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by

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Left-invariant Diffusions on $\mathbb{R}^3 \rtimes S^2$ and their Application to Crossing-preserving Smoothing of HARDI-images

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Abstract

In previous work we studied linear and nonlinear left-invariant diffusion equations on the 2D Euclidean motion group $SE(2)$, for the purpose of crossing-preserving coherence-enhancing diffusion on 2D images. In this article we study left-invariant diffusion on the 3D Euclidean motion group $SE(3)$ and its application to crossing-preserving smoothing of high angular resolution diffusion imaging (HARDI), which is a recent magnetic resonance imaging (MRI) technique for imaging water diffusion processes in fibrous tissues such as brain white matter and muscles.

The linear left-invariant (convection-)diffusions are forward Kolmogorov equations of Brownian motions on the space $\mathbb{R}^3 \rtimes S^2$ of positions and orientations embedded in $SE(3)$ and can be solved by $\mathbb{R}^3 \rtimes S^2$-convolution with the corresponding Green’s functions. We provide analytic approximation formulae and explicit sharp Gaussian estimates for these Green’s functions. In our design and analysis for appropriate (non-linear) convection-diffusions on HARDI-data we put emphasis on the underlying differential geometry on $SE(3)$. We write our left-invariant diffusions in covariant derivatives on $SE(3)$ using the Cartan-connection. This Cartan-connection has constant curvature and constant torsion, and so have the exponential curves which are the auto-parallels along which our left-invariant diffusion takes place. We provide experiments of our crossing-preserving Euclidean-invariant diffusions on artificial HARDI-data containing crossing-fibers.

Keywords: High Angular Resolution Diffusion Imaging (HARDI), Scale spaces, Lie groups, Partial differential equations.

1 Introduction

High angular resolution diffusion imaging (HARDI) is a recent magnetic resonance imaging technique for imaging water diffusion processes in fibrous tissues such as brain white matter and muscles. HARDI provides for each position in 3-space and for each orientation (antipodal pairs on the 2-sphere) an MRI signal attenuation profile, which can be related to the local diffusivity of water molecules in the corresponding direction. It is generally believed that such profiles provide rich information in fibrous tissues. DTI is a related technique, producing a positive symmetric rank-2 tensor field. A DTI tensor (at each position in 3-space) can also be related to a distribution on the 2-sphere, albeit with limited angular resolution. DTI is incapable of representing areas with complex multimodal diffusivity profiles, such
as induced by crossing, “kissing”, or bifurcating fibres. HARDI, on the other hand, does not suffer from this problem, because it is not restricted to functions on the 2-sphere induced by a quadratic form. Cf. Figure 1.

For the purpose of tractography (detection of biological fibers) and visualization, DTI and HARDI data should be enhanced such that fiber junctions are maintained, while reducing high frequency noise in the joined domain of positions and orientations.

Figure 1: DTI versus HARDI: Glyphs reflect the local diffusivity of water in all directions. The rank-2 limitation of a DTI-tensor constrains the corresponding glyph to be ellipsoidal, whereas no such constraint applies to HARDI. Here DTI-tensors are represented by the corresponding ellipsoids \( n^T D n = \lambda_1 \). The color of the ellipsoids in DTI encode the fractional anisotropy factor \( \frac{\sqrt{3(\lambda_1-\lambda_2^2+\lambda_2-\lambda_3)+2\lambda_3^2}}{\lambda_1^2+\lambda_2^2+\lambda_3^2} \), where \( \bar{\lambda} \) is the average of the three eigenvalues \( \lambda_1 \geq \lambda_2 \geq \lambda_3 \) of diffusion tensor field \( D \). HARDI-images \( U : \mathbb{R}^3 \times S^2 \rightarrow \mathbb{R} \) are first linearly re-scaled to \([0,1]\) in the co-domain after which the radius of a point on the surface \( S(x) \) with direction \( n \) equals the value \( U(x,n) \), whereas the color encodes the directions \( n \in S^2 \). The color-coded surface \( S(x) = x + \mu(U(x,n) \ n \ | \ n \in S^2) \), located at the 3D-tangent-space \( T_x(R^3) \) at position \( x \in \mathbb{R}^3 \) is often called HARDI-glyph in the field of visualization. The parameter \( \mu \in \mathbb{R}^+ \) is a scaling factor determining the size of the visualized HARDI-glyph.

Promising research has been done on constructing diffusion (or similar regularization) processes on the 2-sphere defined at each spatial locus separately [10, 22, 23, 43] as an essential pre-processing step for robust fiber tracking. In these approaches position and orientation space are decoupled, and diffusion is only performed over the angular part, disregarding spatial context. Consequently, these methods are inadequate for spatial denoising and enhancement, and tend to fail precisely at the interesting locations where fibres cross or bifurcate.

Therefore in this article we extend recent work on enhancement of elongated structures in 2D greyscale images [2, 27, 26, 28, 21, 20, 13, 16, 14, 15, 19, 18] to the genuinely 3D case of HARDI/DTI, since this approach has proven to be capable of handling all aforementioned problems in various feasibility studies. See Figure 2.

In contrast to the previous works on diffusion of HARDI data [10, 22, 23, 43, 37], we consider both the spatial and the orientational part to be included in the domain, so a HARDI dataset is considered as a function \( U : \mathbb{R}^3 \times S^2 \rightarrow \mathbb{R}^+ \).
Figure 2: Left-invariant diffusion via diffusion on $SE(2) = \mathbb{R}^2 \times S^1$ is the right approach to generically deal with crossings and bifurcations in practice. Left column: original images. Middle column: result of standard coherence enhancing diffusion applied directly in the image domain $\mathbb{R}^2$ (CED), cf. [45]. Right column: coherence enhancing diffusion via the corresponding invertible orientation score (CED-OS) in the 2D-Euclidean motion group $SE(2)$, cf. [19, 27]. Top row: 2-photon microscopy image of bone tissue. Second row: collagen fibers of the heart. Third row: artificial noisy interference pattern. Typically, these 2D-applications clearly show that coherence enhancing diffusion on invertible orientation scores (CED-OS) is capable of handling crossings and bifurcations, whereas (CED) produces spurious artifacts at such junctions. Now in the genuinely 3D-case of HARDI-images $U : \mathbb{R}^3 \times S^2 \to \mathbb{R}$, we do not have to bother about invertibility of the transform between a grey-value image and its orientation score as the input-data itself already gives rise to a function on the 3D Euclidean motion group $SE(3)$. This is now simply achieved by setting $\tilde{U}(x, R) = U(x, Re_z)$, $R \in SO(3)$, $x \in \mathbb{R}^3$, $e_z = (0,0,1)^T$ and the challenge rises to generalize our previous work on crossing preserving diffusion to 3D and to apply the left-invariant diffusion directly on the HARDI-images.

Furthermore, we explicitly employ the proper underlying group structure, that naturally arises by embedding the coupled space of positions and orientations into the group of 3D-rigid motions. The advantage is that we can enhance the data using both orientational and spatial neighborhood information, which potentially leads to improved enhancement and detection algorithms. In this article, the domain of an HARDI-image is parameterized by $(x, n) \in \mathbb{R}^3 \times S^2$, where $x = (x, y, z) \in \mathbb{R}^3$ and $n \in S^2$. Figure 3 shows an example clarifying the structure of a HARDI-image.

This paper is organized as follows. In Section 2 we will start with the introduction of the group structure on the domain of a HARDI-image. Here we will explain that the domain of a HARDI-image of positions and orientations carries a semi-direct product structure rather than a direct Cartesian product structure reflecting a natural coupling between position and orientation. Here we embed the space of positions and orientations into the group of positions and rotations in 3-space, which is commonly denoted by $SE(3) = \mathbb{R}^3 \times SO(3)$. As a result we must write $\mathbb{R}^3 \times S^2 := \mathbb{R}^3 \times SO(3)/(\{0\} \times SO(2))$ rather than $\mathbb{R}^3 \times S^2$ for the domain of an HARDI-image.

In Section 3 we will discuss a few basic tools from group theory which serve as the key ingredients in our diffusions on HARDI-images later on. Within this section we also provide an example to embed a recent paper [6] by Barmopitou et al. on smoothing of HARDI data in our group theoretical framework. We show that their proposed practically designed
kernel operator indeed is a correct left-invariant group-convolution on $\mathbb{R}^3 \rtimes S^2$. However their practically intuitive kernel does not satisfy the semi-group property and does not relate to diffusion or Tikhononov energy minimization on $\mathbb{R}^3 \rtimes S^2$.

Subsequently, in Section 4 we will derive all linear left-invariant convection-diffusion equations on $SE(3)$ and $\mathbb{R}^3 \rtimes S^2$ (the actual domain of HARDI-images) and show that the solutions of these convection-diffusion equations are given by group-convolution with the corresponding Green’s functions, which we explicitly approximate later. Furthermore, in Subsection 4.2, we put an explicit connection with probability theory and random walks in the space of orientations and positions. This connection is established by the fact that the convection-diffusion equations are Fokker-Plank (i.e. forward Kolmogorov) equations of stochastic processes (random walks) on the space of orientations and positions. This in turn brings a nice connection to the actual measurements of water-molecules in oriented fibrous tissues. Symmetry requirements for the linear diffusions on $\mathbb{R}^3 \rtimes S^2$ yields the following four cases:

1. the natural 3D-generalizations of Mumford’s direction process on $\mathbb{R}^2 \rtimes S^1$ [35, 21], which is a contour completion process in the group $SE(2) = \mathbb{R}^2 \rtimes S^1 \equiv \mathbb{R}^2 \rtimes SO(2)$ of 2D-positions and orientations.

2. the natural 3D-generalizations of a (horizontal) random walk on $\mathbb{R}^2 \rtimes S^1$, cf. [18], corresponding to the diffusions proposed by Citti and Sarti [9], which is a contour enhancement process in the group $SE(2) = \mathbb{R}^2 \rtimes S^1 \equiv \mathbb{R}^2 \rtimes SO(2)$ of 2D-positions and orientations,

3. Gaussian scale space [32, 33, 3, 12] over position space, i.e. spatial linear diffusion,

4. Gaussian scale space over angular space (2-sphere), [10, 37, 22, 23, 15, 43], i.e. angular linear diffusion,

or combinations of these four types of convection-diffusions. Note that previous approaches of HARDI-diffusions [10, 37, 22] fit in our framework (third and fourth item), but it is rather the first two cases that are challenging and novel because they involve a natural coupling between position and orientation space and thereby allow appropriate treatment of crossing fibers!

In Section 5 we will explore the underlying differential geometry of our diffusions on HARDI-orientation scores. By means of the Cartan-connection on $SE(3)$ we put a nice relation to rigid body mechanics expressed in moving frames of reference, providing geometrical intuition behind our left-invariant (convection-)diffusions on HARDI-data. Furthermore, we show that our (convection-)diffusion may be expressed in covariant derivatives and we show that both convection and diffusion locally takes place along the exponential curves in $SE(3)$, that are explicitly derived in subsection 5.1. In Section 6 we will derive suitable formulae and Gaussian estimates for the Green’s functions of our linear left-invariant convection-diffusions on HARDI-images. These formula are used in the subsequent section in our numerical convolution-schemes solving the left-invariant diffusions on HARDI-images.
Section 7 explains the basic numerics of our left-invariant PDE- and/or convolution schemes, which we use in the subsequent experimental section, Section 8. Section 8 contains preliminary results of linear left-invariant diffusion on artificial HARDI datasets over the joined coupled domain of positions and orientations (i.e. over $\mathbb{R}^3 \times S^2$).

The final section of this paper provides the theory for non-linear adaptive diffusion on HARDI-images, which is a generalization of our non-linear adaptive diffusion schemes on the 2D-Euclidean motion group [27, 19].

2 The Group Structure on the Domain of a HARDI Image: The Embedding of $\mathbb{R}^3 \times S^2$ into $SE(3)$

In order to generalize our previous work on line/contour-enhancement via left-invariant diffusions on invertible orientation scores of 2D-images we first have to investigate the group structure on the domain of an HARDI-image. Just like orientation scores are scalar-valued functions on the coupled space of 2D-positions and orientations, i.e. the 2D-Euclidean motion group, HARDI-images are scalar-valued functions on the coupled space of 3D-positions and orientations. This generalization involves some technicalities since the 2-sphere $S^2 = \{ x \in \mathbb{R}^3 \mid ||x|| = 1 \}$ is not a Lie-group proper\(^1\) in contrast to the 1-sphere $S^1 = \{ x \in \mathbb{R}^2 \mid ||x|| = 1 \}$. To overcome this problem we will first embed $\mathbb{R}^3 \times S^2$ into $SE(3)$ which is the group of 3D-rotations and translations (i.e. the group of 3D-rigid motions). As a concatenation of two rigid body-movements is again a rigid body movement, the product on $SE(3)$ is given by

$$(x, R)(x', R') = (Rx' + x, RR'), \quad R, R' \in SO(3), x, x' \in \mathbb{R}^3.$$ 

The group $SE(3)$ is a semi-direct product of the translation group $\mathbb{R}^3$ and the rotation group $SO(3)$, since it uses an isomorphism $R \mapsto (x \mapsto Rx)$ from the rotation group onto the automorphisms on $\mathbb{R}^3$. Therefore we write $\mathbb{R}^3 \ltimes SO(3)$ rather than $\mathbb{R}^3 \times SO(3)$ which would yield a direct product. The groups $SE(3)$ and $SO(3)$ are not commutative. Throughout this article we will use Euler-angle parametrization for $SO(3)$, i.e. we write every rotation as a product of a rotation around the $y$-axis, a rotation around the $y$-axis and a rotation around the $z$-axis again.

$$R = R_{e_z, \gamma}R_{e_y, \beta}R_{e_z, \alpha}, \quad (1)$$

where all rotations are counter-clockwise. The advantage of the Euler angle parametrization is that it directly parameterizes $SO(3)/SO(2) \equiv S^2$ as well. Here we recall that $SO(3)/SO(2)$ denotes the partition of all left cosets which are equivalence classes $[g] = \{ h \in SO(3) \mid h \sim g \} = g SO(2)$ under the equivalence relation $g_1 \sim g_2 \iff g_1^{-1}g_2 \in SO(2)$ where we identified $SO(2)$ with rotations around the $z$-axis and we have

$$SO(3)/SO(2) \ni \{ R_{e_z, \gamma}R_{e_y, \beta} \mid \alpha \in [0, 2\pi) \} \leftrightarrow \mathbf{n}(\beta, \gamma) := (\cos \gamma \sin \beta, \sin \gamma \sin \beta, \cos \beta), \quad (2)$$

Like all parameterizations of $SO(3)/SO(2)$, the Euler angle parametrization suffers from the problem that there does not exists a global diffeomorphism from a sphere to a plane. In the Euler-angle parametrization the ambiguity arises at the north and south-pole:

$$R_{e_z, \gamma}R_{e_y, \beta=0}R_{e_z, \alpha} = R_{e_z, \gamma-\delta}R_{e_y, \beta=0}R_{e_z, \alpha+\delta}, \quad \text{and} \quad R_{e_z, \gamma}R_{e_y, \beta=\pi}R_{e_z, \alpha} = R_{e_z, \gamma+\delta}R_{e_y, \beta=0}R_{e_z, \alpha+\delta}, \quad \forall \delta \in [0, 2\pi). \quad (3)$$

Consequently, we occasionally need a second chart to cover $SO(3)$:

$$R = R_{e_z, \bar{\gamma}}R_{e_y, \bar{\beta}}R_{e_z, \bar{\alpha}}, \quad (4)$$

which again implicitly parameterizes $SO(3)/SO(2) \equiv S^2$ using different ball-coordinates $\bar{\beta} \in [-\pi, \pi)$, $\bar{\gamma} \in (-\frac{\pi}{2}, \frac{\pi}{2})$,

$$\mathbf{\bar{n}}(\bar{\beta}, \bar{\gamma}) = R_{e_z, \bar{\gamma}}R_{e_y, \bar{\beta}}e_z = (\sin \bar{\beta}, -\cos \bar{\beta} \sin \bar{\gamma}, \cos \bar{\beta} \cos \bar{\gamma})^T, \quad (5)$$

\(^1\)If $S^2$ were a Lie-group then its left-invariant vector fields are non-zero everywhere, contradicting Poincaré’s “hairy ball theorem” (proven by Brouwer in 1912), or more generally the Poincaré-Hopf theorem (the Euler-characteristic of an even dimensional sphere $S^{2n}$ is 2).
Figure 4: The two charts which together appropriately parameterize the sphere $S^2 \equiv SO(3)/SO(2)$ where the rotation-parameters $\alpha$ and $\tilde{\alpha}$ are free. The first chart (left-image) is the common Euler-angle parametrization (1), the second chart is given by (4). The first chart has singularities at north and south-pole (inducing ill-defined parametrization of the left-invariant vector fields (26) at the unity element) whereas the second chart has singularities at $(\pm 1, 0, 0)$.

but which has ambiguities at the intersection of the equator with the $x$-axis

\[ R_{e_x, \gamma} R_{e_y, \beta = \pm \frac{\pi}{2}} R_{e_z, \tilde{\alpha}} = R_{e_x, \gamma \pm \delta} R_{e_y, \beta = \pm \frac{\pi}{2}} R_{e_z, \tilde{\alpha} \pm \delta}, \text{ for all } \delta \in [0, 2\pi). \quad (6) \]

See Figure 4. Away from the intersection of the $z$ and $x$-axis with the sphere one can accomplish conversion between the two charts by solving for $R_{e_x, \gamma} R_{e_y, \beta} R_{e_z, \tilde{\alpha}} = R_{e_x, \gamma} R_{e_y, \beta} R_{e_z, \alpha}$. 

Now that we have explained the isomorphism $n = Re_z \in S^2 \leftrightarrow SO(3)/SO(2) \ni [R]$ explicitly in charts, we return to the domain of HARDI-images. Considered as a set this domain equals the space of 3D-positions and orientations $\mathbb{R}^3 \times S^2$. However, in order to stress the fundamental embedding of the HARDI-domain in $SE(3)$ and the thereby induced (quotient) group-structure we write $\mathbb{R}^3 \ltimes S^2$, which is given by the following Lie-group quotient:

\[ \mathbb{R}^3 \ltimes S^2 := \mathbb{R}^3 \ltimes SO(3)/\{0\} \times SO(2). \]

Here the equivalence relation on the group of rigid-motions $SE(3) = \mathbb{R}^3 \ltimes SO(3)$ equals

\[ (x, R) \sim (x', R') \iff x = x' \text{ and } R^{-1} R' \text{ is a rotation around } z\text{-axis} \]

and set of equivalence classes within $SE(3)$ under this equivalence relation (i.e. left cosets) equals the space of coupled orientations and positions and is denoted by $\mathbb{R}^3 \ltimes S^2$.

## 3 Tools From Group Theory

In this article we will consider convection-diffusion operators on the space of HARDI-images. We shall model the space of HARDI-images by the space of quadratic integrable functions on the coupled space of positions and orientations, i.e. $L_2(\mathbb{R}^3 \ltimes S^2)$. We will first show that such operators should be left-invariant with respect to the left-action of $SE(3)$ onto the space of HARDI-images. This left-action of the group $SE(3)$ onto $\mathbb{R}^3 \ltimes S^2$ is given by

\[ g \cdot (y, n) = (Ry + x, Rn), \quad g = (x, R) \in SE(3), x, y \in \mathbb{R}^3, n \in S^2, R \in SO(3) \]

and it induces the so-called left-regular action of the same group on the space of HARDI-images similar to the left-regular action on 3D-images (for example orientation-marginals of HARDI-images):
**Definition 1** The left-regular actions of $SE(3)$ onto $L_2(\mathbb{R}^3 \times S^2)$ respectively $L_2(\mathbb{R}^3)$ are A.E. given by

$$
(\mathcal{L}_g)_{(x,r)}(y,n) = U(g^{-1} \cdot (y,n)) = U(R^{-1}(y-x), R^{-1}n), \quad x,y \in \mathbb{R}^3, n \in S^2, U \in L_2(\mathbb{R}^3 \times S^2),
$$

$$
(\mathcal{L}_g)_{(x,r)}f(y) = f(R^{-1}(y-x)),
$$

where $g \in SE(3), y \in \mathbb{R}^3, f \in L_2(\mathbb{R}^3)$.

Intuitively, $\mathcal{L}_g(x,r)$ represents a rigid motion operator on images, whereas $\mathcal{L}_g(x,r)$ represents a rigid motion on HARDI-images.

In order to explain the importance of left-invariance of processing HARDI-images in general we need to define the following operator.

**Definition 2** We define the operator $\mathcal{M}$ which maps a HARDI-image $U : \mathbb{R}^3 \times S^2 \rightarrow \mathbb{R}^+$ to its orientation marginal $\mathcal{M}U : \mathbb{R}^3 \rightarrow \mathbb{R}^+$ as follows (where $\sigma$ denotes the usual surface measure on $S^2$):

$$
(\mathcal{M}U)(y) = \int_{S^2} U(y,n) d\sigma(n).
$$

If $U : \mathbb{R}^3 \times S^2 \rightarrow \mathbb{R}^+$ is a probability density on positions and orientations then $\mathcal{M}U : \mathbb{R}^3 \rightarrow \mathbb{R}^+$ denotes the corresponding probability density on position space only.

