CS Peskin 5/8/2019
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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) $$\underline{X}^k, \quad k = 1 \cdots v$$

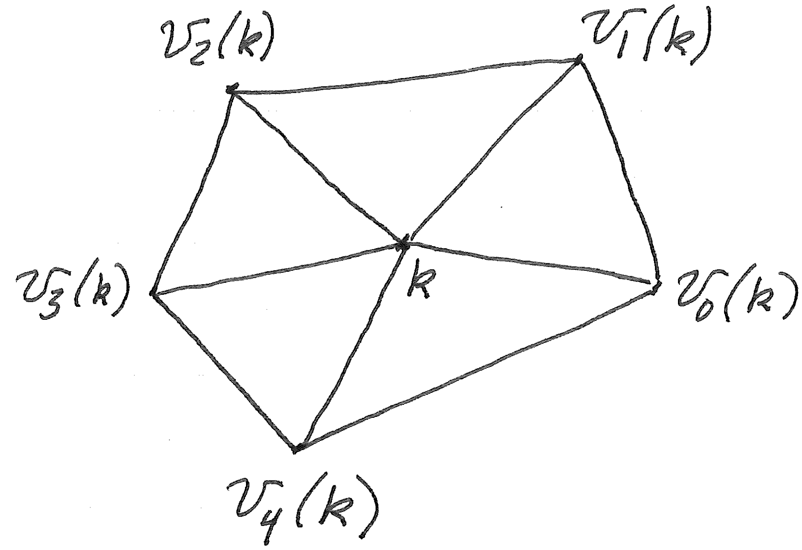
Let the indices of the vertices that are neighbors of vertex k be denoted

(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

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

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:

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

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:

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

by which we mean

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

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 factors of $\frac{1}{3}$. Since these are the only tetrahedra that are affected by a change in $\underline{X}^\ell$, we immediately get

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

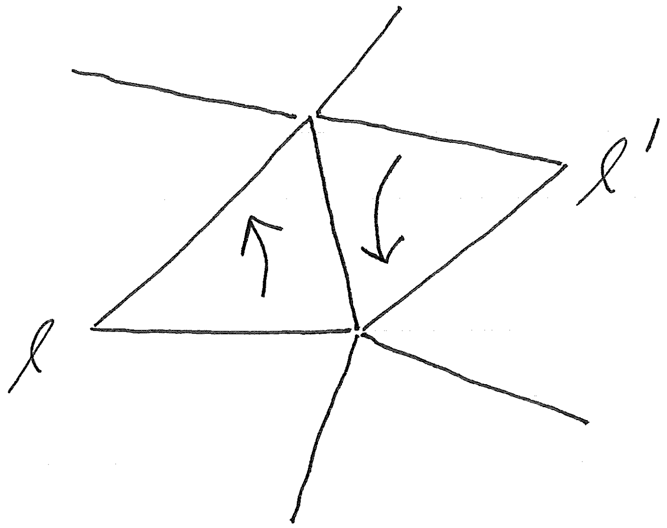
in agreement with (9). In vector notation

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

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

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

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

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

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:

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

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

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

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

If we sum both sides of (16) over $l = 1 \dots v$ 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)

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

= total curvature vector at vertex ℓ

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

= area-preserving energy

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

= 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

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

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),

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

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

$$E_b = \frac{K_b}{2} \sum_{l=1}^{v} \|\underline{A}^l\|^{-1} \frac{\partial A}{\partial X_\beta^l} \frac{\partial A}{\partial X_\beta^l} \tag{26}$$

and from this we get

$$\frac{\partial E_b}{\partial X_\alpha^k} = -\frac{K_b}{2} \sum_{l=1}^{v} \|\underline{A}^l\|^{-2} \frac{\partial \|\underline{A}^l\|}{\partial X_\alpha^k} \frac{\partial A}{\partial X_\beta^l} \frac{\partial A}{\partial X_\beta^l} + K_b \sum_{l=1}^{v} \|\underline{A}^l\|^{-1} \frac{\partial A}{\partial X_\beta^l} \frac{\partial^2 A}{\partial X_\alpha^k \partial X_\beta^l} \tag{27}$$

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

Combining (25) & (27) and making use of the definition of $\underline{H}^\ell$, we get

