleq \tilde{B} - B$. If $\Delta B \equiv 0$, then, $R = R_{\vec{f}}$, $R \in \mathcal{G}_B$. In this case, go to step 19, otherwise, continue to step 11.

(10) If $\mathcal{K}_B$ is Tetrahedric or Icosahedric, then, $\mathcal{G}_B = \mathcal{K}_B$. In this case stop. Otherwise, continue to step 11.

(11) $\tilde{B} \triangleq \Lambda\left(\tilde{R}\right) B$ (see Eq. 9), where $\tilde{R}$ is an arbitrary rotation-inversion.

(12) $\tilde{V} \triangleq \mathcal{F}_{PP}\left(\tilde{B}\right)$.

(13) For each pair of spherical angles (θ_j, ϕ_k) in the pseudo-polar grid, compute $\Delta_{V,\tilde{V}}(\theta_j, \phi_k)$ (see Eq. 15).

(14) List all the vectors $\vec{w}$, which satisfy $\Delta_{V,\tilde{V}}(\vec{w}) = 0$. If no vector was detected, then, $\mathcal{G}_B = \mathcal{K}_B$. In this case stop. Otherwise, continue to step 15.

(15) If $\mathcal{K}_B = \{E\}$, continue to step 15a. Otherwise, go to step 16.

(a) Choose the single vector $\vec{a}$, which satisfies $\Delta_{V,\tilde{V}}(\vec{a}) = 0$.

(b) Solve Eq. 31 for the reflection R using Lemma 3.13. $R \in \mathcal{G}_B$. Go to step 19.

(16) If $\mathcal{K}_B$ is Cyclic, continue to step 16a. Otherwise, go to step 17.

(a) Choose a vector $\vec{w}$, which satisfies $\Delta_{V,\tilde{V}}(\vec{w}) = 0$, and solve Eq. 32 for the reflection S using Lemma 3.13. $R = S$, $R \in \mathcal{G}_B$. Go to step 19.

(17) If $\mathcal{K}_B$ is Octahedric, continue to step 17a. Otherwise, go to step 18.

(a) let $\vec{v}_1$ and $\vec{v}_2$ be a twofold and threefold rotation axes of B, respectively. Compute $\vec{w} = \vec{v}_1 \times \vec{v}_2$, $R = R_{\vec{w}}$, $R \in \mathcal{G}_B$ (see Eq. 6). Go to step 19.

(18) $\mathcal{K}_B$ is Dihedric of order $2m$. If $m > 2$ go to step 18a. Otherwise, go to step 18b.

(a) Define $\vec{v} \triangleq \vec{f}_j + \vec{f}_k$, where $\vec{f}_j$ and $\vec{f}_k$ are two adjacent secondary rotation axes of B and let $\vec{f}$ be the principle rotation axis of B. Compute $\vec{w} = \vec{v} \times \vec{f}$. $R = R_{\vec{w}}$, $R \in \mathcal{G}_B$ (see Eq. 6). Go to step 19.

(b) Let $\left\{\vec{f}_1, \vec{f}_2, \vec{f}_3\right\}$ be the rotation axes of B. For each pair $j, k \in \{1, 2, 3\}$ define $\vec{v} \triangleq \vec{f}_j + \vec{f}_k$. Compute $\vec{w} = \vec{v} \times \vec{f}_l$, $l \neq \{j, k\}$, $R = R_{\vec{w}}$. If $B - \Lambda(R)B \equiv 0$, stop - then, $R \in \mathcal{G}_B$.

(19) $\mathcal{G}_B = \mathcal{K}_B \cup R\mathcal{K}_B \triangleq \mathcal{K}_B \cup \{RO \, : \, O \in \mathcal{K}_B\}$.

Complexity: Based on the complexity of Algorithms 4.16 and 4.20, the complexity of Algorithm 4.21 is also $O\left(N^3 log\left(N\right)\right)$.

5. Experimental Results

In this section, we present the experimental results for different types of volumes. All the intermediate and final results of Algorithm 4.21 are examined in the next examples. According to Eq. 14, the range of the represented frequencies in the pseudo-polar representation is wider as N grows. The tested volumes are all of size $64 \times 64 \times 64$. In addition, the rotated and rotated inverted replicas are approximated on the Cartesian grid, since grid points are not necessarily transformed to grid points. The presented results show that despite of the inaccuracies, which originated from low resolution of the volumes and from the transformation of the volume, the 3DSDA is robust and accurate. The results are summarized in Tables 1-4.

Step-by-step evolution of the application of the 3DSDA to the example in Fig. 8:

Let B be the arrow shown in Fig. 8(a).

Step 1:

$\tilde{B} \triangleq \Lambda\left(\tilde{O}\right)B$, which is shown in Fig. 8 (b), is a rotated replica of B. The rotation axis of $\tilde{O}$ is $\vec{f}_0 = (0.8256\,, 0.2008\,, 0.5273)^t$ and the rotation angle of $\tilde{O}$ is $\delta = 175°$.