The marginal gives us an ordinary 3D image that is a “simplified” version of the HARDI image, containing less information on the orientational structure. This is analogous to taking the trace of a DTI-image. Now that we defined this operator which maps an HARDI-image onto its marginal we formulate the following theorem which tells us that we get a Euclidean invariant operator on the marginal of HARDI-images if the operator on the HARDI-image is left-invariant. This motivates our restriction to left-invariant operators, akin to our framework of invertible orientation scores [2, 27, 26, 28, 21, 20, 13, 16, 14, 15, 19, 18], where invertible orientation scores are complex-valued functions on $SE(2) = \mathbb{R}^2 \times S^1$, just like HARDI-images are real-valued functions on $\mathbb{R}^3 \times S^2$.

**Theorem 1** Suppose $\Phi$ is an operator on the space of HARDI-images to itself. Then the corresponding operator $\mathcal{Y}$ on the orientation marginals given by $\mathcal{Y}(\mathcal{M}(U)) = \mathcal{M}(\Phi(U))$ is Euclidean invariant if operator $\Phi$ is left-invariant, i.e.

$$
(\Phi \circ \mathcal{L}_g = \mathcal{L}_g \circ \Phi, \quad \text{for all } g \in SE(3)) \Rightarrow \mathcal{U}_g \circ \mathcal{Y} = \mathcal{Y} \circ \mathcal{U}_g, \quad \text{for all } g \in SE(3).
$$

**Proof** The result follows directly by the intertwining relation $\mathcal{U}_g \circ \mathcal{M} = \mathcal{M} \circ \mathcal{L}_g$ for all $g \in SE(3)$. Now regardless of the fact if $\Phi$ is bounded or unbounded, linear or non-linear, we have under assumption of left-invariance of $\Phi$ that

$$
\mathcal{Y} \circ \mathcal{U}_g \circ \mathcal{M} = \mathcal{Y} \circ \mathcal{M} \circ \mathcal{L}_g = \mathcal{M} \circ \Phi \circ \mathcal{L}_g = \mathcal{M} \circ \mathcal{L}_g \circ \Phi = \mathcal{U}_g \circ \mathcal{M} \circ \Phi = \mathcal{U}_g \circ \mathcal{Y} \circ \mathcal{M}. \quad \Box
$$

All useful linear operators in image processing can be written as kernel operators. Therefore, we classify all left-invariant kernel operators $\mathcal{K}$ on HARDI-images in the next subsection and we will provide important probabilistic interpretation of these left-invariant kernel operators.

**Lemma 1** Let $\mathcal{K}$ be a bounded operator from $L_2(\mathbb{R}^3 \times S^2)$ into $L_\infty(\mathbb{R}^3 \times S^2)$ then there exists an integrable kernel $k : \mathbb{R}^3 \times S^2 \times \mathbb{R}^3 \times S^2 \rightarrow \mathbb{C}$ such that $\|\mathcal{K}\|^2 = \sup_{(y,n) \in \mathbb{R}^3 \times S^2} \int_{\mathbb{R}^3 \times S^2} |k(y,n ; y',n')|^2 dy' d\sigma(n')$ and we have

$$
(\mathcal{K}U)(y,n) = \int_{\mathbb{R}^3 \times S^2} k(y,n ; y',n') U(y',n') dy' d\sigma(n'),
$$

for almost every $(y,n) \in \mathbb{R}^3 \times S^2$ and all $U \in L_2(\mathbb{R}^3 \times S^2)$. Now $\mathcal{K}_k := \mathcal{K}$ is left-invariant iff $k$ is left-invariant, i.e.

$$
\mathcal{L}_g \circ \mathcal{K}_k = \mathcal{K}_k \circ \mathcal{L}_g \iff \forall g \in SE(3) \forall y,y',n,n' \in S^2 : k(g \cdot (y,n) ; g \cdot (y',n')) = k(y,n ; y',n').
$$
Proof The first part of the Theorem follows by the general Dunford-Pettis Theorem [7, p.113-114]. With respect to the left-invariance we note that on the one hand we have

$$\left( K_{h} \mathcal{L}_{g} U \right)(y, n) = \int \int k(y, n; y', n') U(R^{-1}(y' - x, R^{-1}n')) dy' \, dn'$$

$$= \int \int k(y, n; R y + x, R n') U(y', n') dy' \, dn'$$

$$= \int \int k(y, n; g \cdot (y', n')) U(y', n') dy' \, dn'$$

whereas on the other hand $$(\mathcal{L}_{g} K_{h}) (y, n) = \int \int k(g^{-1}(y, n); y', n') U(y', n') dy' \, dn'$$, for all $g \in SE(3)$, $U \in \mathbb{L}_{2}(\mathbb{R}^{3} \times S^{2})$, $(x, n) \in \mathbb{R}^{3} \times S^{2}$. Now $SE(3)$ acts transitively on $\mathbb{R}^{3} \times S^{2}$ from which the result directly follows. □

From the invariance property (8) we deduce that

$$k(y, n; y', n') = k((R_{e_{x}, \gamma} R_{e_{y}, \beta})^{T}(y - y'), (R_{e_{x}, \gamma} R_{e_{y}, \beta})^{T}n(\beta, \gamma), 0, e_{z}) ,$$

and consequently we obtain the following result:

Corollary 1 If we use the well-known Euler-angle parametrization of SO(3), we have $SO(3)/SO(2) \equiv S^{2}$ with the isomorphism $R_{e_{x}, \gamma} R_{e_{y}, \beta} \rightarrow n(\beta, \gamma) = (\sin \beta \cos \gamma, \cos \beta \sin \gamma, \cos \beta)^{T} = R_{e_{x}, \gamma} R_{e_{y}, \beta} e_{z}$. Then to each positive left-invariant kernel $k : \mathbb{R}^{3} \times \mathbb{S}^{2} \times \mathbb{R}^{3} \times \mathbb{S}^{2} \rightarrow \mathbb{R}^{+}$ with $\int_{\mathbb{S}^{2}} k(\theta, e_{z}; y, n) dy d\sigma(n) = 1$ we can associate a unique probability density $p : \mathbb{R}^{3} \times S^{2} \rightarrow \mathbb{R}^{+}$ with the invariance property

$$p(y, n) = p(R_{e_{x}, \alpha} y, R_{e_{x}, \alpha} n), \quad \text{for all } \alpha \in [0, 2\pi),$$

such that

$$k(y, n(\beta, \gamma); y', n'(\beta', \gamma')) = p((R_{e_{x}, \gamma} R_{e_{y}, \beta})^{T}(y - y'), (R_{e_{x}, \gamma} R_{e_{y}, \beta})^{T}n(\beta, \gamma))$$

with $p(y, n) = k(y, n; 0, e_{z})$. We can briefly rewrite [25, eq. 7.59] and (7), coordinate-independently, as

$$K_{k} U(y, n) = p *_{S^{2} \times S^{2}} U(y, n) = \int_{S^{2}} p(R_{\alpha}^{T}(y - y'), R_{\alpha}^{T}n) U(y', n') d\sigma(n') dy',$$

where $\sigma$ denotes the surface measure on the sphere and where $R_{\alpha}$ is any rotation such that $n' = R_{\alpha} e_{z}$.

By the invariance property (9), the convolution (10) on $\mathbb{R}^{3} \times S^{2}$ may be written as a (full) $SE(3)$-convolution. An $SE(3)$ convolution [8] of two functions $\tilde{p} : SE(3) \rightarrow \mathbb{R}$, $\tilde{U} : SE(3) \rightarrow \mathbb{R}$ is given by:

$$\tilde{p} *_{SE(3)} \tilde{U}(g) = \int_{SE(3)} \tilde{p}(h^{-1}g) \tilde{U}(h) d\mu_{SE(3)}(h) ,$$

where Haar-measure $d\mu_{SE(3)}(x, R) = dx \, d\mu_{SO(3)}(R)$ with $d\mu_{SO(3)}(R_{e_{x}, \gamma} R_{e_{y}, \beta} R_{e_{z}, \alpha}) = \sin \beta d\alpha d\beta d\gamma$. It is easily verified that (9) implies that if we set $\tilde{p}(x, R) := p(x, R e_{z})$ and $\tilde{U}(x, R) := U(x, R e_{z})$ the following identity holds:

$$(\tilde{p} *_{SE(3)} \tilde{U})(x, R) = 2\pi (\tilde{p} *_{S^{2} \times S^{2}} U)(x, R e_{z}) .$$

Later on in this article (in Subsection 4.2 and Subsection 4.3) we will relate scale spaces on HARDI-data and first order Tikhonov regularization on HARDI-data to Markov processes. But in order to provide a road map of how the group-convolutions will appear in the more technical remainder of this article we provide some preliminary explanations on probabilistic interpretation of $\mathbb{R}^{3} \times S^{2}$-convolutions.

In particular we will restrict ourselves to conditional probabilities where $p(y, n) = p_{t}(y, n)$ represents the probability density of finding an oriented random walker at position $y$ with orientation $n$ at time $t > 0$, given that it started at
(0, e_z) at time \( t = 0 \). In such case the probabilistic interpretation of the kernel operator is as follows. The function \((y, n) \mapsto (K_k U)(y, n) = (p_t \ast_{R^3 \times S^2} U)(y, n)\) represents the probability density of finding some oriented particle, starting from the initial distribution \( U : \mathbb{R}^3 \times S^2 \to \mathbb{R}^+ \) at time \( t = 0 \), at location \( y \in \mathbb{R}^3 \) with orientation \( n \in S^2 \) at time \( t > 0 \). Furthermore, in a Markov process traveling time is memoryless, so in such process traveling time is negatively exponentially distributed \( P(T = t) = e^{-\lambda t} \) with expectation \( E(T) = \frac{1}{\lambda} \). Consequently, the probability density \( p^\lambda \) of finding an oriented random walker starting from \((0, e_z)\) at time \( t = 0 \), regardless its traveling time is given by

\[
p^\lambda(y, n) = \int_0^\infty p_t(y, n) P(T = t) dt = \lambda \int_0^\infty p_t(y, n) e^{-\lambda t} dt
\]

Summarizing, we can always take Laplace-transform with respect to time to go from transition densities \( P_t \) to unconditional probability densities \( P^\lambda \). The same holds for the probability density \( P^\lambda_y \) of finding an oriented particle at location \( y \in \mathbb{R}^3 \) with orientation \( n \in S^2 \) starting from initial distribution \( U \) (i.e. the HARDI-data) regardless the traveling time, since

\[
P^\lambda_y(y, n) = \lambda \int_0^\infty e^{-\lambda t} (p_t \ast_{R^3 \times S^2} U)(y, n) dt = \left( \left( \lambda \int_0^\infty e^{-\lambda t} p_t dt \right) \ast_{R^3 \times S^2} U \right)(y, n) = (p^\lambda \ast_{R^3 \times S^2} U)(y, n).
\]

Intuitively, this follows by superposition, left-invariance and \( p^\lambda_{U=\delta_0} = \lambda \ast_{R^3 \times S^2} \delta_0 = p^\lambda \).

### 3.1 Relation of the Method Proposed by Barmpoutis et al. to \( \mathbb{R}^3 \times S^2 \)-convolution

In [6] the authors propose\(^2\) the following practical decomposition for the kernel \( k \):

\[
k^{t, \kappa}_d(y, n; y', n') = \frac{1}{4\pi} k^t_{\text{dist}}(||y - y'||) k^\kappa_{\text{orient}}(n \cdot n') k^\kappa_{\text{fiber}} \left( \frac{1}{||y - y'||} n \cdot (y - y') \right),
\]

where \( k^t_{\text{dist}}(||y - y'||) = \frac{1}{(4\pi t)^2} e^{-\frac{||y - y'||^2}{4t}} \) denotes the Gaussian on \( \mathbb{R}^3 \) and where

\[
k^\kappa_{\text{orient}}(\cos \phi) = k^\kappa_{\text{fiber}}(\cos \phi) = \frac{e^{\kappa \cos(i\phi)}}{2\pi J_0(i\kappa)}
\]

with \( \phi \in (-\pi, \pi] \) angle between respectively \( n \) and \( n' \) between \( n \) and \( y - y' \), which denotes the von Mises distribution on the circle, which is indeed positive and \( \int_{-\pi}^{\pi} \frac{e^{\kappa \cos(x)}}{2\pi J_0(i\kappa)} dx = 1 \). The decomposition (14) automatically implies that the corresponding kernel operator \( K_k \) is left-invariant, regardless the choice of \( k_{\text{dist}}, k^\kappa_{\text{orient}}, k^\kappa_{\text{fiber}} \) since

\[
k^\kappa_{\text{dist}}(||R^{-1}(y - x) - R^{-1}(y' - x)||) k^\kappa_{\text{orient}}(R^{-1}n \cdot R^{-1}n') k^\kappa_{\text{fiber}}(\frac{1}{||R^{-1}(y - x) - R^{-1}(y' - x)||} (R^{-1}n') \cdot (R^{-1}n - (y' - x)))
\]

\[
= k^\kappa_{\text{dist}}(||y - y'||) k^\kappa_{\text{orient}}(n \cdot n') k^\kappa_{\text{fiber}} \left( \frac{1}{||y - y'||} n \cdot (y - y') \right) \iff
\]

\[
k^{t, \kappa}(g^{-1}(y, n); g^{-1}(y', n')) = k^{t, \kappa}(y, n; y', n'), \quad \text{for all } g = (R, x) \in SE(3).
\]

The corresponding probability density (which does satisfy (9))

\[
p(t, \kappa)(y, n) = \frac{1}{4\pi} k^t_{\text{dist}}(||y||) k^\kappa_{\text{orient}}(e_z \cdot n) k^\kappa_{\text{fiber}} (||y||^{-1} n \cdot y), \quad y \neq 0,
\]

should be interpreted as a probability density of finding a oriented particle at position \( y \in \mathbb{R}^3 \) with orientation \( n \in S^2 \) given that it started at location \( 0 \) with orientation \( e_z \). The practical rationale behind the decomposition (14), is that two neighboring local orientations \((y, n) \in \mathbb{R}^3 \times S^2 \) and \((y', n') \in \mathbb{R}^3 \times S^2 \) are supposed to strengthen each other if

\(^2\)We used slightly different conventions as in the original paper to ensure \( L_1 \)-normalizations in (14).
Furthermore the decomposition allows us to reduce computation time by: This motivates our quest (in Section 6) for appropriate diffusion kernels (related to Brownian motion on $\mathbb{R}^3 \times S^2$ by iteration (in the right-image the second glyph on the $z$-axis has a larger radius than the glyph at 0). The effective shape of the convolution kernel is destroyed by iteration, as the kernel (15) does not satisfy the semi-group property. This motivates our quest (in Section 6) for appropriate diffusion kernels (related to Brownian motion on $\mathbb{R}^3 \times S^2$) on $\mathbb{R}^3 \times S^2$ that do satisfy the semigroup property $p^D_t \ast_{\mathbb{R}^3 \times S^2} p^D_s = p^D_{t+s}$, involving only one time-parameter.

the distance between $y$ and $y'$ is close (represented by the first kernel $k_{dist}$), if the orientations are similar (represented by $k_{\text{orient}}$), if the orientation $n$ at position $y$ is nicely aligned according to some a priori fibre model with the local orientation $(y', n')$, i.e. if the orientation of $\|y - y'\|^{-1}(y - y')$ is close to the orientation $n$ (represented by $k_{\text{fiber}}$). Furthermore the decomposition allows us to reduce computation time by:

$$\left(\mathcal{K}_{t,x} \ast U\right)(y, n) = (p_{t,x} \ast_{\mathbb{R}^3 \times S^2} U)(y, n)$$

$$= \frac{1}{\sigma^2} \int_{\mathbb{R}^3} k_{\text{dist}}^{3d}(\|y - y'\|)k_{\text{fiber}}^{\|y - y'\|^{-1}n \cdot (y - y')} \left(\int_{S^2} U(y', n')k_{\text{orient}}^{n \cdot n'}d\sigma(n')\right) dy'$$.  

Despite the fact that the practical kernel (14) gives rise to a reasonable connectivity measure between two local orientations $(y, n)$ and $(y', n') \in \mathbb{R}^3 \times S^2$ and that the associated kernel operator has the right covariance properties, the associated kernel operator is not related to left-invariant diffusion and/or Tikhonov regularization on $\mathbb{R}^3 \times S^2$, as was aimed for in the paper [6]. In this inspiring pioneering paper the authors consider an usual position dependent energy and deal with the Euler-Lagrange equations in an usual way (in particular [6, eq. 7]). The kernel (15) involves two separate time parameters $t, \kappa$ and the probability kernels (14) are not related to Brownian motions and/or Markov-processes on $\mathbb{R}^3 \times S^2$, since they do not satisfy the semi-group property (which happens to be also one of the axioms [3, 12] for diffusion/scale spaces on images). A disadvantage as we will explain next, however, is that the kernel is not entirely suited for iteration unless combined with non-linear operators such as non-linear grey-value transformations. The function $y \mapsto \|y\|^{-1}y \cdot n$ within (15) is discontinuous at the origin, as it depends along which line 0 is approached. If the origin is approached by a straight-line along $n$ the limit-value is 1 and this seems to be a reasonable choice for evaluating the kernel at $y = 0$ (a situation which regularly occurs in the convolution). By Cauchy-Schwarz the finite maximum of the kernel is obtained at $y = 0$ (and $n = e_z$). Since the kernel is single-sided and does not have a singularity at the origin convolution with itself will allow the maximum of the effective kernel to run away\footnote{Set $a := \frac{1}{\pi^2}[\ldots, 0, 1, 0, 0, \ldots]$, then for every $n \in \mathbb{N}$ the sequence $a_n := a \ast (n-1) a \in \ell_1(\mathbb{Z})$ has $n + 1$ non-zero coefficients: $a_k = (1 + \alpha)^{-n}a_k(\binom{n}{k})$, $k = 0, \ldots, n$. So the position of the maximum of $a_n$ increases with $n$ (if $\alpha = 1$ it takes place at $k = \lfloor \frac{n}{2} \rfloor$).} from its center, similar to the following periodic convolution on a finite grid $\{0, 0, 0, 0, 1, \alpha, 0, 0\} \ast \{0, 0, 0, 0, 1, \alpha, 0, 0\} = \{0, 0, 0, 0, 1, 2\alpha, \alpha^2, 0\}$ with $\alpha \leq 1$. See Figure 5, where we numerically $\mathbb{R}^3 \times S^2$-convolved the kernel (14) with itself. However, if the kernel would have satisfied the semigroup-property this problem would not have occurred.
For example the single-sided exact Green’s function of Mumford’s direction process [21] (and its approximations [42, 16, 21]) on \( SE(2) = \mathbb{R}^2 \times S^1 \) has a natural singularity at the origin.

Before we consider scale spaces on HARDI-data whose solutions are given by \( \mathbb{R}^3 \times S^2 \)-convolution (10) with the corresponding Green’s functions (which do satisfy the semigroup-property) we provide, for the sake of clarity, a quick review on scale spaces of periodic signals from a group theoretical PDE-point of view.

### 3.2 Introductory Example: Reviewing Scale Spaces/Tikhonov regularization on the Circle

The Gaussian scale space equation and corresponding resolvent equation (i.e. the solution of Tikhonov regularization) on a circle \( T = \{ e^{i\theta} \mid \theta \in [0, 2\pi) \} \equiv S^1 \) with group product \( e^{i\theta}e^{i\theta'} = e^{i(\theta+\theta')} \), read

\[
\begin{align*}
\partial_t u(\theta, s) &= D_{11} \partial_{\theta}^2 u(\theta, t), \\
u(0, t) &= u(2\pi, t) \quad \text{and} \quad u(\theta, 0) = f(\theta),
\end{align*}
\]

and \( p_\gamma(\theta) = \gamma(D_{11} \partial_{\theta}^2 - \gamma I)^{-1} f(\theta) \), with \( \theta \in [0, 2\pi) \) and \( D_{11} > 0 \) fixed, where we note that the function \( \theta \to p_\gamma(\theta) = \gamma \int_0^\infty u(\theta, t)e^{-\gamma s}dt \) is the minimizer of the Tikhonov-energy

\[
E(p_\gamma) := \int_0^{2\pi} \gamma |p_\gamma(\theta) - f(\theta)|^2 + D_{11} |p_\gamma'(\theta)|^2 d\theta
\]

under the periodicity condition \( p_\gamma(0) = p_\gamma(2\pi) \). By left-invariance the solutions are given by \( T \)-convolution (or “periodic convolution”) with their Green’s function (or “impuls-response”), say \( \gamma \). Recall that the relation between Tikhonov regularization and scale space theory is given by Laplace-transform with respect to time, cf. [24], and we thereby have the following relation between the two regularizations:

\[
u(\cdot, t) = G_t \ast_T f \quad \text{and} \quad p_\gamma = R^{D_{11}}_{\gamma} \ast_T f, \quad \text{with} \; R^{D_{11}}_{\gamma} = \gamma \int_0^\infty G^{D_{11}}_t e^{-\gamma t}dt,
\]

where the \( T \)-convolution is given by \( f \ast_T g(e^{i\theta}) = \int_0^{\pi} f(e^{i(\theta-\theta')})g(e^{i\theta'})d\theta' \). Now orthogonal eigenfunctions of the diffusion process correspond to eigenfunctions of the generator \( (D_{11} \partial_{\theta}^2 - \gamma I)^2 \) and they are given by \( \eta_n(\theta) = \frac{\sqrt{2\pi}}{\sqrt{n(n-1)}}, \) so that

\[
\begin{align*}
u(\theta, t) &= \sum_{n \in \mathbb{Z}} (\eta_n, f)_{L_2(T)} \eta_n(\theta)e^{-n^2D_{11}t}, \quad G^{D_{11}}_{s}\ast f(\theta) = \sum_{n \in \mathbb{Z}} \eta_n(\theta)\eta_n(0)e^{-n^2D_{11}t}, \\
p_\gamma(\theta) &= \sum_{n \in \mathbb{Z}} (\eta_n, f)_{L_2(T)} \eta_n(\theta)\frac{\gamma}{n^2D_{11}+\gamma}, \quad R^{D_{11}}_\gamma(\theta) = \sum_{n \in \mathbb{Z}} \eta_n(\theta)\eta_n(0)\frac{\gamma}{n^2D_{11}+\gamma}.
\end{align*}
\]

A well-known drawback of such an approach is that the series do not converge quickly if \( t > 0 \) resp. \( \gamma > 0 \) are small. In such case one of course prefers a spatial implementation over a Fourier implementation, where one unfolds the circle and calculate modulo \( 2\pi \)-shifts afterwards, i.e.

\[
\begin{align*}
u(\theta, s) &= (G^{D_{11}}_t \ast f)(\theta), \quad \text{where} \; G^{D_{11}}_t(\theta) = \sum_{n \in \mathbb{Z}} G^{D_{11}, \infty}_t(\theta - 2\pi n),
\end{align*}
\]

where the Green’s functions for diffusion and Tikhonov regularization on \( \mathbb{R} \) are \( G^{D_{11}, \infty}_t(\theta) = (4\pi t)^{-1/2}e^{-\frac{\theta^2}{4t}} \) and \( R^{D_{11}, \infty}_\gamma(\theta) = \frac{\sqrt{\gamma}}{2}e^{-\sqrt{\gamma}|\theta|} \). Again the latter formula follows by Laplace transform of the first. The sums in (20) can be computed explicitly, yielding \( G^{D_{11}}_t(\theta) = \frac{1}{2\sqrt{\pi}} \theta_3 \left( \frac{\theta}{2\sqrt{\pi}t}, e^{-1} \right), \) where \( \theta_3 \) is a theta-function of the 3rd kind.

