Automatic Construction of Correspondences for Tubular Surfaces
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Abstract—Statistical shape modeling is an established technique and is used for a variety of tasks in medical image processing, such as image segmentation and analysis. A challenging task in the construction of a shape model is establishing a good correspondence across the set of training shapes. Especially for shapes of cylindrical topology, very little work has been done. This paper describes an automatic method to obtain a correspondence for a set of cylindrical shapes. The method starts from an initial correspondence which is provided by cylindrical parameterization. The quality, measured in terms of the description length, of the obtained correspondence is then improved by deforming the parameterizations using cylindrical b-spline deformations and by optimization of the spatial alignment of the shapes. In order to allow efficient gradient guided optimization, an analytic expression is provided for the gradient of this quality measure with respect to the parameters of the parameterization deformation and the spatial alignment. A comparison is made between models obtained from the correspondences before and after the optimization. The results show that, in comparison with parameterization based correspondences, this new method establishes correspondences that generate models with significantly increased performance in terms of reconstruction error, generalization ability, and specificity.

Index Terms—point correspondence problem, statistical shape models, tubular structures, minimum description length, image segmentation, image shape analysis.

I. INTRODUCTION

SHAPE correspondences and the derived statistical shape models have a wide range of applications in medical image computing [1], [2]. They have been used to analyze shape differences between different classes of objects, for example, the lateral ventricles of schizophrenics versus a healthy group [3]. They have also been employed to gain more knowledge about the anatomical variability of certain organs or bones as for example the human ear canal [4]. Such knowledge can in turn be used to reconstruct malformed, missing, or fractured bone structures [5]. A widespread application of statistical shape models is their use as prior knowledge in automatic image segmentation [6]–[8]. The probability density function of the shape is estimated from a set of manual segmentations. This knowledge is then used to guide the segmentation process of an unseen instance and to restrict the segmentation result to the class of plausible shapes.

The major hurdle in the construction of a statistical shape model is establishing a dense correspondence over the surfaces of a large set of training shapes. These correspondences should be of high quality, i.e., the correspondence should match anatomically equivalent points over the surfaces. If this requirement is not met, artificial modes of variation are introduced into the shape model and this has a negative effect on the performance of the model when used for image segmentation or interpretation [9].

For 2D shapes, a correspondence between the boundary curves of the individual shapes is often defined by manual landmarking [10]. Although this approach is feasible, it turns out to be a time-consuming and error-prone task. In principle, the approach can be extended to 3D but it becomes highly impractical due to the large amount of landmarks that need to be located and the increased level of difficulty in pin-pointing them. Several approaches have been proposed to automate this labor-intensive procedure.

A relatively simple but effective approach is to establish the sought-after correspondence by means of surface parameterization [11]–[17]. Thereby, a one-to-one map is constructed between each surface of the set and some common, predefined and usually mathematically simple parameter domain, such as a planar disc or a sphere. For each surface, the obtained one-to-one map associates a 2D parameter coordinate with each point of the 3D surface. The surface-to-surface correspondence is then defined by the assigned parameter values i.e., points between the surfaces correspond when they share the same parameters.

Although the parameterization approach produces valid correspondences, there is still room for improvement. The parameterization of each shape in the training set is done independently of the other shapes, thus correlations between the shapes are not taken into account. When an approach takes this extra information into account, it can obtain better correspondences. Surface parameterization can provide a good initial correspondence for such a method. Davies et al. developed such a correspondence method in [18]. They use the description length of the derived shape model as a measure of correspondence quality and optimize the correspondences with respect to this criterion. To date, their minimum description length (MDL) approach is considered the method of choice for the construction of correspondences [9].

Most of the aforementioned techniques focus on sets of surfaces of spherical topology since these are prevalent in biomedical image processing, e.g., kidneys, liver, and brain ventricles. Nonetheless, the developed principles can be translated to surfaces of other topologies. More specifically, this paper deals with the translation of these principles to sets of surfaces of cylindrical topology, such as the trachea, cochlear channels, aortic aneurysms, and the rectum. For such surfaces, the cylinder is the natural choice for the parameter domain. An initial correspondence is obtained by specialized cylindrical parameterization techniques. Following this, the correspondence is improved by an optimization framework that adopts
the MDL criterion as a measure of correspondence quality.

The remainder of this paper is organized as follows. Related work is discussed in Section I-A. An overview of the correspondence method is given in Section II. Parameterization of surfaces of cylindrical topology is discussed in Section III. The measure of correspondence quality, namely description length, is treated in Section IV. Section V details the procedure of how an initial correspondence is obtained and Section VI elaborates on the correspondence optimization. Experimental results of applying the method to a number of phantoms and real data sets are presented and discussed in Section VII. Section VIII concludes the paper.

A. Related Work

Parameterization of surfaces with disc-like topology onto a planar convex region has been addressed in [11]. A parameterization technique to parameterize surfaces of spherical topology onto the sphere has been developed by Brechbühler et al. [12] and is known as SPHARM. This was later used to model the shape of brain structures for segmentation [6] and analysis [3]. Conformal parameterization techniques for surfaces of spherical topology were introduced in [19]–[21]. A more efficient alternative to SPHARM, utilizing a progressive surface representation, was provided by Praun and Hoppe [13]. Based on this spherical parameterization technique, Huysmans et al. have developed a cylindrical parameterization technique to parameterize tubular surfaces onto the cylinder in a progressive way [14]. Conformal parameterization of surfaces of cylindrical topology was addressed in [22], [23] and [24]. Algorithms for more complex topologies (genus-n) have also been proposed [15]–[17] but, from a correspondence optimization point of view, these algorithms are suboptimal since they rely on a heuristic or manually defined surface chartification. In [25] Ricci flow is used to construct a seamless periodic tiling of a genus-n surface in the plane, sphere, or hyperbolic space and it is known as the universal covering space. The obtained map is angle preserving and can be used to construct harmonic maps between surfaces of the same topology [32].

In [26], Kottche and Taylor used the determinant of the landmark covariance matrix as an optimization objective. Based on their ideas, Davies et al. developed a minimum description length (MDL) formulation for the assessment of correspondence quality for 2D curves [18], which was later simplified by Thodberg [27]. The method for building MDL correspondences has been extended to surfaces of spherical topology [28], which was later improved by Heimann et al. [29] in terms of computational efficiency. Horkev and Yang applied the MDL principle to surfaces of disk-like topology [30] and an extension to more complex topologies was obtained by cutting surfaces into topological discs prior to optimization [31]. This of course constrains the optimization along the cuts. In the recent work of Li et al. [32], a globally optimal map, in terms of harmonic energy, is obtained between two surfaces sharing arbitrary complex topology. An extension of their method to populations of surfaces and to other correspondence metrics, e.g. MDL, is, however, not addressed. Recently introduced point-based correspondence techniques can also handle arbitrary topology. In [34], Ferrarini et al. use self organizing maps to obtain a pairwise correspondence between each population member and a template. In [33], Cates et al. use particle systems to optimize geometry sampling and groupwise correspondence with respect to an information theoretic measure comparable to MDL. Point-based correspondence techniques are promising but problems occurring with highly convoluted surfaces still need to be addressed.

Little work has been done in shape modeling for cylindrical surfaces. In [35], de Bruijne et al. proposed an improved modeling scheme for tubular objects. They used a manually determined correspondence. Some of the previously discussed techniques could be employed to build a correspondence for a set of cylindrical shapes. For example, the spherical MDL framework can be applied when the holes of the cylindrical shapes are closed but this can result in an invalid correspondence at the boundaries and this approach will not perform well for elongated surfaces [36]. The correspondence methods that rely on chartification [16], [31] could also be applied to cylindrical surfaces but obviously the performance of the chartification heuristic will influence the final quality. The method proposed in this paper does not suffer from these drawbacks since, here, the description length minimization method is translated specifically to treat sets of surfaces of cylindrical topology.

