# Energy Functions for the Representation of Immersed Elastic Boundaries

C. Peskin

Fall 2007

(revised, Spring 2021, in the pages on link structures)

Consider an elastic material, the configuration of which is given by

$$\underline{x} = \underline{X}(q)$$

where $q = (q_1, \dots, q_m)$ are material coordinates.

Let the elastic energy of the configuration $\underline{X}(\;)$ be denoted

$$E[\underline{X}]$$

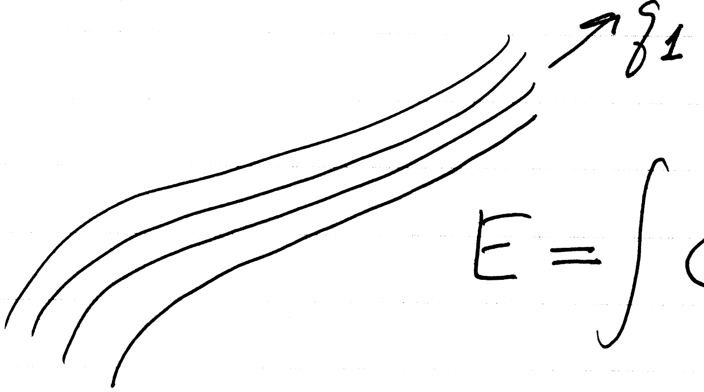
Now consider a perturbation $\underline{X}(q) \to \underline{X}(q) + \delta\underline{X}(q)$

Then, to first order, the corresponding $\delta E$ is a linear functional of $\delta\underline{X}$. As such it may be written

$$\delta E = \int \boxed{\phantom{XXXX}} \cdot \delta\underline{X}(q)\, dq$$

where $dq = dq_1 \cdots dq_m$. By definition, the coefficient of $\delta\underline{X}(q)$ is the "variational derivative" of $E$, and is denoted $\dfrac{\delta E}{\delta \underline{X}}(q)$.

Example: A fiber continuum




$$E = \int \mathcal{E}\left(\left|\frac{\partial \underline{X}}{\partial \xi_1}\right|\right) d\xi$$

Note that $$\left|\frac{\partial \underline{X}}{\partial \xi_1}\right| = \left(\frac{\partial \underline{X}}{\partial \xi_1}\cdot\frac{\partial \underline{X}}{\partial \xi_1}\right)^{1/2},$$

so
$$\delta\left|\frac{\partial \underline{X}}{\partial \xi_1}\right| = \frac{1}{2}\left(\frac{\partial \underline{X}}{\partial \xi_1}\cdot\frac{\partial \underline{X}}{\partial \xi_1}\right)^{-1/2} 2\,\frac{\partial \underline{X}}{\partial \xi_1}\cdot\delta\frac{\partial \underline{X}}{\partial \xi_1}$$

$$= \frac{\partial \underline{X}/\partial \xi_1}{|\partial \underline{X}/\partial \xi_1|}\cdot\frac{\partial}{\partial \xi_1}(\delta \underline{X})$$

and therefore
$$\delta E = \int \mathcal{E}'\left(\left|\frac{\partial \underline{X}}{\partial \xi_1}\right|\right)\frac{\partial \underline{X}/\partial \xi_1}{|\partial \underline{X}/\partial \xi_1|}\cdot\frac{\partial}{\partial \xi_1}\delta \underline{X}\, d\xi$$

$$= -\int \frac{\partial}{\partial \xi_1}\left[\mathcal{E}'\left(\left|\frac{\partial \underline{X}}{\partial \xi_1}\right|\right)\frac{\partial \underline{X}/\partial \xi_1}{|\partial \underline{X}/\partial \xi_1|}\right]\cdot\delta \underline{X}\, d\xi$$

Let

$$T = \mathcal{E}'\left(\left|\frac{\partial \underline{X}}{\partial \xi_1}\right|\right) = \text{tension}$$

$$\underline{\tau} = \frac{\partial \underline{X}/\partial \xi_1}{|\partial \underline{X}/\partial \xi_1|} = \text{unit tangent}$$

and we see that

$$-\frac{\delta E}{\delta \underline{X}} = \frac{\partial}{\partial \xi_1}(T\underline{\tau})$$

In general, the principle of virtual work tells us that the elastic force density is given by

$$\underline{F} = -\frac{\delta E}{\delta \underline{X}}$$

so, in the case of a fiber continuum

$$\underline{F} = \frac{\partial}{\partial \xi_1}(T\underline{\tau})$$

Let $E$ be any elastic energy functional that is invariant under translations.