The unique solution \( u(\theta, t) \) can (at least formally, via Fourier transform on \( T \)) be written as

\[
u(\theta, t) = (e^{i\Delta_{\gamma}} f)(\theta) = (G^{D_{11}}_{t} \ast_T f)(\theta) \quad \text{with} \; \Delta_{\gamma} = (\partial_{\theta})^2
\]

and by \( e^{s \Delta_{\gamma}} e^{t \Delta_{\gamma}} = e^{(s+t) \Delta_{\gamma}} \) the heat-kernel on \( T \) satisfies the for (iterations) important semi-group property:

\[
G^{D_{11}}_{s} \ast_T G^{D_{11}}_{t} = G^{D_{11}}_{s+t}, \quad \text{for all} \; s, t > 0.
\]
In this basic example the generator of a Gaussian scale space on the torus is given by $D_{11}\partial^2_{\theta}$. Just like the solution operator $(D_{11}\partial^2_{\theta} - \lambda I)^{-1}$ of Tikhonov regularization, it is left-invariant. This means that these operators commute with the left-regular representation on $\mathbb{T}$ given by $L_{e^{i\theta'}}f(e^{i\theta}) = f(e^{i(\theta'-\theta)})$, for all $f \in C_c(\mathbb{T})$, i.e. an ordinary (right) shift of complex-valued functions on $\mathbb{T}$, since $\mathbb{T}$ is commutative. Due to this left-invariance, the solutions (18) of a Gaussian Scale Space and Tikhonov regularization are given by $\mathbb{T}$-convolution. This (periodic) convolution is the naturally related to our convolution operators (11), as the only difference is the replacement of the group product and the left-invariant Haar measure. Now in order to generalize scale space representations of functions on a torus to scale space representations of HARDI-data, i.e. functions on $\mathbb{R}^3 \times S^2$ embedded in $SE(3) = \mathbb{R}^3 \times SO(3)$, we simply have to replace the left-invariant vector field $\partial_\theta$ on $\mathbb{T}$ by the left-invariant vector fields on $SE(3)$ (or rather $\mathbb{R}^3 \times S^2$) in the quadratic form which generates the scale space on the group, [14]. In the next section we will compute the left-invariant vector fields on $SE(3)$.

3.3 Left-invariant Vector Fields on $SE(3)$ and their Dual Elements

We will use the following basis for the tangent space $T_e(SE(3))$ at the unity element $e = (0, I) \in SE(3)$:

$$A_1 = \partial_x, A_2 = \partial_y, A_3 = \partial_z, A_4 = \partial_x, A_5 = \partial_\beta, A_6 = \partial_\alpha,$$

where we stress that at the unity element $R = I$, we have $\beta = 0$ and here the tangent vectors $\partial_\beta$ and $\partial_\alpha$ are not defined, which requires a description of the tangent vectors on the $SO(3)$-part by means of the second chart.

The tangent space at the unity element $e = (0, 0, 0, R = I), T_e(SE(3))$, is a 3D Lie algebra equipped with Lie product

$$[A, B] = \lim_{t \to 0} t^{-2}(a(t) b(t)(a(t))^{-1}(b(t))^{-1} - e),$$

where $t \to a(t)$ resp. $t \to b(t)$ are any smooth curves in $G$ with $a(0) = b(0) = e$ and $a'(0) = A$ and $b'(0) = B$, for explanation on the formula (21) which holds for general matrix Lie groups, see [17, App.G]. Define $\{A_1, A_2, A_3\} := \{e_\theta, e_x, e_y\}$. Then $\{A_1, A_2, A_3\}$ form a basis of $T_e(SE(2))$ and their Lie-products are

$$[A_i, A_j] = \sum_{k=1}^{6} c^{k}_{ij} A_k,$$

where the non-zero structure constants for all three isomorphic Lie-algebras are given by

$$-c^{k}_{ij} = c^{k}_{ij} = \begin{cases} \text{sgn perm}\{i-3, j-3, k-3\} & \text{if } i, j, k \geq 4, i \neq j \neq k, \\
\text{sgn perm}\{i, j-3, k\} & \text{if } i \leq 3, j \geq 4, i \neq j \neq k, \end{cases}$$

The corresponding left-invariant vector fields $\{A_i\}_{i=1}^{6}$ are obtained by the push-forward of the left-multiplication $L_{g} h = gh$ by $A_i|_g \phi = (L_g) A_i \phi = A_i(\phi \circ L_g)$ (for all smooth $\phi : \Omega_g \to \mathbb{R}$ which are locally defined on some neighborhood $\Omega_g$ of $g$) and they can be obtained by the derivative of the right-regular representation:

$$A_i|_g \phi = d\mathcal{R}(A_i)\phi(g) = \lim_{h \to 0} \frac{\phi(g e^{h A_i}) - \phi(g)}{h}.$$

Expressed in the first coordinate chart (1) this renders for the left-invariant derivatives at position $g = (x, y, z, R_{x, y, z}, R_{\gamma, \beta, \alpha}) \in SE(3)$ (see also [8, Section 9.10])

$$A_1 = \cos \alpha \cos \beta \cos \gamma - \sin \alpha \sin \gamma \partial_x + \sin \alpha \cos \gamma \partial_y + \cos \alpha \sin \beta \partial_z, $$
$$A_2 = \sin \alpha \cos \beta \cos \gamma - \cos \alpha \sin \gamma \partial_x + \cos \alpha \cos \gamma \sin \beta \partial_y + \sin \alpha \sin \beta \partial_z, $$
$$A_3 = \sin \beta \cos \gamma \partial_x + \sin \gamma \partial_y + \cos \beta \partial_z,$$
$$A_4 = \sin \alpha \cot \beta \partial_x + \sin \alpha \partial_y - \cos \alpha \partial_z,$$
$$A_5 = -\sin \alpha \cot \beta \partial_x + \cos \alpha \partial_y + \sin \alpha \partial_z,$$
$$A_6 = \partial_\alpha.$$
for $\beta \neq 0$ and $\beta \neq \pi$. The explicit formula of the left-invariant vector fields (which are well-defined in north- and south-pole) in the second chart (4) are:

\[
\begin{align*}
\mathcal{A}_1 &= \cos \tilde{\alpha} \cos \tilde{\beta} \partial_x + (\cos \tilde{\gamma} \sin \tilde{\alpha} + \cos \tilde{\alpha} \sin \tilde{\beta} \sin \tilde{\gamma}) \partial_y \\
\mathcal{A}_2 &= -\sin \tilde{\alpha} \cos \tilde{\beta} \partial_x + (\cos \tilde{\alpha} \cos \tilde{\gamma} - \sin \tilde{\alpha} \sin \tilde{\beta} \sin \tilde{\gamma}) \partial_y \\
\mathcal{A}_3 &= \sin \tilde{\beta} \partial_x - \cos \tilde{\beta} \sin \tilde{\gamma} \partial_y + \cos \tilde{\alpha} \cos \tilde{\gamma} \partial_z, \\
\mathcal{A}_4 &= -\cos \tilde{\alpha} \tan \tilde{\beta} \partial_x + \sin \tilde{\alpha} \partial_y + \frac{\cos \tilde{\alpha}}{\cos \tilde{\beta}} \partial_z, \\
\mathcal{A}_5 &= \sin \tilde{\alpha} \tan \tilde{\beta} \partial_x + \cos \tilde{\alpha} \partial_y - \frac{\sin \tilde{\alpha}}{\cos \tilde{\beta}} \partial_z,
\end{align*}
\]

for $\tilde{\beta} \neq \frac{\pi}{2}$ and $\tilde{\beta} \neq -\frac{\pi}{2}$. Note that $dR$ is a Lie-algebra isomorphism, i.e.

\[
[A_i, A_j] = \sum_{k=1}^{6} c_{ij}^k A_k \Leftrightarrow [dR(A_i), dR(A_j)] = \sum_{k=1}^{6} c_{ij}^k dR(A_k) \Leftrightarrow [A_i, A_j] = A_i A_j - A_j A_i = \sum_{k=1}^{6} c_{ij}^k A_k.
\]

These vector fields form a local moving coordinate frame of reference on $SE(3)$, the corresponding dual frame \{d$\mathcal{A}^1, \ldots, d\mathcal{A}^6$\} in $(T(SE(3)))^*$ is defined by

\[
\langle d\mathcal{A}^i, A_j \rangle := d\mathcal{A}^i(A_j) = \delta^i_j, i, j = 1, \ldots, 6,
\]

where $\delta^i_j = 1$ if $i = j$ and zero else. A brief computation yields the following dual frame (in both coordinate charts):

\[
\begin{pmatrix}
d\mathcal{A}^1 \\
d\mathcal{A}^2 \\
d\mathcal{A}^3 \\
d\mathcal{A}^4 \\
d\mathcal{A}^5 \\
d\mathcal{A}^6
\end{pmatrix} = \begin{pmatrix}
(R_{e_\gamma} R_{e_\beta} R_{e_\alpha})^T & 0 \\
0 & M_{\beta, \alpha}
\end{pmatrix} \begin{pmatrix}
\mathrm{d}x \\
\mathrm{d}y \\
\mathrm{d}z \\
\mathrm{d}\alpha \\
\mathrm{d}\beta \\
\mathrm{d}\gamma
\end{pmatrix}
\]

where the $3 \times 3$-zero matrix is denoted by $0$ and where the $3 \times 3$-matrices $M_{\beta, \gamma}$, $M_{\beta, \alpha}$ are given by

\[
M_{\beta, \alpha} = \begin{pmatrix}
0 & \sin \alpha & -\cos \alpha \sin \beta \\
0 & \cos \alpha & \sin \alpha \sin \beta \\
1 & 0 & \cos \beta
\end{pmatrix}, \quad M_{\beta, \alpha} = \begin{pmatrix}
-\cos \tilde{\alpha} \tan \tilde{\beta} & \sin \tilde{\alpha} & \frac{\cos \tilde{\alpha}}{\cos \tilde{\beta}} \\
\sin \tilde{\alpha} \tan \tilde{\beta} & \cos \tilde{\alpha} & -\frac{\sin \tilde{\alpha}}{\cos \tilde{\beta}} \\
1 & 0 & 0
\end{pmatrix}^{-T}.
\]

Finally, we note that by linearity the $i$-th dual vector filters out the $i$-th component of a vector field $v^j A_j$

\[
\langle d\mathcal{A}^i, \sum_{j=1}^{6} v^j A_j \rangle = v^i, \quad \text{for all } i, j = 1, \ldots, 6.
\]

4. Left-Invariant Diffusions on $SE(3) = \mathbb{R}^3 \rtimes SO(3)$ and $\mathbb{R}^3 \rtimes S^2$

In order to apply our general theory on diffusions on Lie groups, [14], to suitable (convection-)diffusions on HARDI-images, we first extend all functions $U : \mathbb{R}^2 \rtimes S^3 \rightarrow \mathbb{R}$ to functions $\tilde{U} : \mathbb{R}^2 \rtimes SO(3) \rightarrow \mathbb{R}$ in the natural way

\[
\tilde{U}(x, R) = U(x, R e_\gamma) \text{ or in Euler angles: } \tilde{U}(x, R_{e_\gamma} R_{e_\beta} R_{e_\alpha}) = U(x, n(\beta, \gamma)).
\]

**Definition 3** We will call $\tilde{U} : \mathbb{R}^3 \rtimes SO(3) \rightarrow \mathbb{R}$, given by (28), the HARDI-orientation score corresponding to HARDI-image $U : \mathbb{R}^3 \rtimes S^2 \rightarrow \mathbb{R}$.
Here we note that the function $\tilde{U}$ in general is not equal to the wavelet transform of some image $f : \mathbb{R}^2 \to \mathbb{R}$, in contrast to our previous works on invertible orientations of 2D-images, [15], [25], [2], [21], [18], [19] and invertible orientation scores of 3D-images, [20], [15].

Then we follow our general construction of scale space representations $W$ of functions $U$ (could be an image, or a score/wavelet transform of an image) defined on Lie groups, [14], where we consider the special case $G = SE(3)$:

$$\begin{align*}
\frac{\partial}{\partial t} W(g, t) &= Q^{D, a}(A_1, A_2, \ldots, A_6) W(g, t), \\
\lim_{t \downarrow 0} W(g, t) &= \tilde{U}(g).
\end{align*}$$

(29)

which is generated by a quadratic form on the left-invariant vector fields:

$$Q^{D, a}(A_1, A_2, \ldots, A_n) = \sum_{i=1}^{6} a_i A_i + \sum_{j=1}^{6} A_i D_{ij} A_j$$

(30)

Now the Hörmander requirement, [31], on the symmetric $^4 D = [D_{ij}] \in \mathbb{R}^{6 \times 6}$, $D \geq 0$ and $a$, which guarantees smooth non-singular scale spaces, for $SE(3)$ tells us that $D$ need not be strictly positive definite. The Hörmander requirement is that all included generators together with their commutators should span the full tangent space$^3$. To this end for diagonal $D$ one should consider the set

$$\mathcal{S} = \{ i \in \{1, \ldots, 6\} \mid D_{ii} \neq 0 \vee a_i \neq 0 \},$$

now if for example 1 is not in here then 3 and 5 must be in $\mathcal{S}$, or if 4 is not in $\mathcal{S}$ then 5 and 6 should be in $\mathcal{S}$. Following the general theory [14] we note that if the Hörmander condition is satisfied the solutions of the linear diffusions (i.e. $D, a$ are constant) are given by $SE(3)$-convolution with a smooth probability kernel $p_t^{D, a} : SE(3) \to \mathbb{R}^+$ such that

$$W(g, t) = (p_t^{D, a} *_{SE(3)} \tilde{U})(g) = \int_{SE(3)} p_t^{D, a}(h^{-1}g)\tilde{U}(h) d\mu_{SE(3)}(h),$$

$$\lim_{t \downarrow 0} p_t^{D, a} *_{SE(3)} \tilde{U} = \tilde{U},$$

with $p_t^{D, a} > 0$ and $\int_{SE(3)} p_t^{D, a}(g) d\mu_{SE(3)}(g) = 1.$

where the limit is taken in $L_2(SE(3))$-sense.

We stress that the left-invariant diffusion on the group (in our case $SE(3)$) also gives rise to left-invariant scale spaces on homogeneous spaces within the group, in our case of $\mathbb{R}^3 \times S^2 = SE(3) / (\{0\} \times SO(2))$. There are however, two important issues to be taken into account.

1. If we apply the diffusions directly to HARDI-orientation scores we can as well delete the last direction in our diffusions because clearly $A_6 = \partial_\alpha$ vanishes on functions which are not dependent on $\alpha$, i.e. $\partial_\alpha \tilde{U} = 0$.

2. In order to naturally relate the (convection-)diffusions on HARDI-orientation scores, to (convection-)diffusions on HARDI-images we have to make sure that the evolution equations are well defined on the cosets $SO(3) / SO(2)$, meaning that they do not depend on the choice of representant in the classes.

Next we will formalize the second condition on diffusions on HARDI-orientation scores more explicitly. A movement along the equivalence classes $SO(3) / SO(2)$ is done by right multiplication with the subgroup $\text{Stab}(e_3) \equiv SO(2)$, it means that our diffusion operator $\Phi_t$ which is the transform that maps the HARDI-orientation score $\tilde{U} : \mathbb{R}^3 \times SO(3) \to \mathbb{R}^+$ to a diffused HARDI-orientation score $\Phi_t(\tilde{U}) = e^{tQ^{D, a}} \tilde{U}$, with stopping time $t > 0$, should satisfy

$$ (\Phi_t \circ R_h)(\tilde{U}) = \Phi_t(\tilde{U}) \quad \text{for all } h \in \text{Stab}(e_3) \equiv SO(2),$$

(31)

$^4$Note if $D$ would have an antisymmetric part we could move it to the convection part by means of the commutator relations (22).

$^5$By left-invariance this means that one only has to consider the tangent space at the unity element.
Analogously, for adaptive non-linear diffusions, that is \( dR_i = 0 \), where \( A = (A_1, \ldots, A_6)^T \) and where

\[
Z_\alpha = \begin{pmatrix}
\cos \alpha & -\sin \alpha & 0 & 0 & 0 & 0 \\
\sin \alpha & \cos \alpha & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & \cos \alpha & -\sin \alpha & 0 \\
0 & 0 & 0 & \sin \alpha & \cos \alpha & 0 \\
0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix} = R_{e_{\alpha}} \oplus R_{\alpha} \oplus Z_\alpha \in SO(6), Z_\alpha \in SO(3).
\]

Now for constant \( D \) and \( a \) (i.e. linear diffusion on the HARDI-data) the requirement (32) simply reads

\[
Q^{D,a}(A) = Q^{D,a}(Z_\alpha A) = Q^{D,a}(Z_\alpha A)^T D Z_\alpha, a \Leftarrow Z_\alpha a \text{ and } D = Z_\alpha^T D Z_\alpha, \quad (34)
\]

which by Schur's lemma is the case if

\[
a^1 = a^2 = a^5 = 0 \text{ and } D = \text{diag}\{D_{11}, D_{11}, D_{33}, D_{44}, D_{44}\}.
\]

Analogously, for adaptive non-linear diffusions, that is \( D \) and \( a \) not constant but depending on the initial condition \( U \), i.e. \( D(U) : SE(3) \rightarrow \mathbb{R}^{3 \times 3} \), with \( (D(U))^T = D(U) > 0 \) and \( a(U) \) the requirement (32) simply reads

\[
a(U) R_{e_{\alpha}} \Rightarrow Z_\alpha^T (a(U)) \text{ and } D(R_{e_{\alpha}}) R_{\alpha} \Rightarrow Z_\alpha D(U) Z_\alpha^T.
\]

Summarizing all these results we conclude on HARDI-data whose domain equals the homogeneous space \( \mathbb{R}^3 \times S^2 \) one has the following scale space representations:

\[
\left\{ \begin{array}{l}
\partial_t W(y, n, t) = Q^{D(U), a(U)}(A_1, A_2, \ldots, A_6) W(y, n, t), \\
W(y, n, 0) = U(y, n).
\end{array} \right.
\]

with \( Q^{D(U), a(U)}(A_1, A_2, \ldots, A_6) = \sum_{i=1}^5 \left( a_i A_i + \sum_{j=1}^5 A_i D_{ij} U(A_j) \right) \), where from now on we assume that \( D(U) \) and \( a(U) \) satisfy (36). Again in the linear case where \( D(U) = D \), \( a(U) = a \) this means that we shall automatically assume (35). In this case the solutions of (37) are given by the following kernel operators on \( \mathbb{R}^3 \times S^2 \):

\[
W(y, n, t) = \left( \frac{\Delta t}{2 \pi} \right) \int_{\mathbb{R}^3} D^{a} \left( (R_{e_{\gamma'}} R_{e_{\gamma''}})^T y - y', (R_{e_{\gamma'}} R_{e_{\gamma''}})^T n \right) U(y', n(\beta', \gamma')) \, dy' \, d\sigma(n(\beta', \gamma'))
\]

where the surface measure on the sphere is given by \( d\sigma(n(\beta', \gamma')) = \sin \beta' \, d\gamma' \, d\beta' \). Now in particular in the linear case, since \( (\mathbb{R}^3, I) \) and \( (\theta, SO(3)) \) are subgroups of \( SE(3) \), we obtain the Laplace-Beltrami operators on these subgroups by means of:

\[
\Delta_{S^2} = Q^D = \text{diag}\{0, 0, 0, 0, 0, 0\}, a = 0 = (A_2)^2 + (A_3)^2 + (A_6)^2 = (\partial_\beta)^2 + \cot(\beta) \partial_\beta + \sin^{-2}(\beta) (\partial_\gamma)^2,
\]

\[
\Delta_{R^3} = Q^D = \text{diag}\{1, 1, 1, 0, 0, 0\}, a = 0 = (A_1)^2 + (A_2)^2 + (A_3)^2 = (\partial_\beta)^2 + (\partial_\gamma)^2 + (\partial_\delta)^2.
\]

Remark: Recall that in the linear case we assumed (35) to ensure (32) so that (31) holds. It is not difficult to show, [25, p.170], that this implies the required symmetry (9) on the convolution kernel.