Step 2:

$V \triangleq \mathcal{F}_{PP}(B)$ and $\tilde{V} \triangleq \mathcal{F}_{PP}\left(\tilde{B}\right)$.

Step 3:

$\Delta_{V,\tilde{V}}$ is the ADF of V and $\tilde{V}$, see Fig. 8 (c).

Step 4:

$\vec{f_0}$ is the only detected vector. As a consequence, we conclude that $\mathcal{K}_V = \{E\}$.

Step 7:

$\tilde{B} \triangleq \Lambda(I)\, B$, where I is the inversion transformation. See Fig. 8 (d).

Step 8:

Since ΔB is not identically zero, $I \notin \mathcal{G}_V$.

Step 11:

$\tilde{B} \triangleq \Lambda\left(\tilde{R}\right) B$, where $\tilde{R} = \begin{pmatrix} -0.9683 & -0.1722 & 0.1811 \\ 0.1522 & -0.9812 & -0.1191 \\ -0.1982 & 0.0877 & -0.9762 \end{pmatrix}$ is a rotation-inversion.

See Fig. 8 (e).

Step 12:

$\tilde{V} \triangleq \mathcal{F}_{PP}\left(\tilde{B}\right)$.

Step 13:

$\Delta_{V,\tilde{V}}$ is the ADF of V and $\tilde{V}$, see Fig. 8 (f).

Step 15:

15a:

$\vec{a} = (0.9931\,, -0.0828\,, 0.0828)^t$ is the only detected vector.

15b:

The solution of the equation $R\vec{a} = \tilde{R}^{-1}\vec{a}$ is the reflection

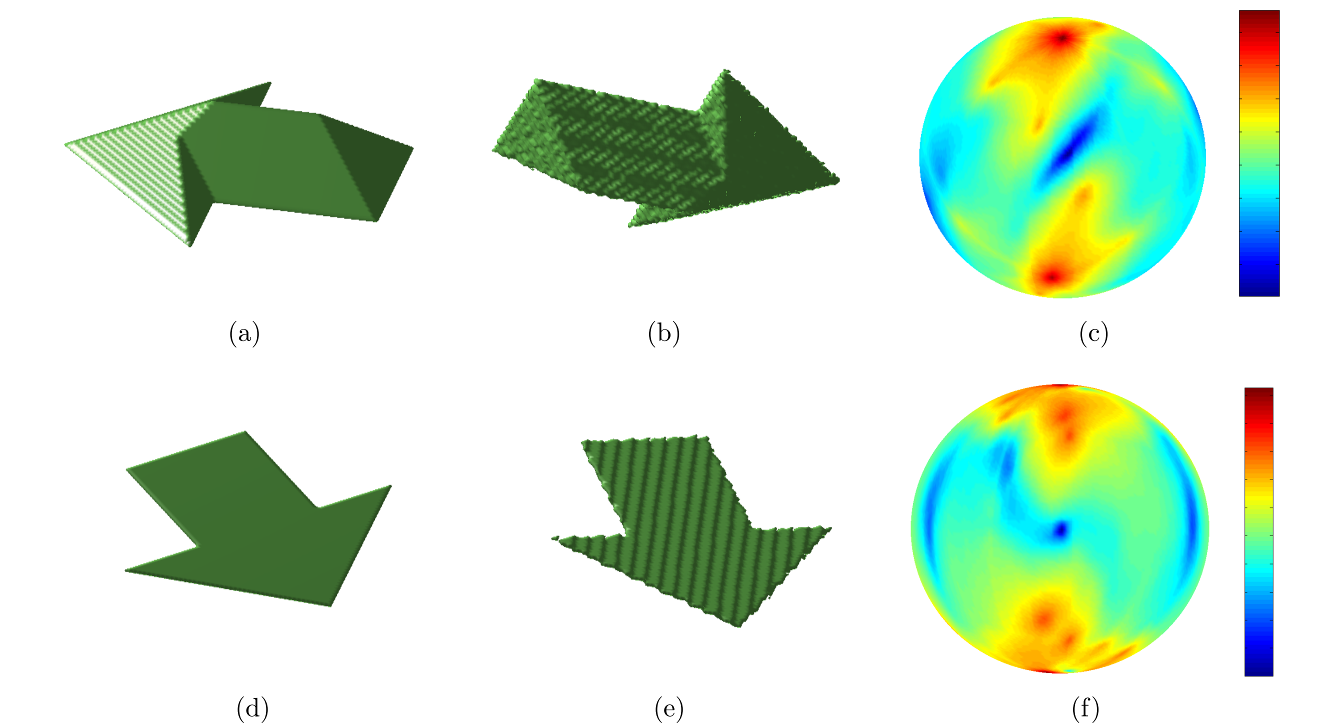
$R = R_{\vec{g}} = \begin{pmatrix} -0.9997 & 0 & 0.0264 \\ 0 & 1 & 0 \\ 0.0264 & 0 & 0.9997 \end{pmatrix}$, whose reflection axis is

$\vec{g} = (0.9999\,, -0.0001\,, -0.0132)^t$.

