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Discrete Differential Geometry

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Preface

Discrete differential geometry (DDG) is a new and active mathematical terrain where differential geometry (providing the classical theory of smooth manifolds) interacts with discrete geometry (concerned with polytopes, simplicial complexes, etc.), using tools and ideas from all parts of mathematics. DDG aims to develop discrete equivalents of the geometric notions and methods of classical differential geometry. Current interest in this field derives not only from its importance in pure mathematics but also from its relevance for other fields such as computer graphics.

Discrete differential geometry initially arose from the observation that when a notion from smooth geometry (such as that of a minimal surface) is discretized "properly", the discrete objects are not merely approximations of the smooth ones, but have special properties of their own, which make them form a coherent entity by themselves. One might suggest many different reasonable discretizations with the same smooth limit. Among these, which one is the best? From the theoretical point of view, the best discretization is the one which preserves the fundamental properties of the smooth theory. Often such a discretization clarifies the structures of the smooth theory and possesses important connections to other fields of mathematics, for instance to projective geometry, integrable systems, algebraic geometry, or complex analysis. The discrete theory is in a sense the more fundamental one: the smooth theory can always be recovered as a limit, while it is a nontrivial problem to find which discretization has the desired properties.

The problems considered in discrete differential geometry are numerous and include in particular: discrete notions of curvature, special classes of discrete surfaces (such as those with constant curvature), cubical complexes (including quad-meshes), discrete analogs of special parametrization of surfaces (such as conformal and curvature-line parametrizations), the existence and rigidity of polyhedral surfaces (for example, of a given combinatorial type), discrete analogs of various functionals (such as bending energy), and approximation theory. Since computers work with discrete representations of data, it is no surprise that many of the applications of DDG are found within computer science, particularly in the areas of computational geometry, graphics and geometry processing.

Despite much effort by various individuals with exceptional scientific breadth, large gaps remain between the various mathematical subcommunities working in discrete differential geometry. The scientific opportunities and potential applications here are very substantial. The goal of the Oberwolfach Seminar "Discrete Differential Geometry" held in May–June 2004 was to bring together mathematicians from various subcommunities working in different aspects of DDG to give lecture courses addressed to a general mathematical audience. The seminar was primarily addressed to students and postdocs, but some more senior specialists working in the field also participated.

There were four main lecture courses given by the editors of this volume, corresponding to the four parts of this book:

I: Discretization of Surfaces: Special Classes and Parametrizations,
II: Curvatures of Discrete Curves and Surfaces,
III: Geometric Realizations of Combinatorial Surfaces,
IV: Geometry Processing and Modeling with Discrete Differential Geometry.

These courses were complemented by related lectures by other participants. The topics were chosen to cover (as much as possible) the whole spectrum of DDG—from differential geometry and discrete geometry to applications in geometry processing.

Part I of this book focuses on special discretizations of surfaces, including those related to integrable systems. Bobenko's "Surfaces from Circles" discusses several ways to discretize surfaces in terms of circles and spheres, in particular a Möbius-invariant discretization of Willmore energy and S-isothermic discrete minimal surfaces. The latter are explored in more detail, with many examples, in Bücking's article. Pinkall constructs discrete surfaces of constant negative curvature, documenting an interactive computer tool that works in real time. The final three articles focus on connections between quad-surfaces and integrable systems: Schief, Bobenko and Hoffmann consider the rigidity of quad-surfaces; Hoffmann constructs discrete versions of the smoke-ring flow and Hashimoto surfaces; and Suris considers discrete holomorphic and harmonic functions on quad-graphs.

Part II considers discretizations of the usual notions of curvature for curves and surfaces in space. Sullivan's "Curves of Finite Total Curvature" gives a unified treatment of curvatures for smooth and polygonal curves in the framework of such FTC curves. The article by Denne and Sullivan considers isotopy and convergence results for FTC graphs, with applications to geometric knot theory. Sullivan's "Curvatures of Smooth and Discrete Surfaces" introduces different discretizations of Gauss and mean curvature for polyhedral surfaces from the point of view of preserving integral curvature relations.

Part III considers the question of realizability: which polyhedral surfaces can be embedded in space with flat faces. Ziegler's "Polyhedral Surfaces of High Genus" describes constructions of triangulated surfaces with n vertices having genus $O(n^2)$ (not known to be realizable) or genus $O(n \log n)$ (realizable). Timmreck gives some new criteria which could be used to show surfaces are not realizable. Lutz discusses automated methods to enumerate triangulated surfaces and to search for realizations. Bokowski discusses heuristic methods for finding realizations, which he has used by hand.

Part IV focuses on applications of discrete differential geometry. Schröder's "What Can We Measure?" gives an overview of intrinsic volumes, Steiner's formula and Hadwiger's theorem. Wardetzky shows that normal convergence of polyhedral surfaces to a smooth limit suffices to get convergence of area and of mean curvature as defined by the cotangent formula. Desbrun, Kanso and Tong discuss the use of a discrete exterior calculus for computational modeling. Grinspun considers a discrete model, based on bending energy, for thin shells.

We wish to express our gratitude to the Mathematisches Forschungsinstitut Oberwolfach for providing the perfect setting for the seminar in 2004. Our work in discrete differential geometry has also been supported by the Deutsche Forschungsgemeinschaft (DFG), as well as other funding agencies. In particular, the DFG Research Unit "Polyhedral Surfaces", based at the Technische Universität Berlin since 2005, has provided direct support to the three of us (Bobenko, Sullivan, Ziegler) based in Berlin, as well as to Bücking and Lutz. Further authors including Hoffmann, Schief, Suris and Timmreck have worked closely with this Research Unit; the DFG also supported Hoffmann through a Heisenberg Fellowship. The DFG Research Center MATHEON in Berlin, through its Application Area F "Visualization", has supported work on the applications of discrete differential geometry. Support from MATHEON went to authors Bücking and Wardetzky as well as to the three of us in Berlin. The National Science Foundation supported the work of Grinspun and Schröder, as detailed in the acknowledgments in their articles.

Our hope is that this book will stimulate the interest of other mathematicians to work in the field of discrete differential geometry, which we find so fascinating.

Alexander I. Bobenko
Peter Schröder
John M. Sullivan
Günter M. Ziegler

Berlin, September 2007

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Part I

Discretization of Surfaces:

Special Classes and Parametrizations

Discrete Differential Geometry, A.I. Bobenko, P. Schröder, J.M. Sullivan and G.M. Ziegler, eds.
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Surfaces from Circles

Alexander I. Bobenko

Abstract. In the search for appropriate discretizations of surface theory it is crucial to preserve fundamental properties of surfaces such as their invariance with respect to transformation groups. We discuss discretizations based on Möbius-invariant building blocks such as circles and spheres. Concrete problems considered in these lectures include the Willmore energy as well as conformal and curvature-line parametrizations of surfaces. In particular we discuss geometric properties of a recently found discrete Willmore energy. The convergence to the smooth Willmore functional is shown for special refinements of triangulations originating from a curvature-line parametrization of a surface. Further we treat special classes of discrete surfaces such as isothermic, minimal, and constant mean curvature. The construction of these surfaces is based on the theory of circle patterns, in particular on their variational description.

Keywords. Circular nets, discrete Willmore energy, discrete curvature lines, isothermic surfaces, discrete minimal surfaces, circle patterns.

1. Why from circles?

The theory of polyhedral surfaces aims to develop discrete equivalents of the geometric notions and methods of smooth surface theory. The latter appears then as a limit of refinements of the discretization. Current interest in this field derives not only from its importance in pure mathematics but also from its relevance for other fields like computer graphics.