II. Method Outline

The method, treated in this paper, constructs a dense surface correspondence together with an optimal spatial alignment for an arbitrary population of cylindrical surfaces. It proceeds in two steps. First, a correspondence is derived from the surface parameterizations by alignment of the surfaces and parameterizations. The result is referred to as the rigid correspondence. Then, the rigid correspondence is improved by applying local, non-rigid, deformations to the parameterizations while keeping the surfaces optimally aligned. The finally obtained correspondence is referred to as the non-rigid correspondence. An overview of these two steps can be found in Figure 1.

The input to the method is a set of \( n_s \) triangle surfaces \( \{M_1, \ldots, M_{n_s}\} \) of cylindrical topology. Each surface \( M_i \) is defined by a tuple \( (V_i, T_i) \), where \( V_i \) is the set of \( n_{\text{verts}} \) vertices \( \{v_1^i, \ldots, v_{n_{\text{verts}}}^i\} \) with \( v_j^i \in \mathbb{R}^3 \) and \( T_i \) is the set of \( n_{\text{tris}} \) triangles \( \{t_1^i, \ldots, t_{n_{\text{tris}}}^i\} \).

The construction of the rigid correspondence is covered by the flow chart in Figure 1(a) and presented in detail in Section V. The rigid correspondence, denoted as \( \{x_1, \ldots, x_{n_s}\} \), is obtained by parameterization of the surfaces \( M_i \), followed by rigid alignment of the surfaces and their parameter spaces. The spatial transformations for the alignment of the surfaces are denoted \( \tau^o(\cdot|\Phi_i^o) \) and the parameterization transformations for the parameter space alignments are denoted \( \rho^o(\cdot|\Phi_i^o) \). In order to avoid convergence to local minima, the optimal parameters \( \Phi_i^o \) and \( \Phi_i^o^\tau \) of these transformations are obtained by a number of consecutive optimizations with respect to the MDL correspondence quality criterion, denoted \( \mu \). The
construction pipeline for the rigid correspondence comprises following steps:

1. A cylindrical parameterization $x_i^p$ is constructed for each surface $M_i$. It constitutes a one-to-one map between the surface $M_i$ and the open-ended cylinder $C^2_h$ of height $h$.

2. A smooth b-spline approximation $\hat{x}_i^p$ is constructed for each surface. The b-spline representation results in smooth optimization objectives and provides a multi-resolution representation of the surface.

3. An initial spatial alignment of the surfaces is obtained by alignment of their principal axes.

4. While keeping the spatial alignment fixed, an alignment of the parameterizations is determined by optimization with respect to MDL.

5. Both the spatial and parameter space alignments are improved by simultaneous optimization with respect to MDL.

In order to obtain the rigid correspondence, the optimal spatial transformations and parameterization transformations are applied to the b-spline approximations of each of the parameterized surfaces:

$$x_i = \hat{\tau}^p(\bullet|\hat{\Phi}_i^{L_0}) \circ \hat{x}_i^p \circ \rho^p(\bullet|\hat{\Phi}_i^{L_0}).$$  \hspace{1cm} (1)

The construction of non-rigid correspondence is covered by the flow chart in Figure 1(b) and is presented in detail in Section VI. The non-rigid correspondence is obtained as an improvement of the rigid correspondence by applying a non-rigid b-spline transformation to the parameter space of each surface and simultaneously optimizing their spatial alignment.

Again, the MDL correspondence criterion was used as the optimization objective. For reasons of efficiency and in order to avoid local minima, the optimization is done successively at a number of resolution levels. With each resolution level $L$, the grid size $n_{L_0} \times n_{L_1}$ for the b-spline approximation $\hat{x}_i^L$ of $x_i$ and the grid size $n_{L_0} \times n_{L_1}$ for the b-spline parameterization deformation $\rho^L(\bullet|\hat{\Phi}_i^{L_0})$ is doubled, allowing for a more detailed correspondence improvement. Also, the number of landmarks $n_p^L$ used to calculate the shape model is increased and the convergence tolerance becomes more strict.

The spatial transformation $\tau(\bullet|\hat{\Phi}_i^{L_0})$ is rigid and has optimal parameters $\hat{\Phi}_i^{L_0}$. The optimization of a resolution level $L$ is initialized with the result from the previous resolution level $L - 1$. The final correspondence is obtained from the optimal transformation parameters $\hat{\Phi}_i^{L_0}$ and $\hat{\Phi}_i^{L_1}$ of the last resolution level:

$$\hat{x}_i^L = \tau(\bullet|\hat{\Phi}_i^{L_0}) \circ \hat{x}_i^L \circ \rho^L(\bullet|\hat{\Phi}_i^{L_0}).$$  \hspace{1cm} (2)

From the final correspondence $\{\hat{x}_1, \ldots, \hat{x}_{n_s}\}$, a map from surface $M_i$ to surface $M_j$ can be obtained by composition of the inverse of parameterization $\hat{x}_i$, with the parameterization $\hat{x}_j$, i.e. $q = \hat{x}_j \circ \hat{x}_i^{-1}(p)$, where $p \in M_i$ and the corresponding point $q \in M_j$.

III. SURFACE REPRESENTATION

A. Parameterization

Starting from a cylindrical surface $M$ defined by its vertices $V$ and triangles $T$, a parameterized version $x$ of $M$ is obtained by assigning a unique pair of cylindrical coordinates to each point of the surface $M$. Usually, the parameter coordinates are only defined explicitly at the vertices of $M$ and the extension over the triangles is implied by barycentric interpolation of the parameter coordinates at the vertices. To be more precise, for surfaces of cylindrical topology, the parameterization $x$ is a homeomorphic function from $C^2_h$ to the surface $M$, i.e.:

$$x : [0, 2\pi] \times [0, h] \to M \subset \mathbb{R}^3,$$

where $C^2_h$ denotes the open-ended two-dimensional cylinder of length $h$ with unit radius, which is parameterized by an angular coordinate $u^0$ and an axial coordinate $u^1$, i.e. $u = (u^0, u^1)$. For $x$ to be a homeomorphism, it must be a bijective, continuous function, and have a continuous inverse.

If the topology of $M$ is consistent, such a homeomorphism can always be obtained although a solution is not unique. This can be seen from the fact that the composition $x \circ \rho$ of any automorphism $\rho$ of the cylinder with the parameterization $x$ of the surface $M$, again is a valid parameterization of the same surface. The particular solution that a parameterization technique will propose is usually the result of the minimization of an energy functional. Different functionals result in different parameterizations, the quality of which depends on the actual application.