A translation may be generated by choosing any fixed $\underline{V}$ independent of $\xi$, and setting

$$\frac{\partial \underline{X}}{\partial t}(\xi,t) = \underline{V}$$

Then

$$0 = \frac{d}{dt} E\left[\underline{X}(\,,t)\right]$$

$$= \int \frac{\delta E}{\delta \underline{X}}(\xi,t) \cdot \frac{\partial \underline{X}}{\partial t}(\xi,t)\, d\xi$$

$$= -\left(\int \underline{F}(\xi,t)\, d\xi\right) \cdot \underline{V}$$

Since $\underline{V}$ is arbitrary

$$\text{total force} = \int \underline{F}(\xi,t)\, d\xi = 0$$

Similarly, let $E$ be any elastic energy functional that is invariant under rotations.

A rotation may be generated by choosing any fixed $\underline{\Omega}$, independent of $q$, and letting

$$\frac{\partial \underline{X}}{\partial t}(q,t) = \underline{\Omega} \times \underline{X}(q,t)$$

Then

$$0 = \frac{d}{dt} E\left[\underline{X}(\cdot,t)\right] = \int \frac{\delta E}{\delta \underline{X}}(q,t) \cdot \left(\underline{\Omega} \times \underline{X}(q,t)\right) dq$$

$$= \underline{\Omega} \cdot \int \underline{X}(q,t) \times \frac{\delta E}{\delta \underline{X}}(q,t)\, dq$$

$$= -\underline{\Omega} \int \left(\underline{X}(q,t) \times \underline{F}(q,t)\right) dq$$

Since $\underline{\Omega}$ is arbitrary

$$0 = \text{total torque} = \int \underline{X}(q,t) \times \underline{F}(q,t)\, dq$$

It is often convenient to discretize the elastic energy first, and then find the force by differentiation. Thus, we construct

$$E_N(\underline{X}_1 \cdots \underline{X}_N) \sim E[\underline{X}]$$

Then

$$\delta E_N = \sum_{k=1}^{N} \frac{\partial E_N}{\partial \underline{X}_k} \cdot \delta \underline{X}_k \sim \int \frac{\delta E}{\delta \underline{X}} \cdot \delta \underline{X} \, dq$$

where $\partial E_N / \partial \underline{X}_k$ denotes the gradient of $E_N$ with respect to $\underline{X}_k$, i.e., the vector with components $\partial E_N / \partial X_{k\alpha}$, where $\alpha = 1,2$ or $\alpha = 1,2,3$.

Therefore

$$\frac{\partial E_N}{\partial \underline{X}_k} \sim \frac{\delta E}{\delta \underline{X}} dq = -\underline{F} \, dq$$

and so we should set

$$\underline{F}_k \Delta q = -\frac{\partial E_N}{\partial \underline{X}_k}$$

(Note that the factor $\Delta q$ is included:

$$-\frac{\partial E_N}{\partial \underline{X}_k} = (\underline{\text{FORCE}})_k$$

As in the continuous case, we have the result that if $E(\underline{X}_1 \cdots \underline{X}_N)$ is invariant under translations and rotations, the total force and the total torque are zero. The proofs are essentially the same as in the continuous case, but the results involve sums instead of integrals

Suppose

$$\frac{\partial \underline{X}_k(t)}{\partial t} = \underline{V}$$

where $\underline{V}$ is independent of $k$. If $E$ is invariant under translations, we have

$$0 = \frac{d}{dt} E(\underline{X}_1 \cdots \underline{X}_N) = \left( \sum_{k=1}^{N} \frac{\partial E}{\partial \underline{X}_k} \right) \cdot \underline{V}$$

Since $\underline{V}$ is arbitrary, it follows that

$$0 = \sum_{k=1}^{N} \frac{\partial E}{\partial \underline{X}_k}$$

i.e., the total force is zero.