Step 19:

$\mathcal{G}_V = \{E, R\}$ (see Table 1).

FIGURE 8. Symmetries detection in an arrow



(a) The volume B. (b) A rotated replica of B, $\tilde{B} \triangleq \Lambda\left(\tilde{O}\right)B$. (c) Pseudo-polar representation of the ADF $\Delta_{B,\tilde{B}}$. $\vec{f_0}$ is the only detected vector. $\vec{f_0}$ is the point of view for both volumes and for the ADF. (d) The inverted replica of B, $\tilde{B} \triangleq \Lambda\left(I\right)B$. (e) A rotated-inverted replica of B, $\tilde{B} \triangleq \Lambda\left(\tilde{R}\right)B$. (f) Pseudo-polar representation of the ADF $\Delta_{B,\tilde{B}}$. $\vec{a}$ is the point of view for the ADF.

Step-by-step evolution of the application of the 3DSDA to the example in Fig. 9:

Let B be the square pyramid, which is shown in Fig. 9(a).

Step 1:

$\tilde{B} \triangleq \Lambda\left(\tilde{O}\right)B$ is the rotated replica of B, which is shown in Fig. 9 (b). The rotation axis of $\tilde{O}$ is $\vec{f_0} = (-0.8370\,, -0.5172\,, 0.1787)^t$ and the rotation angle of O is $\delta = 262°$.

Step 2:

$V \triangleq \mathcal{F}_{PP}\left(B\right)$, $\tilde{V} \triangleq \mathcal{F}_{PP}\left(\tilde{B}\right)$.

Step 3:

$\Delta_{V,\tilde{V}}$ is the ADF of V and $\tilde{V}$, see Fig. 9 (c).

Step 4:

There are four detected vectors: $\vec{f_0}$, $\vec{a_1} = (0.8756\,, -0.2043\,, 0.4378)^t$,
$a_2 = (0.1931\,, 0.7725\,, -0.6051)^t$ and $\vec{a_3} = (0.3961\,, -0.6382\,, 0.6602)^t$.

Step 5:

$\vec{n_1} \triangleq \vec{a_1} \times \vec{f_0} = (-0.2272\,, 0.6255\,, 0.7464)^t$, $\vec{n_2} \triangleq \vec{a_2} \times \vec{f_0} = (-0.2354\,, 0.6351\,, 0.7357)^t$ and $\vec{n_3} \triangleq \vec{a_3} \times \vec{f_0} = (-0.2290\,, -0.6276\,, 0.7441)^t$. The angles between the normal vectors are $\sphericalangle(\vec{n_1}, \vec{n_2}) = 0.95°$, $\sphericalangle(\vec{n_1}, \vec{n_3}) = 0.2°$ and $\sphericalangle(\vec{n_2}, \vec{n_3}) = 0.75°$. As a consequence, there is only one CP $\mathcal{S}_O = \left\{\vec{f_0}, \vec{a_1}, \vec{a_2}, \vec{a_3}\right\}$ where $\mathcal{K}_V$ is Cyclic. See Fig. 9 (d).

Step 6:

$\tilde{O}^{-\frac{1}{2}} = \begin{pmatrix} 0.8970 & 0.0140 & -0.4417 \\ 0.0837 & 0.7481 & 0.5998 \\ 0.3389 & -0.6634 & 0.6671 \end{pmatrix}$ is the rotation of angle $-87.5°$ around $\vec{f_0}$.

Start with $\mathcal{K}_V = \{E\}$.

6a:

$\vec{k} = \tilde{O}^{-\frac{1}{2}} \left(\frac{\vec{a_1} - \langle \vec{a_1}, \vec{f_0} \rangle \vec{f_0}}{\left\| \vec{a_1} - \langle \vec{a_1}, \vec{f_0} \rangle \vec{f_0} \right\|} \right) = (0.1552\,, 0.0888\,, 0.9839)^t.$

6b:

$b = 0.1625$, $c = 0.9867$, $n = 4$, $\gamma = 90°$.

6c:

$\vec{f} = b\vec{f_0} + c\vec{k} = (0.0170\,, 0.0035\,, 0.9998)^t$ and the associated rotation of order four is $O = \begin{pmatrix} 0.0003 & -0.9998 & 0.0205 \\ 0.9999 & 0 & -0.0135 \\ 0.0135 & 0.0205 & 0.9997 \end{pmatrix}$.

6d:

$\mathcal{K}_V = \{E, O\}$

Step 7:

$\tilde{B} = \Lambda(I)\, B$, where I is the inversion transformation, see Fig. 9 (e).

Step 8:

Since $\Delta B \triangleq B - \tilde{B}$ is not identically zero, we have $I \notin \mathcal{G}_V$.