(28) $$\frac{\partial}{\partial X^k_\alpha}\left(E_a + E_b\right) =$$

$$\sum_{\ell=1}^{v}\left(\left(T^\ell - \frac{K_b}{2}\|\underline{H}^\ell\|^2\right)\frac{\partial\|A^\ell\|}{\partial X^k_\alpha} + \frac{K_b}{\|\underline{A}^\ell\|}\frac{\partial A}{\partial X^\ell_\beta}\frac{\partial^2 A}{\partial X^k_\alpha \partial X^\ell_\beta}\right)$$

where

(29) $$T^\ell = K_a\left(\log\frac{\|\underline{A}^\ell\|}{\|\underline{A}^\ell\|_0}\right)\frac{\|\underline{A}^\ell\|_0}{\|\underline{A}^\ell\|}$$

To evaluate the derivatives in (28), we proceed as follows. The starting point is

$$\|\underline{A}^m\|^2 = A^m_\gamma A^m_\gamma \tag{30}$$

Recall that we are using the summation convention on the Greek indices only.

Differentiation with respect to X^ℓ_β gives

$$\cancel{2}\,\|\underline{A}^m\| \frac{\partial \|\underline{A}^m\|}{\partial X^\ell_\beta} = \cancel{2}\,A^m_\gamma \frac{\partial A^m_\gamma}{\partial X^\ell_\beta} \tag{31}$$

and then, dividing by $\|\underline{A}^m\|$, we get the result

$$\frac{\partial \|A^m\|}{\partial X^\ell_\beta} = N^m_\gamma \frac{\partial A^m_\gamma}{\partial X^\ell_\beta} \tag{32}$$

Because of (32), (28) becomes

(33) $$\frac{\partial}{\partial X_\alpha^k}\left(E_a + E_b\right) =$$

$$\sum_{\ell=1}^{\nu}\left(\left(T^\ell - \frac{K_b}{2}\|\underline{H}^\ell\|^2\right) N_\gamma^\ell \frac{\partial A_\gamma^\ell}{\partial X_\alpha^k} + \frac{K_b}{\|\underline{A}^\ell\|}\frac{\partial A}{\partial X_\beta^\ell}\frac{\partial^2 A}{\partial X_\alpha^k \partial X_\beta^\ell}\right)$$

The next step is to sum (32) over m. This gives

(34) $$\frac{\partial A}{\partial X_\beta^\ell} = \sum_{m=1}^{\nu} N_\gamma^m \frac{\partial A_\gamma^m}{\partial X_\beta^\ell}$$

and it follows that

(35) $$H_\beta^\ell = \frac{-1}{\|\underline{A}^\ell\|}\sum_{m=1}^{\nu} N_\gamma^m \frac{\partial A_\gamma^m}{\partial X_\beta^\ell}$$

Now we differentiate on both sides of (34) with respect to X^k_α :

$$(36) \quad \frac{\partial^2 A}{\partial X^k_\alpha \partial X^l_\beta} = \sum_{m=1}^{v} \left(N^m_\gamma \frac{\partial^2 A^m_\gamma}{\partial X^k_\alpha \partial X^l_\beta} + \frac{\partial N^m_\gamma}{\partial X^k_\alpha} \frac{\partial A^m_\gamma}{\partial X^l_\beta} \right)$$

The derivative of N^m_γ is evaluated as follows:

$$(37) \quad \frac{\partial N^m_\gamma}{\partial X^k_\alpha} = \frac{\partial}{\partial X^k_\alpha} \frac{A^m_\gamma}{\|\underline{A}^m\|}$$

$$= \frac{1}{\|\underline{A}^m\|} \frac{\partial A^m_\gamma}{\partial X^k_\alpha} - \frac{A^m_\gamma}{\|\underline{A}^m\|^2} \frac{\partial \|\underline{A}^m\|}{\partial X^k_\alpha}$$

$$= \frac{1}{\|\underline{A}^m\|} \frac{\partial A^m_\gamma}{\partial X^k_\alpha} - \frac{A^m_\gamma}{\|\underline{A}^m\|^2} N^m_{\gamma'} \frac{\partial A^m_{\gamma'}}{\partial X^k_\alpha}$$

$$= \frac{1}{\|\underline{A}^m\|} \left(\delta_{\gamma\gamma'} - N^m_\gamma N^m_{\gamma'} \right) \frac{\partial A^m_{\gamma'}}{\partial X^k_\alpha}$$

$$= \frac{1}{\|\underline{A}^m\|} P^m_{\gamma\gamma'} \frac{\partial A^m_{\gamma'}}{\partial X^k_\alpha}$$

Where

(38) $$P^m = I - (N^m)(N^m)^{\text{Transpose}}$$

which is the projection onto the tangent space at m.