One may suggest many different reasonable discretizations with the same smooth limit. Which one is the best? In the search for appropriate discretizations, it is crucial to preserve the fundamental properties of surfaces. A natural mathematical discretization principle is the invariance with respect to transformation groups. A trivial example of this principle is the invariance of the theory with respect to Euclidean motions. A less trivial but well-known example is the discrete analog for the local Gaussian curvature defined as the angle defect $G(v) = 2\pi - \sum \alpha_i$, at a vertex v of a polyhedral surface. Here the α_i are the angles of all polygonal faces (see Figure 3) of the surface at vertex v. The discrete

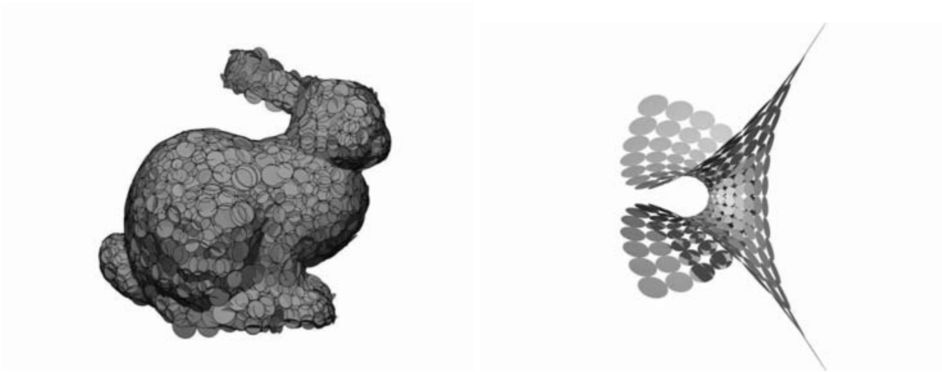

FIGURE 1. Discrete surfaces made from circles: general simplicial surface and a discrete minimal Enneper surface.

Gaussian curvature $G(v)$ defined in this way is preserved under isometries, which is a discrete version of the Theorema Egregium of Gauss.

In these lectures, we focus on surface geometries invariant under Möbius transformations. Recall that Möbius transformations form a finite-dimensional Lie group generated by inversions in spheres; see Figure 2. Möbius transformations can be also thought

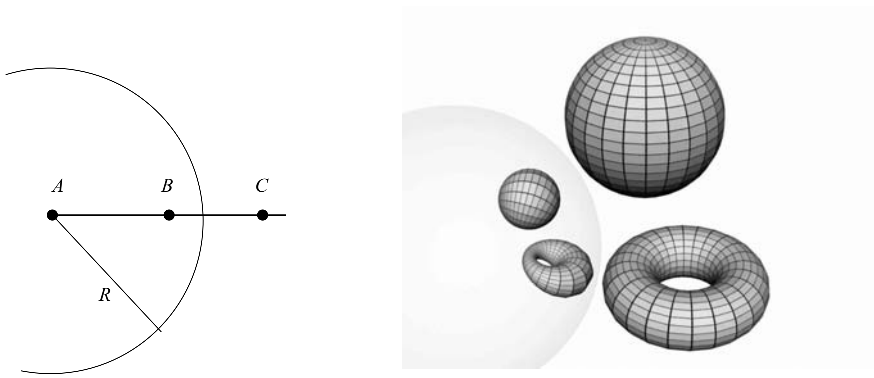

FIGURE 2. Inversion $B \mapsto C$ in a sphere, $|AB||AC| = R^2$. A sphere and a torus of revolution and their inversions in a sphere: spheres are mapped to spheres.

as compositions of translations, rotations, homotheties and inversions in spheres. Alternatively, in dimensions $n \geq 3$, Möbius transformations can be characterized as conformal transformations: Due to Liouville's theorem any conformal mapping $F : U \to V$ between two open subsets $U, V \subset \mathbb{R}^n$, $n \geq 3$, is a Möbius transformation.

Many important geometric notions and properties are known to be preserved by Möbius transformations. The list includes in particular:

- spheres of any dimension, in particular circles (planes and straight lines are treated as infinite spheres and circles),
- intersection angles between spheres (and circles),
- curvature-line parametrization,
- conformal parametrization,
- isothermic parametrization (conformal curvature-line parametrization),
- the Willmore functional (see Section 2).

For discretization of Möbius-invariant notions it is natural to use Möbius-invariant building blocks. This observation leads us to the conclusion that the discrete conformal or curvature-line parametrizations of surfaces and the discrete Willmore functional should be formulated in terms of circles and spheres.

2. Discrete Willmore energy

The Willmore functional [42] for a smooth surface $\mathcal{S}$ in 3-dimensional Euclidean space is

$$\mathcal{W}(S) = \frac{1}{4}\int_{S}(k_1 - k_2)^2 dA = \int_{S} H^2 dA - \int_{S} K dA.$$

Here dA is the area element, k_1 and k_2 the principal curvatures, $H = \frac{1}{2}(k_1 + k_2)$ the mean curvature, and $K = k_1 k_2$ the Gaussian curvature of the surface.

Let us mention two important properties of the Willmore energy:

- $\mathcal{W}(S) \geq 0$ and $\mathcal{W}(S) = 0$ if and only if $\mathcal{S}$ is a round sphere.
- $\mathcal{W}(S)$ (and the integrand $(k_1 - k_2)^2 dA$) is Möbius-invariant [1, 42].

Whereas the first claim almost immediately follows from the definition, the second is a nontrivial property. Observe that for closed surfaces $\mathcal{W}(S)$ and $\int_S H^2 dA$ differ by a topological invariant $\int K dA = 2\pi\chi(S)$. We prefer the definition of $\mathcal{W}(S)$ with a Möbius-invariant integrand.

Observe that minimization of the Willmore energy $\mathcal{W}$ seeks to make the surface "as round as possible". This property and the Möbius invariance are two principal goals of the geometric discretization of the Willmore energy suggested in [3]. In this section we present the main results of [3] with complete derivations, some of which were omitted there.

2.1. Discrete Willmore functional for simplicial surfaces

Let S be a simplicial surface in 3-dimensional Euclidean space with vertex set V, edges E and (triangular) faces F. We define the discrete Willmore energy of S using the circumcircles of its faces. Each (internal) edge $e \in E$ is incident to two triangles. A consistent orientation of the triangles naturally induces an orientation of the corresponding circumcircles. Let $\beta(e)$ be the external intersection angle of the circumcircles of the triangles sharing e, meaning the angle between the tangent vectors of the oriented circumcircles (at either intersection point).

Definition 2.1. The *local discrete Willmore energy* at a vertex v is the sum

$$W(v) = \sum_{e \ni v} \beta(e) - 2\pi.$$

over all edges incident to v. The *discrete Willmore energy* of a compact simplicial surface S without boundary is the sum over all vertices

$$W(S) = \frac{1}{2} \sum_{v \in V} W(v) = \sum_{e \in E} \beta(e) - \pi|V|.$$

Here $|V|$ is the number of vertices of S.

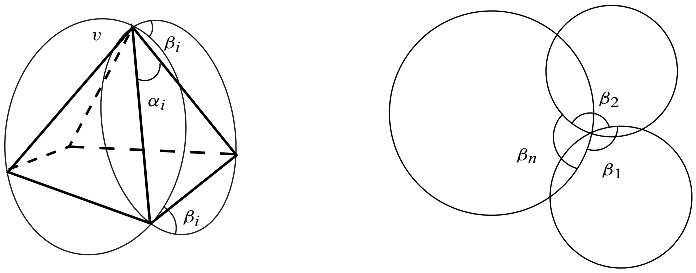

FIGURE 3. Definition of discrete Willmore energy.

Figure 3 presents two neighboring circles with their external intersection angle β_i as well as a view "from the top" at a vertex v showing all n circumcircles passing through v with the corresponding intersection angles $\beta_1, \dots, \beta_n$. For simplicity we will consider only simplicial surfaces without boundary.

The energy $W(S)$ is obviously invariant with respect to Möbius transformations.

The star $S(v)$ of the vertex v is the subcomplex of S consisting of the triangles incident with v. The vertices of $S(v)$ are v and all its neighbors. We call $S(v)$ convex if for each of its faces $f \in F(S(v))$ the star $S(v)$ lies to one side of the plane of f and strictly convex if the intersection of $S(v)$ with the plane of f is f itself.

Proposition 2.2. *The conformal energy $W(v)$ is non-negative and vanishes if and only if the star $S(v)$ is convex and all its vertices lie on a common sphere.*

The proof of this proposition is based on an elementary lemma.

