CS Peskin 5/8/2019

Bending energy and area-preserving energy of a triangulated surface

Consider a closed triangulated surface with the topology of a sphere and with vertices

(1) $$\underline{X}^k, \quad k = 1 \cdots v$$

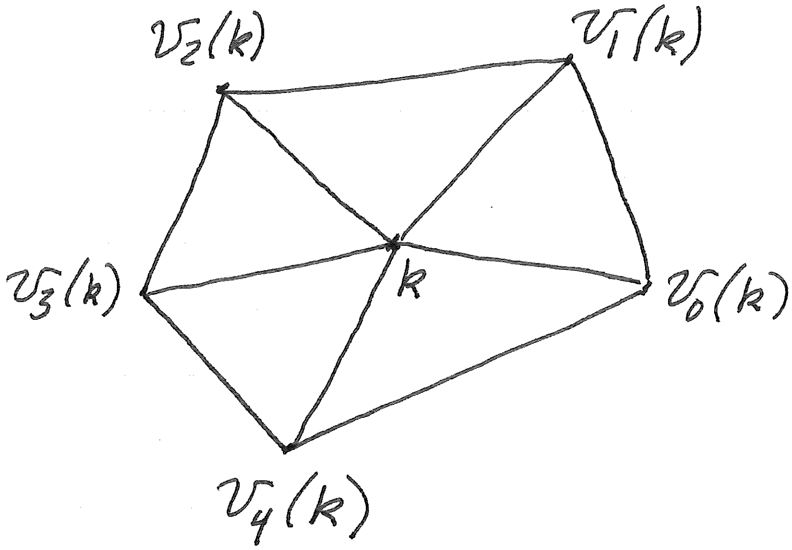
Let the indices of the vertices that are neighbors of vertex k be denoted

(2) $$v_i(k), \quad i = 0 \cdots (n(k) - 1)$$

where $n(k)$ is the number of neighbors of vertex k, and the neighbors are listed in counterclockwise order when viewed from outside of the surface.

In expressions like $v_{i+1}(k)$, "$i+1$" will be understood to mean $i+1$ modulo $n(k)$.

Thus, for example, with $n(k) = 5$, we have the following picture



Let V be the total volume enclosed by the triangulated surface. Each face of the triangulated surface, together with the origin, forms a tetrahedron, and V is the sum of the signed volumes of these tetrahedra. By retaining the sign (and not taking absolute values), we make V independent of the choice of origin, which can even be outside of the surface.

A formula for V in terms of the coordinates of the vertices is as follows

$$(3)\quad V = \frac{1}{3}\sum_{k=1}^{v}\frac{1}{6}\sum_{i=0}^{n(k)-1} \underline{X}^{k}\cdot\left(\underline{X}^{v_i(k)} \times \underline{X}^{v_{i+1}(k)}\right)$$

The factor $\frac{1}{3}$ is needed in this formula because any particular tetrahedron is included three times.

In components

$$(4)\quad V = \frac{1}{3}\sum_{k=1}^{v}\frac{1}{6}\sum_{i=0}^{n(k)-1} \varepsilon_{\alpha\beta\gamma} X^{k}_{\alpha} X^{v_i(k)}_{\beta} X^{v_{i+1}(k)}_{\gamma}$$

Here we use Greek letters taking the values 1,2,3 to indicate the spatial component of a vector, and we also use the summation convention that any particular one of these indices that is repeated in a given term is summed over 1,2,3.

The expression $\varepsilon_{\alpha\beta\gamma}$ is defined by the following statements:

(5) $\begin{cases} \varepsilon_{123} = +1 \\ \varepsilon_{\alpha\beta\gamma} \text{ changes sign if any two of its indices are interchanged.} \end{cases}$

Because of the second part of (5), $\varepsilon_{\alpha\beta\gamma} = 0$ if any two of its indices are the same.

We can associate an area vector $\underline{A}^l$ with each vertex l of the triangulated surface in the following way:

(6) $$\underline{A}^l = \frac{\partial V}{\partial \underline{X}^l} \quad , \; l = 1 \cdots v$$

by which we mean

(7) $$A^l_\lambda = \frac{\partial V}{\partial X^l_\lambda} \quad , \; \begin{matrix} l = 1 \cdots v \\ \lambda = 1,2,3 \end{matrix}$$

To evaluate A_λ^l, we differentiate both sides of (4) with respect to X_λ^l and make use of

(8) $$\frac{\partial X_\alpha^k}{\partial X_\lambda^l} = \delta_{kl}\,\delta_{\alpha\lambda}$$

There are three terms, all of which turn out to be equal, and this cancels the factor $\frac{1}{3}$ that appears in (4). The result is

(9) $$A_\lambda^l = \frac{\partial V}{\partial X_\lambda^l} = \frac{1}{6}\sum_{i=0}^{n(l)-1} \varepsilon_{\lambda\beta\gamma}\, X_\beta^{v_i(l)}\, X_\gamma^{v_{i+1}(l)}$$