Step 9:

9a:

$R_{\vec{f}} = \begin{pmatrix} 0.9994 & -0.0001 & -0.0340 \\ -0.0001 & 1 & -0.0070 \\ -0.0340 & -0.0070 & -0.9994 \end{pmatrix}$. $\tilde{B} = \Lambda\left(R_{\vec{f}}\right) B$. See Fig. 9 (f).

9b:

Since $\Delta B \triangleq B - \tilde{B}$ is not identically zero, then, $R_{\vec{f}} \notin \mathcal{G}_V$.

Step 11:

$\tilde{B}_1 \triangleq \Lambda\left(\tilde{R}\right) B$, where $\tilde{R} = \begin{pmatrix} -0.3333 & -0.9107 & 0.2440 \\ 0.2440 & -0.3333 & -0.9107 \\ -0.9107 & 0.2440 & -0.3333 \end{pmatrix}$ is a rotation-inversion. See Fig. 9 (g).

Step 12:

$\tilde{V}_1 \triangleq \mathcal{F}_{PP}\left(\tilde{B}_1\right)$.

Step 13:

$\Delta_{V,\tilde{V}_1}$ is the ADF of V and $\tilde{V}_1$. See Fig. 9 (h).

Step 14:

There are four detected vectors: $\vec{w_0} = (0.7669\,, -0.4601\,, 0.4474)^t$,
$\vec{w_1} = (0.9662\,, 0.2577\,, 0)^t$, $\vec{w_2} = (0.4500\,, 0.7714\,, -0.4500)^t$ and
$\vec{w_3} = (-0.2211\,, 0.7802\,, 0.5852)^t$.

Step 16:

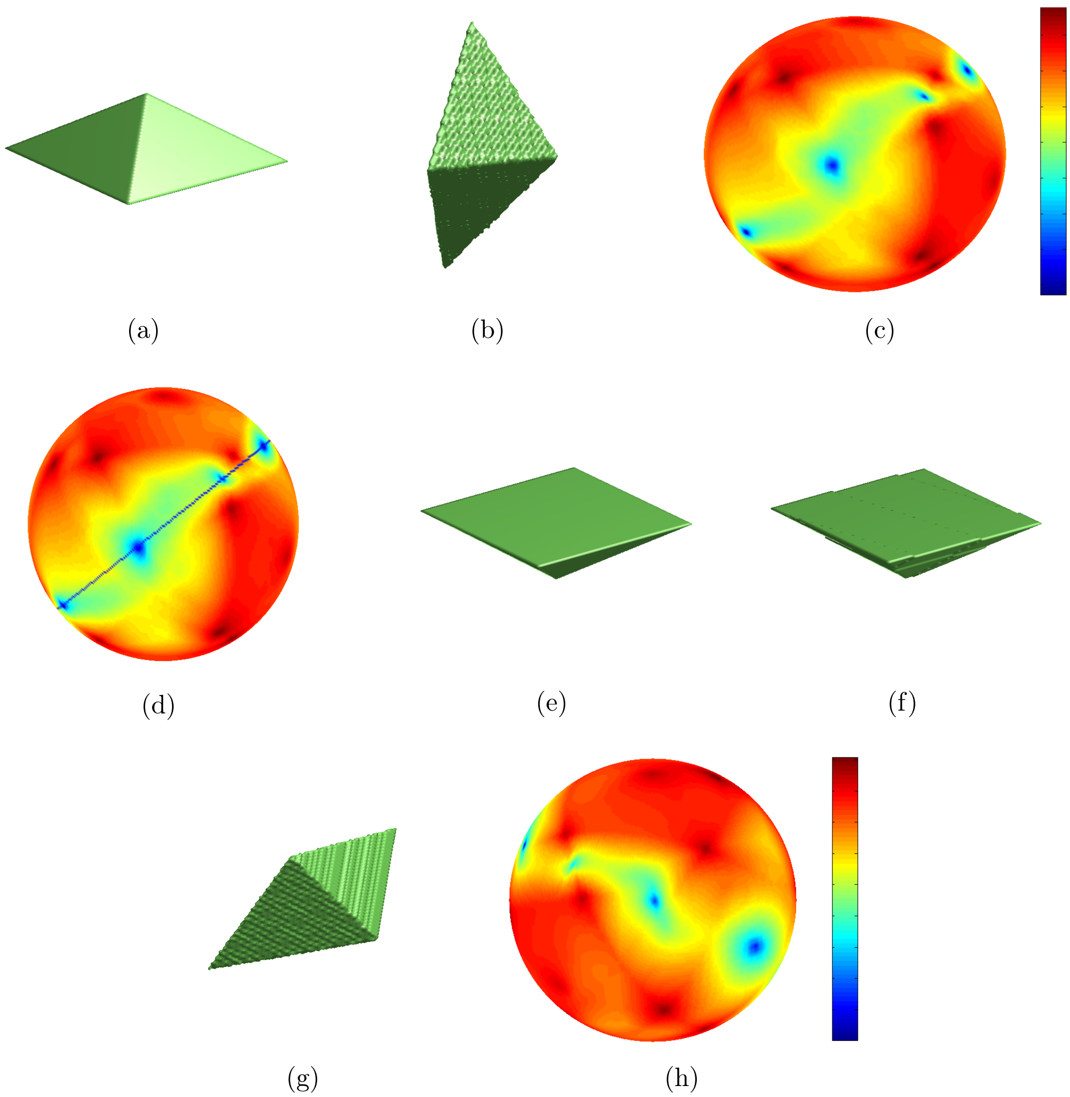
16a:

The solution of the equation $R\vec{w_0} = \tilde{R}^{-1}\vec{w_0}$ is $R = R_{\vec{b}} = \begin{pmatrix} -0.9994 & 0.0315 & 0.0126 \\ 0.0315 & 0.9995 & -0.0002 \\ 0.0126 & -0.0002 & 0.9999 \end{pmatrix}$,
where $\vec{b} = (0.9999\,, -0.0157\,, -0.0063)^t$.

Step 19:

$\mathcal{G}_V = \{E, O, O^2, O^3, R, RO, RO^2, RO^3\}$ (see Table 2).

FIGURE 9. Symmetries detection in a pyramid

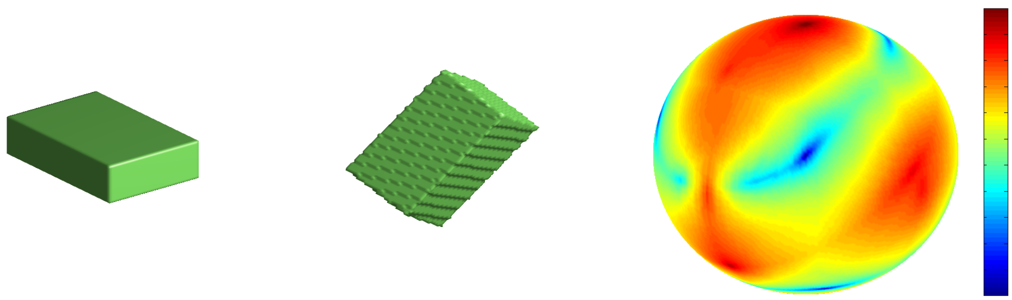


(a) The pyramid B. (b) A rotated replica of B, $\tilde{B} \triangleq \Lambda\left(\tilde{O}\right)B$. (c) Pseudo-polar representation of the ADF $\Delta_{B,\tilde{B}}$. (d) The CP which the detected vectors span. (e) The inverted pyramid $\tilde{B} \triangleq \Lambda\left(I\right)B$. (f) The reflected pyramid $\tilde{B} \triangleq \Lambda\left(R_{\vec{f}}\right)B$. (g) A rotated-inverted replica of B, $\tilde{B}_1 \triangleq \Lambda\left(\tilde{R}\right)B$. (h) $\Delta_{B,\tilde{B}_1}$. $\vec{w}_0$ is the point of view for $\Delta_{B,\tilde{B}_1}$.

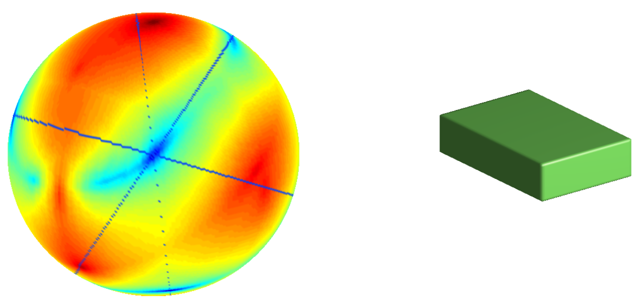
Application of the 3DSDA to the example in Fig. 10:

B is a box (see Fig. 10(a)). Its rotated replica $\tilde{B} \triangleq \Lambda\left(\tilde{O}\right)B$ is shown in Fig. 10 (b). $\tilde{O}$ is the rotation whose axis is $\vec{f}_0$. $V \triangleq \mathcal{F}_{PP}\left(B\right)$, $\tilde{V} \triangleq \mathcal{F}_{PP}\left(\tilde{B}\right)$ and $\Delta_{V,\tilde{V}}$ is the ADF of the volumes, see Fig. 10 (c). There are four detected vectors, $\vec{f}_0$, $\vec{f}_1$, $\vec{f}_2$ and $\vec{f}_4$, which belong to three different CPs (see Fig. 10 (d)) . There are three detected twofold rotation axes: $\vec{v_1} = \left(1\,,0.0056\,,0.0063\right)^t$, $\vec{v_2} = \left(-0.0144\,,0.9999\,,-0.0047\right)^t$ and $\vec{v_3} = \left(-0.0048\,,0.0058\,,1\right)^t$, hence, $\mathcal{K}_V$ is Dihedric with $m = 2$. Let O_1, O_2 and O_3 be the rotations of order two, whose axes are $\vec{v_1}$, $\vec{v_2}$ and $\vec{v_2}$, respectively. Let $\tilde{B_1} = \Lambda(I)\,B$, where I is the inversion transformation, see Fig. 10 (e). Since $\Delta_B \triangleq B - \tilde{B_1} \equiv 0$, $I \in \mathcal{G}_V$ and $\mathcal{G}_V = \{E, O_1, O_2, O_3, I, IO_1, IO_2, IO_3\}$ (see Table 3).