Lemma 2.3. *Let $\mathcal{P}$ be a (not necessarily planar) n-gon with external angles β_i. Choose a point P and connect it to all vertices of $\mathcal{P}$. Let α_i be the angles of the triangles at the tip P of the pyramid thus obtained (see Figure 4). Then*

$$\sum_{i=1}^{n} \beta_i \geq \sum_{i=1}^{n} \alpha_i,$$

and equality holds if and only if $\mathcal{P}$ is planar and convex and the vertex P lies inside $\mathcal{P}$.

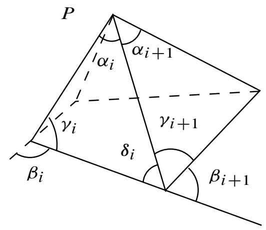

FIGURE 4. Proof of Lemma 2.3

Proof. Denote by γ_i and δ_i the angles of the triangles at the vertices of $\mathcal{P}$, as in Figure 4. The claim of Lemma 2.3 follows from summing over all $i = 1, \ldots, n$ the two obvious relations

$$\beta_{i+1} \geq \pi - (\gamma_{i+1} + \delta_i)$$
$$\alpha_i = \pi - (\gamma_i + \delta_i).$$

All inequalities become equalities only in the case when $\mathcal{P}$ is planar, convex and contains P. □

For P in the convex hull of $\mathcal{P}$ we have $\sum \alpha_i \geq 2\pi$. As a corollary we obtain a polygonal version of Fenchel's theorem [21]:

Corollary 2.4.

$$\sum_{i=1}^{n} \beta_i \geq 2\pi.$$

Proof of Proposition 2.2. The claim of Proposition 2.2 is invariant with respect to Möbius transformations. Applying a Möbius transformation M that maps the vertex v to infinity, $M(v) = \infty$, we make all circles passing through v into straight lines and arrive at the geometry shown in Figure 4 with $P = M(\infty)$. Now the result follows immediately from Corollary 2.4. □

Theorem 2.5. *Let S be a compact simplicial surface without boundary. Then*

$$W(S) \geq 0,$$

and equality holds if and only if S is a convex polyhedron inscribed in a sphere, i.e., a Delaunay triangulation of a sphere.

Proof. Only the second statement needs to be proven. By Proposition 2.2, the equality $W(S) = 0$ implies that the star of each vertex of S is convex (but not necessarily strictly convex). Deleting the edges that separate triangles lying in a common plane, one obtains a polyhedral surface S_P with circular faces and all strictly convex vertices and edges. Proposition 2.2 implies that for every vertex v there exists a sphere S_v with all vertices of the star $S(v)$ lying on it. For any edge (v_1, v_2) of S_P two neighboring spheres S_{v_1} and

S_{v_2} share two different circles of their common faces. This implies $S_{v_1} = S_{v_2}$ and finally the coincidence of all the spheres S_v. □

2.2. Non-inscribable polyhedra

The minimization of the conformal energy for simplicial spheres is related to a classical result of Steinitz [40], who showed that there exist abstract simplicial 3-polytopes without geometric realizations as convex polytopes with all vertices on a common sphere. We call these combinatorial types non-inscribable.

Let S be a simplicial sphere with vertices colored in black and white. Denote the sets of white and black vertices by V_w and V_b, respectively, $V = V_w \cup V_b$. Assume that there are no edges connecting two white vertices and denote the sets of the edges connecting white and black vertices and two black vertices by E_{wb} and E_{bb}, respectively, $E = E_{wb} \cup E_{bb}$. The sum of the local discrete Willmore energies over all white vertices can be represented as

$$\sum_{v \in V_w} W(v) = \sum_{e \in E_{wb}} \beta(e) - 2\pi |V_w|.$$

Its non-negativity yields $\sum_{e \in E_{wb}} \beta(e) \geq 2\pi |V_w|$. For the discrete Willmore energy of S this implies

$$W(S) = \sum_{e \in E_{wb}} \beta(e) + \sum_{e \in E_{bb}} \beta(e) - \pi(|V_w| + |V_b|) \geq \pi(|V_w| - |V_b|). \tag{2.1}$$

Equality here holds if and only if $\beta(e) = 0$ for all $e \in E_{bb}$ and the star of any white vertices is convex, with vertices lying on a common sphere. We come to the conclusion that the polyhedra of this combinatorial type with $|V_w| > |V_b|$ have positive Willmore energy and thus cannot be realized as convex polyhedra all of whose vertices belong to a sphere. These are exactly the non-inscribable examples of Steinitz (see [24]).

One such example is presented in Figure 5. Here the centers of the edges of the tetrahedron are black and all other vertices are white, so $|V_w| = 8, |V_b| = 6$. The estimate (2.1) implies that the discrete Willmore energy of any polyhedron of this type is at least 2π. The polyhedra with energy equal to 2π are constructed as follows. Take a tetrahedron, color its vertices white and chose one black vertex per edge. Draw circles through each white vertex and its two black neighbors. We get three circles on each face. Due to Miquel's theorem (see Figure 10) these three circles intersect at one point. Color this new vertex white. Connect it by edges to all black vertices of the triangle and connect pairwise the black vertices of the original faces of the tetrahedron. The constructed polyhedron has $W = 2\pi$.

To construct further polyhedra with $|V_w| > |V_b|$, take a polyhedron $\hat{P}$ whose number of faces is greater than the number of vertices $|\hat{F}| > |\hat{V}|$. Color all the vertices black, add white vertices at the faces and connect them to all black vertices of a face. This yields a polyhedron with $|V_w| = |\hat{F}| > |V_b| = |\hat{V}|$. Hodgson, Rivin and Smith [27] have found a characterization of inscribable combinatorial types, based on a transfer to the Klein model of hyperbolic 3-space. Their method is related to the methods of construction of discrete minimal surfaces in Section 5.

FIGURE 5. Discrete Willmore spheres of inscribable ($W = 0$) and non-inscribable ($W > 0$) types.

The example in Figure 5 (right) is one of the few for which the minimum of the discrete Willmore energy can be found by elementary methods. Generally this is a very appealing (but probably difficult) problem of discrete differential geometry (see the discussion in [3]).

Complete understanding of non-inscribable simplicial spheres is an interesting mathematical problem. However the existence of such spheres might be seen as a problem for using the discrete Willmore functional for applications in computer graphics, such as the fairing of surfaces. Fortunately the problem disappears after just one refinement step: all simplicial spheres become inscribable. Let $\mathbf{S}$ be an abstract simplicial sphere. Define its refinement $\mathbf{S_R}$ as follows: split every edge of $\mathbf{S}$ in two by inserting additional vertices, and connect these new vertices sharing a face of $\mathbf{S}$ by additional edges ($1 \to 4$ refinement, as in Figure 7 (left)).

Proposition 2.6. *The refined simplicial sphere* $\mathbf{S_R}$ *is inscribable, and thus there exists a polyhedron* S_R *with the combinatorics of* $\mathbf{S_R}$ *and* $W(S_R) = 0$.

Proof. Koebe's theorem (see Theorem 5.3, Section 5) states that every abstract simplicial sphere $\mathbf{S}$ can be realized as a convex polyhedron S all of whose edges touch a common sphere S^2. Starting with this realization S it is easy to construct a geometric realization S_R of the refinement $\mathbf{S_R}$ inscribed in S^2. Indeed, choose the touching points of the edges of S with S^2 as the additional vertices of S_R and project the original vertices of S (which lie outside of the sphere S^2) to S^2. One obtains a convex simplicial polyhedron S_R inscribed in S^2. □

2.3. Computation of the energy

For derivation of some formulas it will be convenient to use the language of quaternions. Let $\{\mathbf{1}, \mathbf{i}, \mathbf{j}, \mathbf{k}\}$ be the standard basis

$$\mathbf{ij} = \mathbf{k}, \quad \mathbf{jk} = \mathbf{i}, \quad \mathbf{ki} = \mathbf{j}, \quad \mathbf{ii} = \mathbf{jj} = \mathbf{kk} = -\mathbf{1}$$

of the quaternion algebra $\mathbb{H}$. A quaternion $q = q_0\mathbf{1} + q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k}$ is decomposed in its real part $\operatorname{Re} q := q_0 \in \mathbb{R}$ and imaginary part $\operatorname{Im} q := q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k} \in \operatorname{Im} \mathbb{H}$. The absolute value of q is $|q| := q_0^2 + q_1^2 + q_2^2 + q_3^2$.