### 4.1 Special Cases of Linear Left-invariant Diffusion on \( \mathbb{R}^3 \times S^2 \)

Now if we consider the singular case \( D = \text{diag}\{1, 1, 1, 0, 0, 0\}, a = 0 \) (not satisfying the Hörmander condition) we get the usual scale space in the position part only

\[
W(y, n, t) = (e^{tU} \cdot n)(y) = \mathcal{F}_{\mathbb{R}^3}^{-1}[\omega \mapsto e^{-\frac{t}{2}||\omega||^2} \mathcal{F}_{\mathbb{R}^3} f(\omega)](y) = (G_t * f)(y), \text{ with } G_t(y) = (4\pi t)^{-\frac{3}{2}} e^{-\frac{||y||^2}{4t}}
\]
and consequently on $\mathbb{R}^3 \times S^2$ we have the singular distributional kernel $p_t^{D,a}(y, n) = G_t(y)\delta_n(y)$, in (38).

If we consider the singular case $D = \text{diag}(0, 0, 0, 1, 1, 1)$, $a = 0$ we get the usual scale space on the sphere:

$$W(y, n; \beta, \gamma, t) = (e^{t \Delta s^2} U(y, \cdot)(x)) = e^{t \Delta s^2} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (Y_{lm}(\beta, \gamma)) e^{t l \alpha s^2} Y_{lm}(\beta, \gamma)$$

$$= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (Y_{lm}(\beta, \gamma)) e^{-t(l+1)} Y_{lm}(\beta, \gamma).$$

where we note that the well-known spherical harmonics $\{Y_{lm}\}_{l=0, \ldots, \infty}$ from an orthonormal basis of $L_2(S^2)$ and $\Delta s^2 Y_{lm} = -l(l+1) Y_{lm}$. Recall

$$Y_l^m(\beta, \gamma) = \sqrt{\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}} P_l^m(\cos \beta) e^{im\gamma} \quad l \in \mathbb{N}, m = -l, \ldots, l. \quad (39)$$

Consequently, on $\mathbb{R}^3 \times S^2$ we have the singular distributional kernel $p_t^{D,a}(y, n) = g_t(n)\delta_0(y)$, in (38), where

$$g_t(n; \beta, \gamma) = \sum_{l=0}^{\infty} (Y_{lm}(\beta, \gamma)) e^{-t(l+1)} = \sum_{l=0}^{\infty} (P_l^m(\cos \beta)) \frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!} e^{-t(l+1)}.$$

Note that in the two cases mentioned above diffusion takes place either only along the spatial part or only along the angular part, which is not desirable as one wants to include line-models which exploit a natural coupling between position and orientation. Such a coupling is naturally included in a smooth way as long as the Hörmander’s condition is satisfied. In the two previous examples, the Hörmander condition is violated since both the span of $\{A_1, A_2, A_3\}$ and the span of $\{A_4, A_5, A_6\}$ are closed Lie-algebra’s, i.e. all commutators are again contained in the same 3-dimensional subspace of the 6-dimensional tangent space.

Therefore we will consider more elaborate simple left-invariant convection, diffusions on $SE(3)$ with natural coupling between position and orientation. To explain what we mean with natural coupling we shall need the next definitions.

**Definition 4** A curve $\gamma : \mathbb{R}^+ \rightarrow \mathbb{R}^3 \times S^2$ given by $s \mapsto \gamma(s) = (y(s), n(s))$ is called horizontal if $n(s) = \frac{\langle y(s) \rangle}{\|y(s)\|} \frac{1}{|y(s)|} y(s)$. A tangent vector to a horizontal curve is called a horizontal tangent vector. A vector field $\mathcal{A}$ on $\mathbb{R}^3 \times S^2$ is horizontal if for all $(y, n) \in \mathbb{R}^3 \times S^2$ the tangent vector $\mathcal{A}(y, n)$ is horizontal. The horizontal part $\mathcal{H}_g$ of each tangent space is the vector-subspace of $T_g(SE(3))$ consisting of horizontal vector fields. Horizontal diffusion is diffusion which only takes place along horizontal curves.

It is not difficult to see that the horizontal part $\mathcal{H}_g$ of each tangent space $T_g(SE(3))$ is spanned by $\{A_3, A_4, A_5\}$. So all horizontal left-invariant convection diffusions are given by (37) where one must set $a_1 = a_2 = 0, D_{2j} = D_{1j} = D_{j1} = 0$ for all $j = 1, 2, \ldots, 5$. Now on a commutative group like $\mathbb{R}^6$ with commutative Lie-algebra $\{\partial_{x_1}, \ldots, \partial_{x_5}\}$ omitting 3-directions (say $\partial_{x_1}, \partial_{x_2}, \partial_{x_3}$) from each tangent space in the diffusion would be a disaster, since this would imply no indirect smoothing would take place along the global $x_1, x_2, x_6$-axes. In $SE(3)$ it is different since the commutators take care of indirect smoothing in the omitted directions $\{A_1, A_2, A_6\}$, since


For example we consider the $SE(3)$-analogues of the Forward-Kolmogorov (or Fokker-Plank) equations of the diirection process for contour-completion and the stochastic process for contour enhancement which we considered in our previous works, [18], on $SE(2)$. Here we provide the resulting PDE’s first and explain the underlying stochastic processes later in subsection 4.2. The Fokker-Plank equation for (horizontal) contour completion on $SE(3)$ is

$$\begin{cases}
\partial_t W(y, n; t) = (A_3 + D ((A_4)^2 + (A_5)^2)) W(y, n; t) = (A_3 + D \Delta s^2) W(y, n, t), \quad D = \frac{1}{2} \sigma^2 > 0, \\
\lim_{t \downarrow 0} W(y, n; t) = U(y, n).
\end{cases} \quad (40)$$
where we note that \((A_0)^2(W(y, n(\beta, \gamma), s)) = 0\). This equation arises from (37) by setting \(D_{44} = D_{55} = D\) and 
\(a_3 = 1\) and all other parameters to zero. The Fokker-Plank equation for (horizontal) contour enhancement is

\[
\begin{align*}
\partial_t W(y, n, t) & = (D_{33}(A_3)^2 + D_{44}(A_4)^2 + (A_5)^2) \, W(y, n, t) = ((A_3)^2 + D \Delta_{S^3}) \, W(y, n, t), \\
\lim_{t \downarrow 0} W(y, n, t) & = U(y, n).
\end{align*}
\]

(41)

The solutions of the left-invariant diffusions on \(\mathbb{R}^3 \times S^2\) given by (37) (with in particular (40) and (41)) are again given by convolution product (38) with a probability kernel \(p_t^{D,a}\) on \(\mathbb{R}^3 \times S^2\).

### 4.2 Brownian Motions on \(SE(3) = \mathbb{R}^3 \rtimes SO(3)\) and on \(\mathbb{R}^3 \times S^2\)

Next we formulate a left-invariant discrete Brownian motion on \(SE(3)\) (expressed in the moving frame of reference). The left-invariant vector fields form a moving frame of reference to the group. Since there are always two ways of considering vector fields. Either one considers them as differential operators on smooth locally defined functions, or one considers them as tangent vectors to equivalent classes of curves. Throughout this article we mainly use the first way of considering vector fields, but in this section we prefer to use the second way. We will write \(\{e_1(g), \ldots, e_n(g)\}\) for the left-invariant vector fields rather than \(\{A_1, \ldots, A_n\}\). We obtain the tangent vector \(e_i\) from \(A_i\) by replacing

\[
\begin{align*}
\partial_x & \leftrightarrow (1, 0, 0, 0, 0, 0), \\
\partial_y & \leftrightarrow (0, 1, 0, 0, 0, 0), \\
\partial_z & \leftrightarrow (0, 0, 1, 0, 0, 0), \\
\partial_u & \leftrightarrow (0, 0, 0, \cos \beta, \cos \gamma, \sin \gamma, -\alpha \sin \beta), \\
\partial_v & \leftrightarrow (0, 0, 0, \alpha \cos \beta, \cos \gamma, \alpha \sin \gamma, 0), \\
\partial_w & \leftrightarrow (0, 0, 0, \cos \gamma \sin \beta, \sin \gamma \sin \beta, \cos \beta),
\end{align*}
\]

(42)

where we identified \(SO(3)\) with a ball with radius \(2\pi\) whose outer-sphere is identified with the origin, using Euler angles \(R_{x, \gamma}R_{y, \beta}R_{z, \alpha} \leftrightarrow \alpha n(\beta, \gamma) \in B_{2\pi}\). Next we formulate left-invariant discrete random walks on \(SE(3)\) expressed in the moving frame of reference \(\{e_i\}_{i=1}^{6}\) given by (26) and (42):

\[
(Y_{n+1}, n_{n+1}) = (Y_n, n_n) + \Delta t \sum_{i=1}^{5} \varepsilon_i \, e_i |(Y_n, n_n) + \sqrt{\Delta s} \sum_{i=1}^{5} \varepsilon_i \, e_i |(Y_n, n_n)
\]

for all \(n = 0, \ldots, N - 1\),

\[
(Y_0, n_0) \sim U^D,
\]

with random variable \((Y_0, n_0)\) is distributed by \(U^D\), where \(U^D\) are the discretely sampled HARDI-data (equidistant sampling in position and second order tesselation of the sphere) and where random variables \((Y_n, n_n)\) are recursively determined using the independently normally distributed random variables \(\varepsilon_{i,n+1}^{n=1,\ldots,N-1}, i=1,\ldots,5\) \(\sim \mathcal{N}(0, 1)\) and where the stepsize equals \(\Delta s = \frac{\pi}{2}\). Now if we apply recursion and let \(N \to \infty\) we get the following continuous Brownian motion processes on \(SE(3)\):

\[
Y(t) = Y(0) + \int_0^t \left( \sum_{i=1}^{3} a_i e_i |(Y(\tau), N(\tau)) + \frac{1}{2} \sigma^2 \sum_{j=1}^{3} \sigma_{ji} e_j |(Y(\tau), N(\tau)) \right) \, d\tau,
\]

\[
N(t) = N(0) + \int_0^t \left( \sum_{i=1}^{5} a_i e_i |(Y(\tau), N(\tau)) + \frac{1}{2} \sigma^2 \sum_{j=1}^{5} \sigma_{ji} e_j |(Y(\tau), N(\tau)) \right) \, d\tau,
\]

(43)

with \(\varepsilon_i \sim \mathcal{N}(0, 1)\) and \((X(0), N(0)) \sim U\) and where \(\sigma = \sqrt{2D} \in \mathbb{R}^{6 \times 6}, \sigma > 0\). Note that \(d\sqrt{\tau} = \frac{1}{2} d\sqrt{\tau} - \frac{i}{2} d\tau\).

Now if we set \(U = \delta_{0}e_i\) (i.e. at time zero ) then suitable averaging of infinitely many random walks of this process yields the transition probability \((y, n) \rightarrow p_t^{D,a}(y, n)\) which is the Green’s function of the left-invariant evolution equations (37) on \(\mathbb{R}^3 \times S^2\). In general the PDE's (37) are the Forward Kolmogorov equation of the general stochastic process (43). This follows by Ito calculus and in particular Ito’s formula for formulas on a stochastic process, for details see [2, app.A] where one should consistently replace the left-invariant vector fields of \(\mathbb{R}^n\) by the left-invariant vector fields on \(\mathbb{R}^3 \times S^2\).
In particular we have now formulated the direction process for contour completion in \( \mathbb{R}^3 \times S^2 \) (i.e. non-zero parameters in (43) are \( D_{44} = D_{55} > 0, D_{33} > 0 \) with Fokker-Planck equation (40)) and the (horizontal) Brownian motion for contour-enhancement in \( \mathbb{R}^3 \times S^2 \) (i.e. non-zero parameters in (43) are \( D_{33} > 0, D_{44} = D_{55} > 0 \) with Fokker-Planck equation (41)).

4.3 Tikhonov-regularization of HARDI-images

In the previous subsection we have formulated the Brownian-motions (43) underlying all linear left-invariant convection-diffusion equations on HARDI-data, with in particular the direction process for contour completion and (horizontal) Brownian motion for contour-enhancement. However, we only considered the time dependent stochastic processes and as mentioned before in Markov-processes traveling time is memoryless and thereby negatively exponentially distributed \( T \sim NE(\lambda) \), i.e. \( P(T = t) = \lambda e^{-\lambda t} \) with expectation \( E(T) = \lambda^{-1} \), for some \( \lambda > 0 \). Now recall our observations (12) and (13) and thereby by means of Laplace-transform with respect to time we relate the time-dependent Fokker-Plank equations to their resolvent equations, as at least formally we have

\[
W(y, n, t) = (e^{((Q^{D,a}(\mathbb{A}))U)}(y, n) \text{ and } P_{\gamma}(y, n, t) = \lambda \int_0^\infty e^{-\lambda t}(e^{((Q^{D,a}(\mathbb{A}))U)}(y, n) = \lambda (\lambda I - Q^{D,a}(\mathbb{A}))^{-1} U(y, n),
\]

for \( t, \lambda > 0 \) and all \( y \in \mathbb{R}^3, n \in S^2 \), where the negative definite generator \( Q^{D,a} \) is given by (30). This is similar to our introductory example on the torus in Subsection 3.2. Typically the resolvent operator \( \lambda (\lambda I - Q^{D,a}(\mathbb{A}))^{-1} \) occurs in a first order Tikhonov regularization as we show in the next theorem.

**Theorem 2** Let \( U \in L_2(\mathbb{R}^3 \times S^2) \) and \( \lambda, D_{33} > 0, D_{44} = D_{55} > 0 \). Then the unique solution of the variational problem

\[
\text{arg min}_{P \in \mathcal{M}(\mathbb{R}^3 \times S^2)} \int_{\mathbb{R}^3 \times S^2} \frac{\lambda}{2} (P(y, n) - U(y, n))^2 + \sum_{k=3}^5 D_{kk}(A_k P(y, n))^2 \, dy \, d\sigma(n)
\]

is given by \( P_0^U(y, n) = (R_D^{\mathbb{A}} \ast U)(y, n) \), where the Green’s function \( R_0^D : \mathbb{R}^3 \times S^2 \rightarrow \mathbb{R}^+ \) is the Laplace-transform of the heat-kernel with respect to time: \( R_0^D(y, n) = \lambda \int_0^\infty \rho^{D,a=0}(y, n) e^{-\lambda t} \, dt \) with \( D = \text{diag}(D_{11}, \ldots, D_{55}) \).

\( P^U_0(y, n) \) equals the probability of finding a random walker in \( \mathbb{R}^3 \times S^2 \) regardless its traveling time at position \( y \in \mathbb{R}^3 \) with orientation \( n \in S^2 \) starting from initial distribution \( U \) at time \( t = 0 \).

**Proof** By convexity of the energy (44) (together with hypo-ellipticity of the operator \( \sum_{k=3}^5 (A_k)^2 \)) the solution of this variational problem is unique. Along the minimizer \( W = P_0^U \) we have

\[
\lim_{h \downarrow 0} \frac{\mathcal{E}(P_{h\delta}^\lambda) - \mathcal{E}(P_0^U)}{h} = 0
\]

for all pertubations \( \delta \in H^1(\mathbb{R}^3 \times S^2) \). So by integration by parts we find

\[
\left( \lambda(W - U) - \sum_{k=3}^5 (A_k)^2 W, \delta \right)_{L_2(\mathbb{R}^3 \times S^2)} = 0
\]

for all \( \delta \in H^1(\mathbb{R}^3 \times S^2) \). Now \( H^1(\mathbb{R}^3 \times S^2) \) is dense in \( L_2(\mathbb{R}^3 \times S^2) \) and therefore \( \lambda U = \left( \lambda I - \sum_{k=3}^5 (A_k)^2 \right) W \), so \( W = \lambda \left( \lambda I - \sum_{k=3}^5 (A_k)^2 \right)^{-1} U \) and by left-invariance and linearity this resolvent equation is solved by a \( \mathbb{R}^3 \times S^2 \)-convolution with the smooth Green’s function \( R_{\lambda, D=\text{diag}(D_{ii})} : \mathbb{R}^3 \times S^2 \setminus \{e\} \rightarrow \mathbb{R}^+ \). By (13) this Green’s function follows by the smooth Green’s function \( G_{s = \text{diag}(D_{ii})} \) by Laplace tranform with respect to time. \( \square \)
5 Differential Geometry: The underlying Cartan-connection on $\text{SE}(3)$ and the auto-parallels in $\text{SE}(3)$

Now that we have constructed all left-invariant scale space representations on HARDI-images, generated by means of a quadratic form (30) on the left-invariant vector fields on $\text{SE}(3)$. The question rises what is the underlying differential geometry for these evolutions?

For example, as the left-invariant vector fields clearly vary per position in the group yielding a moving frame of reference attached to luminosity particles (random walkers in $\mathbb{R}^3 \times S^2$ embedded in $\text{SE}(3)$) with both a position and an orientation, the question rises along which trajectories in $\mathbb{R}^3 \times S^2$ do these particles move? Furthermore, as the left-invariant vector fields are obtained by the push-forward of the left-multiplication on the group, an orientation, the question rises along which trajectories in $\text{SE}(3)$ do these particles move?

$$A_g = (L_g)_* A_e, \text{ i.e. } A_g \hat{\phi} = A_e (\hat{\phi} \circ L_g), \text{ where } L_g h = gh, \ g, h \in \text{SE}(3), \hat{\phi} : \text{SE}(3) \rightarrow \mathbb{R} \text{ smooth},$$

the question rises whether this defines a connection between all tangent spaces, such that these trajectories are auto-parallel with respect to this connection? Finally, we need a connection to rigid body mechanics described in a moving frame of reference, to get some physical intuition in the choice of the fundamental constants$^6 \{a_i\}_{i=1}^6$ and $\{D_{ij}\}_{i=1,j=1}^6$ within our generators (30).

In order to get some first physical intuition on analysis and differential geometry along the moving frame within our generators (30).

In words: The absolute acceleration equals the relative acceleration (which is zero, since $\hat{\epsilon}^{(1)}$ is constant) plus the Coriolis acceleration $2\hat{\epsilon}^{(2)} \times \hat{\epsilon}^{(1)}$ and the centrifugal acceleration $\hat{\epsilon}^{(2)} \times (\hat{\epsilon}^{(2)} \times y(s))$. Now in case of uniform circular motion the speed is constant but the velocity is always tangent to the orbit of acceleration and the acceleration has constant magnitude and always points to the center of rotation. In this case, the total sum of Coriolis acceleration and centrifugal acceleration add up to the well-known centripetal acceleration,

$$\ddot{y}(s) = 2\hat{\epsilon}^{(2)} \times (-\hat{\epsilon}^{(2)} \times R \hat{r}(s)) + \hat{r}^2 \times (\hat{\epsilon}^{(2)} \times R \hat{r}(s)) = -||\hat{\epsilon}^{(2)}||^2 R \hat{r}(s) = -\frac{||\hat{\epsilon}^{(2)}||^2}{R} \hat{r}(s),$$

where $R$ is the radius of the circular orbit $y(s) = m + R \hat{r}(s), \ ||\hat{r}(s)|| = 1$. The centripetal acceleration equals a half times the Coriolis acceleration, i.e. $\ddot{y}(s) = \hat{\epsilon}^{(2)} \times \hat{\epsilon}^{(1)}$.

In our previous work [19] on contour-enhancement and completion via left-invariant diffusions on invertible orientation scores (complex-valued functions on $\text{SE}(2)$) we have put a lot of emphasis on the underlying differential geometry in $\text{SE}(2)$. All results straightforwardly generalize to the case of HARDI-images, which can be considered as functions on $\mathbb{R}^3 \times S^2$ embedded in $\text{SE}(3)$. These rather technical results are summarized in Theorem 3, which

$^6$Or later in Subsection 9 to get some intuition in the choice of functions $\{a_i\}_{i=1}^6$ and $\{D_{ij}\}_{i=1,j=1}^6$. 