An easier way to derive (9) is to define V^l as the sum of the volumes of all of the tetrahedra that touch vertex l. This is given by

(10) $$V^l = \frac{1}{6}\sum_{i=0}^{n(l)-1} \varepsilon_{\alpha\beta\gamma}\, X_\alpha^l\, X_\beta^{v_i(l)}\, X_\gamma^{v_{i+1}(l)}$$

without any factor of $\frac{1}{3}$. Since these are the only tetrahedra that are affected by a change in $\underline{X}^\ell$, we immediately get

$$(11)\qquad A^\ell_\lambda = \frac{\partial V}{\partial X^\ell_\lambda} = \frac{\partial V^\ell}{\partial X^\ell_\lambda} = \frac{1}{6}\sum_{i=0}^{n(\ell)-1} \varepsilon_{\lambda\beta\gamma} X_\beta^{v_i(\ell)} X_\gamma^{v_{i+1}(\ell)}$$

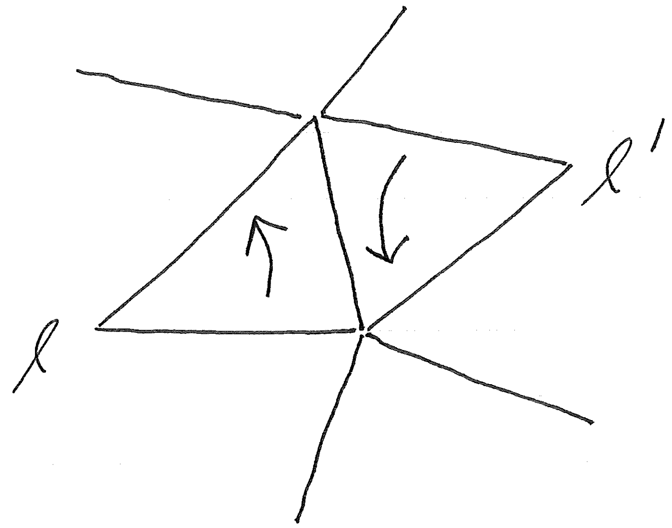
in agreement with (9). In vector notation

$$(12)\qquad \underline{A}^\ell = \frac{1}{6}\sum_{i=0}^{n(\ell)-1} \underline{X}^{v_i(\ell)} \times \underline{X}^{v_{i+1}(\ell)}$$

The sum of all of the vectors $\underline{A}^\ell$ is equal to zero, since

$$(13)\qquad \sum_{\ell=1}^{v} \underline{A}^\ell = \frac{1}{6}\sum_{\ell=1}^{v}\sum_{i=0}^{n(\ell)-1} \underline{X}^{v_i(\ell)} \times \underline{X}^{v_{i+1}(\ell)}$$

and on the right-hand side of (13) every edge of the triangulated surface appears twice, traversed in opposite directions because of the counterclockwise ordering, as shown in the figure:



So the cross products cancel and we get the result that

$$\sum_{\ell=1}^{v} \underline{A}^{\ell} = 0 \tag{14}$$

as claimed above. Because of the definition of $\underline{A}^{\ell}$, this is equivalent to the statement that

$$\sum_{\ell=1}^{v} \frac{\partial V}{\partial \underline{X}^{\ell}} = 0 \tag{15}$$

which states that V is invariant under translations of the whole triangulated surface. Since such a translation is equivalent to a change of origin, we have now proved the assertion made earlier that the volume enclosed by the surface as defined by eq. (3) or (4) is independent of the choice of origin.

The area vector $\underline{A}^l$ is $\frac{1}{3}$ of the sum of the area vectors of the triangular faces that touch vertex l. This is shown as follows:

(16)
$$\frac{1}{3}\sum_{i=0}^{n(l)-1}\frac{1}{2}\left(\underline{X}^{v_i(l)}-\underline{X}^l\right)\times\left(\underline{X}^{v_{i+1}(l)}-\underline{X}^l\right)$$

$$=\frac{1}{6}\sum_{i=0}^{n(l)-1}\left(\underline{X}^{v_i(l)}\times\underline{X}^{v_{i+1}(l)}\right)$$

$$-\frac{1}{6}\underline{X}^l\times\sum_{i=0}^{n(l)-1}\left(\underline{X}^{v_{i+1}(l)}-\underline{X}^{v_i(l)}\right)$$

$$=\underline{A}^l+\underline{0}=\underline{A}^l$$

If we sum both sides of (16) over $l = 1 \ldots v$ and make use of (14), then we reach the conclusion that $\oint \underline{n}\, da$ over the whole triangulated surface is zero. This can be proved for any closed surface by the divergence theorem, but here we have proved it in a purely algebraic way for the special case of a triangulated surface.