In order to obtain good correspondences between surfaces, a parameterization technique should create similar maps for similar surfaces. In addition, it is also desirable that it retains relative areas and angles as much as possible (i.e. distortion). When the parameterizations systematically suffer from large area distortions, undersampling of parts of the surface can occur in the final correspondence. For a tubular surface with an approximately constant width, the use of an harmonic parameterization technique is recommended, e.g. [22], [23]. The harmonic cylindrical parameterization is uniquely defined as the solution of a system of linear equations. As a consequence, it is computationally very efficient. However, it fails to keep...
Fig. 1. (a) Flow chart visualization of the rigid correspondence construction. First, each surface is equipped with a cylindrical parameterization and approximated with a b-spline surface. Then, the surfaces are brought into a reference coordinate system by alignment of their principal axes. This is followed by the alignment of the parameter spaces of the surfaces by optimization w.r.t. the correspondence quality i.e., model description length. Finally, the rigid correspondence is obtained after a second optimization, where both the spatial and parameterization alignment parameters are set free. (b) Flow chart visualization of the non-rigid correspondence improvement. The correspondence is improved by simultaneously optimizing the parameters of the spatial alignments and the b-spline parameterization deformations w.r.t. the correspondence quality. The optimization is performed at multiple resolution levels sequentially, starting at the lowest level with coarse deformations and gradually adding more detail with each new level. Finally, the non-rigid correspondence is obtained.
area distortions within acceptable bounds when large variation in cross-sectional diameter is present. For these cases, the progressive non-linear cylindrical parameterization technique from [14] is a better alternative. It allows control over the trade-off between angle and area distortions, at the cost of an increased computation time. See Figure 2 for a comparison of the two methods.

B. B-Spline Representation

Since the surface $\mathcal{M}$ is a piecewise linear surface, the partial derivatives of the surface coordinates with respect to the parameter coordinates ($\frac{\partial x}{\partial u}$ and $\frac{\partial x}{\partial v}$) are discontinuous at the triangle boundaries, excluding boundaries between coplanar triangles. This is undesirable since these partial derivatives are utilized in the gradient guided optimization of the correspondences. Using cubic b-splines, approximation of $x$ will result in a surface $\tilde{x}$ that is $C^2$ continuous within the b-spline patches and $C^1$ continuous at the patch boundaries. By varying the number of control points used for the approximation, a multi-resolution representation of the surface can be obtained. Moreover, evaluation of the b-spline representation $\tilde{x}$ is much faster than evaluation of the triangle based representation $x$. This is because point location in a regular grid is far more efficient than point location in a triangulation. A good b-spline approximation of $x$ can be achieved with a number of control points much lower than the original number of vertices that $x$ comprises, resulting also in better memory efficiency.

The approximation uses a 2D tensor product b-spline surface. The cubic b-spline kernel, denoted $\beta$, is defined as in [37]:

$$
\beta(u) = \begin{cases} 
\frac{1}{6}(3u^3 - 6u^2 + 4), & |u| \leq 1 \\
\frac{1}{2} - |u|, & |u| \in [1, 2] \\
0, & |u| \geq 2.
\end{cases}
$$

The b-spline surface is defined by a uniform grid of knots $K = \{k_{ij}\}$ positioned on the cylinder $C^2_h$ and a corresponding grid of control points $P = \{p_{ij}\}$ in $\mathbb{R}^3$. An example knot grid is shown in Figure 4(a). The b-spline surface then has the following form:

$$
\tilde{x}(u|K, P) = \sum_{i=-1}^{m_u(0)} \sum_{j=-1}^{m_v(1)} \beta\left(\frac{u - k_{ij}}{\Delta}\right) p_{ij},
$$

where $m_u(0)$ is the number of knots in the $u^{(0)}$-direction and $m_u(1)$ is the number of knots in $u^{(1)}$-direction that are within the range $[0, 2\pi] \times [0, h]$. The 2D cubic b-spline kernel $\beta(u)$ is separable, i.e. $\beta(u) = \beta(u^{(0)})\beta(u^{(1)})$ and the grid spacing is denoted as $\Delta = \frac{\Delta u^{(0)}}{m_u(0)}\frac{\Delta u^{(1)}}{m_u(1)}$. The division in the argument of the b-spline kernel is executed element-wise. In order to obtain a closed and smooth surface at the parameter boundary $u^{(0)} = 2\pi$, the control points satisfy the following conditions:

$$
\begin{align*}
P_{-1,j} &= P_{m_u(0)-1,j} \\
P_{m_u(0)-1,j} &= P_{0,j} \\
P_{m_u(0)+1,j} &= P_{1,j}
\end{align*}
$$

IV. CORRESPONDENCE QUALITY MEASURE

Least squares fitting is used in order to find a set of $m_u(0)(m_u(1) + 2)$ control points that provides a good approximation to the surface $x$. For this purpose, a set of $m_p$ uniformly distributed parameter locations is chosen on the cylinder: $U^{mp} = \{u_1, \ldots, u_{mp}\} \subset C^2_h$. Using these parameter locations, the approximation error can be determined as the sum of the squared distances between the points on the original surface and the points on the approximating surface at corresponding parameter locations. The set of control points $\hat{P}$ for which this error is minimal, is regarded as the optimal set in a least squares sense:

$$
\hat{P} = \arg\min_P \sum_{i=1}^{mp} ||\tilde{x}(u_i|K, P) - x(u_i)||^2
$$

The minimum is found as the solution of the system $BP = X$, where $X$ is a $m_p \times 3$ matrix having surface points $\{x(u_i)\}$ as its rows, $P$ is a $m_u(0)(m_u(1) + 2) \times 3$ matrix having the control points $\{p_{ij}\}$ as its rows, and $B$ is a $m_p \times m_u(0)(m_u(1) + 2)$ matrix. Note that $B_{kl}$ is the contribution of the $l$-th control point $p_l$ to the approximation of the $k$-th surface point $x_k$. The solution is obtained efficiently from the normal equations $B^TBP = B^TX$ [38]. In Figure 3, a surface is shown together with four cylindrical b-spline approximations obtained using an increasing number of control points.

A. Statistical Modeling

In order to build a statistical shape model or a point distribution model [1] for a set of $n_s$ surfaces $\{\mathcal{M}_i\}$, a correspondence needs to be established and the surfaces have to be aligned in a common reference coordinate system. Suppose that $\{x_i\}$ are the parameterizations that express this correspondence in the common reference coordinate system.
Then, the goal of statistical shape modeling is to capture the shape present in the set of surfaces with a probability density function. Here, a distribution is assumed that is symmetric about its mean namely a multivariate Gaussian distribution and the actual distribution parameters are obtained using principal components analysis (PCA) [39].

In this work, the computation of the PCA is done by means of singular value decomposition (SVD). This is more efficient than the traditional method where an eigenvalue decomposition of the large covariance matrix is used. The SVD method also allows the computation of the partial derivatives of the shape mode variances w.r.t. the landmark positions, which is important for the gradient based optimization. A matrix representation of the set of surfaces \( \{x_i\} \) is obtained by sampling each surface at a set of uniformly distributed cylindrical parameter locations \( U^np = \{u_1, \ldots, u_{np}\} \). For each surface, the coordinates of the \( n_s \) landmarks are concatenated and a \( 3np \times n_s \) column vector \( \hat{x}_i \), representing the surface \( x_i \), is obtained:

\[
\hat{x}_i = [x_i(u_1) \ldots x_i(u_{np})].
\]

The landmark matrix \( X \) is then obtained from the \( n_s \) shape vectors as \( X = [\hat{x}_1^T \ldots \hat{x}_n^T] \), resulting in a matrix of dimensions \( 3np \times n_s \). The mean shape vector \( \bar{x} \) is computed as

\[
\bar{x} = \frac{1}{n_s} \sum_{i=1}^{n_s} \hat{x}_i
\]

and the row centered landmark matrix is obtained by subtracting this mean shape from each column of \( X \), i.e.

\[
X_c = [\hat{x}_1^T - \bar{x}^T \ldots \hat{x}_n^T - \bar{x}^T].
\]

Now, let the SVD of the centered landmark matrix be defined as

\[
\frac{1}{\sqrt{n_s}} X_c = PSQ^T,
\]

where \( P \) is a \( 3np \times 3np \) orthonormal matrix containing the left singular vectors \( p_j \) as its columns, \( S \) is a \( 3np \times n_s \) diagonal matrix where the diagonal elements are the singular values \( \sigma_j \) in descending order, and \( Q \) is an \( n_s \times n_s \) orthonormal matrix with the right singular vectors \( q_j \) as its columns. The \( n_s \times n_s \) surface covariance matrix \( D \) is defined as

\[
D = \frac{1}{n_s-1} X_c^T X_c = QS^2Q^T
\]

and its SVD can be calculated efficiently. The first \( m \) columns of \( P \), denoted as \( P_m \), contain the \( m \) shape modes \( p_j \) and they are obtained from the SVD of \( D \) as

\[
P_m = \frac{1}{\sqrt{n_s-1}} X_c Q S_m^{-1},
\]

where \( S_m \) is the matrix that contains the first \( m \) rows of \( S \). The first \( m \) corresponding shape mode variances \( \lambda_j \) are also obtained from Eq. (11) as the first \( m \) squared non-zero singular values \( \sigma_j^2 \).