Substituting (37) into (36), we get the result that

$$(39) \quad \frac{\partial^2 A}{\partial X^k_\alpha \partial X^\ell_\beta} =$$

$$\sum_{m=1}^{\nu} \left(N^m_\gamma \frac{\partial^2 A^m_\gamma}{\partial X^k_\alpha \partial X^\ell_\beta} + \frac{1}{\|\underline{A}^m\|} P^m_{\gamma\gamma'} \frac{\partial A^m_{\gamma'}}{\partial X^k_\alpha} \frac{\partial A^m_\gamma}{\partial X^\ell_\beta} \right)$$

To complete the evaluation of (33), all that we now need are formulae for the first and second derivatives of the components of the area vectors.

From equation (11)

(40) $$A^m_\gamma = \frac{1}{6}\sum_{i=0}^{n(m)-1} \varepsilon_{\gamma\lambda\mu} X_\lambda^{v_i(m)} X_\mu^{v_{i+1}(m)}$$

and it follows that

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

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

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

(42) $$\frac{\partial^2 A^m_\gamma}{\partial X^k_\alpha\, \partial X^l_\beta} = \frac{1}{6}\sum_{i=0}^{n(m)-1} \varepsilon_{\gamma\beta\alpha}\left(\delta_{l,v_{i-1}(m)} - \delta_{l,v_{i+1}(m)}\right)\delta_{k,v_i(m)}$$

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

There are hidden symmetries in equations (41–42), since

$$\frac{\partial A^m_\gamma}{\partial X^l_\beta} = \frac{\partial^2 V}{\partial X^l_\beta \, \partial X^m_\gamma} = \frac{\partial A^l_\beta}{\partial X^m_\gamma} \tag{43}$$

and

$$\frac{\partial^2 A^m_\gamma}{\partial X^k_\alpha \, \partial X^l_\beta} = \frac{\partial^3 V}{\partial X^k_\alpha \, \partial X^l_\beta \, \partial X^m_\gamma} \tag{44}$$

$$= \frac{\partial^2 A^l_\beta}{\partial X^k_\alpha \, \partial X^m_\gamma} = \frac{\partial^2 A^k_\alpha}{\partial X^l_\beta \, \partial X^m_\gamma}$$

but it is not obvious that the right-hand sides of (41–42) are symmetrical in these ways.

We can now use the symmetry (43) and then the formula (41) to evaluate the first term on the right-hand side of (33) and also to evaluate the right hand sides of (34) & (35).

We begin with the latter pair of equations and note that

(45) $$\frac{\partial A^m_\gamma}{\partial X^l_\beta} = \frac{\partial A^l_\beta}{\partial X^m_\gamma}$$

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

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

Substituting (45) into (34) & (35), we get

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

(47) $$H^{l}_{\beta} = -\frac{1}{6\|A^{l}\|} \sum_{i=0}^{n(l)-1} \varepsilon_{\beta\gamma\mu} N_{\gamma}^{v_i(l)} \left(X_{\mu}^{v_{i+1}(l)} - X_{\mu}^{v_{i-1}(l)} \right)$$

In vector notati~

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

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

The first term on the right-hand side of (33) is of the same form as each of the expressions that we have just evaluated, and from this observation we see that this term is equal to the α component of the vector

(50) $$\frac{1}{6}\sum_{i=0}^{n(k)-1}\left(\left(T-\frac{K_b}{2}\|\underline{H}\|^2\right)\underline{N}\right)^{v_i(k)}\times\left(\underline{X}^{v_{i+1}(k)}-\underline{X}^{v_{i-1}(k)}\right)$$

It may be worth mentioning that sums like those in (48-50) can be rewritten in several different ways, for example

(51) $$\sum_{i=0}^{n(k)-1}\underline{Z}^{v_i(k)}\times\left(\underline{X}^{v_{i+1}(k)}-\underline{X}^{v_{i-1}(k)}\right)$$

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

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

On the last two lines of (51), each term makes reference to one edge of the polygon surrounding vertex k, and on the last line the edge vectors appear explicitly. Note that the sum of these edge vectors is zero.