19
The Maurer-Cartan form

Theorem 3 The Maurer-Cartan form $\omega$ on $SE(3)$ is given by

$$\omega_g(X_g) = \sum_{i=1}^{6} (\mathfrak{d}A^i)_{g} \cdot X_g \cdot A_i, \quad X_g \in T_g(SE(2)),$$

where the dual vectors $\{dA^i\}_{i=1}^3$ are given by (27) and $A_i = A_i|_{e}$. It is a Cartan Ehresmann connection form on the principal fiber bundle $P = (SE(3), e, SE(3), \mathcal{L}(SE(3)))$, where $\pi(g) = e$, $\mathcal{R}_g u = u g$, $u, g \in SE(3)$. Let $Ad$ denote the adjoint action of $SE(3)$ on its own Lie-algebra $T_e(SE(3))$, i.e. $Ad(g) = (R_g^{-1} L_g)$, i.e. the push-forward of conjugation. Then the adjoint representation of $SE(3)$ on the vector space $\mathcal{L}(SE(3))$ of left-invariant vector fields is given by

$$\tilde{Ad}(g) = d\mathcal{R} \circ Ad(g) \circ \omega. \quad (46)$$

This adjoint representation gives rise to the associated vector bundle $SE(3) \times_{\tilde{Ad}} \mathcal{L}(SE(3))$. The corresponding connection form on this vector bundle is given by

$$\tilde{\omega} = \sum_{j=1}^{6} \tilde{ad}(A_j) \otimes dA_j = \sum_{i,j,k=1}^{6} c^k_{ij} A_k \otimes dA^i \otimes dA^j, \quad (47)$$

Then $\tilde{\omega}$ yields the following $6 \times 6$-matrix valued matrix 1-form

$$\tilde{\omega}^k_j(\cdot) := -\tilde{\omega}(dA^k, \cdot, A_j) \quad k,j = 1,2,3. \quad (48)$$

on the frame bundle, [40, p.353,p.359], where the sections are moving frames [40, p.354]. Let $\{\mu_k\}_{k=1}^{3}$ denote the sections in the tangent bundle $E := (SE(3), T(SE(3)))$ which coincide with the left-invariant vector fields $\{A_k\}_{k=1}^{3}$. Then the matrix-valued 1-form (48) yields the Cartan connection given by the covariant derivatives

$$D_{X|_{\gamma(t)}}(\mu(\gamma(t))) = D_{\mu(\gamma(t))}(X|_{\gamma(t)})$$

$$= \sum_{k=1}^{6} a^k(t) \mu_k(\gamma(t)) + \sum_{j=1}^{6} \tilde{\omega}^k_j(X|_{\gamma(t)}) \mu_j(\gamma(t))$$

$$= \sum_{k=1}^{6} a^k(t) \mu_k(\gamma(t)) + \sum_{k,l,m=1}^{6} \tilde{\omega}^k_j(t) a^k(\gamma(t)) \Gamma^{j}_{lk} \mu_j(\gamma(t)) \quad (49)$$

7The torsion-tensor $T_\gamma$ of a connection $\nabla$ is given by $T[X, Y] = \nabla_X Y - \nabla_Y X - [X, Y]$. The torsion-tensor $T_\gamma$ of a Levi-Civita connection vanishes, whereas the torsion-tensor of our Cartan-connection $\nabla$ on $SE(3)$ is given by $T_\gamma = 3c^i_{jk} dA^i \otimes dA^j$.

8In a Levi-Civita connection one has $\Gamma^i_{kl} = \frac{1}{2} \mathcal{R}^m (9_{mkl} + g_{ml,k} - g_{kl,m})$ with respect to a holonomic basis.
with \( \dot{a}^k(t) = \sum_{i=6}^{6} \dot{\gamma}^i(t) A_i |_{\gamma(t)} a^k \), for all tangent vectors \( X |_{\gamma(t)} = \sum_{i=6}^{6} \dot{\gamma}^i(t) A_i |_{\gamma(t)} \) along a curve \( t \mapsto \gamma(t) \in SE(2) \) and all sections \( \mu(\gamma(t)) = \sum_{k=1}^{6} a^k(\gamma(t)) \mu_k(\gamma(t)) \). The Christoffel symbols in (49) are constant \( \Gamma_{ik}^{j} = -c_{ik}^{j} \), with \( c_{ik}^{j} \) the structure constants of Lie-algebra \( T_e(SE(3)) \). Consequently, the connection \( D \) has constant curvature and constant torsion and the left-invariant evolution equations (29) can be rewritten in covariant derivatives (using short notation \( \nabla_j := D A_j \)):

\[
\left\{ \begin{aligned}
\partial_s W(g,s) &= \sum_{i,j=1}^{6} A_i ((D_{ij}(W))(g,s)A_j W)(g,s) \\
W(g,0) &= U(g), \quad \text{for all } g \in SE(2), s > 0.
\end{aligned} \right. (50)
\]

Both convection and diffusion in the left-invariant evolution equations (29) take place along the exponential curves \( \gamma_{c,g}(t) = g \cdot e^{t \sum_{i=1}^{6} c_i A_i} \) in \( SE(3) \) which are the covariantly constant curves (i.e. auto-parallel) with respect to the Cartan connection. These spatial projections \( \mathbb{P} R^2 \gamma(0) \) of these curves \( \gamma \) are circular spirals with constant curvature and constant torsion. The curvature magnitude equals \( ||\dot{c}^2|| ||\dot{c}^1|| \) and the curvature vector equals

\[
\kappa(t) = \frac{1}{||\dot{c}^1||} \left( \cos(t ||\dot{c}^2||) \, \dot{c}^2 \times \dot{c}^1 + \sin(t ||\dot{c}^2||) \, \hat{c}^2 \times \dot{c}^2 \times \hat{c}^1 \right),
\]

where \( c = (c^1, c^2, c^3, c^4, c^5, c^6) = (\dot{c}^1; \dot{c}^2) \). The torsion vector equals \( \tau(t) = [\dot{c}_1 \cdot \dot{c}_2] \kappa(t) \).

**Proof** The proof is a straightforward generalization from our previous results [19, Thm 3.8 and Thm 3.9] on the \( SE(2) \)-case to the case \( SE(3) \). The formulas of the constant torsion and curvature of the spatial part of the exponential curves (which are the exponential curves) follow by the formula for (54) for the spatial part \( x(s) \) of the exponential curves, which we will derive in Section 5.1. Here we stress that \( s(t) = t \sqrt{(c^1)^2 + (c^2)^2 + (c^3)^2} \) is the arc-length of the spatial part of the exponential curve and where we recall that \( \kappa(s) = \ddot{x}(s) \) and \( \tau(s) = \frac{d}{ds} (\dot{x}(s) \times \ddot{x}(s)) \). Note that both the formula (54) for the exponential curves in the next section and the formulas for torsion and curvature are simplifications of our earlier formulas [25, p.175-177].

### 5.1 The Exponential Curves and the Logarithmic Map explicitly in Euler Angles

Next we compute the exponential curves in \( SE(3) \) by an isomorphism of the group \( SE(3) \) to matrix group \( \mathbb{SE}(3) \)

\[
SE(3) \ni (x, R_{\gamma, \beta, \alpha}) \mapsto \begin{pmatrix} R_{\gamma, \beta, \alpha} \end{pmatrix} \in \mathbb{SE}(3) \text{ with } R_{\gamma, \beta, \alpha} = R_{e_x, \gamma} R_{e_x, \beta} R_{e_x, \alpha}.
\]

This isomorphism induces the following isomorphism between the respective Lie-algebra's

\[
\sum_{i=1}^{6} c_i A_i \in \mathcal{L}(SE(3)) \leftrightarrow T_e(SE(3)) \ni \sum_{i=1}^{6} c_i A_i \leftrightarrow \sum_{i=1}^{6} c_i X_i \in \mathbb{R}^{3 \times 3}.
\]

where \( \{ c_i \}_{i=1}^{6} \in \mathbb{R}^6 \) and with matrices \( \{ X_i \}_{i=1}^{6} \in \mathbb{R}^{3 \times 3} \) are given by

\[
\begin{align*}
X_1 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, & X_2 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, & X_3 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\
X_4 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, & X_5 &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & X_6 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}.
\end{align*}
\]
Note that $A_i \leftrightarrow A_i \not\leftrightarrow X_i \Rightarrow [A_i, A_j] \not\leftrightarrow [A_i, A_j] \not\leftrightarrow X_i, X_j$ and indeed direct computation yields:

$$\sum_{k=1}^{6} c^k_i A_k = [A_i, A_j] \not\leftrightarrow [X_i, X_j] = \sum_{k=1}^{6} c^k_i X_k$$

with commutator table

$$\begin{bmatrix}
0 & 0 & 0 & 0 & X_3 & -X_2 \\
0 & 0 & 0 & -X_3 & 0 & X_1 \\
0 & 0 & 0 & X_2 & -X_1 & 0 \\
0 & X_3 & -X_2 & 0 & X_6 & -X_5 \\
-X_3 & X_1 & -X_6 & 0 & X_4 \\
X_2 & -X_1 & 0 & X_5 & -X_4 & 0
\end{bmatrix},$$

where $i$ enumerates vertically and $j$ horizontally and $[A_i, A_j] = A_i A_j - A_j A_i$ and $[X_i, X_j] = X_i X_j - X_j X_i$.

Each element in the Lie-algebra of the matrix group $\mathfrak{g} \in \mathfrak{gl}(3)$ can be written

$$A = \sum_{i=1}^{6} e^i X_i = \begin{pmatrix} \Omega & \xi^{(1)} \\ 0 & 0 \end{pmatrix}, \Omega = \begin{pmatrix} e^6 & -e^5 & e^5 \\ -e^5 & e^4 & -e^4 \\ e^4 & -e^3 & 0 \end{pmatrix} \in so(3), \quad \xi^{(1)} = (e^1, e^2, e^3) \in \mathbb{R}^3.$$

Note that $\Omega x = \xi^{(2)} \times x$ and set $\tilde{q} = \|\xi^{(2)}\| = \sqrt{(e^4)^2 + (e^5)^2 + (e^6)^2}$ so that $\Omega^3 = -\tilde{q}^2 \Omega$ and therefore

$$A^k = \begin{pmatrix} \Omega^k & \Omega^{k-1} \xi^{(1)} \\ 0 & 0 \end{pmatrix} \Rightarrow e^A = \sum_{k=1}^{\infty} \frac{1}{k!} A^k = \begin{pmatrix} e^{\Omega t} & t \int_0^t e^{s \Omega} ds \\ 0 & 1 \end{pmatrix} \xi^{(1)} = \begin{pmatrix} R & x \\ 0 & 1 \end{pmatrix} \in \mathfrak{g} \in \mathfrak{gl}(3),$$

with $\int_0^1 e^{ts \Omega} ds = \sum_{k=0}^{\infty} \frac{(ts \Omega)^k}{k!} = I + \frac{1-\cos(\tilde{q}t)}{\tilde{q}^2} \Omega + \frac{\tilde{q}^2 - \sin(\tilde{q}t)}{\tilde{q}^4} \Omega^2$,

and $R = e^{\Omega t} = I + \frac{\sin(\tilde{q}t)}{\tilde{q}} \Omega + \frac{1-\cos(\tilde{q}t)}{\tilde{q}^2} \Omega^2$.

so that the exponential curves are given by

$$\gamma(t) = \begin{cases}
\frac{t}{\tilde{q}} \sum_{i=1}^{6} e^i A_i, \\
(e_1 t, e_2 t, e_3 t, I)
\end{cases} \begin{pmatrix} (\xi^{(1)}) + \frac{1-\cos(\tilde{q}t)}{\tilde{q}^2} \Omega \xi^{(1)} + (\tilde{q}^2 - \sin(\tilde{q}t)) \Omega^2 \xi^{(1)}, I + \frac{\sin(\tilde{q}t)}{\tilde{q}} \Omega + \frac{1-\cos(\tilde{q}t)}{\tilde{q}^2} \Omega^2 \\
\sin(\alpha \sin \gamma) \\
2 \cos^2 \left(\frac{\beta}{2}\right) \sin(\alpha + \gamma)
\end{pmatrix}$$

if $\xi^{(2)} \neq 0$, 

if $\xi^{(2)} = 0$. 

Here we stress that the vectors $\Omega \xi^{(1)}$ and $\Omega \xi^{(2)}$ are orthogonal to each other since $(\Omega)^T = -\Omega$.

As the exponential map is surjective we are also interested in the logarithmic map. This means we have to solve for $\xi^{(1)} \in \mathbb{R}^3$ and $\Omega \in so(3)$ if we are given group element $g = (x, R_{\gamma, \beta, \alpha}) \in SE(3)$. Note that $\Omega T = -\Omega$, $(\Omega^2)^T = \Omega^2$ so that $R = R^T = 2 \frac{\sin(\tilde{q}t)}{\tilde{q}} \Omega$ from which the logarithmic map $\Omega = \log_{SO(3)} R, R = R_{\gamma, \beta, \alpha}$ follows explicitly:

$$e^4 = c^4_{\gamma, \beta, \alpha} := \frac{\tilde{q}}{2 \sin q} \sin \beta (\sin \alpha - \sin \gamma), \\
e^5 = c^5_{\gamma, \beta, \alpha} := \frac{\tilde{q}}{2 \sin q} \sin \beta (\cos \alpha - \cos \gamma), \\
e^6 = c^6_{\gamma, \beta, \alpha} := \frac{\tilde{q}}{2 \sin q} (2 \cos^2 \left(\frac{\beta}{2}\right) \sin(\alpha + \gamma)).$$

and thereby $\tilde{q} = \sqrt{(e^4)^2 + (e^5)^2 + (e^6)^2} = \tilde{q}_{\gamma, \beta, \alpha} = \arcsin \sqrt{\cos^2 \left(\frac{\alpha + \gamma}{2}\right) \sin^2 \beta + \cos^4 \left(\frac{\beta}{2}\right) \sin^2(\alpha + \gamma)}$. So it remains to express $\xi^{(1)} = (e^1, e^2, e^3)^T$ in Euler angles $(\gamma, \beta, \alpha)$. Now $\Omega^3 = -\tilde{q}^2 \Omega$ implies that

$$\begin{pmatrix} I + \tilde{q}^{-2}(1 - \cos \tilde{q}) \Omega + \tilde{q}^{-3}(\tilde{q} - \sin \tilde{q}) \Omega^2 \end{pmatrix} \xi^{(1)} = x \leftrightarrow$$

$$\xi^{(1)} = \xi^{(1)}_{\gamma, \beta, \alpha} := \begin{pmatrix} (I - \frac{1}{2} \Omega_{\gamma, \beta, \alpha} + \tilde{q}^{-2}(1 - \tilde{q}^{\gamma, \beta, \alpha}) \cot \left(\frac{\tilde{q}^{\gamma, \beta, \alpha}}{2}\right))(\Omega_{\gamma, \beta, \alpha})^2 \\
(x, y, z) \end{pmatrix}.$$

Now equality (55) and (56) provide the explicit logarithmic mapping on $SE(3)$:

$$\log_{SE(3)}(x, R_{\gamma, \beta, \alpha}) = \sum_{i=1}^{3} c^i_{\gamma, \beta, \alpha} A_i + \sum_{i=4}^{6} c^i_{\gamma, \beta, \alpha} A_i. \quad (57)$$
Remark: It can be shown that $\|a\|_2 \mathbb{P}_{\mathbb{R}^3} \gamma_c(t) = \sqrt{(c_1)^2 + (c_2)^2 + (c_3)^2}$. Consequently the arc-length parameter $s > 0$ is expressed in $t$ by means of $s(t) = t \sqrt{(c_1)^2 + (c_2)^2 + (c_3)^2}$. If we want to impose spatial arc-length parameterizations of curves in $SE(3)$ we must rescale all $c_i \rightarrow \frac{c_i}{\sqrt{(c_1)^2 + (c_2)^2 + (c_3)^2}}$ so that $\|c(1)\| = \sqrt{(c_1)^2 + (c_2)^2 + (c_3)^2} = 1$.

Remark: The group $SE(3)$ is isomorphic to the group of rigid motions in $\mathbb{R}^3$ well-known in mechanics. The vector $\epsilon(1)$ denotes constant velocity in the moving coordinate frame $\{a_i\}_{i=1}^3$ whereas $\epsilon(2)$ denotes constant angular velocity with respect to the same moving coordinate frame attached to a particle on a moving rigid body in $\mathbb{R}^3$. Note that $\kappa(0)$ equals the centripetal acceleration at the moving frame of reference $\{A_1, A_2, A_3\}_{|_{\kappa(0)=e}} = \{A_1, A_2, A_3\}$, whereas $\kappa(s)$ equals the centripetal acceleration at the moving frame of reference $\{A_1, A_2, A_3\}_{|_{\kappa(s)}}$, but again expressed in the global coordinate system $\{A_1, A_2, A_3\} = \{\partial_x, \partial_y, \partial_z\}$ of the spatial part $= \mathbb{R}^3$ of the group, which is for $s > 0$ no longer aligned with the moving frame of reference. In order to re-express $\kappa(0)$ over an angle of $s\|\epsilon(2)\|$ around the angular velocity axis $\epsilon_3^2$, which explains (51).

6 Analysis of the Convolution Kernels of Scale Spaces on HARDI-images

It is notorious problem to find explicit formulas the exact Green’s functions $p_{t}^{D, a} : \mathbb{R}^3 \times S^2$ of the left-invariant diffusions (37) on $R^3 \times S^2$. Explicit, tangible and exact formulas for heat-kernels on $SE(3)$ do not seem to exist in literature. Nevertheless, there does exist a nice general theory overlapping the fields of functional analysis and group theory, see for example [41, 36], which at least provides Gaussian estimates for Green’s functions of left-invariant diffusions on Lie groups, generated by subcoercive operators. In the remainder of this section we will employ this general theory to our special case where $SE(3)$ is not nilpotent. This makes it hard to get tangible explicit formulae for the heat-kernels. Therefore we shall generalize our Heisenberg approximations of the Green’s functions on $SE(2)$, [21], [42], [15],[2], to the case $SE(3)$. Again we will follow the general work by ter Elst and Robinson [41] on semigroups on Lie groups generated by weighted subcoercive operators. In their general work we consider a particular case by setting the Hilbert space $L_2(SE(3))$, the group $SE(3)$ and the right-regular representation $R$. Furthermore we consider the algebraic basis
\{A_3, A_4, A_5\} leading to the following filtration of the Lie algebra
\[ g_1 = \text{span}\{A_3, A_4, A_5\} \subset g_2 = \text{span}\{A_1, A_2, A_3, A_4, A_5, A_6\} = L(SE(3)). \]

Now that we have this filtration we have to assign weights to the generators
\[ w_3 = w_4 = w_5 = 1 \text{ and } w_1 = w_2 = w_6 = 2. \]

For example \( w_3 = 1 \) since \( A_3 \) already occurs in \( g_1 \), \( w_6 = 2 \) since \( A_6 \) is within in \( g_2 \) and not in \( g_1 \).