Using the obtained shape modes \( p_j \) and the corresponding mode variances \( \lambda_j \), a new shape instance \( \hat{x} \) can be obtained by adding a linear combination of the principal shape modes to the mean surface:

\[
\hat{x} = \bar{x} + \sum_{j=1}^{n_s-1} p_j b_j,
\]

where \( b_j \) is the contribution of the \( j \)-th principal shape mode to \( \hat{x} \). Equation (13) defines a shape space spanned by the shape parameters \( b_j \) and with the mean shape as the origin. The bounds on the shape parameters of the shape space are usually chosen as a small multiple of the standard deviation of the point cloud along that direction, i.e. \(-3\sqrt{\lambda_j} \leq b_j \leq +3\sqrt{\lambda_j}\).

In what follows, \( \Lambda \) will denote the function that maps a set of corresponded surfaces to the mode variances of their derived shape model:

\[
(\lambda_1, \ldots, \lambda_{n_s-1}) = \Lambda(x_1, \ldots, x_{n_s}[U^np]).
\]

B. Description Length

In Davies et al. [18], a correspondence measure for curves and surfaces is introduced which is regarded as the current standard for correspondence optimization. Their measure is adopted here but in a simplified form. The original measure is based on the minimum description length principle: the sampled surfaces are coded in a message where the encoding is determined by the PCA model built from the correspondence. The total message length of the encoded surfaces, together with the encoded model, determine the quality of the model and therefore also the quality of the correspondence. In this way, a trade-off is made between model complexity and goodness-of-fit. Over the years, the MDL measure has been tuned and in this work the simplified MDL measure, introduced by Thodberg [27], is used. It is a function of the shape mode variances \( \lambda_j \) and is defined as follows:

\[
\mu(\lambda_1, \ldots, \lambda_{n_s-1}) = \sum_{\lambda_i \geq \lambda_c} \left( 1 + \frac{\lambda_i}{\lambda_c} \right) + \sum_{\lambda_i < \lambda_c} \frac{\lambda_i}{\lambda_c},
\]

The free parameter \( \lambda_c \) is set to be the expected noise variance in the data. The variation captured by all modes with an eigenvalue (variance) below \( \lambda_c \) is thus considered noise. As can be seen from the first and the second term in Equation (15) respectively, the benefit of decreasing normal modes is logarithmic while for noise modes it is constant. Furthermore, the quality measure \( \mu \) goes to zero when all eigenvalues go to zero, i.e. it favors compact models. Also, both \( \mu \) and its partial derivatives \( \frac{\partial \mu}{\partial \lambda_i} \) are continuous. This is an attractive property for optimization. Note that shorter description length, i.e. a lower value of \( \mu \), indicates better quality of correspondence.

C. Gradient of Description Length

The L-BFGS minimizer used in this work requires not only the value of the objective \( \mu \) but also the gradient \( \nabla \mu \). In this section, the gradient with respect to the landmark positions \( x_{ij} \) is derived. In [40], Ericsson and Kalle explain how to obtain the partial derivatives of the description length \( \mu \) w.r.t. centered the landmark positions \( x_{ij} \). Their derivation is based on a result obtained by Papadopoulos and Lourakis in [41].
This result is a simple expression, in function of the elements $p_{ik}$ of $P$ and $q_{kj}$ of $Q$, for the derivative of the singular values $\sigma_k$ of $X_c$ w.r.t. the matrix values $x_{ij}^c$, namely:

$$\frac{\partial \sigma_k}{\partial x_{ij}^c} = p_{ik}q_{kj}. \quad (16)$$

The partial derivatives of the description length w.r.t. the non-centered landmarks $x_{ij}$ can be obtained as:

$$\frac{\partial \mu}{\partial x_{ij}} = \sum_{\lambda_k \geq \lambda_c} \frac{1}{\lambda_k} \frac{\partial \lambda_k}{\partial x_{ij}} + \sum_{\lambda_k < \lambda_c} \frac{1}{\lambda_c} \frac{\partial \lambda_k}{\partial x_{ij}}. \quad (17)$$

The derivatives of the shape mode variances $\lambda_k$ can be refined into:

$$\frac{\partial \lambda_k}{\partial x_{ij}} = 2\sigma_k p_{ik} q_{kj} - \frac{2}{n_s} \sigma_k p_{ik} \sum_j q_{kj}, \quad (18)$$

where Equation (16) was used together with the fact that

$$\frac{\partial x_{ij}^c}{\partial x_{ij}} = \begin{cases} 1 & \text{if } i = j \\
\frac{1}{n_s} & \text{if } i = j \text{ and } j \neq i \\
0 & \text{if } i \neq i \end{cases}. \quad (19)$$

Hereby the gradient of the description length w.r.t. the landmarks are obtained. The gradient with respect to the transformation parameters $\Phi$ can be obtained by multiplying the landmark gradient with the Jacobian of the function that maps the transformation parameters to the landmark positions.

V. RIGID CORRESPONDECE

Establishing an initial correspondence for a set of surfaces $\{M_1, \ldots, M_n\}$ starts by parameterizing each surface onto the cylinder. The parameterized piece-wise linear surfaces $\{x_1^c, \ldots, x_n^c\}$ are then approximated using b-splines, resulting in the smooth surfaces $\{\hat{x}_1^c, \ldots, \hat{x}_n^c\}$. Details on this can be found in Section III. The approximation uses a grid of $m_{x(0)}^o \times m_{y(1)}^o$ control points. It was observed that accurate approximations are achieved with a grid size of the order $32 \times 32$ for all surfaces considered in this work. An initial correspondence, denoted $\{\hat{x}_1^c, \ldots, \hat{x}_n^c\}$, is obtained from the b-spline surfaces after applying a spatial alignment $\tau^o(\Phi^r, \Phi^c)$ and parameter space rotation $\rho^o(\Phi^r)$ to each of the surfaces $\hat{x}_i^c$. The optimal transformation parameters $\Phi^o$ and $\Phi^c$ are determined by optimization w.r.t. the model description length $\mu$. The objective $\mu$ contains multiple local minima and therefore suitable initialization for the transformation parameters is required. First the spatial transformation parameters are initialized by principal axes alignment of the surfaces. This is followed by initialization of the parameterization rotation parameters by running a description length optimization for the parameterization rotations while keeping the spatial transformation parameters fixed. Finally, starting from these initial parameters, the full optimization of the description length, where both spatial transformation parameters and parameterization rotation parameters are set free, is executed. This results in the desired rigid correspondence $\{\hat{x}_1^c, \ldots, \hat{x}_n^c\}$. An overview of establishing a rigid correspondence is given in the flow chart of Figure 1(a).