Similarly, if

$$\frac{\partial \underline{X}_k}{\partial t} = \underline{\Omega} \times \underline{X}_k \,.$$

where $\underline{\Omega}$ is independent of $k$, and if $E$ is invariant under rotations, we have

$$0 = \frac{d}{dt} E(\underline{X}_1 \cdots \underline{X}_N) = \sum_{k=1}^{N} \frac{\partial E}{\partial \underline{X}_k} \cdot (\underline{\Omega} \times \underline{X}_k)$$

$$= \underline{\Omega} \cdot \sum_{k=1}^{N} \left( \underline{X}_k \times \frac{\partial E}{\partial \underline{X}_k} \right)$$

Since $\underline{\Omega}$ is arbitrary

$$0 = \sum_{k=1}^{N} \underline{X}_k \times \frac{\partial E}{\partial \underline{X}_k}$$

i.e., the total torque is zero.

Remarks :

1) In general, the concept of torque is origin-dependent: the torque may be zero with respect to one origin and non-zero with respect to another. In the case that the elastic energy is invariant with respect to translation and rotation, the above result is true for torque measured with respect to <u>any</u> origin. To check this, note that

$$\sum_{k=1}^{N} \left( \underline{X}_k - \underline{Z} \right) \times \frac{\partial E}{\partial \underline{X}_k}$$

$$= \sum_{k=1}^{N} \left( \underline{X}_k \times \frac{\partial E}{\partial \underline{X}_k} \right) - \underline{Z} \times \sum_{k=1}^{N} \frac{\partial E}{\partial \underline{X}_k}$$

The first term is zero by rotational invariance with respect to $\underline{0}$, and the second term is zero by translational invariance.

2) The function $\delta_h$ of the immersed boundary method is constructed in such a manner that total force and total torque are preserved during the force-spreading operation:

<u>Homework</u>: Prove the following result in $d = 2$ or $3$ space dimensions:

If
$$\underline{f}(\underline{x}) = \sum_{k=1}^{N} \underline{F}_k \, \delta_h(\underline{x} - \underline{X}_k) \, \Delta q$$
for all $\underline{x} \in g_h$, then
$$\sum_{\underline{x} \in g_h} \underline{f}(\underline{x}) h^d = \sum_{k=1}^{N} \underline{F}_k \, \Delta q$$

$$\sum_{\underline{x} \in g_h} \underline{x} \times \underline{f}(\underline{x}) h^d = \sum_{k=1}^{N} \left( \underline{X}_k \times \underline{F}_k \right) \Delta q$$

where $\times$ denotes the cross product of two vectors, and where $g_h$ is an infinite Cartesian lattice of mesh width $h$.

Hint: The properties of $\delta_h$ that are needed to prove the above result are

$$\delta_h(\underline{x}) = \frac{1}{h^2}\varphi\left(\frac{x_1}{h}\right)\varphi\left(\frac{x_2}{h}\right) \quad \text{when } d=2$$

$$\delta_h(\underline{x}) = \frac{1}{h^3}\varphi\left(\frac{x_1}{h}\right)\varphi\left(\frac{x_2}{h}\right)\varphi\left(\frac{x_3}{h}\right) \quad \text{when } d=3$$

where, in both cases

$$\sum_i \varphi(r-i) = 1, \quad \text{all } r$$

$$\sum_i (r-i)\varphi(r-i) = 0, \quad \text{all } r$$

As a special case of the above result, we see that when $\underline{F}_k \Delta q = -\partial E/\partial \underline{X}_k$ and when $E$ is invariant under translations and rotations, then $\sum_{\underline{x}\in g_h} \underline{f}(\underline{x})h^d = 0$ and $\sum_{\underline{x}\in g_h} \underline{x}\times\underline{f}(\underline{x})h^d = 0$.

We now consider some examples of elastic energy functions $E(\underline{X}_1 \cdots \underline{X}_N)$ that are useful in the representation of immersed elastic boundaries.

Where possible, we write $E(\underline{X}_1 \cdots \underline{X}_N)$ as the discretization of some functional. This makes it clear how to refine parameters as the mesh width is refined.