We now make a series of definitions based on $\underline{A}^l$:

(17) $$\underline{N}^l = \frac{\underline{A}^l}{\|\underline{A}^l\|} = \text{unit normal to the surface at vertex } l$$

(18) $$\|\underline{A}^l\| = \text{amount of area associated with vertex } l$$

(19) $$A = \sum_{l=1}^{v} \|\underline{A}^l\| = \text{area of the triangulated surface}$$

(but note that A is not equal to the sum of the areas of the triangular faces, see below)

$$\underline{H}^{\ell} = -\frac{1}{\|\underline{A}^{\ell}\|} \frac{\partial A}{\partial \underline{X}^{\ell}} \tag{20}$$

= total curvature vector at vertex ℓ

$$E_a = \frac{K_a}{2} \sum_{\ell=1}^{v} \left(\log \frac{\|\underline{A}^{\ell}\|}{\|\underline{A}^{\ell}\|_0} \right)^2 \|\underline{A}^{\ell}\|_0 \tag{21}$$

= area-preserving energy

$$E_b = \frac{K_b}{2} \sum_{\ell=1}^{v} \|\underline{H}^{\ell}\|^2 \|\underline{A}^{\ell}\| \tag{22}$$

= bending energy

In the definition of E_a, $\|\underline{A}^{\ell}\|_0$ denotes the value of $\|\underline{A}^{\ell}\|$ in a reference configuration of the triangulated surface. The definition of E_b does not involve any reference configuration.

Note that K_a has units of energy/area and that K_b has units of energy.

$$(23) \qquad \underline{F}^k \|\underline{A}^k\| = -\frac{\partial E_a}{\partial \underline{X}^k} - \frac{\partial E_b}{\partial \underline{X}^k}$$

= force on vertex k from the energy $E_a + E_b$.

(Here $\underline{F}^k$ is the force per unit area, but the quantity that we actually need is the force.)

This completes the list of definitions.

As remarked above, the area A defined by (19) is not equal to the sum of the areas of the triangular faces. Indeed, from (16) and the triangle inequality, we conclude that

$$(24) \quad \|\underline{A}^{l}\| \le \frac{1}{3}\sum_{i=0}^{n(l)-1} \left\| \frac{1}{2}\left(\underline{X}^{v_i(l)} - \underline{X}^{l}\right) \times \left(\underline{X}^{v_{i+1}(l)} - \underline{X}^{l}\right) \right\|$$

with equality only if all of the faces that touch vertex l are coplanar, so that their normal vectors all point in the same direction.

Although the equality case might hold for some vertices, it cannot hold for all vertices on a closed triangulated surface.

Therefore, by summing both sides of (24) over $l = 1 \cdots V$, we conclude that A as defined by (19) is strictly less than the sum of the areas of all of the triangular faces.

Note, however, that A is exactly equal to the rate of change of the enclosed volume if all of the vertices move in the normal direction as defined by (17) at unit speed.

We now derive explicit formulae for the force on a vertex, as defined by the right-hand side of (23). From (21),

$$(25)\qquad \frac{\partial E_a}{\partial X^k_\alpha} = K_a \sum_{l=1}^{v} \left(\log \frac{\|\underline{A}^l\|}{\|\underline{A}^l\|_0} \right) \frac{\|\underline{A}^l\|_0}{\|\underline{A}^l\|} \frac{\partial \|\underline{A}^l\|}{\partial X^k_\alpha}$$

Before differentiating E_b, we use (20) to rewrite (22) as follows

$$(26)\qquad E_b = \frac{K_b}{2} \sum_{l=1}^{v} \|\underline{A}^l\|^{-1} \frac{\partial A}{\partial X^l_\beta} \frac{\partial A}{\partial X^l_\beta}$$

and from this we get

$$(27)\qquad \frac{\partial E_b}{\partial X^k_\alpha} = -\frac{K_b}{2} \sum_{l=1}^{v} \|\underline{A}^l\|^{-2} \frac{\partial \|\underline{A}^l\|}{\partial X^k_\alpha} \frac{\partial A}{\partial X^l_\beta} \frac{\partial A}{\partial X^l_\beta}$$

$$+ K_b \sum_{l=1}^{v} \|\underline{A}^l\|^{-1} \frac{\partial A}{\partial X^l_\beta} \frac{\partial^2 A}{\partial X^k_\alpha \partial X^l_\beta}$$

Recall that $A = \sum_{m=1}^{v} \|\underline{A}^m\|$. Thus, we need to evaluate the first and second derivatives of $\|\underline{A}^m\|$.

To evaluate these derivatives, we proceed as follows:

(28) $$\|\underline{A}^m\|^2 = \left(A_\gamma^m\right)^2$$

(Recall that the summation convention applies to the Greek indices only.)