We still have to evaluate the second term on the right-hand side of (33). Making use of the definition of H^l and also of equation (39), we have

(52) $$\sum_{l=1}^{v} \frac{K_b}{\|\underline{A}^l\|} \frac{\partial A}{\partial X_\beta^l} \frac{\partial^2 A}{\partial X_\alpha^k \partial X_\beta^l} =$$

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

$$+K_b \sum_{l,m=1}^{v} \frac{-1}{\|\underline{A}^m\|} H_\beta^l P_{\gamma\gamma'}^m \frac{\partial A_{\gamma'}^m}{\partial X_\alpha^k} \frac{\partial A_\gamma^m}{\partial X_\beta^l}$$

We consider the two terms in the right-hand side of (52) separately. Because of (42), the first term becomes

(53)
$$-\frac{K_b}{6}\sum_{l,m=1}^{v}\sum_{i=0}^{n(m)-1}\varepsilon_{\alpha\beta\gamma}H_\beta^l N_\gamma^m$$

$$\left(\delta_{l,v_{i+1}(m)}-\delta_{l,v_{i-1}(m)}\right)\delta_{k,v_i(m)}$$

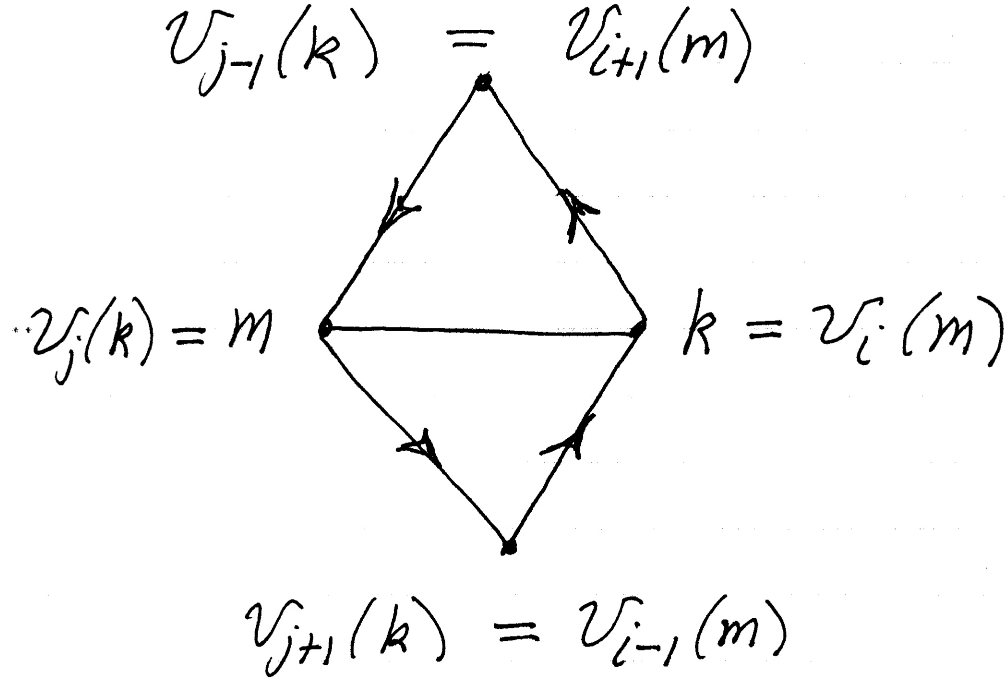
$$=-\frac{K_b}{6}\sum_{m=1}^{v}\sum_{i=0}^{n(m)-1}\left(\underline{H}^{v_{i+1}(m)}\times\underline{N}^m\right)_\alpha\delta_{k,v_i(m)}$$

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

Note that

(54)
$$k=v_i(m)\iff\exists j\text{ such that }m=v_j(k)$$

and moreover j is uniquely determined by k and m



Also, as we can see from the diagram, when k and m are neighbors and i and j are such that $k = v_i(m)$ and $m = v_j(k)$, then we also have

(55) $$v_{j-1}(k) = v_{i+1}(m)$$

(56) $$v_{j+1}(k) = v_{i-1}(m)$$

Taking these relationships into account, we can rewrite the right-hand side of (53) as follows

$$\frac{K_b}{6}\sum_{j=0}^{n(k)-1}\left(\left(\underline{H}^{v_{j+1}(k)}-\underline{H}^{v_{j-1}(k)}\right)\times\underline{N}^{v_j(k)}\right)_\alpha \tag{57}$$