We identify vectors in $\mathbb{R}^3$ with imaginary quaternions

$$v = (v_1, v_2, v_3) \in \mathbb{R}^3 \quad \longleftrightarrow \quad v = v_1\mathbf{i} + v_2\mathbf{j} + v_3\mathbf{k} \in \mathrm{Im}\,\mathbb{H}$$

and do not distinguish them in our notation. For the quaternionic product this implies

$$vw = -\langle v, w\rangle + v \times w, \tag{2.2}$$

where $\langle v, w\rangle$ and $v \times w$ are the scalar and vector products in $\mathbb{R}^3$.

Definition 2.7. Let $x_1, x_2, x_3, x_4 \in \mathbb{R}^3 \cong \mathrm{Im}\,\mathbb{H}$ be points in 3-dimensional Euclidean space. The quaternion

$$q(x_1, x_2, x_3, x_4) := (x_1 - x_2)(x_2 - x_3)^{-1}(x_3 - x_4)(x_4 - x_1)^{-1}$$

is called the *cross-ratio* of x_1, x_2, x_3, x_4.

The cross-ratio is quite useful due to its Möbius properties:

Lemma 2.8. *The absolute value and real part of the cross-ratio $q(x_1, x_2, x_3, x_4)$ are preserved by Möbius transformations. The quadrilateral x_1, x_2, x_3, x_4 is circular if and only if $q(x_1, x_2, x_3, x_4) \in \mathbb{R}$.*

Consider two triangles with a common edge. Let $a, b, c, d \in \mathbb{R}^3$ be their other edges, oriented as in Figure 6.

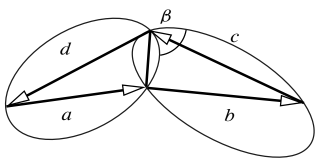

FIGURE 6. Formula for the angle between circumcircles.

Proposition 2.9. *The external angle $\beta \in [0, \pi]$ between the circumcircles of the triangles in Figure 6 is given by any of the equivalent formulas:*

$$\begin{aligned}\cos(\beta) &= -\frac{\mathrm{Re}\, q}{|q|} = -\frac{\mathrm{Re}\,(abcd)}{|abcd|} \\ &= \frac{\langle a,c\rangle\langle b,d\rangle - \langle a,b\rangle\langle c,d\rangle - \langle b,c\rangle\langle d,a\rangle}{|a||b||c||d|}.\end{aligned} \tag{2.3}$$

Here $q = ab^{-1}cd^{-1}$ is the cross-ratio of the quadrilateral.

Proof. Since $\mathrm{Re}\, q$, $|q|$ and β are Möbius-invariant, it is enough to prove the first formula for the planar case $a, b, c, d \in \mathbb{C}$, mapping all four vertices to a plane by a Möbius transformation. In this case q becomes the classical complex cross-ratio. Considering the arguments $a, b, c, d \in \mathbb{C}$ one easily arrives at $\beta = \pi - \arg q$. The second representation follows from the identity $b^{-1} = -b/|b|$ for imaginary quaternions. Finally applying (2.2) we obtain

$$\begin{aligned}\text{Re}\,(abcd) &= \langle a,b\rangle\langle c,d\rangle - \langle a\times b, c\times d\rangle \\ &= \langle a,b\rangle\langle c,d\rangle + \langle b,c\rangle\langle d,a\rangle - \langle a,c\rangle\langle b,d\rangle.\end{aligned}$$

□

2.4. Smooth limit

The discrete energy W is not only a discrete analogue of the Willmore energy. In this section we show that it approximates the smooth Willmore energy, although the smooth limit is very sensitive to the refinement method and should be chosen in a special way. We consider a special infinitesimal triangulation which can be obtained in the limit of $1 \to 4$ refinements (see Figure 7 (left)) of a triangulation of a smooth surface. Intuitively it is clear that in the limit one has a regular triangulation such that almost every vertex is of valence 6 and neighboring triangles are congruent up to sufficiently high order in ϵ (ϵ being of the order of the distances between neighboring vertices).

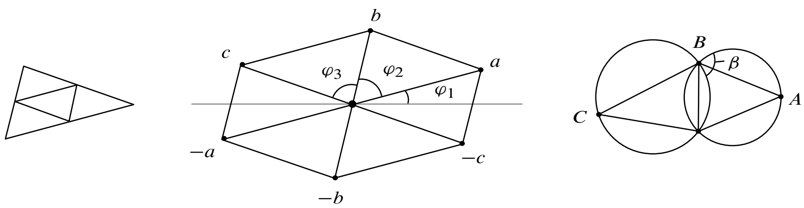

FIGURE 7. Smooth limit of the discrete Willmore energy. *Left:* The $1 \to 4$ refinement. *Middle:* An infinitesimal hexagon in the parameter plane with a (horizontal) curvature line. *Right:* The β-angle corresponding to two neighboring triangles in $\mathbb{R}^3$.

We start with a comparison of the discrete and smooth Willmore energies for an important modeling example. Consider a neighborhood of a vertex $v \in \mathcal{S}$, and represent the smooth surface locally as a graph over the tangent plane at v:

$$\mathbb{R}^2 \ni (x,y) \mapsto f(x,y) = \left(x, y, \frac{1}{2}(k_1x^2 + k_2y^2) + o(x^2+y^2)\right) \in \mathbb{R}^3, \quad (x,y) \to 0.$$

Here x, y are the curvature directions and k_1, k_2 are the principal curvatures at v. Let the vertices $(0,0)$, $a = (a_1, a_2)$ and $b = (b_1, b_2)$ in the parameter plane form an acute triangle. Consider the infinitesimal hexagon with vertices $\epsilon a, \epsilon b, \epsilon c, -\epsilon a, -\epsilon b, -\epsilon c$, (see Figure 7 (middle)), with $b = a + c$. The coordinates of the corresponding points on the smooth surface are

$$\begin{aligned} f(\pm\epsilon a) &= \epsilon(\pm a_1, \pm a_2, \epsilon r_a + o(\epsilon)), \\ f(\pm\epsilon c) &= \epsilon(\pm c_1, \pm c_2, \epsilon r_c + o(\epsilon)), \\ f(\pm\epsilon b) &= (f(\pm\epsilon a) + f(\pm\epsilon c)) + \epsilon^2 R, \quad R = (0,0,r+o(\epsilon)), \end{aligned}$$

where

$$r_a = \frac{1}{2}(k_1 a_1^2 + k_2 a_2^2), \quad r_c = \frac{1}{2}(k_1 c_1^2 + k_2 c_2^2), \quad r = (k_1 a_1 c_1 + k_2 a_2 c_2)$$

and $a = (a_1, a_2), c = (c_1, c_2)$.

We will compare the discrete Willmore energy W of the simplicial surface comprised by the vertices $f(\epsilon a), \dots, f(-\epsilon c)$ of the hexagonal star with the classical Willmore energy $\mathcal{W}$ of the corresponding part of the smooth surface $\mathcal{S}$. Some computations are required for this. Denote by $\epsilon A = f(\epsilon a), \epsilon B = f(\epsilon b), \epsilon C = f(\epsilon c)$ the vertices of two corresponding triangles (as in Figure 7 (right)), and also by $|a|$ the length of a and by $\langle a, c\rangle = a_1 c_1 + a_2 c_2$ the corresponding scalar product.