(29) $$\cancel{2}\|\underline{A}^m\| \frac{\partial \|\underline{A}^m\|}{\partial X_\beta^l} = \cancel{2} A_\gamma^m \frac{\partial A_\gamma^m}{\partial X_\beta^l}$$

(30) $$\frac{\partial \|\underline{A}^m\|}{\partial X_\alpha^k} \frac{\partial \|\underline{A}^m\|}{\partial X_\beta^l} + \|\underline{A}^m\| \frac{\partial^2 \|\underline{A}^m\|}{\partial X_\alpha^k \partial X_\beta^l}$$

$$= \frac{\partial A_\gamma^m}{\partial X_\alpha^k} \frac{\partial A_\gamma^m}{\partial X_\beta^l} + A_\gamma^m \frac{\partial^2 A_\gamma^m}{\partial X_\alpha^k \partial X_\beta^l}$$

Now we divide both sides of (29) and both sides of (30) by $\|\underline{A}^m\|$ and make use of the definition of the unit normal, equation (17), to get the following results

$$\frac{\partial \|\underline{A}^m\|}{\partial X^l_\beta} = N^m_\gamma \frac{\partial A^m_\gamma}{\partial X^l_\beta} \tag{31}$$

$$\frac{\partial^2 \|\underline{A}^m\|}{\partial X^k_\alpha \, \partial X^l_\beta} = N^m_\gamma \frac{\partial^2 A^m_\gamma}{\partial X^k_\alpha \, \partial X^l_\beta} \tag{32}$$

$$+ \frac{1}{\|\underline{A}^m\|}\left(\frac{\partial A^m_\gamma}{\partial X^k_\alpha}\frac{\partial A^m_\gamma}{\partial X^l_\beta} - \frac{\partial \|\underline{A}^m\|}{\partial X^k_\alpha}\frac{\partial \|\underline{A}^m\|}{\partial X^l_\beta} \right)$$

Note that we can make use of (31) to evaluate the last term on the right-hand side of (32). Also, the derivatives of A^m_γ can be rewritten in terms of derivatives of V by making use of the definition (7).

This gives

$$(33)\qquad \frac{\partial \|\underline{A}^m\|}{\partial X^l_\beta} = N^m_\gamma \frac{\partial^2 V}{\partial X^l_\beta \, \partial X^m_\gamma}$$

$$(34)\qquad \frac{\partial^2 \|\underline{A}^m\|}{\partial X^k_\alpha \, \partial X^l_\beta} =$$

$$N^m_\gamma \frac{\partial^3 V}{\partial X^k_\alpha \, \partial X^l_\beta \, \partial X^m_\gamma}$$

$$+ \frac{1}{\|\underline{A}^m\|} \left(\frac{\partial^2 V}{\partial X^k_\alpha \, \partial X^m_{\gamma'}} \left(\delta_{\gamma'\gamma''} - N^m_{\gamma'} N^m_{\gamma''} \right) \frac{\partial^2 V}{\partial X^l_\beta \, \partial X^m_{\gamma''}} \right)$$

Summing these results over $m = 1 \cdots v$, we get the corresponding derivatives of A:

(35) $$\frac{\partial A}{\partial X^l_\beta} = \sum_{m=1}^{v} N^m_\gamma \frac{\partial^2 V}{\partial X^l_\beta \partial X^m_\gamma}$$

(36) $$\frac{\partial^2 A}{\partial X^k_\alpha \partial X^l_\beta} =$$

$$\sum_{m=1}^{v} \left(N^m_\gamma \frac{\partial^3 V}{\partial X^k_\alpha \partial X^l_\beta \partial X^m_\gamma} \right.$$

$$\left. + \frac{1}{\|\underline{A}^m\|} \left(\frac{\partial^2 V}{\partial X^k_\alpha \partial X^m_{\gamma'}} \left(\delta_{\gamma'\gamma''} - N^m_{\gamma'} N^m_{\gamma''} \right) \frac{\partial^2 V}{\partial X^l_\beta \partial X^m_{\gamma''}} \right) \right)$$

Now we need to evaluate the second and third derivatives of V. We start from equation (11), reindexed as follows

(37) $$\frac{\partial V}{\partial X^{\ell}_{\beta}} = \frac{1}{6} \sum_{i=0}^{n(\ell)-1} \varepsilon_{\beta\lambda\mu} X^{v_i(\ell)}_{\lambda} X^{v_{i+1}(\ell)}_{\mu}$$