Now that we have these weights we define the following dilations on the Lie algebra \( T_e(SE(3)) \) (recall \( A_i = A_i|_e \)):
\[
\gamma_q^{\alpha}(\sum_{i=1}^6 q^{w_i} c_i A_i) = \sum_{i=1}^6 q^{w_i} c_i A_i, \quad \text{for all } c_i \in \mathbb{R},
\]
\[
\tilde{\gamma}_q(x, y, z, R_{\tilde{\gamma}, \tilde{\beta}, \tilde{\alpha}}) = \left( \frac{x}{q^3}, \frac{y}{q^3}, \frac{z}{q^3}, R_{\tilde{\gamma}, \tilde{\beta}, \tilde{\alpha}} \right), \quad q > 0,
\]
and for \( 0 < q \leq 1 \) we define the Lie product \([A, B]_q = \gamma_q^{-1}[\gamma_q(A), \gamma_q(B)]\). Now let \( (SE(3))_q \) be the simply connected Lie group generated by the Lie algebra \( (T_e(SE(3)), [\cdot, \cdot]) \). This Lie group is isomorphic to the matrix group with group product:
\[
(x, R_{\tilde{\gamma}, \tilde{\beta}, \tilde{\alpha}}) \quad \gamma_q'(x', R_{\tilde{\gamma}', \tilde{\beta}', \tilde{\alpha}'} = \left( x + S_q \cdot R_{\tilde{\gamma}, \tilde{\beta}, \tilde{\alpha}} \cdot q \cdot S_q^{-1} \cdot x', \quad R_{\tilde{\gamma}, \tilde{\beta}, \tilde{\alpha}} \cdot R_{\tilde{\gamma}', \tilde{\beta}', \tilde{\alpha}'} \right) \]
where the diagonal \( 3 \times 3 \)-matrix is defined by \( S_q := \text{diag}\{1, 1, q\} \) and we used short-notations \( R_{\tilde{\gamma}, \tilde{\beta}, \tilde{\alpha}} = R_{e, \tilde{\gamma}, \tilde{\beta}, \tilde{\alpha}} = R_{e, \tilde{\gamma}} \) for all \( q \in (SE(3))_q \) and we used short-notations \( R_{\tilde{\gamma}, \tilde{\beta}, \tilde{\alpha}} = R_{e, \tilde{\gamma}, \tilde{\beta}, \tilde{\alpha}} = R_{e, \tilde{\gamma}} \), i.e. our elements of \( SO(3) \) are expressed in the second coordinate chart (4). Now the left-invariant vector fields on the group \((SE(3))_q\) are given by
\[
A_i^q|_q = (\tilde{\gamma}_q^{-1} \circ L_{\gamma_q}) A_i, \quad i = 1, \ldots, 6.
\]
Straightforward (but intense) calculations yield (for each \( g = (x, R_{\tilde{\gamma}, \tilde{\beta}, \tilde{\alpha}}) \in (SE(3))_q \)):
\[
A_1^q|_q = \cos(q^2 \tilde{\alpha}) \cos(q \tilde{\beta}) \partial_x + (\cos(q \tilde{\gamma}) \sin(\tilde{\alpha}^2) + \cos(\tilde{\alpha}^2) \sin(q \tilde{\gamma}) \sin(q \tilde{\gamma})) \partial_y + \qquad + q \sin(\tilde{\alpha}^2) \sin(q \tilde{\gamma}) \sin(q \tilde{\gamma}) \partial_z
\]
\[
A_2^q|_q = - \sin(q \tilde{\gamma}) \sin(\tilde{\alpha}^2) \sin(\tilde{\gamma}) \partial_x + (\cos(q \tilde{\gamma}) \cos(\tilde{\alpha}^2) \sin(q \tilde{\gamma}) \sin(q \tilde{\gamma})) \partial_y + \qquad + q \sin(q \tilde{\gamma}) \sin(q \tilde{\gamma}) \partial_z
\]
\[
A_3^q|_q = q^{-1} \sin(q \tilde{\beta}) \partial_y - q^{-1} \cos(q \tilde{\beta}) \sin(q \tilde{\gamma}) \partial_y + \cos(q \tilde{\beta}) \cos(q \tilde{\gamma}) \partial_z - \sin(q \tilde{\gamma}) \partial_z
\]
\[
A_4^q|_q = q^{-1} \cos(q \tilde{\alpha}^2) \tan(q \tilde{\gamma}) \partial_x + \sin(q \tilde{\gamma}) \partial_y + \frac{\cos(q \tilde{\alpha}^2) \cos(q \tilde{\gamma})}{\sin(q \tilde{\beta})} \partial_z
\]
\[
A_5^q|_q = q^{-1} \sin(q \tilde{\alpha}^2) \tan(q \tilde{\gamma}) \partial_x + \cos(q \tilde{\alpha}^2) \partial_y - \frac{\sin(q \tilde{\gamma})}{\cos(q \tilde{\beta})} \partial_z
\]
\[
A_6^q|_q = \partial_z.
\]
Now note that \([A_i, A_j]_q = \gamma_q^{-1}[\gamma_q(A_i), \gamma_q(A_j)] = \gamma_q^{-1} q^{w_i + w_j} [A_i, A_j] = \sum_{k=1}^6 q^{w_i + w_j - w_k} c_{ij}^k A_k\) and thereby we have
\[
[A_4, A_5]_q = A_6, \quad [A_4, A_6]_q = - q^2 A_3, \quad [A_5, A_6]_q = q A_4, \quad [A_4, A_4]_q = - A_2, \quad [A_4, A_2]_q = q^2 A_3, \quad [A_5, A_1]_q = - q^2 A_3, \quad [A_5, A_3]_q = A_1, \quad [A_6, A_1]_q = q^2 A_2 \text{ and } [A_6, A_2]_q = - q^2 A_1.
\]
Analogously to the case \( q = 1 \), \((SE(3))_{q=1} = SE(3)\) we have an isomorphism of the common Lie algebra at the unity element \( T_e(SE(3)) = T_e((SE(3))_q) \) and left-invariant vector fields on the group \((SE(3))_q\) :
\[
(A_1 \leftrightarrow A_1^q \text{ and } A_2 \leftrightarrow A_2^q) \Rightarrow [A_1, A_2]_q \leftrightarrow [A_1^q, A_2^q].
\]
It can be verified that the left-invariant vector fields \(A_1^q \) satisfy the same commutation relations (61). Now let us consider the case \( q \downarrow 0 \), then we get a nilpotent-group \((SE(3))_0\) with left-invariant vector fields
\[
A_1^q = \partial_x, \quad A_2^q = \partial_y, \quad A_3^q = \tilde{\beta} \partial_x - \tilde{\gamma} \partial_y + \partial_z, \quad A_4^q = - \tilde{\beta} \partial_x + \partial_y, \quad A_5^q = \partial_y, \quad A_6^q = \partial_z.
\]
6.1.1 The Heisenberg-approximation of the Contour Completion Kernel

Recall that the generator of contour completion diffusion was given by \( A_3 + D_{44}((A_4)^2 + (A_5)^2) \). So let us replace the true left-invariant vector fields \( \{A_i\}_{i=3}^5 \) on \( SE(3) = (SE(3))_q=1 \) by their Heisenberg-approximations \( \{A_i^{(0)}\}_{i=3}^5 \) that are given by (62) and compute the Green’s function \( p^3_t = D_{44} = D_{55} \) on \( (SE(3))_0 \) i.e. the convolution kernel which yields the solutions of contour completion on \( (SE(3))_0 \) by group convolution on \( (SE(3))_0 \). For \( 0 < D_{44} \ll 1 \) this kernel is a local approximation of the true contour completion kernel\(^9\) in \( \mathbb{R}^3 \times S^2 \):

\[
\overline{\Phi}^{t=1, D_{44} = D_{55}}(x, y, z, \tilde{\gamma}, \tilde{\beta}) = \delta(t - z) e^{t(\tilde{\beta} \partial_t + D_{44}(\tilde{\beta} \partial_z)^2)} e^{e^{t(\tilde{\gamma} \partial_y + D_{44}(\tilde{\gamma} \partial_y)^2)}} (y, \tilde{y}, \tilde{\gamma}) = \delta(t - z) e^{-\frac{3}{4}D_{44}^{x^2+y^2+z^2}} e^{-\frac{12(x-1/2)\beta^2 + 2y^2}{4D_{44}}} e^{-\frac{12\beta y (1/2)\gamma^2}{4D_{44}}} \quad \text{if } z > 0
\]

(63)

where \( \tilde{\gamma} = D_{\epsilon, \gamma} D_{\epsilon, \beta} e_z = (\sin \beta, -\sin \gamma \cos \beta, \cos \gamma \cos \beta)^T \). The corresponding resolvent kernel on the group \( (SE(3))_0 \) is now directly obtained by Laplace transform with respect to time\(^10\):

\[
\overline{R}^{t=1, D_{44} = D_{55}}_{\lambda}(x, y, z, \tilde{\gamma}, \tilde{\beta}) = \left\{ \begin{array}{ll}
\frac{3}{4D_{44}^{x^2+y^2+z^2}} e^{-\frac{12(x-1/2)\beta^2 + 2y^2}{4D_{44}}} e^{-\frac{12\beta y (1/2)\gamma^2}{4D_{44}}} & \text{if } z > 0 \\
0 & \text{if } z \leq 0 \text{ and } (x, y) \neq (0, 0).
\end{array} \right.
\]

(64)

So we make a remarkable observation: The Heisenberg-approximation (67) of the contour completion kernel in \( (SE(3)) \) is a direct product of two Heisenberg approximations of contour completion kernels in \( SE(2) \), \([21],[15, \text{ eq. 4.113}])\), where one of the kernels is in \((x, \tilde{\gamma})\) coordinates and where the other one is expressed in \((y, -\tilde{\gamma})\) coordinates:

\[
p^3_t = D_{44} : (SE(3))_0 (x, y, z, \tilde{\gamma}, \tilde{\beta}) = p^3, D_{44} : (SE(2))_0 (x, y, \tilde{\beta}) \cdot p^3, D_{44} : (SE(2))_0 (z, -y, \tilde{\gamma}).
\]

(65)

Now since the Heisenberg approximation kernel \( p^3, D_{44} : (SE(2))_0 \) is for reasonable parameter settings (that is \( D_{44} < D_{53} \ll 1 \)) close to the exact kernel \( p^3, D_{44} : (SE(2))_0 \) we heuristically propose for these reasonable parameter settings the same direct-product approximation for the exact contour-enhancement kernels on \( \mathbb{R}^3 \times S^2 \):

\[
p^3_t = D_{44} : (SE(2))_0 (x, y, z, \tilde{\gamma}, \tilde{\beta}) = p^3, D_{44} : (SE(2))_0 (x, y, \tilde{\beta}) \cdot p^3, D_{44} : (SE(2))_0 (z, -y, \tilde{\gamma}),
\]

(66)

where the exact kernels \( p^3_t = D_{44} : (SE(2))_0 \) for contour completion in \( SE(2) \) can be found in [21].

6.1.2 The Heisenberg-approximation of the Contour Enhancement Kernel

Recall that the generator of contour completion diffusion was given by \( D_{53}(A_3)^2 + D_{44}((A_4)^2 + (A_5)^2) \). So let us replace the true left-invariant vector fields \( \{A_i\}_{i=3}^5 \) on \( SE(3) = (SE(3))_q=1 \) by their Heisenberg-approximations \( \{A_i^{(0)}\}_{i=3}^5 \) given by (62) and consider the Green’s function \( p^{t=1, D_{44} = D_{55}} \) on \( (SE(3))_0 \):

\[
p^{t=1, D_{44} = D_{55}} : e^{t(\tilde{\beta} \partial_t + D_{44}(\tilde{\beta} \partial_z)^2)} e^{e^{t(\tilde{\gamma} \partial_y + D_{44}(\tilde{\gamma} \partial_y)^2)}} (y, \tilde{y}, \tilde{\gamma}) = \delta(t - z) e^{-\frac{3}{4}D_{44}^{x^2+y^2+z^2}} e^{-\frac{12(x-1/2)\beta^2 + 2y^2}{4D_{44}}} e^{-\frac{12\beta y (1/2)\gamma^2}{4D_{44}}},
\]

(67)

which is not easy to compute. However we follow the same approach as we applied previously \([18]\) to the diffusion kernels on the 2D-Euclidean motion group \( (SE(2))_0 \), which follows the coordinate substitutions as proposed by Citti and Sarti \([9]\). The group \( (SE(3))_0 \) however is not (entirely) a direct product of two \( H_3 \) groups and application of the coordinate-translation

\[
x'_1 = x'_2 = \frac{z}{\sqrt{2}D_{44}}, \omega'_1 = \frac{\tilde{\beta}}{\sqrt{2}D_{44}} \text{ and } \omega'_2 = \frac{\tilde{\gamma}}{\sqrt{2}D_{44}}, t'_1 = \frac{2(x - \tilde{\beta})}{\sqrt{D_{44}D_{53}}}, t'_2 = \frac{-2(y + \tilde{\gamma})}{\sqrt{D_{44}D_{53}}},
\]

\(^9\)The superscript for the kernel is actually \( p^{D_t} \) so in the superscript-labels, for the sake of simplicity, we only mention the non-zero coefficients \( D_{ij}, a_t \) of (37).

\(^{10}\)Note that the delta distribution \( \delta(s - z) \) allowed us to replace all \( s \) by \( z \) in the remaining factor in (67) which makes it easy to apply the Laplace-transform.
expressed the generator into
\[
(D_{33}(A_2^0)^2 + D_{44}((A_2^0)^2 + (A_2^0)^2)) = \frac{1}{2}(\partial_{x_1'} - 2x_1'\partial_{t_1'})^2 + \frac{1}{2}(\partial_{x_2'} - 2x_2'\partial_{t_2'})^2 + \frac{1}{2}(\partial_{x_1'} + 2x_1'\partial_{t_1'})^2 + (\partial_{x_1'} - 2x_1'\partial_{t_1'}) (\partial_{x_2'} - 2x_2'\partial_{t_2'}) =: \Delta_K + \tilde{A}_2 \tilde{A}_4 ,
\]
where \( \Delta_K = (1/2)((\tilde{A}_2)^2 + (\tilde{A}_4)^2 + \tilde{A}_3)^2 + (\tilde{A}_4)^2 \) equals the Kohn’s Laplacian, \([29]\), on the group \( H_5 \), which is a sum of the four horizontal left-invariant vector fields on \( H_5 \), \([29, 17]\). Note that \( \Delta_K \) is also the Kohn’s Laplacian on the group \( H_3 \times H_3 \) (with extra imposed identification \( x_1' = x_2' \)). If we neglect the cross-term \( \tilde{A}_2 \tilde{A}_4 \) in the generator we get the following approximation
\[
\bar{p}_t^{D_{33}, D_{44} = D_{55}}, \mathbb{R}^3 \times S^2 (x, y, z, \theta(\tilde{\beta}, \tilde{\gamma})) \approx \bar{p}_t^{D_{33}, D_{44} = D_{55}} \mathbb{R}^2 \times (SE(2))_0 (z/2, x, \tilde{\beta}) \cdot \bar{p}_t^{D_{33}, D_{44} = D_{55}} \mathbb{R}^2 \times (SE(2))_0 (z/2, -y, \tilde{\gamma}) .
\]
So similar to the contour-completion kernel on \( \mathbb{R}^3 \times S^2 \) derived in the previous section, recall \((65)\), the Heisenberg-approximation kernel on \( \mathbb{R}^3 \times S^2 \) is a direct product of two Heisenberg-approximation kernels on \( (SE(2))_0 \).

Now since the Heisenberg approximation kernel \( \bar{p}_t^{D_{33}, D_{44} = D_{55}} \mathbb{R}^2 \times (SE(2))_0 \) is for reasonable parameter settings (that is \( 0 < \frac{D_{33}}{D_{55}} \ll 1 \)) close to the exact kernel \( \bar{p}_t^{D_{33}, D_{44} = D_{55}} \mathbb{R}^2 \times (SE(2))_0 \), we heuristically propose for these reasonable parameter settings the same direct-product approximation for the exact contour-enhancement kernels on \( \mathbb{R}^3 \times S^2 \):
\[
\bar{p}_t^{D_{33}, D_{44} = D_{55} \mathbb{R}^3 \times S^2 (x, y, z, \theta(\tilde{\beta}, \tilde{\gamma})) \approx \bar{p}_t^{D_{33}, D_{44} = D_{55}} \mathbb{R}^2 \times (SE(2))_0 (z/2, x, \tilde{\beta}) \cdot \bar{p}_t^{D_{33}, D_{44} = D_{55}} \mathbb{R}^2 \times (SE(2))_0 (z/2, -y, \tilde{\gamma}) .
\]
In \([18, 9]\) one can find the exact solutions of the Green’s function \( \bar{p}_t^{D_{33}, D_{44} = D_{55}} \mathbb{R}^2 \times (SE(2))_0 \) related to the Green’s function \([29]\) on \( H(3) \) by means of a coordinate transform and in \([18]\) one can find the exact solutions of the Green’s function, \( p_t^{D_{33}, D_{44} = D_{55}} \mathbb{R}^2 \times (SE(2))_0 \), but these exact formulae are not as tangible as the following asymptotical formulae:
\[
\begin{align*}
\bar{p}_t^{D_{33}, D_{44} = D_{55}} \mathbb{R}^3 \times S^2 (x, y, \theta) & \equiv -\frac{1}{4\pi t} e^{-\frac{1}{4\pi t} \sqrt{\left(\frac{x_1^2}{\tau_1} + \frac{x_2^2}{\tau_2} + \frac{|y+\theta|}{\tau_4} \right)^2 + \frac{2\theta}{\tau_4} + \frac{2\theta}{\tau_4} \sin \theta + \frac{\theta^2}{\tau_4} \sin \theta} } , \\
\bar{p}_t^{D_{33}, D_{44} = D_{55}} \mathbb{R}^3 \times S^2 (x, y, \tau_4, \theta) & \equiv \begin{cases} e^{-\frac{1}{4\pi t} \sqrt{\left(\frac{x_1^2}{\tau_1} + \frac{x_2^2}{\tau_2} + \frac{|y+\theta|}{\tau_4} \right)^2 + \frac{2\theta}{\tau_4} + \frac{2\theta}{\tau_4} \sin \theta + \frac{\theta^2}{\tau_4} \sin \theta} } , & \text{if } \theta \neq 0 , \\
e^{-\frac{1}{4\pi t} \sqrt{\left(\frac{x_1^2}{\tau_1} + \frac{x_2^2}{\tau_2} + \frac{|y|}{\tau_4} \right)^2 + \frac{2\theta}{\tau_4} + \frac{2\theta}{\tau_4} \sin \theta + \frac{\theta^2}{\tau_4} \sin \theta} } , & \text{if } \theta = 0 .
\end{cases}
\end{align*}
\]
which are globally sharp estimates, with \( \frac{1}{2} < c < \sqrt{2} \), for details see \([18, \text{ch 5.4}]\).

### 6.2 Gaussian Estimates for the Heat-kernels on \( SE(3) \)

According to the general theory \([41]\) the heat-kernels \( p_t^{SE(3); q : D = \text{diag}(D_{33}, D_{44}, D_{55})} (SE(3))_q \rightarrow \mathbb{R}^+ \) (i.e. kernels for contour enhancement whose convolutions yield horizontal\(^{11}\) diffusion on \( (SE(3))_q \)) on the parameterized class of groups \( (SE(3))_q \), \( q \in [0, 1] \) in between \( SE(3) \) and its nilpotent Heisenberg approximation \( (SE(3))_0 \) satisfy the following Gaussian estimates (for \( D \) equal to the \( 3 \times 3 \) identity matrix \( I_3 \))
\[
C_1 e^{-\frac{C_2 |g|_2^2}{8t}} \leq p_t^{SE(3); q : D = I_3} (g) \leq C_3 e^{-\frac{C_4 |g|_2^2}{4t}} ,
\]
with \( 0 < C_1 < C_3 \) and \( 0 < C_4 < C_2 \), where the norm \( \| \cdot \|_1 : (SE(3))_q \rightarrow \mathbb{R}^+ \) is given by
\[
\| g \|_1 = | \log(SE(3))_q (g) |_q ,
\]
where \( \log(SE(3))_q : (SE(3))_q \rightarrow T_c ((SE(3))_q) \) is the logarithmic mapping on \( (SE(3))_q \) (which we computed explicitly for \( (SE(3))_q = SE(3) \) in Section 5.1 and which we will compute for \( q = 0 \) as well) and where the

\(^{11}\)Horizontal diffusion in \( SE(3) \) is diffusion which takes place along horizontal curves in \( \mathbb{R}^3 \times S^2 \rightarrow SE(3) \).
weighted modulus, [41], in our special case of interest is given by

$$\left| \sum_{i=1}^{6} c_i^q A_i^q \right|_q = \sqrt{|c_1^q| + |c_0^q| + |c_0^q|^2 + |c_1^q|^2 + |c_5^q|^2},$$

where $c_i^q \in \mathbb{R}$ and where we recall our weighting (59). However, similar to our work [18, ch:] on estimating (horizontal diffusion) heat-kernels on $SE(2)$, we estimate the weighted modulus by an equivalent differentiable modulus:

$$\left| \sum_{i=1}^{6} c_i^q A_i^q \right|_q = \sqrt{|c_1^q|^2 + |c_0^q|^2 + (|c_0^q|^2 + |c_1^q|^2 + |c_5^q|^2)^2},$$

where we note that $\sqrt{2}|g|^q \geq |g|_q \geq |g|^q$ for all $g \in (SE(3))_q$, $q \in [0, 1]$.

Now suppose $(c_1^q, \ldots, c_6^q) = (c_1^q(g), \ldots, c_6^q(g)) := \log_{(SE(3))_q}(g)$, then there exist constants $0 < \tilde{C}_1 < \tilde{C}_3$ and $0 < \tilde{C}_4 < \tilde{C}_5$ such that the following Gaussian estimates hold:

$$\tilde{C}_1 e^{-c_2 4 c_2} \leq \mathcal{P}_t \leq \tilde{C}_3 e^{-c_2 4 c_2},$$

(71)

where we again use short notation $c_i^q = c_i^q(g)$, $i = 1, \ldots, 6$. Now, from the applied point of view $D = I_3$ is an un-realistic situation and only for $q = 0$ there exist dilations on the group $(SE(3))_q$ so that we can easily generalize the estimates to the diagonal case $D = \text{diag}(D_{33}, D_{44}, D_{55})$.