Lemma 2.10. *The external angle $\beta(\epsilon)$ between the circumcircles of the triangles with the vertices $(0, A, B)$ and $(0, B, C)$ (as in Figure 7 (right)) is given by*

$$\beta(\epsilon) = \beta(0) + w(b) + o(\epsilon^2), \quad \epsilon \to 0, \quad w(b) = \epsilon^2 \frac{g \cos\beta(0) - h}{|a|^2 |c|^2 \sin\beta(0)}. \tag{2.4}$$

Here $\beta(0)$ is the external angle of the circumcircles of the triangles $(0, a, b)$ and $(0, b, c)$ in the plane, and

$$g = |a|^2 r_c (r + r_c) + |c|^2 r_a (r + r_a) + \frac{r^2}{2}(|a|^2 + |c|^2),$$
$$h = |a|^2 r_c (r + r_c) + |c|^2 r_a (r + r_a) - \langle a, c\rangle (r + 2r_a)(r + 2r_c).$$

Proof. Formula (2.3) with $a = -C, b = A, c = C + \epsilon R, d = -A - \epsilon R$ yields for $\cos\beta$

$$\frac{\langle C, C + \epsilon R\rangle\langle A, A + \epsilon R\rangle - \langle A, C\rangle\langle A + \epsilon R, C + \epsilon R\rangle - \langle A, C + \epsilon R\rangle\langle A + \epsilon R, C\rangle}{|A||C||A + \epsilon R||C + \epsilon R|},$$

where $|A|$ is the length of A. Substituting the expressions for A, C, R we see that the term of order ϵ of the numerator vanishes, and we obtain for the numerator

$$|a|^2 |c|^2 - 2\langle a, c\rangle^2 + \epsilon^2 h + o(\epsilon^2).$$

For the terms in the denominator we get

$$|A| = |a|\left(1 + \frac{r_a^2}{2|a|^2}\epsilon^2 + o(\epsilon^2)\right), \quad |A + \epsilon R| = |a|\left(1 + \frac{(r + r_a)^2}{2|a|^2}\epsilon^2 + o(\epsilon^2)\right)$$

and similar expressions for $|C|$ and $|C + \epsilon R|$. Substituting this to the formula for $\cos\beta$ we obtain

$$\cos\beta = 1 - 2\left(\frac{\langle a, c\rangle}{|a||c|}\right)^2 + \frac{\epsilon^2}{|a|^2|c|^2}\Big(h - g\big(1 - 2\big(\frac{\langle a, c\rangle}{|a||c|}\big)^2\big)\Big) + o(\epsilon^2).$$

Observe that this formula can be read as

$$\cos\beta(\epsilon) = \cos\beta(0) + \frac{\epsilon^2}{|a|^2|c|^2}\big(h - g\cos\beta(0)\big) + o(\epsilon^2),$$

which implies the asymptotics (2.4). □

The term $w(b)$ is in fact the part of the discrete Willmore energy of the vertex v coming from the edge b. Indeed the sum of the angles $\beta(0)$ over all 6 edges meeting at v is 2π. Denote by $w(a)$ and $w(c)$ the parts of the discrete Willmore energy corresponding to the edges a and c. Observe that for the opposite edges (for example a and $-a$) the terms w coincide. Denote by $W_\epsilon(v)$ the discrete Willmore energy of the simplicial hexagon we consider. We have

$$W_\epsilon(v) = (w(a) + w(b) + w(c)) + o(\epsilon^2).$$

On the other hand the part of the classical Willmore functional corresponding to the vertex v is

$$\mathcal{W}_\epsilon(v) = \frac{1}{4}(k_1 - k_2)^2 S + 0(\epsilon^2),$$

where the area S is one third of the area of the hexagon or, equivalently, twice the area of one of the triangles in the parameter domain

$$S = \epsilon^2 |a||c| \sin\gamma.$$

Here γ is the angle between the vectors a and c. An elementary geometric consideration implies

$$\beta(0) = 2\gamma - \pi. \tag{2.5}$$

We are interested in the quotient $W_\epsilon/\mathcal{W}_\epsilon$ which is obviously scale-invariant. Let us normalize $|a| = 1$ and parametrize the triangles by the angles between the edges and by the angle to the curvature line; see Figure 7 (middle).

$$\begin{aligned} (a_1, a_2) &= (\cos\phi_1, \sin\phi_1), \qquad (2.6)\\ (c_1, c_2) &= \Big(\frac{\sin\phi_2}{\sin\phi_3}\cos(\phi_1 + \phi_2 + \phi_3), \frac{\sin\phi_2}{\sin\phi_3}\sin(\phi_1 + \phi_2 + \phi_3)\Big). \end{aligned}$$

The moduli space of the regular lattices of acute triangles is described as follows,

$$\Phi = \{\phi = (\phi_1, \phi_2, \phi_3) \in \mathbb{R}^3 | \, 0 \le \phi_1 < \frac{\pi}{2},\ 0 < \phi_2 < \frac{\pi}{2},\ 0 < \phi_3 < \frac{\pi}{2},\ \frac{\pi}{2} < \phi_2 + \phi_3\}.$$

Proposition 2.11. *The limit of the quotient of the discrete and smooth Willmore energies*

$$Q(\phi) := \lim_{\epsilon \to 0} \frac{W_\epsilon(v)}{\mathcal{W}_\epsilon(v)}$$

is independent of the curvatures of the surface and depends on the geometry of the triangulation only. It is

$$Q(\phi) = 1 - \frac{(\cos 2\phi_1 \cos\phi_3 + \cos(2\phi_1 + 2\phi_2 + \phi_3))^2 + (\sin 2\phi_1 \cos\phi_3)^2}{4\cos\phi_2 \cos\phi_3 \cos(\phi_2 + \phi_3)}, \tag{2.7}$$

and we have $Q > 1$. The infimum $\inf_\Phi Q(\phi) = 1$ corresponds to one of the cases when two of the three lattice vectors a, b, c are in the principal curvature directions:

- $\phi_1 = 0$, $\phi_2 + \phi_3 \to \frac{\pi}{2}$,
- $\phi_1 = 0$, $\phi_2 \to \frac{\pi}{2}$,
- $\phi_1 + \phi_2 = \frac{\pi}{2}$, $\phi_3 \to \frac{\pi}{2}$.

Proof. The proof is based on a direct but rather involved computation. We used the *Mathematica* computer algebra system for some of the computations. Introduce

$$\tilde{w} := \frac{4w}{(k_1 - k_2)^2 S}.$$

This gives in particular

$$\tilde{w}(b) = 2\frac{h + g(2\cos^2\gamma - 1)}{(k_1 - k_2)^2|a|^3|c|^3\cos\gamma\sin^2\gamma} = 2\frac{h + g\left(2\frac{\langle a,c\rangle^2}{|a|^2|c|^2} - 1\right)}{(k_1 - k_2)^2\langle a,c\rangle(|a|^2|c|^2 - \langle a,c\rangle^2)}.$$

Here we have used the relation (2.5) between $\beta(0)$ and γ. In the sum over the edges $Q = \tilde{w}(a) + \tilde{w}(b) + \tilde{w}(c)$ the curvatures k_1, k_2 disappear and we get Q in terms of the coordinates of a and c:

$$\begin{aligned} Q = 2\Big(&(a_1^2c_2^2 + a_2^2c_1^2)(a_1c_1 + a_2c_2) + a_1^2c_1^2(a_2^2 + c_2^2) + a_2^2c_2^2(a_1^2 + c_1^2) \\ &+ 2a_1a_2c_1c_2\big((a_1 + c_1)^2 + (a_2 + c_2)^2\big)\Big)/ \\ &\Big((a_1c_1 + a_2c_2)\big(a_1(a_1 + c_1) + a_2(a_2 + c_2)\big)\big((a_1 + c_1)c_1 + (a_2 + c_2)c_2\big)\Big). \end{aligned}$$

Substituting the angle representation (2.6) we obtain

$$Q = \frac{\sin 2\phi_1 \sin 2(\phi_1 + \phi_2) + 2\cos\phi_2 \sin(2\phi_1 + \phi_2)\sin 2(\phi_1 + \phi_2 + \phi_3)}{4\cos\phi_2\cos\phi_3\cos(\phi_2 + \phi_3)}.$$