Then

(38) $$\frac{\partial^2 V}{\partial X^{\ell}_{\beta} \partial X^{m}_{\gamma}} = \frac{1}{6} \sum_{i=0}^{n(\ell)-1} \varepsilon_{\beta\gamma\mu} \delta_{m, v_i(\ell)} X^{v_{i+1}(\ell)}_{\mu}$$

$$+ \frac{1}{6} \sum_{i=0}^{n(\ell)-1} \varepsilon_{\beta\lambda\gamma} X^{v_i(\ell)}_{\lambda} \delta_{m, v_{i+1}(\ell)}$$

$$= \frac{1}{6} \sum_{i=0}^{n(\ell)-1} \varepsilon_{\mu\beta\gamma} \left(\delta_{m, v_i(\ell)} X^{v_{i+1}(\ell)}_{\mu} - \delta_{m, v_{i+1}(\ell)} X^{v_i(\ell)}_{\mu} \right)$$

and

(39) $$\frac{\partial^3 V}{\partial X^{k}_{\alpha} \partial X^{\ell}_{\beta} \partial X^{m}_{\gamma}} = \frac{1}{6} \sum_{i=0}^{n(\ell)-1} \varepsilon_{\alpha\beta\gamma} \left(\delta_{m, v_i(\ell)} \delta_{k, v_{i+1}(\ell)} - \delta_{m, v_{i+1}(\ell)} \delta_{k, v_i(\ell)} \right)$$

Substituting (38) into (35) gives the result

$$(40)\quad \frac{\partial A}{\partial X^{\ell}_{\beta}} = \frac{1}{6}\sum_{i=0}^{n(\ell)-1} \varepsilon_{\beta\gamma\mu}\left(N_{\gamma}^{v_i(\ell)} X_{\mu}^{v_{i+1}(\ell)} - N_{\gamma}^{v_{i+1}(\ell)} X_{\mu}^{v_i(\ell)}\right)$$

or, in vector notation,

$$(41)\quad \frac{\partial A}{\partial \underline{X}^{\ell}} = \frac{1}{6}\sum_{i=0}^{n(\ell)-1}\left(\underline{N}^{v_i(\ell)} \times \underline{X}^{v_{i+1}(\ell)} - \underline{N}^{v_{i+1}(\ell)} \times \underline{X}^{v_i(\ell)}\right)$$

This result can be rewritten in several different ways by re-indexing and making use of the periodicity of the index i.
One interesting way is

$$(42)\quad \frac{\partial A}{\partial \underline{X}^{\ell}} = \frac{1}{6}\sum_{i=0}^{n(\ell)-1}\left(\underline{N}^{v_{i+1}(\ell)} + \underline{N}^{v_i(\ell)}\right) \times \left(\underline{X}^{v_{i+1}(\ell)} - \underline{X}^{v_i(\ell)}\right)$$

This seems to have two extra terms in comparison to (41) but the extra terms cancel upon summation over i.

The first term on the right-hand side of (36) can be evaluated by using (39):

$$(43) \qquad \sum_{m=1}^{v} N_\gamma^m \frac{\partial^3 V}{\partial X_\alpha^k \partial X_\beta^\ell \partial X_\gamma^m}$$

$$= \frac{1}{6} \sum_{i=0}^{n(\ell)-1} \varepsilon_{\alpha\beta\gamma} \left(N_\gamma^{v_i(\ell)} \delta_{k, v_{i+1}(\ell)} - N_\gamma^{v_{i+1}(\ell)} \delta_{k, v_i(\ell)} \right)$$

Since the left-hand side of this expression is symmetrical under the interchange $\binom{k}{\alpha} \leftrightarrow \binom{\ell}{\beta}$ and since $\varepsilon_{\alpha\beta\gamma} = -\varepsilon_{\beta\alpha\gamma}$, we also have the following alternate version of (43):

$$(44) \qquad \sum_{m=1}^{v} N_\gamma^m \frac{\partial^3 V}{\partial X_\alpha^k \partial X_\beta^\ell \partial X_\gamma^m}$$

$$= \frac{1}{6} \sum_{i=0}^{n(k)-1} \varepsilon_{\alpha\beta\gamma} \left(N_\gamma^{v_{i+1}(k)} \delta_{\ell, v_i(k)} - N_\gamma^{v_i(k)} \delta_{\ell, v_{i+1}(k)} \right)$$

$$= \frac{1}{6} \sum_{i=0}^{n(k)-1} \varepsilon_{\alpha\beta\gamma} \left(N_\gamma^{v_{i+1}(k)} - N_\gamma^{v_{i-1}(k)} \right) \delta_{\ell, v_i(k)}$$

To evaluate the second term on the right-hand side of (36), we need to use equation (38) twice. To prepare for this, we first note that (38) can be rewritten as follows

$$\frac{\partial^2 V}{\partial X^l_\beta \, \partial X^m_\gamma} = \frac{1}{6} \sum_{i=0}^{n(l)-1} \delta_{m, v_i(l)} \, \varepsilon_{\beta\gamma\mu} \left(X_\mu^{v_{i+1}(l)} - X_\mu^{v_{i-1}(l)} \right) \tag{45}$$