FIGURE 10. Symmetries detection in a box



(a) (b) (c)



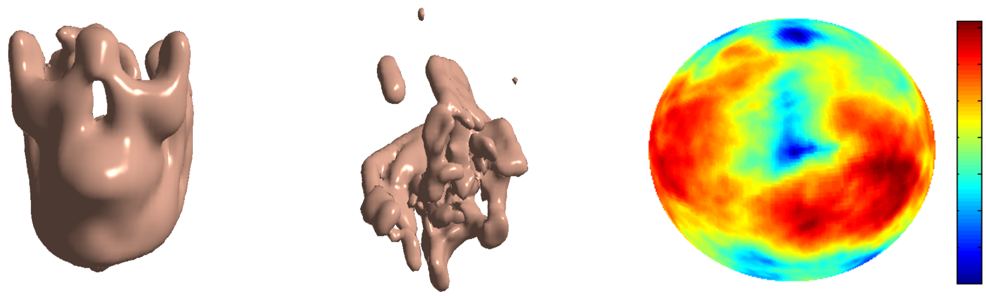
(d) (e)

(a) The volume B. (b) A rotated replica of B, $\tilde{B} \triangleq \Lambda\left(\tilde{O}\right)B$. (c) Pseudo-polar representation of the ADF $\Delta_{B,\tilde{B}}$. $\vec{f_0}$ is the point of view. (d) The three CPs. The common vector is $\vec{f_0}$. (e) The inverted replica of B, $\tilde{B} \triangleq \Lambda\left(\tilde{I}\right)B$.

Application of the 3DSDA to the example in Fig. 11:

B is a MRI skull model (see Fig. 11(a)). Its rotated-inverted replica $\tilde{B} \triangleq \Lambda\left(\tilde{R}\right)B$ is shown in Fig. 11 (b), where $\tilde{R} = \begin{pmatrix} -0.6667 & -0.6667 & 0.3333 \\ 0.3333 & -0.6667 & -0.6667 \\ -0.6667 & 0.3333 & -0.6667 \end{pmatrix}$ is a rotation-inversion. $V \triangleq \mathcal{F}_{PP}(B)$, $\tilde{V} \triangleq \mathcal{F}_{PP}\left(\tilde{B}\right)$ and $\Delta_{V,\tilde{V}}$ is the ADF of the volumes, see Fig. 11 (c). The detected vector is $\vec{a} = (0.8498,\ -0.3983,\ 0.3452)^t$, and the corresponding detected reflection is $R_{\vec{a}} = \begin{pmatrix} -0.9175 & 0.2354 & -0.0294 \\ 0.2354 & 0.9719 & 0.0035 \\ -0.0294 & 0.0035 & 0.9996 \end{pmatrix}$. The volume $\Lambda(R)B$ is shown in Fig. 11 (d).

FIGURE 11. Symmetries detection in a skull model



(a) (b) (c)

(a) The volume B. (b) A rotated replica of B, $\tilde{B} \triangleq \Lambda\left(\tilde{R}\right) B$. (c) Pseudo-polar representation of the ADF $\Delta_{B,\tilde{B}}$. $\vec{a}$ is the point of view.

Tables 1-4 present the detected symmetries of an arrow, a pyramid a box, and a skull model, respectively. Column (a) shows the known symmetries of the volume B, i.e., the elements of $\mathcal{G}_B$, in matrix representation. Column (b) describes the detected elements of $\mathcal{G}_B$ in matrix representation. Column (c) is the SVD distance between the known and the detected symmetries, which is the maximal singular value of the difference matrix. Column (d) describes only rotations and reflections. $\epsilon = \sphericalangle\left(\vec{a}, \vec{d}\right)$, where $\vec{a}$ is the actual axis and $\vec{d}$ is the detected one. Column (e) is $\Lambda\left(D\right)B$, where D is the detected isometry.