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

Finally, we need to evaluate the last term in the right-hand side of (52). Since our goal is to collapse the sums over l and m, we make the substitutions

$$\frac{\partial A^m_\gamma}{\partial X^l_\beta}=\frac{1}{6}\sum_{i=0}^{n(m)-1}\varepsilon_{\gamma\beta\mu}\,\delta_{l,v_i(m)}\left(X_\mu^{v_{i+1}(m)}-X_\mu^{v_{i-1}(m)}\right) \tag{58}$$

and

$$(59)\quad \frac{\partial A^m_{\gamma'}}{\partial X^k_\alpha} = \frac{1}{6}\sum_{j=0}^{n(k)-1} \varepsilon_{\alpha\gamma'\mu'}\,\delta_{m,v_j(k)}\left(X^{v_{j+1}(k)}_{\mu'} - X^{v_{j-1}(k)}_{\mu'}\right)$$

Note that (59) is not merely a reindexed version of (58). Equation (58) is essentially equation (41), and equation (59) is a re-indexed version of (45). Equations (41) and (45) are related by the hidden symmetry (43).

When we substitute (58) into the last term of (52), the sum over l collapses into $l = v_i(m)$, and the following new variable makes an appearance

(60) $$Q_\gamma^m = \frac{1}{6\|\underline{A}^m\|} \sum_{i=0}^{n(m)-1} \varepsilon_{\gamma\beta\mu} H_\beta^{v_i(m)} \left(X_\mu^{v_{i+1}(m)} - X_\mu^{v_{i-1}(m)} \right)$$

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

In terms of Q, the last term of (52) takes the form

(62) $$-K_b \sum_{m=1}^{v} Q_\gamma^m P_{\gamma\gamma'}^m \frac{\partial A_{\gamma'}^m}{\partial X_\alpha^k}$$

Now we use (59) and the symmetry of P^m to rewrite this as

(63) $$-\frac{K_b}{6} \sum_{j=0}^{n(k)-1} \varepsilon_{\alpha\gamma'\mu'} \left(P_{\gamma'\gamma} Q_\gamma \right)^{v_j(k)} \left(X_{\mu'}^{v_{j+1}(k)} - X_{\mu'}^{v_{j-1}(k)} \right)$$

and this is the α component of

$$(64)\quad -\frac{K_b}{6}\sum_{j=0}^{n(k)-1}(P\underline{Q})^{v_j(k)}\times\left(\underline{X}^{v_{j+1}(k)}-\underline{X}^{v_j(k)}\right)$$

Then, at last, putting everything together, we can write a formula for the force on vertex k:

$$(65)\quad \underline{F}^k\,\|\underline{A}^k\| = -\frac{\partial}{\partial\underline{X}^k}\left(E_a+E_b\right) =$$

$$\frac{1}{6}\sum_{j=0}^{n(k)-1}\left(\underline{S}^{v_j(k)}\times\left(\underline{X}^{v_{j+1}(k)}-\underline{X}^{v_{j-1}(k)}\right)\right.$$
$$\left.+K_b\,\underline{H}^{v_j(k)}\times\left(\underline{N}^{v_{j+1}(k)}-\underline{N}^{v_{j-1}(k)}\right)\right)$$

where

(66) $$\underline{S}^m = \left(-T^m + \frac{K_b}{2}\|\underline{H}^m\|^2\right)\underline{N}^m + K_b\, P^m \underline{Q}^m$$

(67) $$T^m = K_a \left(\log \frac{\|\underline{A}^m\|}{\|\underline{A}^m\|_0}\right)\frac{\|\underline{A}^m\|_0}{\|\underline{A}^m\|}$$

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

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

(70) $$P^m = I - \underline{N}^m \left(\underline{N}^m\right)^{\text{Transpose}}$$

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

(71) $$E_{st} = K_{st} A$$

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

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

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 (68).

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

$$f - e + v = 2 \qquad (1)$$

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 triangulation of a sphere 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

$$2e = 3f \tag{3}$$

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

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

This system has determinant 1, and its solution is

$$e = 3(v-2) \tag{5}$$

$$f = 2(v-2) \tag{6}$$

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

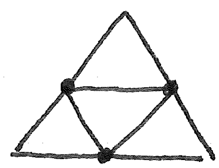
which is equivalent to (7), and elimination of e gives

(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.