This can be expressed in another way by noting that the left-hand side is symmetric under the interchange $(l,\beta) \Leftrightarrow (m,\gamma)$, so we may make this interchange on the right-hand side and then use $\varepsilon_{\gamma\beta\mu} = -\varepsilon_{\beta\gamma\mu}$ to obtain

$$\frac{\partial^2 V}{\partial X^l_\beta \, \partial X^m_\gamma} = -\frac{1}{6} \sum_{i=0}^{n(m)-1} \delta_{l, v_i(m)} \, \varepsilon_{\beta\gamma\mu} \left(X_\mu^{v_{i+1}(m)} - X_\mu^{v_{i-1}(m)} \right) \tag{46}$$

We will use both (45) and (46) in the following, re-indexed as follows:

$$(47)\quad \frac{\partial^2 V}{\partial X^k_\alpha \partial X^m_{\gamma'}} = \frac{1}{6}\sum_{i=0}^{n(k)-1} \delta_{m,v_i(k)}\, \varepsilon_{\alpha\gamma'\mu'} \left(X^{v_{i+1}(k)}_{\mu'} - X^{v_{i-1}(k)}_{\mu'} \right)$$

$$(48)\quad \frac{\partial^2 V}{\partial X^l_\beta \partial X^m_{\gamma''}} = -\frac{1}{6}\sum_{j=0}^{n(m)-1} \delta_{l,v_j(m)}\, \varepsilon_{\beta\gamma''\mu''} \left(X^{v_{j+1}(m)}_{\mu''} - X^{v_{j-1}(m)}_{\mu''} \right)$$

Note the factor $\delta_{m,v_i(k)}$ in (47) and the factor $\delta_{l,v_j(m)}$ in (48). When we sum over m, the first such factor will allow us to replace the whole sum by the term $m = v_i(k)$. Later, we will also sum over l, and then we will be able to replace that whole sum by the term $l = v_j(m) = v_j(v_i(k))$.

We now use (47) & (48) to evaluate the second term on the right-hand side of (36):

$$(49)\quad \sum_{m=1}^{v} \frac{1}{\|\underline{A}^m\|} \left(\frac{\partial^2 V}{\partial X_\alpha^k \partial X_{\gamma'}^m} \left(\delta_{\gamma'\gamma''} - N_{\gamma'}^m N_{\gamma''}^m\right) \frac{\partial^2 V}{\partial X_\beta^\ell \partial X_{\gamma''}^m} \right)$$

$$= -\frac{1}{36} \sum_{i=0}^{n(k)-1} \sum_{j=0}^{n(v_i(k))-1} \delta_{\ell, v_j(v_i(k))} \frac{1}{\|\underline{A}^{v_i(k)}\|}$$

$$\varepsilon_{\alpha\gamma'\mu'} \left(X_{\mu'}^{v_{i+1}(k)} - X_{\mu'}^{v_{i-1}(k)} \right)$$

$$\left(\delta_{\gamma'\gamma''} - N_{\gamma'}^{v_i(k)} N_{\gamma''}^{v_i(k)} \right)$$

$$\varepsilon_{\beta\gamma''\mu''} \left(X_{\mu''}^{v_{j+1}(v_i(k))} - X_{\mu''}^{v_{j-1}(v_i(k))} \right)$$

In the series of definitions made earlier, equations (17-23), the variables for which we do not yet have explicit formulae in terms of the coordinates of the vertices are $\underline{H}^l$, E_b, and the first derivatives of E_a and E_b. These formulae will now be provided.

Substituting (42) into (20), we immediately get

(50) $$\underline{H}^l = -\frac{1}{6\|\underline{A}^l\|}\sum_{i=0}^{n(l)-1}\left(\underline{N}^{v_{i+1}(l)} + \underline{N}^{v_i(l)}\right)\times\left(\underline{X}^{v_{i+1}(l)} - \underline{X}^{v_i(l)}\right)$$

With $\underline{H}^l$ known, equation (22) becomes an explicit formula for E_b.

Next, we evaluate $\partial E_a/\partial X^k_\alpha$. From (25), we see that we need $\partial\|\underline{A}^l\|/\partial X^k_\alpha$, and from (33) this is given by

(51) $$\frac{\partial\|\underline{A}^l\|}{\partial X^k_\alpha} = N^l_\beta \frac{\partial^2 V}{\partial X^k_\alpha\,\partial X^l_\beta}$$

By making use of (47), we can write this as

$$\frac{\partial \|\underline{A}^{\ell}\|}{\partial X_\alpha^k} = \tag{52}$$

$$\frac{1}{6}\sum_{i=0}^{n(k)-1} \delta_{\ell, v_i(k)}\, \varepsilon_{\alpha\beta\gamma}\, N_\beta^\ell \left(X_\gamma^{v_{i+1}(k)} - X_\gamma^{v_{i-1}(k)} \right)$$

