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A discrete-to-continuum approach to the curvatures of membrane networks and parametric surfaces

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ABSTRACT

The present work deals with a scale bridging approach to the curvatures of discrete models of structural membranes, to be employed for an effective characterization of the bending energy of flexible membranes, and the optimal design of parametric surfaces and vaulted structures. We fit a smooth surface model to the data set associated with the vertices of a patch of an unstructured polyhedral surface. Next, we project the fitting function over a structured lattice, obtaining a 'regularized' polyhedral surface. The latter is employed to define suitable discrete notions of the mean and Gaussian curvatures. A numerical convergence study shows that such curvature measures exhibit strong convergence in the continuum limit, when the fitting model consists of polynomials of sufficiently high degree. Comparisons between the present method and alternative approaches available in the literature are given.

1. Introduction

The elastic response in bending of structural and biological membrane models is often described through surface energies depending on the curvature tensor of the membrane ('curvature energy', refer, e.g., to Helfrich, 1973; Seung and Nelson, 1988; Helfrich and Kozlov, 1993; Gompper and Kroll, 1996; Discher et al., 1997; Hartmann, 2010; Fraternali and Marcelli, 2012; Schmidt and Fraternali, 2012). One of the most frequently employed bending energy models is the so-called Helfrich energy, which has the following structure

$$E^{bend} = \int_S \left(\frac{\kappa_H}{2} \hat{H}^2 + \kappa_G K \right) dS$$

where S is the current configuration of the membrane; $\hat{H}$ is twice the mean curvature H (i.e., the sum of the two principal curvatures); K is the Gaussian curvature (the product of the two principal curvatures); and κ_H and κ_G are suitable stiffness parameters (Helfrich, 1973; Seung and Nelson, 1988). Once κ_H and κ_G are given, it is clear that the computation of such an energy entirely relies on the estimates of the curvatures H and K. Membrane network models often make use of triangulated membrane networks, and short-range or long-range pair interactions (Seung and Nelson, 1988; Marcelli et al., 2005; Dao et al., 2006; Fraternali and Marcelli, 2012; Schmidt and Fraternali, 2012). A correct estimation of the curvature energy of such models plays a special role when modeling the mechanics of heavily deformed networks (Espriu, 1987; Seung and Nelson, 1988; Bailiie et al., 1990; Gompper and Kroll, 1996). Energy minimization, surface smoothing and curvature estimation of discrete surface models are also challenging problems of computational geometry, and their physical, structural, and architectural implications attract the interest of researchers working in different areas (refer, e.g., to Bartesaghi and Sapiro, 2001; Bechthold, 2004; Pottman et al., 2007; El Sayed et al., 2009; Pottman, 2010; Stratil, 2010; Fraternali, 2010; Datta et al., 2011; Raney et al., 2011; Sullivan, 2008; Wardetzky, 2008). Polyhedral surfaces are frequently employed to discretize parametric surfaces within CAD, CAE and CAM systems (Rypl and Bittnar, 2006), and their regularization at the continuum is important when dealing, e.g., with the parametric design and/or the prototype fabrication of structural surfaces and vaulted structures (Bechthold, 2004; Fu et al., 2008; Pottman et al., 2007; Stratil, 2010; Datta et al., 2011).

The present work deals with a discrete-to-continuum approach to the curvatures of discrete membranes models, which looks at the continuum limits of suitable discrete definitions of such quantities. It is known from the literature that numeric approaches of the curvatures of polyhedral surfaces may feature oscillating behavior in the continuum limit (weak convergence), in presence of arbitrary

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tessellation patterns (cf. e.g., the example in Fig. 4 of Wardetzky, 2008). The present approach aims to circumvent such convergence issues, by fitting a smooth surface model to the data set associated with the vertices of a patch of an arbitrary polyhedral surface. We evaluate the fitting function at the nodes of a structured lattice, generating a new polyhedral surface with ordered structure, and 'regularized' discrete definitions of the membrane curvatures. The remainder of the paper is organized as follows. We begin by briefly recalling the mathematical definitions of the curvatures of smooth membranes in Section 2. Next, we formulate the proposed regularization procedure in Section 3. We study the convergence behavior of the given curvature measures with reference to a model problem (Section 4). We draw the main conclusions the present work in Section 5, where we also discuss potential applications and future extensions of the current research.