Since $(SE(3))_0$ is a nilpotent Lie-group isomorphic to the matrix group (60) (where we take the limit $q \downarrow 0$) it is not difficult (this is much easier than the case $q = 1$, recall Section 5.1) to compute the exponent (recall (61)):

$$\exp \begin{pmatrix} 0 & -c_0^q & c_0^q & c_0^q \\ 0 & 0 & -c_0^q & c_0^q \\ 0 & 0 & 0 & c_0^q \\ 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & -c_0^q & c_0^q & c_0^q \\ 0 & 1 & -c_0^q & c_0^q \\ 0 & 0 & 1 & -c_0^q \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & -\tilde{\alpha} \tilde{\beta} x \\ 0 & 1 & -\tilde{\gamma} y \\ 0 & 0 & 1 & z \end{pmatrix}$$

and inverting these relations we find the simple formulas for the functions $c_i^q$ that we use in our estimates (73)

$$c_0^q(g) = x + \frac{1}{2} y \tilde{\alpha} - \frac{1}{2} z \tilde{\beta} + \frac{1}{2} z \tilde{\alpha} \tilde{\gamma}, \quad c_1^q(g) = \tilde{\gamma}, \quad c_2^q(g) = \tilde{\beta} - \frac{1}{2} \tilde{\alpha} \tilde{\gamma}, \quad c_3^q(g) = \tilde{\alpha}.$$

(72)

defined for all $g = (x, y, z, \begin{pmatrix} \tilde{\alpha} & \tilde{\beta} & \tilde{\gamma} \\ 0 & 1 & 0 \end{pmatrix}) \in (SE(3))_0$. By our embedding $\mathbb{R}^3 \times S^2$ into $SE(3)$, we must set $\tilde{\alpha} = 0$ and thereby $c_0^q = 0$. Consequently, for the Heisenberg approximations of the diffusion kernels on $\mathbb{R}^3 \times S^2$ we have

$$\tilde{C}_1 e^{-c_2 4 c_2} \leq \mathcal{P}_t (x, y, z, \tilde{\alpha}, \tilde{\beta}, \tilde{\gamma}) \leq \tilde{C}_3 e^{-c_2 4 c_2},$$

(73)

where we used short notation $\mathcal{P}_t = \mathcal{P}_t^{(SE(3))_0,D=I_3} : \mathbb{R}^3 \times S^2 \to \mathbb{R}^+$ for the Heisenberg approximation $q = 0$ of the contour enhancement kernel with $D_{33} = D_{44} = D_{55} = 1$. Now by application of the following dilation:

$$z' = \frac{z}{\sqrt{D_{33}}}, \quad x' = \frac{x}{\sqrt{D_{33}D_{44}}}, \quad \beta' = \frac{\beta}{\sqrt{D_{44}}}, \quad y' = \frac{y}{\sqrt{D_{33}D_{44}}}, \quad \tilde{\gamma}' = \frac{\tilde{\gamma}}{\sqrt{D_{44}}}$$

the generator of the corresponding diffusion on $\mathbb{R}^3 \times S^2$ for the general case where $D = \text{diag}(D_{33}, D_{44}, D_{55} = D_{44})$ relates to the diffusion generator for the case $D = I_3$, recall (62):

$$\sum_{i=3}^{5} D_{ii} (A_i^q)^2 = D_{33} (\tilde{\beta} \partial_x - \tilde{\gamma} \partial_y + \partial_z)^2 + D_{44} (\partial_x)^2 + D_{44} (\partial_y)^2 \leftrightarrow (\beta' \partial_x' - \tilde{\gamma}' \partial_y' + \partial_z')^2 + (\partial_x')^2 + (\partial_y')^2,$$
consequently, we find the following estimates for the general Heisenberg approximation kernels

\[ C_1 e^{-\frac{c_2}{4n}(\frac{|x_1|^2+|x_2|^2}{\sigma_{x_1}^2} + \frac{|x_3|^2+|x_4|^2}{\sigma_{x_2}^2})^2} \leq \tilde{p}_t^{D,q=0}(x, \tilde{n}(\tilde{\beta}, \tilde{\gamma})) \leq C_3 e^{-\frac{c_4}{4n}(\frac{|x_1|^2+|x_2|^2}{\sigma_{x_1}^2} + \frac{|x_3|^2+|x_4|^2}{\sigma_{x_2}^2})^2}, \]

(74)

where we used short notation \( c_k^q = c_k^q(x, R_{\tilde{\gamma}, \tilde{\beta}, 0}), k = 1, \ldots, 5, x = (x, y, z)^T \in \mathbb{R}^3 \), recall (72).

The exact value of the constants \( C_1 \) and \( C_2 \) is not crucial since in our convolution algorithms we normalize the convolution kernels anyway. Also the constants \( C_3 \) and \( C_4 \) can be taken into account by re-scaling time \( t \). Nevertheless, in order to guarantee the sharpness of our estimates the constants \( C_3 \) and \( C_4 \) resp. the constants \( C_1 \) and \( C_2 \) should be close. This indeed seems to be the case, as our previously derived approximation (68) can be re-expressed as

\[ p_t^{D_{33}, D_{44}=D_{55}}(x, y, 2z, \tilde{n}(\tilde{\beta}, \tilde{\gamma})) \approx \frac{1}{(4\pi t^2 D_{33} D_{44})^2} e^{-\frac{1}{4\pi t^2}(\frac{2|c_2|^2}{|\sigma_{x_1}|^2} + \frac{|c_3|^2}{|\sigma_{x_2}|^2} + \frac{|c_4|^2}{|\sigma_{x_3}|^2})}, \]

with constant \( \frac{1}{4} \leq c \leq \sqrt{2} \approx 1.19 \) due to our Gaussian estimates for contour-enhancement in \( SE(2), \) [18, ch:5.4]). Consequently, by the general results in [41, Prop.6.1] we conclude (similar to the \( SE(2) \)-case [18, ch:5.4,eq.5.28]) that a reasonable approximation and upperbound of the horizontal diffusion kernel on \( \mathbb{R}^3 \times S^2 \) is given by

\[ p_t^{D=\text{diag}(0,0,D_{33},D_{44},D_{55},0)}(x, \tilde{n}(\tilde{\beta}, \tilde{\gamma})) \approx \frac{1}{(4\pi t^2 D_{33} D_{44})^2} e^{-\frac{1}{4\pi t^2}(\frac{2|c_2|^2}{|\sigma_{x_1}|^2} + \frac{|c_3|^2}{|\sigma_{x_2}|^2} + \frac{|c_4|^2}{|\sigma_{x_3}|^2})}, \]

(75)

where we again use short notation \( c_k^q := c_k^q(x, R_{\tilde{\gamma}, \tilde{\beta}, 0}), k = 1, \ldots, 6 \). Recall from Section 5.1 that these constants are computed by the logarithm (57) on \( SE(3) \) or more explicitly by (55) and (56). The latter two equalities are analogously expressed in the second coordinate chart yielding formulas for the functions \( c_k^q : \mathbb{R}^3 \times S^2 \rightarrow \mathbb{R} \) in (75):

\[
\begin{align*}
\tilde{q} &= \arcsin \sqrt{\cos^2(\tilde{\gamma}/2) \sin^2(\tilde{\beta}) + \cos^4(\tilde{\beta}/2) \sin^2(\tilde{\gamma}/2)},

c^{(2)} &= (c^1, c^2, c^3)^T = \tilde{q} \left( \frac{\sin(\tilde{\gamma}) \cos\left(\tilde{\gamma}/2\right)}{\sin(\tilde{q})}, \frac{\sin\tilde{\beta} \cos\left(\tilde{\gamma}/2\right)}{\sin(\tilde{q})}, \frac{1}{2} \sin\tilde{\gamma} \sin\tilde{\beta} \right)^T,

c^{(1)} &= (c^1, c^2, c^3)^T = x - \frac{1}{2} c^{(2)} \times x + \tilde{q}^{-2}(1 - \left(\frac{\tilde{q}}{2}\right)^2) c^{(2)} \times (c^{(2)} \times x).
\end{align*}
\]

(76)

These functions \( c_k^q \) (the case \( q = 1 \)) are indeed consistent with the functions \( c_0^k \) (the case \( q = 0 \)) in the sense that \( \lim_{q \to 0} c^k(x, y, z, q, \beta) = c_0^k(x, y, z, \beta, \gamma) \), where we recall (59) for \( k = 1, 2, \ldots, 5 \).

7 Implementation of the Left-Invariant Derivatives and \( \mathbb{R}^3 \times S^2 \)-Diffusion

In our implementations we do not use the two charts (among which the Euler-angles parametrization) of \( S^2 \) because this would involve cumbersome and expensive bookkeeping of mapping the coordinates from one chart to the other (which becomes necessary each time the singularities (3) and (6) are arrived).

Instead we recall that the left-invariant vector fields on HARDI-orientation scores \( \tilde{U} : SE(3) \rightarrow \mathbb{R} \), which by definition (recall Definition 3) automatically satisfy

\[ \tilde{U}(R R e_{\tilde{\gamma}, \beta}) = \tilde{U}(R), \]

(77)

are constructed by the derivative of the right-regular representation

\[ A_i \tilde{U}(g) = (dR(A_i) \tilde{U})(g) = \lim_{h \downarrow 0} \frac{\tilde{U}(g e^{h A_i}) - \tilde{U}(g)}{h} = \lim_{h \downarrow 0} \frac{\tilde{U}(g e^{h A_i}) - 2 \tilde{U}(g e^{-h A_i})}{2h}, \]

are constructed by the derivative of the right-regular representation

\[ A_i \tilde{U}(g) = (dR(A_i) \tilde{U})(g) = \lim_{h \downarrow 0} \frac{\tilde{U}(g e^{h A_i}) - \tilde{U}(g)}{h} = \lim_{h \downarrow 0} \frac{\tilde{U}(g e^{h A_i}) - 2 \tilde{U}(g e^{-h A_i})}{2h}, \]

are constructed by the derivative of the right-regular representation

\[ A_i \tilde{U}(g) = (dR(A_i) \tilde{U})(g) = \lim_{h \downarrow 0} \frac{\tilde{U}(g e^{h A_i}) - \tilde{U}(g)}{h} = \lim_{h \downarrow 0} \frac{\tilde{U}(g e^{h A_i}) - 2 \tilde{U}(g e^{-h A_i})}{2h}, \]
where in the numerics we can take finite step-sizes in the righthand side. Now in order to avoid a redundant computation we can also avoid taking the de-tour via HARDI-orientation scores and actually work with the left-invariant vector fields on the HARDI-data itself. To this end we need the consistent right-action $\mathfrak{R}$ of $SE(3)$ acting on the space of HARDI-images $L_2(\mathbb{R}^3 \times S^2)$. To construct this consistent right-action we formally define $S : L_2(\mathbb{R}^3 \times S^2) \to H$, where $H$ denotes the space of HARDI-orientation scores, that equals the space of quadratic integrable functions on the group $SE(3)$ which are $\alpha$ right-invariant, i.e. satisfying (77) by
\[(SU)(x, R) = \hat{U}(x, R) = U(x, Re_z)\].

This mapping is injective and its left-inverse is given by $(S^{-1})U(x, n) = \hat{U}(x, R_n)$, where again $R_n \in SO(3)$ is some rotation such that $R_ne_z = n$. Now the consistent right-action $\mathfrak{R} : SE(3) \to B(L_2(\mathbb{R}^3 \times S^2))$, where $B(L_2(\mathbb{R}^3 \times S^2))$ stands for all bounded linear operators on the space of HARDI-images, is (almost everywhere) given by
\[(\mathfrak{R}(x, R)U)(y, n) = (S^{-1} \circ R_{(x, R)} \circ S)U(y, n) = U(R_n x + y, R_n Re_z)\].

This yields the left-invariant vector fields (directly) on sufficiently smooth HARDI-images:
\[
A_i U(y, n) = (d\mathfrak{R}(A_i))U(y, n) = \lim_{h \to 0} \frac{\mathfrak{R}_{y,h,A}(U)(y, n) - U(y, n)}{h} = \lim_{h \to 0} \frac{\mathfrak{R}_{y,h,A}(U)(y, n) - (\mathfrak{R}_{y,h,A}(U))(y, n)}{2h}.
\]

Now in our algorithms we take finite step-sizes and elementary computations (using the exponent (54)) yield the following simple expressions for the (horizontal) left-invariant vector fields:
\[
\begin{align*}
A_1 U(y, n) &\approx \frac{U(y+hRne_z, n) - U(y-hRne_z, n)}{2h}, \\
A_2 U(y, n) &\approx \frac{U(y+hRe_\gamma, e_\gamma) - U(y-hRe_\gamma, e_\gamma)}{2h}, \\
A_3 U(y, n) &\approx \frac{U(y+hRe_\beta, e_\beta) - U(y-hRe_\beta, e_\beta)}{2h}.
\end{align*}
\]

The left-invariant vector fields $\{A_1, A_2, A_4, A_5\}$ clearly depend on the choice of $R_n \in SO(3)$ which maps $R_ne_z = n$. Now functions in the space $H$ are $\alpha$-right invariant, so thereby we may assume that $R$ can be written as $R = R_{e_\gamma, e_\beta}$, now if we choose $R_n$ again such that $R_{\alpha, \beta} = R_{e_\gamma, e_\beta} R_{e_\gamma, e_\beta} \alpha \equiv 0 = 0$ then we take consistent sections in $SO(3)/SO(2)$ and we get full invertibility $S^{-1} \circ S = S \circ S^{-1} = I$.

In our diffusion schemes, however, the choice of representant $R_n$ is irrelevant, because we impose $\alpha$-right invariance (32) on the diffusion generator (which in the linear case boils down to (35)) and as a result we have $D_{44} = D_{55}$, $D_{11} = D_{22}$. The thereby obtained operators $(A_1)^2 + (A_3)^2 = \Delta_{S^2}|_H$ and $D_{11} = D_{22}$ and $(A_1)^2 + (A_5)^2$ are invariant under transformations of the type $A \to Z_{\alpha_0}A$ for all $\alpha_0 \in [0, 2\pi)$, recall (33).

In the computation of (78) one would have liked to work with discrete subgroups of $SO(3)$ acting on $S^2$ in order to avoid interpolations, but unfortunately the platonic solid with the largest amount of vertices (only 20) is the dodecahedron and the platonic solid with the largest amount of faces (again only 20) is the icosahedron. Nevertheless, we would like to sample the 2-sphere such that the distance between sampling points should be as equal as possible and simultaneously the area around each sample point should be as equal as possible. Therefore we follow the common approach by regular triangulations (i.e. each triangle is regularly divided into $(o + 1)^2$ triangles) of the icosahedron, followed by a projection on the sphere. This leads to $N_o = 2 + 10(o + 1)^2$ vertices. We typically considered $o = 1, 2, 3$, for further motivation regarding uniform spherical sampling, see [28, ch.7.8.1].

For the required interpolations to compute (78) within our spherical sampling there are two simple options. Either one uses a triangular interpolation of using the three closest sampling points, or one uses a discrete spherical harmonic interpolation. The disadvantage of the first and simplest approach is that it introduces additional blurring, whereas the second approach can lead to overshoots and undershoots. In the latter approach a $\pi$-symmetric function on the sphere only requires even values for $l \in \{0, 2, 4, \ldots, L\}$ in which case the total amount of spherical harmonics is $n_{SH} = \frac{1}{2}(L+1)(L+2)$. Now for decent reconstruction of the spherical sampling we need at least $n_{SH} > N_o$, which puts a lower bound on $L$ but on the other hand $L$ should not become too large as this would induce aliasing artefacts.
and instability. Although, there exist more efficient and accurate algorithms for discrete harmonic transforms (DSHT), [11, 34], we next give a brief explanation of the basic algorithm we used. To this end we first recall that the continuous spherical harmonic transform is given by

\[ (SHT(f))(l, m) = (Y^l_m, f)_{L^2(s_2)} = \int_0^{2\pi} \int_0^\pi Y^l_m(\beta, \gamma) f(\beta, \gamma) \sin \beta \, d\beta d\gamma. \]

The spherical harmonics (39) form a complete orthonormal basis in \( L^2(S^2) \), so the inverse is given by

\[ f(n(\beta, \gamma)) = \sum_{l=0}^\infty \sum_{m=-l}^l (SHT(f))(l, m) Y^l_m(\beta, \gamma) \]

for almost every \( \beta \in [0, \pi) \) and almost every \( \gamma \in [0, 2\pi) \). As mentioned before (in Subsection 4.1) the function \( f \) becomes a regular smooth function (which is defined everywhere) if we apply a slight diffusion on the 2-sphere:

\[ e^{t_{reg} \Delta L_B} f(n(\beta, \gamma)) = \sum_{l=0}^\infty \sum_{m=-l}^l e^{-t_{reg}(l+1)^2}(SHT(f))(l, m) Y^l_m(\beta, \gamma), \tag{79} \]

with \( 0 < t_{reg} \ll 1 \). Next we explain the discrete version of this transform.

**Discrete Spherical Harmonic Transform:** Given a sampling \( \{n_k\}_{k=1}^{N_o} \) of the sphere, we compute a matrix \( M = \left[ \frac{1}{\sqrt{c}} Y_{m(j)}^{l(j)} \right] \) with \( j \) an index that enumerates the spherical harmonics, which equals \( j(l, m) = 1 + l^2 + (m + l) \) if we want all values of \( l \) and \( j(l, m) = 1 + \frac{1}{2}(l - 1) + (m + l) \) if we only need even values of \( l \). The functions \( j \mapsto l(j), j \mapsto m(j) \) denote the inverse relations (uniquely determined since \( m \in \{-l, \ldots, l\} \)). Factor \( C = \sum_{j=1}^{N_o} |Y_{m(j)}^{l(j)}(0, 0)| \) is chosen such that \( \sum_{j=1}^{n_{SH}} M_{jk}M_{jk} = 1 \) for all \( k = 1, \ldots, N_o \). The DSHT of a sampled function \( f = (f_1, \ldots, f_{N_o}) \) on the sampled sphere equals \( s := DSHT[f] = (M \cdot \text{diag}(A))f \), where \( A = (A_S(n_1), \ldots, A_S(n_{N_o})) \) is a vector of weighting factors (to compensate for differences in the sampling densities of the sampling points) where the effective area surrounding \( n_i \) (i.e. the sum of all areas of direct-neighbor-triangles containing \( n_i \) as a vertex) is given by \( A_S(n_i) \). The inverse DSHT is given by \( DSHT^{-1}[s] = (\text{diag}(A))^{-1}M^{-1}s \), but is approximated by \( (\text{diag}(A^{-1}))M^T s \). Now as \( n_{SH} \) increases the matrix \( M \) becomes more and more unitary and the approximate inverse tends to the true inverse, see Figure 6. However if \( n_{SH} \) becomes too large aliasing artifacts arise.

Now we can approximate the continuous spherical harmonics coefficients by the discrete spherical harmonics coefficients and we can use (79) for interpolation.

### 7.1 Finite Difference Scheme for Linear \( \mathbb{R}^3 \times S^2 \) Diffusion

The linear diffusion system on \( \mathbb{R}^3 \times S^2 \) can be rewritten as

\[
\begin{cases}
\partial_t W(y, n, t) = (D_{11}((A_1)^2 + (A_2)^2) + (A_3)^2 + D_{44} \Delta_{S^2}) W(y, n, t) \\
W(y, n, 0) = U(y, n)
\end{cases}
\]

Figure 6: Effect of increasing spherical harmonic bandwidth \( L \) on the net operator matrix \( M^T M \) for the case \( N_o = 32 \) (first order tessellation of dodecahedron). Clearly, if one takes higher order spherical harmonics than strictly required, reconstruction of the sampled function on the sphere improves.
This system equals the Fokker-Plank equations of horizontal Brownian motion on $\mathbb{R}^3 \times S^2$ in case $D_{11} = 0$.

Spatially, we take second order centered finite differences for $\langle A_1 \rangle^2$, $\langle A_2 \rangle^2$ and $\langle A_3 \rangle^2$, i.e. we applied the discrete operators in the right-hand side of (78) twice, so for example we have

$$((\langle A_3 \rangle^2 W)(y, n, t) \approx \frac{W(y + 2hR_a e_z, n, t) - 2W(y, n, t) + W(y - 2hR_a e_z, n, t)}{2h},$$

where we apply the earlier mentioned interpolation methods (trilinear or by means of (79)). In our algorithm we apply a first order approximation in time (i.e. Euler-forward scheme)

$$\partial_t W(y, n, t) \approx \frac{W(y, n, t + \Delta t) - W(y, n, t)}{\Delta t},$$

where we choose $\Delta t$ small enough such that the algorithm is stable. In the orientation dimensions we calculate the Laplace operator on the sphere $\Delta_{S^2}$ via the spherical harmonic transform, where for stability purposes a small diffusion-regularization (79) is applied via the spherical harmonic domain as well, so we approximated

$$\Delta_{S^2} W(y, n(\beta, \gamma), t) \approx \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (l + 1)! e^{-t \rho_2 (l+1)} \left( SHT(W(y, n(\beta, \gamma), t)) \right) (l, m) Y_{lm}(\beta, \gamma). \quad (80)$$

For efficiency, the chain of operators, SHT- (80)-inverse SHT, is stored in a $N_o \times N_o$-matrix, so that calculation of $\Delta_{S^2}$ consists of a simple matrix-vector multiplication.

### 7.2 Convolution Schemes for Linear $\mathbb{R}^3 \times S^2$-Diffusion

Instead of a finite difference scheme one can use the theoretical fact that the solutions of the linear diffusions (37) are given by $\mathbb{R}^3 \times S^2$-convolution (38) with the corresponding (smooth) Green’s function $p_t^{D,a}$ that we derived analytically in Section 6. The convolution scheme is a straightforward discretization of $W(y, n, t) = (p_t^{D,a} *_{\mathbb{R}^3 \times S^2} U)(y)$ given by (10), where the integrals are usually replaced by sums using the mid-point rule (unless one has to deal with the singularity at the origin of the contour-completion kernel). This approach has computational advantages (in contrast to the $SE(2)$-convolutions) over the highly technical steerable $SE(3)$-convolutions [2, p.174-179]. We propose the following options to evaluate the Green’s function for contour enhancement (i.e. non-zero parameters are $D_{33} > 0$, $D_{44} = D_{55} > 0$ and $D_{11} = D_{22} \geq 0$) in the integration (38):

1. Use the finite difference scheme to numerically compute the Green’s function. Disadvantage: This requires interpolation. Advantage: If the time step $\Delta t << 1$ the numeric approximation of the kernel is very accurate.

2. if $D_{11} = D_{22} = 0$ we can use the analytic approximation formulae for the contour enhancement kernel. Here one can either use (75) where the functions $(x, n) \rightarrow \phi^k(x, n)$ are computed by means of the algorithm (76), or one may use the simpler but less accurate formula (69) using the asymptotical formula (70). In case $0 < D_{44}/D_{33} << 1$ one may want to use the fast Heisenberg approximation kernel (68) together with (70).