Substituting (52) into (25) gives the result

$$\frac{\partial E_a}{\partial X_\alpha^k} = \frac{K_a}{6}\sum_{i=0}^{n(k)-1} \left(\log \frac{\|\underline{A}^{v_i(k)}\|}{\|\underline{A}^{v_i(k)}\|_0} \right) \frac{\|\underline{A}^{v_i(k)}\|_0}{\|\underline{A}^{v_i(k)}\|} \tag{53}$$

$$\varepsilon_{\alpha\beta\gamma}\, N_\beta^{v_i(k)} \left(X_\gamma^{v_{i+1}(k)} - X_\gamma^{v_{i-1}(k)} \right)$$

or, in vector notation

$$\frac{\partial E_a}{\partial \underline{X}^k} = \frac{K_a}{6}\sum_{i=0}^{n(k)-1} \left(\log \frac{\|\underline{A}^{v_i(k)}\|}{\|\underline{A}^{v_i(k)}\|_0} \right) \frac{\|\underline{A}^{v_i(k)}\|_0}{\|\underline{A}^{v_i(k)}\|} \tag{54}$$

$$\underline{N}^{v_i(k)} \times \left(\underline{X}^{v_{i+1}(k)} - \underline{X}^{v_{i-1}(k)} \right)$$

Finally, we evaluate $\partial E_b / \partial X_\alpha^k$, which is given by (27). By making use of the definition of $\underline{H}^l$, equation (20), we can rewrite (27) as follows

(55) $$\frac{\partial E_b}{\partial X_\alpha^k} = -\frac{K_b}{2} \sum_{l=1}^{v} \|\underline{H}^l\|^2 \frac{\partial \|\underline{A}^l\|}{\partial X_\alpha^k}$$

$$- K_b \sum_{l=1}^{v} H_\beta^l \frac{\partial^2 A}{\partial X_\alpha^k \partial X_\beta^l}$$

We evaluate these two terms separately. From (52), the first term becomes

(56) $$-\frac{K_b}{12} \sum_{i=0}^{n(k)-1} \|\underline{H}^{v_i(k)}\|^2 \varepsilon_{\alpha\beta\gamma} N_\beta^{v_i(k)} \left(X_\gamma^{v_{i+1}(k)} - X_\gamma^{v_{i-1}(k)} \right)$$

and from (36), (44), and (49), the second term becomes

(57) $$-\frac{K_b}{6}\sum_{i=0}^{n(k)-1}\varepsilon_{\alpha\beta\gamma}H_\beta^{v_i(k)}\left(N_\gamma^{v_{i+1}(k)}-N_\gamma^{v_{i-1}(k)}\right)$$

$$-\frac{K_b}{36}\sum_{i=0}^{n(k)-1}\frac{\varepsilon_{\alpha\gamma'\mu'}\left(X_{\mu'}^{v_{i+1}(k)}-X_{\mu'}^{v_{i-1}(k)}\right)}{\|\underline{A}^{v_i(k)}\|}$$

$$\left(\delta_{\gamma'\gamma''}-N_{\gamma'}^{v_i(k)}N_{\gamma''}^{v_i(k)}\right)$$

$$\sum_{j=0}^{n(v_i(k))-1}\varepsilon_{\gamma''\beta\mu''}H_\beta^{v_j(v_i(k))}\left(X_{\mu''}^{v_{j+1}(v_i(k))}-X_{\mu''}^{v_{j-1}(v_i(k))}\right)$$

We can write this in vector notation by introducing the projection operator

(58) $$P^k = I - N^k(N^k)^T$$

which is the projection onto the tangent space at vertex k.

Then, putting everything together,

$$(59)\quad \frac{\partial E_b}{\partial \underline{X}^k} =$$

$$- \frac{K_b}{12} \sum_{i=0}^{n(k)-1} \left\| \underline{H}^{v_i(k)} \right\|^2 \left(\underline{N}^{v_i(k)} \times \left(\underline{X}^{v_{i+1}(k)} - \underline{X}^{v_{i-1}(k)} \right) \right)$$

$$- \frac{K_b}{6} \sum_{i=0}^{n(k)-1} \underline{H}^{v_i(k)} \times \left(\underline{N}^{v_{i+1}(k)} - \underline{N}^{v_{i-1}(k)} \right)$$

$$- \frac{K_b}{36} \sum_{i=0}^{n(k)-1} \left(P^{v_i(k)} \sum_{j=0}^{n(v_i(k))-1} \underline{H}^{v_j(v_i(k))} \times \left(\underline{X}^{v_{j+1}(v_i(k))} - \underline{X}^{v_{j-1}(v_i(k))} \right) \right)$$

$$\times \left(\underline{X}^{v_{i+1}(k)} - \underline{X}^{v_{i-1}(k)} \right) \frac{1}{\left\| \underline{A}^{v_i(k)} \right\|}$$

This completes the derivation of the forces need to simulate the bending energy and area-preserving energy of a triangulated surface.

Surface Tension

Since it is closely related to the foregoing, we also define a surface tension energy and the corresponding force.