A. Spatial Alignment Initialization

The spatial transformation $\tau^o(\Phi^r) : \mathbb{R}^3 \rightarrow \mathbb{R}^3$, used for the alignment of the surfaces, is a 3D rigid transformation. It is composed of a 3D rotation around the surface center followed by a 3D translation. The rotation is parameterized by a unit quaternion $q = (w, q_x, q_y, q_z) \in S^3$, where $S^3$ is the three-sphere. In order to be of unit length, the quaternion should adhere to the following constraint:

$$\sqrt{w^2 + q_x^2 + q_y^2 + q_z^2} = 1. \quad (20)$$

Quaternion parameterization for rotation does not suffer from the singularities encountered with Euler angles. The translation is parameterized by a 3d vector $t = (t_x, t_y, t_z)$. The transformation $\tau^o$ is thus controlled by seven parameters: $\Phi^r = (q, t)$.

Let

$$\hat{x}_i^o(\Phi^r) = \tau^o(\Phi^r) \circ \hat{x}_i^o \quad (21)$$

be a shorthand notation for the surface obtained after applying the spatial transformation $\tau^o$ to the surface $\hat{x}_i^o$, for given parameters $\Phi^r$. Then, the parameters $\{\Phi^r_1, \ldots, \Phi^r_n\}$ are chosen so that the surfaces $\{\hat{x}_1^o(\Phi^r_1), \ldots, \hat{x}_n^o(\Phi^r_n)\}$ have their principal axes aligned with the axes of the reference coordinate system. The translation vector $t_i$ for surface $\hat{x}_i^o$ centers the surface at the origin of the coordinate system, i.e. $t_i = -\hat{v}_i = -\frac{1}{n_v} \sum_{j=1}^{n_v} v_{ij}$ where $\hat{v}_i$ is the average of the vertices $v_{ij}$ of surface $\hat{x}_i^o$. The rotation for the surface is obtained using singular value decomposition. Let $V_i = [v_{ij} - \hat{v}_i]^T \ldots [v_{ij} - \hat{v}_i]^T$ be the matrix that has the centered vertices of $M_i$ as its rows and let the singular value decomposition of the coordinate covariance matrix be defined as $\frac{1}{n_v} V_i^T V_i = U_i S_i^2 U_i^T$. Then, $U_i$ is the rotation matrix that aligns the principal axes of the surface with the reference coordinate axes. Note that the rotation matrix $U_i$ is not uniquely defined since the singular vectors are defined up to their sign. Thus there are eight possible rotations, from which four can be eliminated since they produce a mirrored surface. From the four remaining rotations, the one is chosen that best matches a reference surface $M_r$ in terms of the following error:

$$\sum_{j=1}^{n_p} [D(\hat{x}_i^o(u_j, \Phi^o), M_r)]^2, \quad (22)$$

where $D(p, M)$ measures the distance from $p$ to the closest point on $M$. The quaternion $q_i$ that represents the best rotation together with the translation $t_i$ form the initialization for the spatial transformation parameter set, i.e. $\Phi^r_i = (q_i, t_i)$.

B. Parameterization Alignment Initialization

The parameterization transformation $\rho^o(\Phi^c)$, used to align the parameterizations, is a parameter space rotation and it is controlled by a single parameter $\Phi^c \in [0, 2\pi]$, defining the angle of rotation. The transformation has the following form:

$$\rho^o(\Phi^c) : C_h^2 \rightarrow C_h^2 \quad (23)$$

$$u \mapsto (u(0) + \Phi^c, u(1)). \quad (24)$$
Similar to Equation (21), a shorthand notation for the surface obtained after applying the spatial and parameterization transformation, for given parameters $\Phi_i^{(s)}$ and $\Phi_i^{(r)}$, is as follows:

$$\hat{x}_i^{(i)}(\bullet; \Phi_i^{(s)}, \Phi_i^{(r)}) = \tau^i(\bullet; \Phi_i^{(s)}) \circ \hat{x}_i^{(0)} \circ \rho^i(\bullet; \Phi_i^{(r)}). \quad (25)$$

The initial values for the parameterization rotation parameters $\{\Phi_1^{(r)}, \ldots, \Phi_n^{(r)}\}$ are then obtained by solving the following optimization problem:

$$\arg \min_{\Phi_i^{(r)}, \forall i} \mu \circ \Lambda(\ldots, \hat{x}_i^{(i)}(\bullet; \Phi_i^{(s)}, \Phi_i^{(r)}), \ldots) \mid U^{n_{\sigma}}, \quad (26)$$

where the $\Phi_i^{(r)}$ are the initial spatial alignment parameters obtained in the previous section.

C. Full Alignment

Now, starting from the initial spatial transformation parameters $\{\Phi_1^{(s)}, \ldots, \Phi_n^{(s)}\}$ and the initial parameterization rotation parameters $\{\Phi_1^{(r)}, \ldots, \Phi_n^{(r)}\}$, obtained in the previous two sections, the full description length minimization with rigid transformations can be solved:

$$\arg \min_{\Phi_i^{(s)}, \Phi_i^{(r)}, \forall i} \mu \circ \Lambda(\ldots, \hat{x}_i^{(i)}(\bullet; \Phi_i^{(s)}, \Phi_i^{(r)}), \ldots) \mid U^{n_{\sigma}} \quad + \rho^T \frac{\alpha}{n_{\sigma}} \sum_j \eta^T(\Phi_j^{(r)}). \quad (27)$$

Here, the regularization term $\eta^T(\Phi_j^{(r)})$ penalizes parameter sets with a quaternion that violates Equation (20). The penalty for a quaternion $q$ is measured as $(1 - \sqrt{q^T q})^2$. The regularization term attains its minimum when all quaternions are in $S^3$ and smoothly penalizes any deviation from this. In all the experiments a regularization factor $\alpha = 10^6$ was used. The parameters that solve Equation (27) are denoted $\{\Phi_1^{(s)}, \Phi_1^{(r)}, \ldots, \Phi_n^{(s)}, \Phi_n^{(r)}\}$ and they provide the final rigid correspondence $\{\hat{x}_1^{(i)}(\bullet; \Phi_1^{(s)}, \Phi_1^{(r)}), \ldots, \hat{x}_n^{(i)}(\bullet; \Phi_n^{(s)}, \Phi_n^{(r)})\}$.

VI. Non-Rigid Correspondence

In the previous section, an rigid correspondence $\{x_1, \ldots, x_n\}$ was produced by applying the optimal rigid spatial transformations and rigid parameterization transformations to the parameterized surfaces. An improvement over this rigid correspondence can be obtained by allowing local deformations of the parameterizations. Such local deformations can be realized by a non-rigid parameterization transformation. Here, a cylindrical b-spline parameterization deformation $\rho^L$ is used, where $L$ indicates the level of resolution of the deformation. The spatial transformation $\tau$ is the same as in Section V. The optimal non-rigid parameterization deformations, together with the spatial transformation parameters, are determined by optimization. The optimization is done at increasing levels of resolution, sequentially, to avoid convergence to a local optimum. The flow chart in Figure 1(b) gives an overview of the multi-resolution correspondence optimization.