TABLE 1. Detected symmetries of the arrow

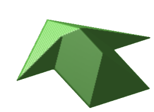
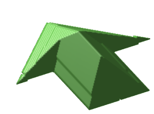
(a) Known Symmetry K	(b) Detected Symmetry D	(c) $\|K-D\|$	(d) $\|\epsilon\|$	(e) $\Lambda\left(D\right)B$
$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	0	0	
$R_{\vec{x}} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$R_{\vec{g}} = \begin{pmatrix} -0.9997 & 0 & 0.0264 \\ 0 & 1 & 0 \\ 0.0264 & 0 & 0.9997 \end{pmatrix}$	0.0264	0.7561°	

Table 2. Detected symmetries of the pyramid

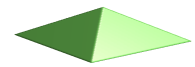
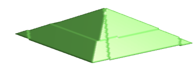
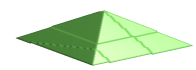
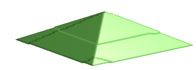
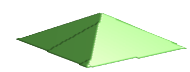
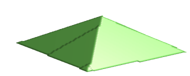
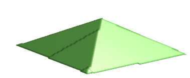
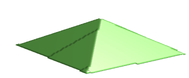
(a) Known Symmetry K	(b) Detected Symmetry D	(c) $\|K-D\|$	(d) $\|\epsilon\|$	(e) $\Lambda(D)B$
$E=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$E=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	0	0	
$o=\begin{pmatrix}0&-1&0\\1&0&0\\0&0&1\end{pmatrix}$	$O=\begin{pmatrix}0.0003&-0.9998&0.0205\\0.9999&0&-0.0135\\0.0135&0.0205&0.9997\end{pmatrix}$	0.0245	0.9946°	
$o^2=\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}$	$O^2=\begin{pmatrix}-0.9994&0.0001&0.0340\\0.0001&-1&0.0070\\0.0340&0.0070&0.9994\end{pmatrix}$	0.0347	0.9946°	
$o^3=\begin{pmatrix}0&1&0\\-1&0&0\\0&0&1\end{pmatrix}$	$O^3=\begin{pmatrix}0.0003&0.9999&0.0135\\-0.9998&0&0.0205\\0.0205&-0.0135&0.9997\end{pmatrix}$	0.0245	0.9946°	
$r=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$R=\begin{pmatrix}-0.9994&0.0315&0.0126\\0.0315&0.9995&-0.0002\\0.0126&-0.0002&0.9999\end{pmatrix}$	0.0339	0.9713°	
$ro=\begin{pmatrix}0&1&0\\1&0&0\\0&0&1\end{pmatrix}$	$RO=\begin{pmatrix}0.0315&0.9994&0.0126\\0.9995&-0.0315&-0.0002\\-0.0002&-0.0126&0.9999\end{pmatrix}$	0.0339	0.9373°	
$ro^2=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&1\end{pmatrix}$	$RO^2=\begin{pmatrix}0.9994&-0.0315&0.0126\\-0.0315&-0.9995&-0.0002\\-0.0126&0.0002&0.9999\end{pmatrix}$	0.0339	0.9020°	
$ro^3=\begin{pmatrix}0&-1&0\\-1&0&0\\0&0&1\end{pmatrix}$	$RO^3=\begin{pmatrix}-0.0315&-0.9994&0.0126\\-0.9995&0.0315&-0.0002\\0.0002&0.0126&0.9999\end{pmatrix}$	0.0339	0.9373°	

Table 3. Detected symmetries of the box

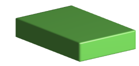
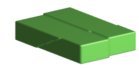
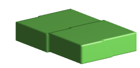
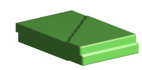
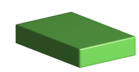
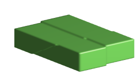
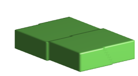
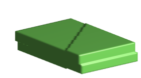
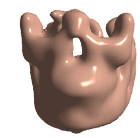
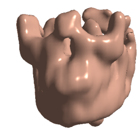
(a) Known Symmetry K	(b) Detected Symmetry D	(c) $\|K-D\|$	(d) $\|\epsilon\|$	(e) $\Lambda(D)\,B$
$E=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$E=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	0	0	
$o_1=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&-1\end{pmatrix}$	$O_1=\begin{pmatrix}0.9999&0.0112&0.0126\\0.0112&-0.9999&0.0001\\0.0126&0.0001&-0.9999\end{pmatrix}$	0.0169	0.4835°	
$o_2=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix}$	$O_2=\begin{pmatrix}-0.9996&-0.0288&0.0001\\-0.0288&0.9995&-0.0094\\0.0001&-0.0094&-1\end{pmatrix}$	0.0303	0.8681°	
$o_3=\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix}$	$O_3=\begin{pmatrix}-1&-0.0001&-0.0097\\-0.0001&-0.9999&0.0115\\-0.0097&0.0115&0.9999\end{pmatrix}$	0.0151	0.4319°	
$I=\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&-1\end{pmatrix}$	$I=\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&-1\end{pmatrix}$	0	0	
$Io_1=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$IO_1=\begin{pmatrix}-0.9999&-0.0112&-0.0126\\-0.0112&0.9999&-0.0001\\-0.0126&-0.0001&0.9999\end{pmatrix}$	0.0169	0.4835°	
$Io_2=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&1\end{pmatrix}$	$IO_2=\begin{pmatrix}0.9996&0.0288&-0.0001\\0.0288&-0.9995&0.0094\\-0.0001&0.0094&1\end{pmatrix}$	0.0303	0.8681°	
$Io_3=\begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix}$	$IO_3=\begin{pmatrix}1&0.0001&0.0097\\0.0001&0.9999&-0.0115\\0.0097&-0.0115&-0.9999\end{pmatrix}$	0.0151	0.4319°	