The energy is proportional to the total area of the surface

$$(60) \qquad E_{st} = K_{st} A$$

where A is given by (19). The constant K_{st} has units of energy/area = force/length.

The force on vertex k is given by

$$(61) \qquad -\frac{\partial E_{st}}{\partial \underline{X}^k} = -K_{st} \frac{\partial A}{\partial \underline{X}^k} = K_{st} \|\underline{A}^k\| \, \underline{H}^k$$

see (20). Thus $K_{st} \underline{H}^k$ is the force per unit area, and $K_{st} \|\underline{A}^k\| \underline{H}^k$ is the force.

To evaluate $\|\underline{A}^k\| \underline{H}^k$, see (50).

Topology of a triangulated sphere

A spherical graph is a graph that can be drawn on the surface of a sphere without any edges crossing.

Such a graph partitions the surface of the sphere into a number of faces.

Let

$f = \#$ of faces

$e = \#$ of edges

$v = \#$ of vertices

of a spherical graph. If the graph is connected, then Euler has proved that

$$f - e + v = 2 \tag{1}$$

Proof by induction: Start with one vertex and no edges, and grow the graph by adding one edge at a time*. At the start, $e = 0$ and $f = v = 1$, so equation (1) is satisfied. For each edge that is added, there are two

*such that the graph is always connected possibilities:

i) The new edge connects two existing vertices. In that case it cuts an existing face into two faces, and we have

$$\Delta f = +1, \quad \Delta e = +1, \quad \Delta v = 0$$

So equation (1) continues to be satisfied..

ii) The new edge connects an existing vertex to a new vertex. Then

$$\Delta f = 0, \quad \Delta e = 1, \quad \Delta v = 1$$

so equation (1) continues to be satisfied.

Note that the new edge cannot connect two new vertices, since it would not then be connected to the rest of the graph, and the procedure is to grow the graph in such a way that it is connected at every stage.

From the proof of Euler's formula, we can also derive the following generalization:

Any spherical graph, connected or not, satisfies

(2) $$f - e + v = 1 + n$$

where n is the number of connected components. The proof is by induction, as before, starting from zero edges, one face, and one vertex in each of the connected components.

Note that (2) is correct even in the case of zero connected components, which has $f = 1$ and $e = v = 0$.

A <u>triangulation of a sphere</u> is a connected spherical graph with the property that every face has exactly three edges. Since each edge is shared by two faces, we then have the equation

(3) $$2e = 3f$$

Combining (1) & (3), we have a linear system for the numbers of edges and faces in terms of the number of vertices

(4) $$\begin{cases} 2e - 3f = 0 \\ e - f = v - 2 \end{cases}$$

This system has determinant 1, and its solution is

(5) $$e = 3(v-2)$$

(6) $$f = 2(v-2)$$

Thus, the numbers of edges and faces of a triangulation of the sphere is determined by the number of vertices.

An interesting generalization that includes the above result and its converse is the following:

If a connected spherical graph has
(i) no self loops, and
(ii) no pair of vertices that is connected by more than one edge

Then

(7) $$e \leq 3(v-2)$$

(8) $$f \leq 2(v-2)$$

with equality in each case if and only if the graph is a triangulation of the sphere.

Proof: Because of the restrictions (i) and (ii), every face has at least three edges. Therefore,

(9) $$2e \geq 3f$$

with equality if and only if the graph is a triangulation of the sphere.

We can eliminate e or f from this inequality by using Euler's formula, equation (1).

Elimination of f gives

(10) $$2e \geq 3(e - v + 2)$$

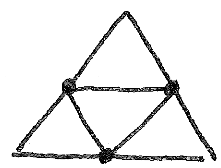
which is equivalent to (7), and elimination of e gives

(11) $$2(f + v - 2) \geq 3f$$

which is equivalent to (8). Also, we have equality in (10) & (11) if and only if we have equality in (9), and this happens if and only if the graph is a triangulation.

In summary, for any given number of vertices, triangulations maximize the numbers of edges and faces over all connected spherical graphs that respect the conditions (i) and (ii), and moreover the numbers of edges and faces of a triangulation are determined by the number of vertices. Any connected spherical graph that respects (i) and (ii) and has $e = 3(v-2)$ or $f = 2(v-2)$ <u>is</u> a triangulation!

We can construct a nice triangulation of the sphere in the following way. Start from an icosahedron which has 12 vertices, 30 edges, and 20 faces. Each triangular face can then be refined by cutting it into four triangles



and then projecting the new vertices out onto the sphere. (After projection, the central triangle is different from the other three. To minimize these differences and keep the triangulation as uniform as possible, it is best to start from an icosahedron, rather than a tetrahedron or an octahedron.)

The above procedure can be done recursively to reach any level of refinement that may be needed. The original 12 vertices each have 5 neighbors, and this remains true of them during refinement, but all of the subsequently-created vertices have 6 neighbors.