At every resolution level $L$, the optimal transformation parameters for that level are determined in the following manner:

First, each surface $x_i$, obtained from the rigid correspondence procedure, is approximated with a b-spline surface, denoted $\hat{x}_i^{(L)}$. The approximation uses a $m_n^{L(0)} \times m_n^{L(1)}$ grid of control points. Here, $m_n^{L(0)} = 3 \cdot 2^{L-1}$ and $m_n^{L(1)} = \lceil \frac{n_p}{L} \rceil$ is used, thus the resolution is approximately isotropic and doubled from one level to the next. Each surface $\hat{x}_i^{(L)}$ is transformed according to the spatial transformation parameters $\Phi_i^{(r)}$ and parameterization transformation parameters $\Phi_i^{(r)}$ as follows:

$$\hat{x}_i^{(i)}(\bullet; \Phi_i^{(r)}, \Phi_i^{(r)}) = \tau(\bullet; \Phi_i^{(r)}) \circ \hat{x}_i^{(0)} \circ \rho(\bullet; \Phi_i^{(r)}). \quad (28)$$

The level-$L$ b-spline parameterization transformation $\rho^L$ is defined by a grid of $n_p^{L(0)} \times n_p^{L(1)}$ control points. Similar to the approximation b-spline, the transformation b-spline has an isotropic resolution that is doubled at each new level, i.e. $n_p^{L(0)} = 3 \cdot 2^{L-1}$ and $n_p^{L(1)} = \lceil \frac{n_p}{L} \rceil$. Using the notation from Equation (28), the optimal level-$L$ transformation parameters are determined by solving the following optimization problem:

$$\arg \min_{\Phi_i^{(r)}, \Phi_i^{(r)} \mid U^{n_{\sigma}}, \forall i} \mu \circ \Lambda(\ldots, \hat{x}_i^{(i)}(\bullet; \Phi_i^{(r)}, \Phi_i^{(r)}), \ldots) \mid U^{n_{\sigma}} \quad + \rho^T \frac{\alpha^T}{n_{\sigma}} \sum_j \eta^T(\Phi_j^{(r)}). \quad (29)$$

Here, $\eta^T$ is the regularization for the spatial transformations, as defined in Section V-C, and $\eta^T$ is the regularization for the parameterization deformations in order to avoid overfitting. The experimentally determined regularization constants are $\alpha^T = 10^6$ and $\alpha^T = 0.2$. The set of parameter coordinates $U^{n_{\sigma}}$, used to estimate the shape covariance matrix, contains $n_p^{L-1} = 250 \cdot 4^{L-1}$ parameter locations. Thus, the number of samples per area increases fourfold with every new level. This mirrors the doubling of the resolution of the surface approximation and parameterization transformation. Note that the optimal transformation parameters for the optimization problem of level $L - 1$ are used to initialize the parameters of the current the level $L$. To initialize the b-spline parameterization transformation parameters $\Phi_i^{(r)}$ from $\Phi_i^{(r)}$, the b-spline upsampling technique from [42] is used. The initialization of the spatial transformations is trivial, i.e $\Phi_i^{(r)} = \Phi_i^{(r)}$. In this work, three levels of resolution were used and thus the optimal transformation parameters $\{\Phi_1^{(r)}, \Phi_1^{(r)}, \ldots, \Phi_n^{(r)}, \Phi_n^{(r)}\}$ of the third level optimization problem are the final transformation parameters. These provide the final correspondence $\{\hat{x}_1, \ldots, \hat{x}_n\}$.

In the following two sections, the actual form of the parameterization transformation will be detailed and a suitable regularizer is introduced.

A. Reparameterization Transformation

The parameterization space $C_2^L$ is deformed using a parameterization transformation $\rho^L(u; \Phi_i^{(s)})$, where $L$ denotes the level of resolution. The transformation is an automorphism of the parameter space, i.e. $\rho^L$ constitutes a continuous one-to-one map of $C_2^L$. The space of possible reparameterizations is spanned by the transformation parameters $\Phi_i^{(s)}$. Different bases can be used to represent a reparameterization function
In this work, \( \rho^L \) is a 2d cubic b-spline function with knot positions on a regular grid. Such a representation has a number of convenient properties: (1) cubic b-spline deformations are \( C^2 \) continuous with respect to their parameters within the patches and \( C^1 \) continuous at the patch boundaries. This is required for efficient, gradient guided, optimization. (2) it has compact support which makes it fast to evaluate and allows local control. And, (3) it can be used in a multi-resolution method by refining the grid that controls the shape of the deformation.

The b-spline deformation function \( \rho^L \) is defined by a set of knots \( K^L = \{ \kappa^L_{ij} \} \) and a set of control point displacements \( \Phi^{iL} = \{ \delta^L_{ij} \} \):

\[
\rho^L(u|\Phi^L) = \sum_{i=-1}^{n^L_{u(0)}+1} \sum_{j=-1}^{n^L_{u(1)}} \beta \left( \frac{u - \kappa^L_{ij}}{\Delta^L} \right) (\kappa^L_{ij} + \delta^L_{ij}) \mod(0) 2\pi \tag{30}
\]

Where the modulo operator, \( \mod(0) \), acts on the first coordinate of the parameter space and keeps the deformed parameter within the bounds \([0, 2\pi]\). \( \beta \) is the 2D separable cubic b-spline kernel from Equation (3). The knots and the corresponding control points are arranged on a regular \( n^L_{u(0)} \times n^L_{u(1)} \) grid on the cylinder \( C^L_h \). The spacing between the knots is denoted as \( \Delta^L = \left( \frac{2\pi}{n^L_{u(0)}}, \frac{2\pi}{n^L_{u(1)}} \right) \).

The following constraints on the control point displacements \( \delta^L_{ij} \) make sure that \( \rho^L \) is periodic and continuous at the parameter boundary \( u(0) = 2\pi \):

\[
\begin{align*}
\delta_{-1,j} &= \delta_{n^L_{u(0)}-1,j} \\
\delta_{0,j} &= \delta_{n^L_{u(0)},j}, \forall j. \\
\delta_{1,j} &= \delta_{n^L_{u(0)}+1,j}
\end{align*}
\tag{31}
\]

In order to make \( \rho^L \) one-to-one along the boundaries of \( C^L_h \), the following constraints are also enforced:

\[
\begin{align*}
\delta^{(1)}_{-1,1} &= -\delta^{(1)}_{1,1} \\
\delta^{(1)}_{i,n^L_{u(0)}-2} &= -\delta^{(1)}_{i,n^L_{u(0)}}, \forall i. \\
\delta^{(1)}_{1,1} &= 0 \\
\delta^{(1)}_{i,n^L_{u(0)}-1} &= 0
\end{align*}
\tag{32}
\]

In this work, the same arrangement of knots \( K^L \) is used for the reparameterization of each surface \( x_k \). Only the control point displacements \( \Phi_k^{L} = \{ \delta^L_{ij,k} \} \) differ from surface to surface. Figure 4(a) shows a 3 \times 4 cylindrical grid of knots in an unfolded view and Figure 4(b) shows a grid of control points for that knot grid, where the control points are obtained by adding the control point displacement to the knot location, i.e. \( \kappa^L_{ij} + \delta^L_{ij} \). Observe that both the knots and the control points reside on the parameter domain \( C^L_h \). The b-spline function \( \rho^L \) thus defines a reparameterization function of the cylindrical parameter domain \( C^2_h \).

**B. Reparameterization Regularization**

From Equation (30), it can be seen that the reparameterization transformation \( \rho^L \) is a linear combination of translated versions of the cubic b-spline kernel \( \beta \). As a result, the reparameterization transformation is \( C^2 \) continuous within the patches and \( C^1 \) continuous at the patch boundaries. The inherent smoothness of the b-spline transformation is convenient but it does not avoid overfitting by the b-spline transform. Overfitting is perceived as an irregular local deformation and occurs in regions where \( \mu \) is insensitive to local deformations, e.g. when a b-spline kernel is not supported by any landmark samples in the calculation of \( A \).