One can check that this formula is equivalent to (2.7). Since the denominator in (2.7) on the space Φ is always negative we have $Q > 1$. The identity $Q = 1$ holds only if both terms in the nominator of (2.7) vanish. This leads exactly to the cases indicated in the proposition when the lattice vectors are directed along the curvature lines. Indeed the vanishing of the second term in the nominator implies either $\phi_1 = 0$ or $\phi_3 \to \frac{\pi}{2}$. Vanishing of the first term in the nominator with $\phi_1 = 0$ implies $\phi_2 \to \frac{\pi}{2}$ or $\phi_2 + \phi_3 \to \frac{\pi}{2}$. Similarly in the limit $\phi_3 \to \frac{\pi}{2}$ the vanishing of

$$\big(\cos 2\phi_1 \cos\phi_3 + \cos(2\phi_1 + 2\phi_2 + \phi_3)\big)^2/\cos\phi_3$$

implies $\phi_1 + \phi_2 = \frac{\pi}{2}$. One can check that in all these cases $Q(\phi) \to 1$. □

Note that for the infinitesimal equilateral triangular lattice $\phi_2 = \phi_3 = \frac{\pi}{3}$ the result is independent of the orientation ϕ_1 with respect to the curvature directions, and the discrete Willmore energy is in the limit $Q = 3/2$ times larger than the smooth one.

Finally, we come to the following conclusion.

Theorem 2.12. *Let $\mathcal{S}$ be a smooth surface with Willmore energy $\mathcal{W}(\mathcal{S})$. Consider a simplicial surface S_ϵ such that its vertices lie on $\mathcal{S}$ and are of degree 6, the distances between the neighboring vertices are of order ϵ, and the neighboring triangles of S_ϵ meeting at a vertex are congruent up to order ϵ^3 (i.e., the lengths of the corresponding edges differ by terms of order at most ϵ^4), and they build elementary hexagons the lengths of whose* *opposite edges differ by terms of order at most ϵ^4. Then the limit of the discrete Willmore energy is bounded from below by the classical Willmore energy*

$$\lim_{\epsilon \to 0} W(S_\epsilon) \geq \mathcal{W}(\mathcal{S}). \tag{2.8}$$

Moreover, equality in (2.8) *holds if S_ϵ is a regular triangulation of an infinitesimal curvature-line net of $\mathcal{S}$, i.e., the vertices of S_ϵ are at the vertices of a curvature-line net of $\mathcal{S}$.*

Proof. Consider an elementary hexagon of S_ϵ. Its projection to the tangent plane of the central vertex is a hexagon which can be obtained from the modeling one considered in Proposition 2.11 by a perturbation of vertices of order $o(\epsilon^3)$. Such perturbations contribute to the terms of order $o(\epsilon^2)$ of the discrete Willmore energy. The latter are irrelevant for the considerations of Proposition 2.11. □

Possibly minimization of the discrete Willmore energy with the vertices constrained to lie on S could be used for computation of a curvature-line net.

2.5. Bending energy for simplicial surfaces

An accurate model for bending of discrete surfaces is important for modeling in computer graphics. The bending energy of smooth thin shells (compare [22]) is given by the integral

$$E = \int (H - H_0)^2 dA,$$

where H_0 and H are the mean curvatures of the original and deformed surface, respectively. For $H_0 = 0$ it reduces to the Willmore energy.

To derive the bending energy for simplicial surfaces let us consider the limit of fine triangulations, where the angles between the normals of neighboring triangles become small. Consider an isometric deformation of two adjacent triangles. Let θ be the external dihedral angle of the edge e, or, equivalently, the angle between the normals of these triangles (see Figure 8) and $\beta(\theta)$ the external intersection angle between the circumcircles of the triangles (see Figure 3) as a function of θ.

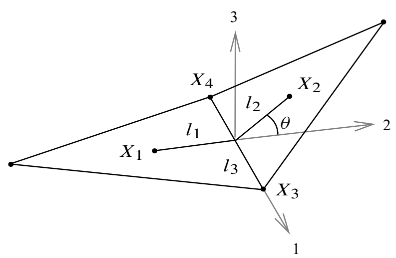

FIGURE 8. Defining the bending energy for simplicial surfaces.

Proposition 2.13. *Assume that the circumcenters of two adjacent triangles do not coincide. Then in the limit of small angles $\theta \to 0$ the angle β between the circles behaves as follows:*

$$\beta(\theta) = \beta(0) + \frac{l}{4L}\theta^2 + o(\theta^3).$$

Here l is the length of the edge and $L \neq 0$ is the distance between the centers of the circles.

Proof. Let us introduce the orthogonal coordinate system with the origin at the middle point of the common edge e, the first basis vector directed along e, and the third basis vector orthogonal to the left triangle. Denote by X_1, X_2 the centers of the circumcircles of the triangles and by X_3, X_4 the end points of the common edge; see Figure 8. The coordinates of these points are $X_1 = (0, -l_1, 0)$, $X_2 = (0, l_2 \cos\theta, l_2 \sin\theta)$, $X_3 = (l_3, 0, 0)$, $X_4 = (-l_3, 0, 0)$. Here $2l_3$ is the length of the edge e, and l_1 and l_2 are the distances from its middle point to the centers of the circumcirlces (for acute triangles). The unit normals to the triangles are $N_1 = (0, 0, 1)$ and $N_2 = (0, -\sin\theta, \cos\theta)$. The angle β between the circumcircles intersecting at the point X_4 is equal to the angle between the vectors $A = N_1 \times (X_4 - X_1)$ and $B = N_2 \times (X_4 - X_2)$. The coordinates of these vectors are $A = (-l_1, -l_3, 0)$, $B = (l_2, -l_3 \cos\theta, -l_3 \sin\theta)$. This implies for the angle

$$\cos\beta(\theta) = \frac{l_3^2 \cos\theta - l_1 l_2}{r_1 r_2}, \tag{2.9}$$

where $r_i = \sqrt{l_i^2 + l_3^2}$, $i = 1, 2$ are the radii of the corresponding circumcircles. Thus $\beta(\theta)$ is an even function, in particular $\beta(\theta) = \beta(0) + B\theta^2 + o(\theta^3)$. Differentiating (2.9) by θ^2 we obtain

$$B = \frac{l_3^2}{2 r_1 r_2 \sin\beta(0)}.$$

Also formula (2.9) yields

$$\sin\beta(0) = \frac{l_3 L}{r_1 r_2},$$

where $L = |l_1 + l_2|$ is the distance between the centers of the circles. Finally combining these formulas we obtain $B = l_3/(2L)$. □

This proposition motivates us to define the bending energy of simplicial surfaces as

$$E = \sum_{e \in E} \frac{l}{L}\theta^2.$$

For discrete thin-shells this bending energy was suggested and analyzed by Grinspun et al. [23, 22]. The distance between the barycenters was used for L in the energy expression, and possible advantages in using circumcenters were indicated. Numerical experiments demonstrate good qualitative simulation of real processes.

Further applications of the discrete Willmore energy in particular for surface restoration, geometry denoising, and smooth filling of a hole can be found in [8].

3. Circular nets as discrete curvature lines

Simplicial surfaces as studied in the previous section are too unstructured for analytical investigation. An important tool in the theory of smooth surfaces is the introduction of (special) parametrizations of a surface. Natural analogues of parametrized surfaces are quadrilateral surfaces, i.e., discrete surfaces made from (not necessarily planar) quadrilaterals. The strips of quadrilaterals obtained by gluing quadrilaterals along opposite edges can be considered as coordinate lines on the quadrilateral surface.

We start with a combinatorial description of the discrete surfaces under consideration.

Definition 3.1. A cellular decomposition $\mathcal{D}$ of a two-dimensional manifold (with boundary) is called a *quad-graph* if the cells have four sides each.