2. Monge description of a membrane network

Let us consider a given discrete set X_N of N nodes (or particles) extracted from a membrane network, which have Cartesian coordinates $\{x_{a_1}, x_{a_2}, z_a\}$ $(a = 1, \ldots, N)$ with respect to a given frame $\{O, x_1, x_2, z \equiv x_3\}$ (Fig. 1). We introduce a continuum regularization of X_N through the following Monge chart

$$z_N(\mathbf{x}) = \sum\nolimits_{a=1}^{N} z_a g_a(\mathbf{x}), \tag{1}$$

where g_a are suitable *shape functions*, and $\mathbf{x} = \{x_1, x_2\}$ denotes the position vector in the x_1, x_2 plane.

The Monge map (1) is defined locally when dealing with complex surfaces and/or closed membranes. In such a case, the axes $\{x_1, x_2\}$ are conveniently drawn on a plane perpendicular to a local estimate of the normal to the corresponding surface (refer, e.g., to (Fraternali et al., 2012) for a detailed illustration of such a covering technique). We name 'platform' the orthogonal projection of X_N onto the x_1, x_2 plane, and we look at x_1 and x_2 as *curvilinear coordinates* of the membrane. If the shape functions g_a are sufficiently smooth, it is an easy task to compute the first fundamental forms $a_{\alpha\beta}$ and the second fundamental forms $b_{\alpha\beta}$ of z_N (refer, e.g. to Kühnel, 2002; Fraternali et al., 2012). The unit tangents $\boldsymbol{\nu}_{\langle 1\rangle}$, $\boldsymbol{\nu}_{\langle 2\rangle}$ to the lines of curvature, and the principal curvatures k_1, k_2 are then obtained from the eigenvalue problem

$$(b_{\alpha\beta} - k_\gamma a_{\alpha\beta})\nu^{\beta}_{\langle\gamma\rangle} = 0 \quad (\gamma = 1, 2) \tag{2}$$

3. A bridging scale approach to the curvatures of polyhedral surfaces

In the special case of a polyhedral membrane, the definition of the fundamental forms and principal curvatures relies on a suitable generalized definition of the *hessian* of z_N, i.e., the second order tensor $\mathbf{H}z_N$ with Cartesian components $z_{N,\alpha\beta}$ (we let $z_{N,\alpha}$ denote the partial derivative of z_N with respect to x_α). Indeed, in such a case, the shape function g_a are piecewise linear functions, and the second-order derivatives of the Monge map (1) exist only in the distributional sense (refer, e.g., to Davini and Paroni, 2003; Sullivan, 2008; Wardetzky, 2008). Throughout the rest of the paper, we focus our attention on a triangulated membrane network, letting Π_N indicate the triangulation that is obtained by projecting such a network over the platform Ω. We denote the position vector of the generic node of Π_N by $\mathbf{x}_n$, and the corresponding coordination number by S_n. In addition, we indicate the edges attached to $\mathbf{x}_n$ by $\Gamma_n^1, \ldots, \Gamma_n^{S_n}$; and the unit vectors perpendicular and tangent to such edges by $\mathbf{h}_n^1, \ldots, \mathbf{h}_n^{S_n}$, and $\mathbf{k}_n^1, \ldots, \mathbf{k}_n^{S_n}$, respectively (Fig. 1). Beside Π_N, we introduce a dual mesh of Ω, which is formed by polygons connecting the barycenters of the triangles attached to $\mathbf{x}_n$ to the mid-points of the edges $\Gamma_n^1, \ldots, \Gamma_n^{S_n}$ ('barycentric' dual mesh, cf. Fig. 1). We say that Π_N is a *structured triangulation* of Ω if, given any tensor $\mathbf{H}$ independent of position, it results

$$\sum_{j=1}^{S_n+1} \int_{G_n} \mathbf{H}(\mathbf{x} - \mathbf{x}_n^j) \cdot (\mathbf{x} - \mathbf{x}_n^j) \nabla g_n^j \otimes \nabla g_n = \mathbf{0} \tag{3}$$

in correspondence with each node $\mathbf{x}_n$. Here, $\mathbf{x}_n^1, \ldots, \mathbf{x}_n^{S_n}$ are the nearest neighbors of $\mathbf{x}_n$; $\mathbf{x}_n^{S_n+1} = \mathbf{x}_n$; G_n is the union of the triangles attached to $\mathbf{x}_n$; and g_n^j is the shape function associated with $\mathbf{x}_n^j$ (refer, e.g., to the benchmark examples shown in Fig. 2).