To counter these irregularities, a regularization term is introduced, denoted \( \eta^\rho \). For b-splines, a number of regularization terms have been used in the past [44], [45]. Here, a simple regularizer is chosen that measures the Dirichlet energy of the parameterization displacement function. This displacement function, denoted \( \varphi \) can be derived easily from Equation 30:

\[
\varphi(u|\Phi^L) = \sum_{i=-1}^{n^L_{u(0)}+1} \sum_{j=-1}^{n^L_{u(1)}} \beta \left( \frac{u - \kappa^L_{ij}}{\Delta^L} \right) \delta^L_{ij} \tag{33}
\]

The regularization term \( \eta^\rho \) for the deformation is then defined as:

\[
\eta^\rho(\Phi^L) = \int \int_{C^L_h} \left( \left| \frac{\partial \varphi(u|\Phi^L)}{\partial u^{(0)}} \right|^2 + \left| \frac{\partial \varphi(u|\Phi^L)}{\partial u^{(1)}} \right|^2 \right) \Delta u
\tag{34}
\]

In what follows, \( \beta^{(c)}_{u(\cdot)} = \beta \left( \frac{u^{(c)}}{\Delta u^{(c)} - 1} \right) \) is used as a shorthand notation and the prime mark symbol denotes the derivative. Substituting the b-spline transformation into Equation (34) results in:

\[
\eta^\rho(\Phi^L) = \sum_{ij} \sum_{kl} \delta^L_{ij}\delta^L_{kl} \left( \frac{1}{\Delta(u^{(0)})^2} \int_0^{2\pi} \beta^{(c)}_{u(0)} \beta^{(c)}_{u(0)} du^{(0)} \right) \int_0^h \beta^{(1)}_{u(1)} \beta^{(1)}_{u(1)} du^{(1)} + \frac{1}{\Delta(u^{(1)})^2} \int_0^{2\pi} \beta^{(c)}_{u(1)} \beta^{(c)}_{u(1)} du^{(0)} \right) \int_0^h \beta^{(1)}_{u(1)} \beta^{(1)}_{u(1)} du^{(1)} \tag{35}
\]

From this, the derivatives of the smoothness energy w.r.t. the control point displacements are easily derived:

\[
\frac{\partial \eta}{\partial \delta^L_{kl}} = 2 \sum_{ij} \delta^L_{ij} \left( \frac{1}{\Delta(u^{(0)})^2} \int_0^{2\pi} \beta^{(c)}_{u(0)} \beta^{(c)}_{u(0)} du^{(0)} \right) \int_0^h \beta^{(1)}_{u(1)} \beta^{(1)}_{u(1)} du^{(1)} + \frac{1}{\Delta(u^{(1)})^2} \int_0^{2\pi} \beta^{(c)}_{u(1)} \beta^{(c)}_{u(1)} du^{(0)} \right) \int_0^h \beta^{(1)}_{u(1)} \beta^{(1)}_{u(1)} du^{(1)} \tag{36}
\]

Equations (35) and (36) can be evaluated analytically and, as a result, they can be used efficiently with a gradient based optimization method.

**VII. RESULTS AND DISCUSSION**

**A. Data Sets**

In this work, six populations of surfaces were used to test the proposed correspondence method. Three of these are phantom populations, each consisting of 30 surfaces: a
from the corresponding knots $\kappa$ on the knot grid. Together these define a cylindrical parameterization transformation. The shape of the transformation is controlled by the displacements $\delta_{ij}$ from the corresponding knots $\kappa_{ij}$.

population of disks where the position of the disk on the cylinder is variable, a population of beams with varying width and depth, and a population of cylinder-like bent surfaces with elliptic cross-section where the width and height of the cross-section is variable together with the amount of bending. A sample surface of each of these populations is shown in Figure 5(a). There are also three populations of synthetic surfaces, in clockwise order in (a) are cylinders, disks, and beams. The three populations of real surfaces, in clockwise order in (b) are clavicles, tracheas, and thrombi.

### B. Performance Measures

In what follows, different correspondences will be constructed for the above-mentioned populations. The quality of the established correspondences is evaluated by deriving a PCA-model from the correspondence and reporting performance measures for the obtained model. The performance of a model is measured here by the compactness, reconstruction ability, generalization ability and specificity of the model. The performance measures are reported for the full $k$-mode model and all restricted $m$-mode, $m < k$, versions of the PCA-model. In a comparison, the correspondence having the best performance measures, for its derived model, is considered the best correspondence.

Now, given a set of surfaces $\{M_1, \ldots, M_n\}$, let the correspondence be denoted as $\{x_1, \ldots, x_n\}$ and the derived shape model as $\hat{x}^m$, where $m$ is the number of modes of the shape model. Then the compactness of a model is measured as the cumulative variance:

$$C(m) = \sum_{i=1}^{m} \lambda_i,$$

where $\lambda_i$ is the variance of the $i$-th shape mode. The reconstruction ability indicates how good a model is able to reconstruct the surfaces that were used to build the model. It is measured as the average approximation error after fitting the model to each of the surfaces $\{M_1, \ldots, M_n\}$:

$$R(m) = \frac{1}{n_s} \sum_{i=1}^{n_s} \min_{\Phi^T, b} D(\tau(\Phi^T) \circ \hat{x}^m(b), M_i),$$

where $\Phi^T$ are the parameters of the rigid transformation $\tau$, $b$ are model parameters, and $D(x, y)$ measures the average closest point distance from surface $y$ to surface $x$. The optimal parameters $\Phi^T$ and $b$, resulting in the best model-to-surface
fit, are determined iteratively by alternately estimating $\Phi^T$ and $\mathbf{b}$ in a least squares sense. The generalization ability of a model determines how well the model generalizes to unseen instances of the modeled class. It is measured as the average approximation error after fitting leave-one-out versions of the model to the left out surfaces:

$$G(m) = \frac{1}{n_a} \sum_{i=1}^{n_a} \min_{\Phi^T, \mathbf{b}} D(\tau(\Phi^T) \circ \hat{x}^m_i(\mathbf{b}), \mathcal{M}_i),$$  
(39)$$

where $\hat{x}^m_i$ is the $m$-mode model where the $i$-th surface was left out, i.e. it is built from the corresponded surfaces $\{x_1, \ldots, \tilde{x}_{i-1}, x_{i+1}, \ldots, x_{n_a}\}$. The model specificity measures how much random samples, generated by the model, resemble the original surfaces:

$$S(m) = \frac{1}{n_t} \sum_{i=1}^{n_t} \min_{\Phi^T, \mathbf{b}} D(\tau(\Phi^T) \circ \hat{x}^m_i(\mathbf{b}^n_i), \mathcal{M}_j),$$  
(40)$$

where the $\mathbf{b}^n_i$ are random Gaussian model parameters for the sample of the $i$-th trial and $n_t$ is the number of random samples used to estimate the specificity. Note that the model performance measures from [18] result in a bias towards the MDL-optimized models. The model performance measures in Eq. (38), (39), and (40) do not suffer from this drawback. The compactness measure from Eq. (37) is closely related to the MDL-measure and therefore biased. It is, however, reported here because it contains important information of how a model captures the variation of a population.