For the contour-completion case where the non-zero parameters are $a_3^3 = 1$, $D_{44} = D_{55} > 0$ generalizations of the finite difference scheme of the previous section are questionable due to the trade-off between accuracy of convection and stability of diffusion. Alternation of convection and diffusion with very small time steps (like described in [46] for the $SE(2)$-case) is probably preferable here. To avoid these highly technical issues we propose kernel-implémentations for the contour completion case, where we distinguish between the following options:

---

12 By means of the Gershgorin circle theorem one can guarantee stability, akin to left-invariant diffusions on $SE(2)$, cf. [27], [28, p.145-146].
$D_{44} = 0.005, t = 2$  $D_{44} = 0.005, t = 4$  $D_{44} = 0.005, t = 8$  $D_{44} = 0.015, t = 4$  Gaussian $D_{44} = 0.005, t = \frac{1}{\sqrt{2}}$

Figure 7: Left four figures: HARDI-Glyph visualization of the analytic approximations (for $0 < D_{44}/D_{33} << 1$) (69) using asymptotical formula (70) of the Green’s function $p_t^{D_{33},D_{44}:R^3\times S^2}$ for contour enhancement, which satisfies the semigroup property: $p_t^{D_{33},D_{44}:R^3\times S^2} * p_s^{D_{33},D_{44}:R^3\times S^2} = p_{t+s}^{D_{33},D_{44}:R^3\times S^2}$ and consequently there arise no artefacts (such as in Figure 5) in the iterative diffusion. We normalized the stretching parameter $D_{33} = 1$ and the values of $D_{44}$ and $t$ are depicted on top. The size of the kernel is controlled by $t > 0$, whereas $D_{44}$ controls the bending of the kernel. Right figure: HARDI-Glyph visualization of the close Gaussian estimation formula (75) using (76) for the Green’s function $p_t^{D_{33},D_{44}:R^3\times S^2}$ for $t = \frac{4}{\sqrt{2}}$ and $D_{44} = 0.005$.

1. For the more interesting resolvent of the contour-completion process use analytic formula (64) (which is accurate in case $0 < 4\lambda D_{44} << 1$).

2. For the time-dependent contour completion process use analytical formula (65) (which is accurate in case $0 < 4t D_{44} << 1$).

3. For both time-dependent and resolvent contour completion process one can use the accurate (at least in the neighborhood of the $z$-axis) relation (88) (in the spatial Fourier domain) to contour-completion on $SE(2)$, together with earlier developed algorithms [4, 5, 46, 18, 21] for contour completion on $SE(2)$.

Figure 7 shows HARDI-glyph visualizations of several contour enhancement kernels and Figure 8 shows HARDI-glyph visualizations of a contour completion kernel.

8 Experiments of Linear Crossing-preserving Diffusion on HARDI-images

We implemented linear, left-invariant diffusion on HARDI-data with diagonal diffusion matrix $D = \text{diag}(D_{ii})$ with $D_{11} = D_{22}, D_{44} = D_{55}$ (and $D_{66}=0$) using an explicit numerical scheme as explained in Subsubsection 7.1. Figure 9 and 10 show results of the linear diffusion process. In these examples an artificial three-dimensional HARDI dataset is created, to which Rician noise is added. Next, we apply two different $\mathbb{R}^3 \times S^2$-diffusions on both the noise-free and the noisy dataset. To visualize our results we used the DTI tool (see http://www.bmia.bmt.tue.nl/software/dtitool/) which can visualize HARDI glyphs using the Q-ball visualization method [10]. In the results, all glyphs are scaled.
$D_{44} = 0.07, \lambda = 0.05$

Singularity at $z = x = y = 0$

Figure 8: Left: HARDI-Glyph visualization of the analytic approximations (accurate for $0 < 4\lambda D_{44} << 1$) given by (64) of the Green’s function $p_{k}^{\lambda, D_{44}; R^{3} \times S^{2}}$ for contour completion. Top right: HARDI-glyphs at $(0, 0, z)$ with from left to right $z = 0.1, 0.5, 1, 1.5$. The contour completion kernel is single-sided (i.e. $p_{k}^{\lambda, D_{44}; R^{3} \times S^{2}}(x, y, z, n) = 0$ for $z < 0$), in contrast to the contour enhancement kernel depicted in Figure 7. The positive probability density kernel $p_{k}^{\lambda, D_{44}; R^{3} \times S^{2}}$ is $L_{1}$-normalized but has a singularity (bottom right) at the origin, akin to its 2D-equivalent [21, 35].
equivalently. The isotropic diffusion \( D_{43} = D_{22} = D_{11} \) does not preserve the anisotropy of the glyphs well; especially in the noisy case we observe that we get almost isotropic glyphs. With anisotropic diffusion, the anisotropy of the HARDI glyphs is preserved much better and in the noisy case the noise is clearly reduced. The resulting glyphs are, however, less directed than in the noise-free input image. This would improve when using nonlinear diffusion, which we will implement and test in future work. The basic theoretical PDE-framework for non-linear diffusions, analogue to non-linear diffusions on orientation scores of 2D-images, [27, 19], is the subject of the next section. As an alternative to non-linear adaptive diffusion, we are currently investigating the inclusion of thinning steps by means of left-invariant erosions (solutions of left-invariant Hamilton-Jakobi PDE’s on HARDI-data). See Figures 9 and 10.

9 Non-Linear, Adaptive, Left-Invariant Diffusions on HARDI-images

Our first aim is to estimate the locally best fitting exponential curve (54) to the probability density (for example HARDI data) \((y, n) \mapsto U(y, n) \in \mathbb{R}^+\) at each position \((y, n) \in \mathbb{R}^3 \times S^2\). Recall that such a distribution gives rise to a probability distribution \((x, R) \mapsto \tilde{U}(x, R)\) on \(SE(3)\) (which we call HARDI-orientation score) by means of (28).

To achieve our goal, we follow the same approach as in our previous works on non-linear diffusions on invertible orientation scores (of 2D-images) defined on \(SE(2)\) [25, p.118-120], [19, ch:3.4], [27, ch:5.2]. We again formulate a minimization problem that minimizes the “iso-contours” of the left-invariant gradient vector at position \(g\), leading to the optimal tangent vector \(c_*(y, n) = (c_1^*(y, n), \ldots, c_5^*(y, n), 0)^T\):

\[
    c_*(y, n) = \arg \min_{c(y, n)} \left\{ \left\| \frac{d}{dt} (\nabla \tilde{U}(g e^{c(y, n)}) \right\|_{\mu}^2 \left| \|c(y, n)\|_{\mu} = 1 \right. \right\},
\]

where the left-invariant gradient \(d\tilde{U} = \sum_{i=1}^5 A_i(\tilde{U}) \ dA_i\), a co-vector, is represented by row-vector given by

\[
    \nabla \tilde{U} = A\tilde{U} = (A_1\tilde{U}, \ldots, A_5\tilde{U}, 0).
\]

where \(\| \cdot \|_{\mu}\) denotes the norm on a vector in tangent space \(T_g(SE(3))\) (i.e. the norm at the right side) resp. on a covector in the dual tangent space \(T^*_g(SE(3))\) (the norm on the left side). We represent tangent vectors

\[
    c(y, n) = \sum_{i=1}^5 c_i^*(y, n) \ A_i|_{g=(y, R_n)}
\]

as column-vector \(c(y, n) = (c_1^*(y, n), \ldots, c_5^*(y, n), 0)^T\) and their norm is defined by \(\|c\|_{\mu} := \sqrt{(c, c)_\mu}\) with the inner product \((c, c)_\mu := \mu^2 \left( \sum_{j=1}^3 c_j^2 c_j^2 \right) + \sum_{j=4}^6 c_j^2 c_j^2\). where parameter\(^{13}\) \(\mu\) ensures that all components of the inner product are dimensionless. The value of the parameter determines how the distance in the spatial dimensions relates to distance in the orientation dimension. Implicitly, this also defines the norm on covectors by \(\|\tilde{c}\|_{\mu} = \sqrt{(\tilde{c}, \tilde{c})_{\mu}}\), \((\tilde{c}, \tilde{c})_{\mu} = (\tilde{c}, G_{\mu}^{-1}\tilde{c}) = \mu^2 \left( \sum_{j=1}^3 c_j c_j \right) + \sum_{j=4}^6 c_j c_j\). By means of the calculus of variations it follows that the minimizer \(c_*(y, n)\) satisfies

\[
    (M_{\mu} \mathcal{H}\tilde{U}(g) M_{\mu})^T (M_{\mu} \mathcal{H}\tilde{U}(g) M_{\mu}) \tilde{c}^*(y, n) = \lambda \tilde{c}^*(y, n),
\]

where \(M_{\mu} := \text{diag}(1/\mu, 1/\mu, 1/\mu, 1, 1, 1)\) and \(\tilde{c} = M_{\mu}^{-1}c\) and where the 6 × 6 Hessian of \(\tilde{U}\) on \(\mathbb{R}^3 \times S^2\) is given by

\[
    \mathcal{H}\tilde{U}(g) = [A_j A_i U(g)]^i_{\text{row-index}} j_{\text{column index}}, \quad g = (y, R) \in SE(3).
\]

\(^{13}\)In some of our previous works on \(SE(2)\) we denoted this fundamental parameter by \(\beta > 0\), but here we use \(\mu > 0\) to avoid confusion with Euler-angle \(\beta > 0\) in \(SO(3)\).
Figure 9: Result of $\mathbb{R}^3 \times S^2$-diffusion on an artificial HARDI dataset of two crossing straight lines where one of the lines is curved, with and without added Rician noise with $\sigma = 0.17$ (signal amplitude 1). Image size: $10 \times 10 \times 10$ spatial and 162 orientations. Parameters of the isotropic diffusion process: $D_{11} = D_{22} = D_{33} = 1, D_{44} = D_{55} = 0.01$. Parameters of the anisotropic diffusion process: $D_{11} = D_{22} = 0.01, D_{33} = 1, D_{44} = D_{55} = 10^{-4}$. In both cases we have set $t_{reg} = 0.01$ in (79).
Figure 7.10: Result of $R^3 \rtimes S^2$-diffusion on an artificial HARDI dataset of two crossing lines where one of the lines is curved, with and without added Rician noise with $\sigma = 0.17$ (signal amplitude 1). Image size: $10 \times 10 \times 10$ spatial and 162 orientations. Parameters of the isotropic diffusion process: $D_{11} = D_{22} = D_{33} = 1, D_{44} = D_{55} = 0.01$. Parameters of the anisotropic diffusion process: $D_{11} = D_{22} = 0.01, D_{33} = 1, D_{44} = D_{55} = 10^{-4}$. In both cases we have set $t_{reg} = 0.01$ in (79).
where the last row contains of zero’s only. This amounts to eigensystem analysis of the symmetric $6 \times 6$ matrix-valued function $g \mapsto (M_{\mu} \mathcal{H} \hat{U}(g) M_{\mu})^7 (M_{\mu} \mathcal{H} \hat{U}(g) M_{\mu})$, where one of the three eigenvectors gives $\mathbf{c}_e(y, n)$. The eigenvector with the smallest corresponding eigenvalue is selected as tangent vector $\mathbf{c}_e(y, n)$, and the desired tangent vector $\mathbf{c}_e(y, n)$ is then given by $\mathbf{c}_e(y, n) = M_{\mu} \mathbf{c}_e(y, n)$.

Now that we have computed the optimal tangent vector $\mathbf{c}(y, n)$ at $(y, n) \mapsto U(y, n)$ (and thereby the best fitting exponential curve $t \mapsto g e^{\sum_{i=1}^d e^{A_i t}}$ in $\mathbb{R}^3 \times S^2$) we construct the non-linear adaptive diffusion function as follows:

$$
D(U)(y, n) = c_e(y, n) \mathbf{c}(y, n) \left( \frac{\|c(y, n)\|^2}{\mu} + D_o(U)(y, n) \left( \begin{array}{ccc} I_3 & 0 & 0 \\ 0 & \mu^2 I_3 \\ \end{array} \right) \right),
$$

where $D_o(U)(y, n)$ is a locally adaptive anisotropy factor. Finally, we note that the conditions (34) are satisfied so our final well-defined non-linear diffusion system on the HARDI-data are:

$$
\begin{cases}
\partial_t W(y, n, t) = (A_i [D(U)(y, n)]_{ij} A_j W)(y, n, t), \\
\lim_{t \to 0} W(y, n, t) = U(y, n).
\end{cases}
$$

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### A Towards an Exact Analytic Formula for the Direction Process in 3D

Recall from Section 4.1 that the Fokker-Plank equation of the direction process (for contour completion) in $\mathbb{R}^3 \times S^2$ is given by (40), which is a special case of (37) with $D = \text{diag} \{0, 0, 0, D_{44}, D_{55} = D_{44} \}$ and $a = (0, 0, 1, 0, 0)$. Now in order to derive its Green’s function (i.e. “impulse response”) we must set the initial condition as a single Dirac-delta at the unity element $(0, e_z) \in \mathbb{R}^3 \times S^2$. So we must derive

$$
p_s(y, n, s) = e^{\rho((A_4)^2 + (A_5)^2 - A_3)} \delta_{\rho} \otimes \delta_{e_z},
$$

explicitly. To this end we should get a grip on the spectrum of the generator $A_4^2 + A_5^2 - A_3$, which is an unbounded operator on the space of HARDI-images $\mathcal{L}_2(\mathbb{R}^3 \times S^2)$. Analogously to our derivation of the exact Green’s function for contour completion in $SE(2)$ we apply a spatial Fourier transform. So we would like to find the exact solutions of

$$
\mathcal{F}_{\mathbb{R}^3} (D_{44}((A_4)^2 + (A_5)^2 - A_3))^{-1} \hat{U} = \lambda \hat{U},
$$

where $\hat{U}(\omega, n) = [\mathcal{F}_{\mathbb{R}^3} Q(\cdot, n)](\omega)$. We use the following parametrization for the variable in Fourier domain

$$
\omega = (\omega_x, \omega_y, \omega_z) = \rho (\sin \beta, \sin \gamma, \cos \beta \cos \gamma), \text{ with } \beta, \gamma \in [-\pi, \pi], \rho = \|\omega\| > 0,
$$

since it is consistent with our parametrization $n = n(\beta, \gamma) \in S^2$ given by (5). Now note that $\mathcal{F} A_3 \mathcal{F}^{-1} = i \omega \cdot n$ and thereby we can rewrite (84) as

$$
(B_\omega \hat{U})(\omega, n(\beta, \gamma)) = \lambda \hat{U}(\omega, n(\beta, \gamma)), \text{ where the generator in the spatial Fourier domain equals}
$$

$$
B_\omega = \frac{D_{44}^2}{\cos^2(\beta)} (\partial_\theta)^2 + D_{44}(\partial_\beta)^2 - \rho \left( \cos(\beta - \bar{\beta}) - 2 \cos \beta \cos \bar{\beta} \sin^2 \left( \frac{\beta - \bar{\beta}}{2} \right) \right)
$$

(85)
which is rather difficult to solve. Therefore, we apply the approximation $\cos \tilde{\beta} = 1 + O(\tilde{\beta}^2) \approx 1$ while maintaining all other dependencies on $\tilde{\beta}$. This is somewhat similar to the Heisenberg-approximations, [21, ch:4.3] but this time without destroying the periodicity. So we must solve

\[
(D_{44}(\beta)^2 - i\rho \cos(\beta - \tilde{\beta}) + D_{44}(\beta)^2 - i\rho \cos(\gamma - \tilde{\gamma}) - i\rho \cos \beta) \hat{U}_{\text{approx}}(\omega, \tilde{n}(\beta, \tilde{\gamma})) = \lambda \hat{U}_{\text{approx}}(\omega, \tilde{n}(\beta, \tilde{\gamma})),
\]

so for each $\omega \in \mathbb{R}^3$ fixed, the operator on the left is a sum of two commuting Mathieu-operators, so we can apply the method of separation. To this end we write

\[
\hat{U}_{\text{approx}}(\omega, \tilde{n}(\beta, \tilde{\gamma})) = B(\beta)C(\tilde{\gamma}),
\]

So by the periodicity constraints we find

\[
D_{44} \left( \frac{B''(\beta)}{B(\beta)} + \frac{C''(\tilde{\gamma})}{C(\tilde{\gamma})} \right) - i\rho (\cos(\beta - \tilde{\beta}) + \cos(\gamma - \tilde{\gamma})) = \lambda_1 + \lambda_2 = \lambda + i\rho \cos \beta,
\]

where the eigenvalue $\lambda$ of the generator equals the sum of $-i\rho \cos \beta$ and the separations constants $\lambda_1, \lambda_2$. So we have the following Sturm-Liouville-type of system for $C$:

\[
\begin{cases}
C''(\tilde{\gamma}) - i\frac{D_{44}}{B(\beta)} \cos(\gamma - \tilde{\tau})C(\tilde{\gamma}) = \lambda_1 \\
C(-\pi) = C(\pi)
\end{cases}
\]

where we evaluate $C : [-\pi, \pi] \to \mathbb{R}$ later only from $[-\frac{\tilde{\tau}}{2}, \frac{\pi}{2}]$ whose the countable eigen-solutions are given by

\[
C_n(\tilde{\gamma}) = \frac{1}{2\pi} ce_n(\frac{\tilde{\gamma} - \tilde{\tau}}{2}, \frac{2\rho i}{D_{44}}) \quad \text{with eigenvalue } \lambda_1 = \lambda_1^n = a_n\left(\frac{2\rho i}{D_{44}}\right), \quad n = 0, 1, 2, 3, \ldots,
\]

where the function $q \mapsto a_n(q)$ denotes the Mathieu-characteristics, [39, 1] and where $ce_n(., q)$ denotes the cosine elliptic Mathieu-function (with Floquet exponent $n$), [39, 1], which is a $\pi$-periodic solution of Mathieu’s equation $y''(z) + 2q \cos(2z)y(z) = a_n(q)y(z)$. Similarly, the eigensystem of

\[
\begin{cases}
B''(\beta) - i\frac{D_{44}}{B} \cos(\beta - \tilde{\tau})B(\beta) = \lambda_1 \\
B(-\pi) = B(\pi)
\end{cases}
\]

is given by $B_m(\beta) = \frac{1}{2} \frac{\sqrt{D_{44}}}{D_{44}} ce_n\left(\frac{3\beta - \tilde{\tau}}{2}, \frac{2\rho i}{D_{44}}\right)$ with eigenvalue $\lambda_1^n = a_m\left(\frac{2\rho i}{D_{44}}\right), \quad m = 0, 1, 2, 3, \ldots$. Consequently, a complete set of bi-orthogonal\textsuperscript{14} eigenfunctions (with eigen values $\lambda_{mn}$) of the generator $B_\omega$ is given by

\[
\hat{U}_{mn}(\omega, \tilde{n}(\beta, \tilde{\gamma})) = ce_n\left(\frac{\beta - \tilde{\tau}}{2}, \frac{2\rho i}{D_{44}}\right) ce_n\left(\frac{\gamma - \tilde{\tau}}{2}, \frac{2\rho i}{D_{44}}\right) \quad \text{and} \quad \lambda_{mn}(\omega) = -i\rho \cos \beta - \frac{a_m(\frac{2\rho i}{D_{44}})}{4} < 0.
\]

Consequently, we have the following approximation formula for $p_{44}^{SE(2), D_{44}}$ of the Green’s function $p_{44}^{SE(2), D_{44}} : (SE(2) \setminus \{e\}) \to \mathbb{R}^+$ of the direction process in $SE(2)$. In fact we have the following intriguing geometrical relation

\[
\mathcal{F}_{\mathbb{R}^3}\left(e^{t((A_4)^2+(A_5)^2-A_3)}|_{\cos \beta=1} \delta_{\theta} \otimes \delta_{\varphi}\right)(\omega, \tilde{n}(\beta, \tilde{\gamma})) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} e^{t\lambda_{mn}(\omega)} \hat{U}_{mn}(\omega, \tilde{n}(\beta, \tilde{\gamma})) \hat{U}_{mn}(0, \tilde{n}(\beta, \tilde{\gamma})).
\]  

Now this expression is quite similar to one of our exact formulas for the (spatial) Fourier transform $\mathcal{F}_{\mathbb{R}^3} p_{44}^{SE(2), D_{44}}$ of the Green’s function $p_{44}^{SE(2), D_{44}}$ of the Green’s function of the contour completion process in $SE(2)$ for the computation of the approximation (88) of the Green’s function of the contour completion process in $SE(3)$.

\textsuperscript{14}Here bi-orthogonality means that the conjugation is omitted in the $L_2$ inner-product, i.e. $\int_{-\pi}^{\pi} \int_0^{2\pi} \int_{0}^{2\pi} \hat{U}_{mn}(\beta, \varphi) \hat{U}_{mn}(\beta, \varphi) d\beta d\varphi = \delta_{m'n'} \delta_{nn'}$, which follows from the fact that $(B_\omega)^* \phi = B_\omega^2 \phi$ for all $\phi \in H^2([-\pi, \pi] \times [0, 2\pi])$. 

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References


[18] R. Duits, and E.M. Franken Left invariant parabolic evolution equations on SE(2) and contour enhancement via invertible orientation scores, part I: Linear left-invariant diffusion equations on SE(2) Accepted for publication in the Quarterly on Applied mathematics, AMS, to appear in 2009.


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