A discrete definition of the hessian of a polyhedral surface z_N is obtained by introducing a piecewise constant tensor field $\mathbf{H}_N z_N$ over the dual mesh $\hat{\Pi}_N$, which takes the following value over the generic dual cell $\hat{\Omega}_n$ (cf. e.g., Fraternali et al., 2002; Fraternali, 2007)

$$\mathbf{H}_N z_N(n) = \frac{1}{|\hat{\Omega}_n|} \sum_{j=1}^{S_n} \frac{\ell_n^j}{2} \left[\left[\frac{\delta z_N}{\delta h} \right]\right]_n^j \mathbf{h}_n^j \otimes \mathbf{h}_n^j \tag{4}$$

Here, $[[\delta z_N/\delta h]]_n^j$ indicates the jump in the directional derivative $\nabla z_N \cdot \mathbf{h}_n^j$ across the edge Γ_n^j, and ℓ_n^j denotes the length of Γ_n^j. It is worth noting that the trace of $\mathbf{H}_N z_N(n)$ provides a discrete definition of the Lapalacian of z_N (refer to Davini and Paroni, 2003; Fraternali, 2007 for further details). We associate the discrete hessian $\mathbf{H}_N z_N(n)$, and the following weighted gradient (Taubin, 1995)

$$\nabla_N z_N(n) = \frac{1}{3|\hat{\Omega}_n|} \sum_{j=1}^{S_n} \nabla z_N^j |T_n^j| \tag{5}$$

to the generic node of Π_N. In (5), ∇z_N^j denotes the gradient of z_N over the jth triangle attached to $\mathbf{x}_n$, and $|T_n^j|$ denotes the area of such a triangle.

Let us consider now families of triangulations Π_N that show increasing numbers of nodes N, and are such that the *mesh size* $h_N = \sup_{\Omega_m \in \Pi_N} \{\mathrm{diam}(\Omega_m)\}$ approaches zero, as N goes to infinity. We associate a polyhedral surface $z_N(\mathbf{x})$ to each of such triangulations, by projecting a given smooth surface map $z_0(\mathbf{x})$ over Π_N. Referring to structured triangulations, it can be proved that the sequence of the discrete hessians $\mathbf{H}_N z_N$ converges to the hessian of z_0, as N goes to infinity (cf. Lemma 2 of Fraternali, 2007). Unfortunately, such a nice convergence property is not guaranteed if the triangulations Π_N do not match the property (3) ('*unstructured triangulations*'). Let K_n denote a 'patch' of an unstructured triangulation Π_N, which is formed by the k nearest neighbors of $\underline{x}_n$, $k \geq 1$ being a given integer. In order to tackle convergence issues, we construct a smooth fitting function $\tilde{f}_n(\mathbf{x})$ of the values taken by z_N at the vertices of K_n. Next, we evaluate $\tilde{f}_n(\mathbf{x})$ at the vertices $\tilde{\mathbf{x}}_1, \ldots, \tilde{\mathbf{x}}_{\tilde{N}}$ of a second, structured triangulation $\tilde{\Pi}_n$ of the platform (or a portion of Ω comprising $\mathbf{x}_n$), and build up the following 'regularized' polyhedral surface

$$\tilde{z}_n = \sum_{m=1}^{\tilde{N}} \tilde{f}_n(\tilde{\mathbf{x}}_m) \tilde{g}_m \tag{6}$$

The fitting model $\tilde{f}_n$ might consist of suitable interpolation polynomials associated with K_n, local maximum entropy shape functions, B-Splines, Non-Uniform Rational B-Splines (NURBS), or other fitting functions available in standard software libraries. In (6), $\tilde{g}_m$ denotes the shape function associated with the current node $\tilde{\mathbf{x}}_m \in \tilde{\Pi}_n$. By replacing z_N with $\tilde{z}_n$ in Eqs. (4) and (5), we finally endow $\mathbf{x}_n$ with a regularized discrete hessian $\mathbf{H}_N \tilde{z}_N(n)$, and a regularized discrete gradient $\nabla_N \tilde{z}_N(n)$. Straightforward manipulations of the above gradients and hessians lead us to generalized notions of the