Table 4. Detected symmetries of a skull model

(a) Known Symmetry K	(b) Detected Symmetry D	(c) $\|K-D\|$	(d) $\|\epsilon\|$	(e) $\Lambda(D)B$
$E=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$E=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	0	0	
$R_{\vec{a}}=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$R_{\vec{a}}=\begin{pmatrix}-0.9175&0.2354&-0.0294\\0.2354&0.9719&0.0035\\-0.0294&0.0035&0.9996\end{pmatrix}$	0.2389	6.8615°	

6. Conclusions

This paper presents an algorithm for detection of $3D$ finite symmetries. These symmetries are invariant under the Fourier transform, hence, symmetries detection in the volume is equivalent to symmetries detection in the transformed volume. We use the pseudo-polar Fourier representation, in order to convert the volume from Cartesian to pseudo-polar representation. The pseudo-polar grid enables an accurate polar analysis of the ADF of a given volume and a rotated or rotated-inverted replica. We prove that the ADF encapsulates the whole information needed for symmetry detection, where the isometric replicas were chosen arbitrarily. The algorithm was tested on several volumes and the detected symmetries were very close to the correct symmetries, even when the symmetries were imperfect.

This work can be extended into several directions: Detection of infinite symmetries and checking the robustness of the algorithm in the presence of noise.

References

[1] D. W. Thompson, On Growth and Form. Cambridge, 1961.

[2] A. Averbuch and Y. Shkolnisky, "3D Fourier based discrete Radon transform", *Applied and Computational Harmonic Analysis*, vol. 15, pp. 33-69, 2003.

[3] W. Miller, Symmetry groups and their applications. Academic Press, 1972.

[4] Y. Keller, Y. Shkolnisky and A. Averbuch, "Volumes registration using 3D pseudo-polar Fourier transform", *IEEE Trans. on Signal Processing,* 54(11), 4323-4331, 2006.

[5] H. Zabrodsky, S. Peleg and D. Avnir, "Symmetry as a Continuous Feature", *IEEE Trans. Pattern Analysis and Machine Intelligence,* vol. 17, no. 12, pp. 1154-1165, Dec. 1995.

[6] H. Zabrodsky, S. Peleg and D. Avnir, "Hierarchical Symmetry", *Proc. Int'l Conf. Pattern Recognition,* Aug. 30 - Sept. 3, The Hague, The Netherlands, 1992, vol. III, pp. 9-11.

[7] S. Parry-Barwick and A. Bowyer, "Symmetry Analysis and Geometric Modeling", *Digital Image Computing: Techniques and Applications,* K.K. Fung and A. Ginige, eds. Dec. 1993, vol. I, pp. 39-46, Australian Pattern Recognition Society.

[8] P. Brass and C. Knauer, "Testing congruence and symmetry for general 3-dimensional objects", *Comput. Geom. Theory Appl.,* vol. 27, no. 1, pp. 3-11, 2004.

[9] C. Sun and J. Sherrah, "3D Symmetry Detection using the Extended Gaussian Image", *IEEE Trans. Pattern Analysis and Machine Intelligence,* vol. 19, no. 2, pp. 164-168, Feb. 1997.

[10] A. Martinet, C. Soler, N. Holzschuch, F. X. Sillion, "Accurate Detection of Symmetries in 3D Shapes", *ACM Transactions on Graphics,* vol. 25, no. 2, pp. 439-464, Apr. 2006.

[11] H. Alt, K. Mehlhorn, H. Wagener and Welzl, "Congruence, Similarity, and Symmetries of Geometric Objects", *Discrete and Computational Geometry*, vol. 3, pp. 237-256, 1988.

[12] M. Kazhdan, T. Funkhouser and S. Rusinkiewicz "Symmetry Descriptors and 3D Shape Matching", *Eurographics Symposium on Geometry Processing (2004).*

[13] J. Podolak, P. Shilane, A. Golovinsky, S. Rusinkiewicz and T. Funkhouser "A Planar-Reflective Symmetry Transform for 3D Shapes", *ACM Transactions on Graphics,* vol. 25, no. 3, pp. 549-559, Jul. 2006.

[14] N. J. Mitra, L. J. Guibas and M. Pauly "Partial and Approximate Symmetry Detection for 3D Geometry", *ACM Transactions on Graphics,* vol. 25, no. 3, pp. 560-568, Jul. 2006.

[15] E. Trucco and A. Verri, Introductory Techniques for 3-D Computer Vision. New Jersey: Prentice-Hall, 1998, pp.333-334.

[16] P. M. Neumann, G. A. Stoy, E.C. Thompson, Groups and Geometry. Oxford University Press, 1995.

[17] A. Holden, Shapes, space and symmetry. Columbia University Press, 1971.

[18] M. Jeger, B. Eckmann, Vector Geometry & Linear Algebra. John Wiley & Sons, 1967.