A quadrilateral surface is a mapping f of a quad-graph to $\mathbb{R}^3$. The mapping f is given just by the values at the vertices of $\mathcal{D}$, and vertices, edges and faces of the quad-graph and of the quadrilateral surface correspond. Quadrilateral surfaces with planar faces were suggested by Sauer [35] as discrete analogs of conjugate nets on smooth surfaces. The latter are the mappings $(x, y) \mapsto f(x, y) \in \mathbb{R}^3$ such that the mixed derivative f_{xy} is tangent to the surface.

Definition 3.2. A quadrilateral surface $f : \mathcal{D} \to \mathbb{R}^3$ all faces of which are circular (i.e., the four vertices of each face lie on a common circle) is called a *circular net* (or discrete orthogonal net).

Circular nets as discrete analogues of curvature-line parametrized surfaces were mentioned by Martin, de Pont, Sharrock and Nutbourne [32, 33] . The curvature-lines on smooth surfaces continue through any point. Keeping in mind the analogy to the curvature-line parametrized surfaces one may in addition require that all vertices of a circular net are of even degree.

A smooth conjugate net $f : D \to \mathbb{R}^3$ is a curvature-line parametrization if and only if it is orthogonal. The angle bisectors of the diagonals of a circular quadrilateral intersect orthogonally (see Figure 9) and can be interpreted [14] as discrete principal curvature directions.

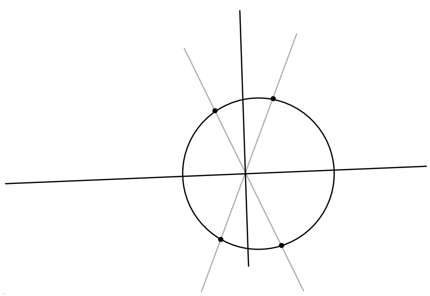

FIGURE 9. Principal curvature directions of a circular quadrilateral.

There are deep reasons to treat circular nets as a discrete curvature-line parametrization.

- The class of circular nets as well as the class of curvature-line parametrized surfaces is invariant under Möbius transformations.
- Take an infinitesimal quadrilateral $(f(x,y), f(x+\epsilon), y), f(x+\epsilon), y+\epsilon), f(x,y+\epsilon))$ of a curvature-line parametrized surface. A direct computation (see [14]) shows that in the limit $\epsilon \to 0$ the imaginary part of its cross-ratio is of order ϵ^3. Note that circular quadrilaterals are characterized by having real cross-ratios.
- For any smooth curvature-line parametrized surface $f : D \to \mathbb{R}^3$ there exists a family of discrete circular nets converging to f. Moreover, the convergence is C^∞, i.e., with all derivatives. The details can be found in [5].

One more argument in favor of Definition 3.2 is that circular nets satisfy the *consistency principle*, which has proven to be one of the organizing principles in discrete differential geometry [10]. The consistency principle singles out fundamental geometries by the requirement that the geometry can be consistently extended to a combinatorial grid one dimension higher. The consistency of circular nets was shown by Cieśliński, Doliwa and Santini [19] based on the following classical theorem.

Theorem 3.3 (Miquel). *Consider a combinatorial cube in $\mathbb{R}^3$ with planar faces. Assume that three neighboring faces of the cube are circular. Then the remaining three faces are also circular.*

Equivalently, provided the four-tuples of black vertices coming from three neighboring faces of the cube lie on circles, the three circles determined by the triples of points corresponding to three remaining faces of the cube all intersect (at the white vertex in Figure 10). It is easy to see that all vertices of Miquel's cube lie on a sphere. Mapping the vertex shared by the three original faces to infinity by a Möbius transformation, we obtain an equivalent planar version of Miquel's theorem. This version, also shown in Figure 10, can be proven by means of elementary geometry.

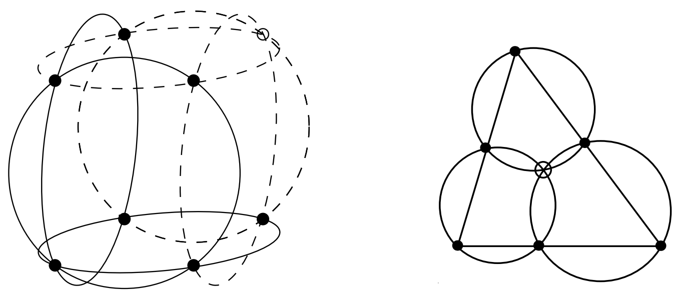

FIGURE 10. Miquel's theorem: spherical and planar versions.

Finally note that circular nets are also treated as a discretization of triply orthogonal coordinate systems. Triply orthogonal coordinate systems in $\mathbb{R}^3$ are maps $(x, y, z) \mapsto f(x, y, z) \in \mathbb{R}^3$ from a subset of $\mathbb{R}^3$ with mutually orthogonal f_x, f_y, f_z. Due to the classical Dupin theorem, the level surfaces of a triply orthogonal coordinate system intersect along their common curvature lines. Accordingly, discrete triply orthogonal systems are defined as maps from $\mathbb{Z}^3$ (or a subset thereof) to $\mathbb{R}^3$ with all elementary hexahedra lying on spheres [2]. Due to Miquel's theorem a discrete orthogonal system is uniquely determined by the circular nets corresponding to its coordinate two-planes (see [19] and [10]).

4. Discrete isothermic surfaces

In this section and in the following one, we investigate discrete analogs of special classes of surfaces obtained by imposing additional conditions in terms of circles and spheres.

We start with minor combinatorial restrictions. Suppose that the vertices of a quad-graph $\mathcal{D}$ are colored black or white so that the two ends of each edge have different colors. Such a coloring is always possible for topological discs. To model the curvature lines, suppose also that the edges of a quad-graph $\mathcal{D}$ may consistently be labelled '+' and '−', as in Figure 11 (for this it is necessary that each vertex has an even number of edges). Let f_0 be a vertex of a circular net, $f_1, f_3, \ldots, f_{4N-1}$ be its neighbors, and

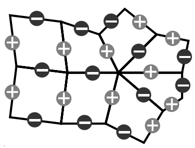

FIGURE 11. Labelling the edges of a discrete isothermic surface.

$f_2, f_4, \ldots, f_{4N}$ its next-neighbors (see Figure 12 (left)). We call the vertex f_0 generic if it is not co-spherical with all its neighbors and a circular net $f : \mathcal{D} \to \mathbb{R}^3$ generic if all its vertices are generic.

Let $f : \mathcal{D} \to \mathbb{R}^3$ be a generic circular net such that every vertex is co-spherical with all its next-neighbors. We will call the corresponding sphere *central*. For an analytical description of this geometry let us map the vertex f_0 to infinity by a Möbius transformation $\mathcal{M}(f_0) = \infty$, and denote by $F_i = \mathcal{M}(f_i)$, the images of the f_i, for $i = 1, \ldots, 4N$. The points $F_2, F_4, \ldots, F_{4N}$ are obviously coplanar. The circles of the faces are mapped to straight lines. For the cross-ratios we get

$$q(f_0, f_{2k-1}, f_{2k}, f_{2k+1}) = \frac{F_{2k} - F_{2k+1}}{F_{2k} - F_{2k-1}} = \frac{z_{2k+1}}{z_{2k-1}},$$

where z_{2k+1} is the coordinate of F_{2k+1} orthogonal to the plane $\mathcal{P}$ of $F_2, F_4, \ldots, F_{4N}$. (Note that since f_0 is generic none of the z_i vanishes.) As a corollary we get for the product of all cross-ratios:

$$\prod_{k=1}^{n} q(f_0, f_{2k-1}, f_{2k}, f_{2k+1}) = 1. \tag{4.1}$$

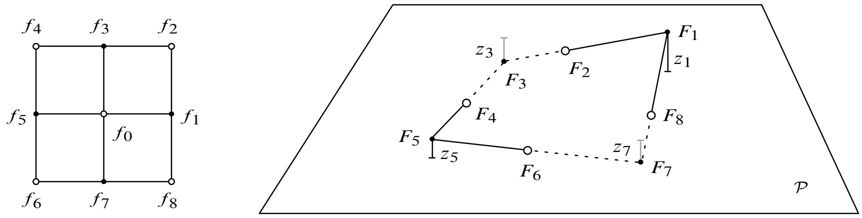

FIGURE 12. Central spheres of a discrete isothermic surface: combinatorics *(left)*, and the Möbius normalized picture for $N = 2$ *(right)*.