C. Rigid versus Non-Rigid Correspondence

The surfaces of each of the six phantom and real populations were parameterized using the progressive parameterization technique of [14]. The chosen height $h$ of the cylinder for each of the populations can be found in Table I. From the parameterized surfaces, a $16 \times 16 \times h$ b-spline representation was computed for each surface using $m_p = 10.000$ points. This was followed by the construction of the rigid correspondence. The number of landmarks to estimate the covariance was $n_p = 4000$ for all populations. Starting from the rigid correspondence, the non-rigid correspondence was calculated. In this construction, a b-spline regularization factor of $\alpha^0 = 0.2$ was used for all populations. Three levels of scale were used for the b-spline surface, the reparameterization transformation and for the number of landmarks. On the coarsest scale, a $4 \times 4$ b-spline surface, together with a $4 \times 4$ reparameterization transformation, was the covariance matrix was estimated based
Fig. 7. The model performance measures, together with the standard error, for the phantom populations. From left to right: beams, disks and cylinders populations. From top to bottom: compactness, reconstruction, generalization and specificity measure. In each graph a comparison is made of the ideal correspondence (green), the rigid correspondence (red) is and the non-rigid correspondence (black). For each model, the first $m$ modes are shown that capture 99% of the total variance in the model.

on 250 landmarks. At each new resolution level the values are increased as detailed in Section VI. All optimizations problems were solved with the L-BFGS routine [46]. For the alignment initialization (Eq. 26) and full alignment (Eq. 27) a gradient tolerance of 0.01 was used to determine convergence. For the multi-resolution correspondence optimization (Eq. 29) a gradient tolerance of $0.01 \times 2^{-L}$ was used. The quality of the obtained correspondences was assessed using the above-mentioned model performance measures. The results are shown in Figure 7 for the phantom populations and in Figure 8 for the real populations.

In Figure 7, the ideal (intuitive), the rigid and the non-rigid correspondence for the phantom populations are compared. For the disk population, it can be seen that the non-rigid and the ideal correspondence are of comparable quality. The rigid correspondence on the other hand is much worse. This is due to the fact that the parameterization technique maps the disk part of the surfaces to a different location in the parameter space. The non-rigid correspondence improvement, on the other hand, moves the disks to the same part of the parameter space and this results in an optimal correspondence. See Figure 6 for a visualization of the rigid and b-spline optimized model. The improved compactness of the non-rigid over the ideal correspondence can be attributed to the reduced area that the disk part of the surface for the non-rigid correspondence takes in the parameter-space. For the beam population, the quality of the correspondences is comparable, with a slight advantage for the ideal, since the parameterization technique already
generates a good correspondence. The most notable difference is the improved specificity of the ideal model, which is due to the fact that the other models can generate samples with rounded corners. For the cylinders population, it can be seen that the non-rigid correspondence is an improvement over the ideal, which is mainly due to the improved spatial alignment of the surfaces.

In Figure 6, a visualization of the first few modes of the models of the CT-scanned populations can be found. In Figure 8, the model performance measures for the rigid and the non-rigid correspondence are shown for the CT-scanned populations. It is more difficult to analyze these results because there is no ideal correspondence available. It can be seen though that the rigid correspondence generates good models for all three populations and that the non-rigid correspondence is a significant improvement in most cases. Compared to the clavicle and trachea populations, the approximation errors for the thrombi population errors are higher. This can be attributed to the large variability that is present in the thrombi population, together with the lower resolution of the ct-scans, that is $0.5 \times 0.5 \times 0.5 mm^3$ versus $0.5 \times 0.5 \times 2.0 mm^3$.

In Table I, the MDL values for the ideal (when available), the rigid, and the non-rigid correspondences can be found for all populations. It can be seen that the b-spline correspondence optimization always succeeds in decreasing the MDL-value. Such a decrease indicates that the resulting shape model became less complex. This is most apparent for the disk population: the five modes of the rigid model (MDL-value of 17.2) are reduced to a single mode by the b-spline optimization (MDL-value of 4.6). Table I also reports the execution time
for the construction of the correspondences, once the parameterizations are obtained. About 10\% of the time is taken by the rigid correspondence construction. The correspondences for the phantom populations are constructed more efficiently compared with the CT-scanned populations. This is because the phantom shape models are relatively simple, i.e. they have a small number of modes. The construction for the CT-scanned populations takes a couple of hours. Toghether with the construction of the parameterizations, a correspondence can easily be established overnight.

\subsection*{D. Influence of Parameters}

In this section, the influence of the method parameters on the resulting correspondence is investigated. Figure 9 shows the model performance parameters for the clavicle population when using different values for the most important parameters: (a) the b-spline deformation regularization controlled by factor $\alpha^p$ in Eq. (29), (b) the number of landmarks to estimate the shape covariance matrix, controlled by $n_p$ in Eq. (14), and (c) the number of scale levels $L$ for the b-spline surface approximation, the b-spline parameterization transform and the
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**Table II**

**Influence of the multi-level scheme for the clavicle population.**

landmarks.

In the first column of Figure 9, the influence of the b-spline regularization factor $\alpha^p$ is shown and it can be seen that, as expected, lower regularization, i.e. smaller $\alpha^p$, generates better models. However, the regularization can not be lowered too much since then irregularities can appear. No irregularities were noted with regularization factors $\alpha^p \leq 0.2$ for all considered populations.

In the second column of Figure 9, it can be seen that the influence of the number of landmarks $n_p$ is negligible for the clavicle population. It can, however, happen that using too few landmarks results in undersampling of highly variable parts of the surface, which, in turn, will result in a degraded correspondence. This was observed for the thorbini population, where $n_p^L = 250 \cdot 4^{L-1}$ landmarks generated a significantly better correspondence than $n_p^L = 31 \cdot 4^{L-1}$ landmarks (result not shown). Using less landmarks reduces computation time, but it can also result in a degraded correspondences.

In the last column of Figure 9, the model performance measures for different multi-scale schemes are shown and in Table II the corresponding MDL values are listed. Four different schemes are shown: 1D-1O-1L optimizes the correspondence using a single resolution, 3D-1O-1L uses three resolution levels for the deformations, 3D-3O-1L uses three levels for the deformations and the surfaces, and 3D-3O-3L is the full multi-resolution scheme using three levels for the deformations, the surfaces, and the landmarks. It can be seen that, for the clavicle, the single scale scheme generates a degraded correspondence and the three other schemes generate comparable correspondences. However, the full 3-scale scheme is considerably faster. For the disk population, the performance degradation of the single scale method was even more notable since, as opposed to the three other schemes, it did not successfully correspond the disk parts of the surface (result not shown).

**VIII. Conclusions**

In this work, the minimum description length approach for shape modeling was translated to surfaces of cylindrical topology. The proposed method establishes an alignment and a correspondence for a population of surfaces of cylindrical topology. It generates a rigid correspondence based on cylindrical surface parameterizations and an improved correspondence using multi-level b-spline reparameterizations. Care was taken to ensure that the objective functions are differentiable with respect to the alignment and reparameterization parameters and, where necessary, an expression for the gradient was provided. It was shown that the method produces correspondences that agree with the intuitive correspondence and that the derived shape models generate small approximation errors.

The cylindrical correspondence method of this paper, together with the spherical correspondence methods from [28] and [29], and the disc-like correspondence method of [30], already cover a wide range of biomedical surfaces. However, it would be interesting to extend the method to other topologies. The method of this paper can be trivially extended to surfaces of genus-1 topology where the torus can be used as the parametric domain. More complex topologies can be treated by decomposing the surfaces in a consistent set of discs and tubes. Populations of tubular structures with bifurcations could be handled well with this approach. However, arbitrary complex surfaces will suffer from the boundary constraints imposed by the surface decomposition. The development of a method that can handle arbitrary topology, without constraints, is a very challenging problem to be solved in the future.

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**References**