Definition 4.1. A circular net $f : \mathcal{D} \to \mathbb{R}^3$ satisfying condition (4.1) at each vertex is called a *discrete isothermic surface*.

This definition was first suggested in [6] for the case of the combinatorial square grid $\mathcal{D} = \mathbb{Z}^2$. In this case if the vertices are labelled by $f_{m,n}$ and the corresponding cross-ratios by $q_{m,n} := q(f_{m,n}, f_{m+1,n}, f_{m+1,n+1}, f_{m,n+1})$, the condition (4.1) reads

$$q_{m,n}q_{m+1,n+1} = q_{m+1,n}q_{m,n+1}.$$

Proposition 4.2. *Each vertex $f_{m,n}$ of a discrete isothermic surface $f : \mathbb{Z}^2 \to \mathbb{R}^3$ has a central sphere, i.e., the points $f_{m,n}$, $f_{m-1,n-1}$, $f_{m+1,n-1}$, $f_{m+1,n+1}$ and $f_{m-1,n+1}$ are co-spherical. Moreover, for generic circular maps $f : \mathbb{Z}^2 \to \mathbb{R}^3$ this property characterizes discrete isothermic surfaces.*

Proof. Use the notation of Figure 12, with $f_0 \equiv f_{m,n}$, and the same argument with the Möbius transformation $\mathcal{M}$ which maps f_0 to ∞. Consider the plane $\mathcal{P}$ determined by the points F_2, F_4 and F_6. Let as above z_k be the coordinates of F_k orthogonal to the plane $\mathcal{P}$. Condition (4.1) yields

$$\frac{F_8 - F_1}{F_8 - F_7} = \frac{z_1}{z_7}.$$

This implies that the z-coordinate of the point F_8 vanishes, thus $F_8 \in \mathcal{P}$. □

The property to be discrete isothermic is also 3D-consistent, i.e., can be consistently imposed on all faces of a cube. This was proven first by Hertrich-Jeromin, Hoffmann and Pinkall [26] (see also [10] for generalizations and modern treatment).

An important subclass of discrete isothermic surfaces is given by the condition that all the faces are conformal squares, i.e., their cross ratio equals -1. All conformal squares are Möbius equivalent, in particular equivalent to the standard square. This is a direct discretization of the definition of smooth isothermic surfaces. The latter are immersions $(x, y) \mapsto f(x, y) \in \mathbb{R}^3$ satisfying

$$\|f_x\| = \|f_y\|, \qquad f_x \perp f_y, \qquad f_{xy} \in \text{span}\{f_x, f_x\}, \tag{4.2}$$

i.e., conformal curvature-line parametrizations. Geometrically this definition means that the curvature lines divide the surface into infinitesimal squares.

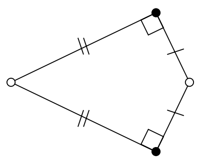

FIGURE 13. Right-angled kites are conformal squares.

The class of discrete isothermic surfaces is too general and the surfaces are not rigid enough. In particular one can show that the surface can vary preserving all its black vertices. In this case, one white vertex can be chosen arbitrarily [7]. Thus, we introduce a more rigid subclass. To motivate its definition, let us look at the problem of discretizing the class of conformal maps $f : D \to \mathbb{C}$ for $D \subset \mathbb{C} = \mathbb{R}^2$. Conformal maps are characterized by the conditions

$$|f_x| = |f_y|, \qquad f_x \perp f_y. \tag{4.3}$$

To define discrete conformal maps $f : \mathbb{Z}^2 \supset D \to \mathbb{C}$, it is natural to impose these two conditions on two different sub-lattices (white and black) of $\mathbb{Z}^2$, i.e., to require that the edges meeting at a white vertex have equal length and the edges at a black vertex meet orthogonally. This discretization leads to the circle patterns with the combinatorics of the square grid introduced by Schramm [37]. Each circle intersects four neighboring circles orthogonally and the neighboring circles touch cyclically; see Figure 14 (left).

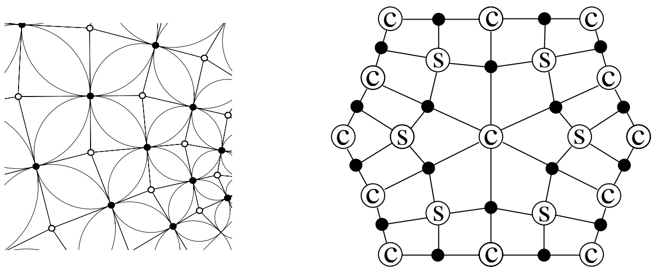

FIGURE 14. Defining discrete S-isothermic surfaces: orthogonal circle patterns as discrete conformal maps *(left)* and combinatorics of S-quad-graphs *(right)*.

The same properties imposed for quadrilateral surfaces with the combinatorics of the square grid $f : \mathbb{Z}^2 \supset \mathcal{D} \to \mathbb{R}^3$ lead to an important subclass of discrete isothermic surfaces. Let us require for a discrete quadrilateral surface that:

- the faces are orthogonal kites, as in Figure 13,
- the edges meet at black vertices orthogonally (black vertices are at orthogonal corners of the kites),
- the kites which do not share a common vertex are not coplanar (locality condition).

Observe that the orthogonality condition (at black vertices) implies that one pair of opposite edges meeting at a black vertex lies on a straight line. Together with the locality condition this implies that there are two kinds of white vertices, which we denote by ⓒ and ⓢ. Each kite has white vertices of both types and the kites sharing a white vertex of the first kind ⓒ are coplanar.

These conditions imposed on the quad-graphs lead to S-quad-graphs and S-isothermic surfaces (the latter were introduced in [7] for the combinatorics of the square grid).

Definition 4.3. An *S-quad-graph* $\mathcal{D}$ is a quad-graph with black and two kinds of white vertices such that the two ends of each edge have different colors and each quadrilateral has vertices of all kinds; see Figure 14 (right). Let $V_b(\mathcal{D})$ be the set of black vertices. A *discrete S-isothermic surface* is a map

$$f_b : V_b(\mathcal{D}) \to \mathbb{R}^3,$$

with the following properties:

1. If $v_1, \dots, v_{2n} \in V_b(\mathcal{D})$ are the neighbors of a ⓒ-vertex in cyclic order, then $f_b(v_1), \dots, f_b(v_{2n})$ lie on a circle in $\mathbb{R}^3$ in the same cyclic order. This defines a map from the ⓒ-vertices to the set of circles in $\mathbb{R}^3$.
2. If $v_1, \dots, v_{2n} \in V_b(\mathcal{D})$ are the neighbors of an ⓢ-vertex, then $f_b(v_1), \dots, f_b(v_{2n})$ lie on a sphere in $\mathbb{R}^3$. This defines a map from the ⓢ-vertices to the set of spheres in $\mathbb{R}^3$.
3. If v_c and v_s are the ⓒ- and ⓢ-vertices of a quadrilateral of $\mathcal{D}$, then the circle corresponding to v_c intersects the sphere corresponding to v_s orthogonally.

Discrete S-isothermic surfaces are therefore composed of tangent spheres and tangent circles, with the spheres and circles intersecting orthogonally. The class of discrete S-isothermic surfaces is obviously invariant under Möbius transformations.

Given a discrete S-isothermic surface, one can add the centers of the spheres and circles to it giving a map $V(\mathcal{D}) \to \mathbb{R}^3$. The discrete isothermic surface obtained is called the *central extension* of the discrete S-isothermic surface. All its faces are orthogonal kites.

An important fact of the theory of isothermic surfaces (smooth and discrete) is the existence of a dual isothermic surface [6]. Let $f : \mathbb{R}^2 \supset D \to \mathbb{R}^3$ be an isothermic immersion. Then the formulas

$$f_x^* = \frac{f_x}{\|f_x\|^2}, \quad f_y^* = -\frac{f_y}{\|f_y\|^2}$$