1) Elastic fiber (no bending rigidity)

$$E(\underline{X}_1 \cdots \underline{X}_N) = \frac{K_s}{2} \sum_{k=1}^{N-1} \left( \frac{|\underline{X}_{k+1} - \underline{X}_k|}{\Delta \xi} - 1 \right)^2 \Delta \xi$$

$$\frac{\partial E}{\partial X_{l\alpha}} = K_s \sum_{k=1}^{N-1} \left( \frac{|\underline{X}_{k+1} - \underline{X}_k|}{\Delta \xi} - 1 \right) \frac{1}{2 \Delta \xi} \left| \underline{X}_{k+1} - \underline{X}_k \right|^{-1} 2 (X_{k+1,\alpha} - X_{k\alpha})(\delta_{k+1,l} - \delta_{k,l}) \Delta \xi$$

$$-\frac{\partial E}{\partial \underline{X}_l} = + K_s \sum_{k=1}^{N-1} \left( \frac{|\underline{X}_{k+1} - \underline{X}_k|}{\Delta \xi} - 1 \right) \frac{\underline{X}_{k+1,\alpha} - \underline{X}_{k\alpha}}{|\underline{X}_k - \underline{X}_k|} (\delta_{k,l} - \delta_{l,k+1})$$

Let

$$T_{k+1/2} = K_s \sum_{k=1}^{N-1} \left( \frac{|\underline{X}_{k+1} - \underline{X}_k|}{\Delta q} - 1 \right)$$

$$\underline{\tau}_{k+1/2} = \frac{\underline{X}_{k+1} - \underline{X}_k}{|\underline{X}_{k+1} - \underline{X}_k|}$$

Then

$$\underline{F}_l \, \Delta q = \sum_{k=1}^{N-1} T_{k+1/2} \, \underline{\tau}_{k+1/2} \left( \delta_{kl} - \delta_{k+1,l} \right)$$

We can collapse the sums if we are careful about the ends of the fiber

$$\underline{F}_l = \frac{(l \neq N)\, T_{l+1/2}\, \underline{\tau}_{l+1/2} - T_{l-1/2}\, \underline{\tau}_{l-1/2}\, (l \neq 1)}{\Delta q}$$

$l = 1 \cdots N$, where a condition like $(l \neq N)$ evaluates to 1 when it is true and zero when false.

The collapsed form looks like a discretization of

$$\frac{\partial}{\partial \xi}(T \underline{\tau})$$

which indeed it is, but because we have derived the force from a discretized energy function, we also get a specific recipe what to do at the ends of the fiber.

We can program the above without special cases at the ends. The expression we need to evaluate is of the form

$$B_l = \sum_{k=1}^{N-1} A_{k+1/2}(\delta_{kl} - \delta_{k+1,l})$$

for $l = 1 \cdots N$. Note that $B$ contains $N$ elements, whereas $A$ contains only $N-1$. The result can be obtained as follows:

$$B = [A, 0] - [0, A]$$

where

$$A = [A_{1+1/2}, \ldots, A_{N-1/2}]$$

2) Elastic fibers with bending rigidity

$$E(\underline{X}_1 \cdots \underline{X}_N) = \frac{K_b}{2} \sum_{k=2}^{N-1} |\underline{C}_k|^2 \Delta q$$

where

$$\underline{C}_k = \frac{\underline{X}_{k+1} - 2\underline{X}_k + \underline{X}_{k-1}}{(\Delta q)^2} , \quad k = 2, \dots, N-1$$

Then

$$F_{l\alpha} \Delta q = -\frac{\partial E}{\partial X_{l\alpha}} = -K_b \sum_{k=2}^{N-1} C_{k\alpha} \frac{\delta_{k+1,l} - 2\delta_{kl} + \delta_{k-1,l}}{(\Delta q)^2} \Delta q$$

$$\underline{F}_l = -K_b \frac{(l \ge 3)\underline{C}_{l-1} - (2 \le l \le N-1) 2\underline{C}_l + (l \le N-2)\underline{C}_{l+1}}{(\Delta q)^2}$$

which is a discretization of $\underline{F} = -K_b \dfrac{\partial^4 \underline{X}}{\partial q^4}$, except that a specific recipe is included on what to do at the ends of the fiber. For each component of C, F, the above is neatly programmed as

```
C=(X(3:N)-2*X(2:(N-1))+X(1:(N-2)))/dq^2
F=([0,0,C]-2*[0,C,0]+[C,0,0])/dq^2
```

Remark: The elastic energy we have just defined is zero whenever the points

$$\underline{X}_1 \cdots \underline{X}_N$$

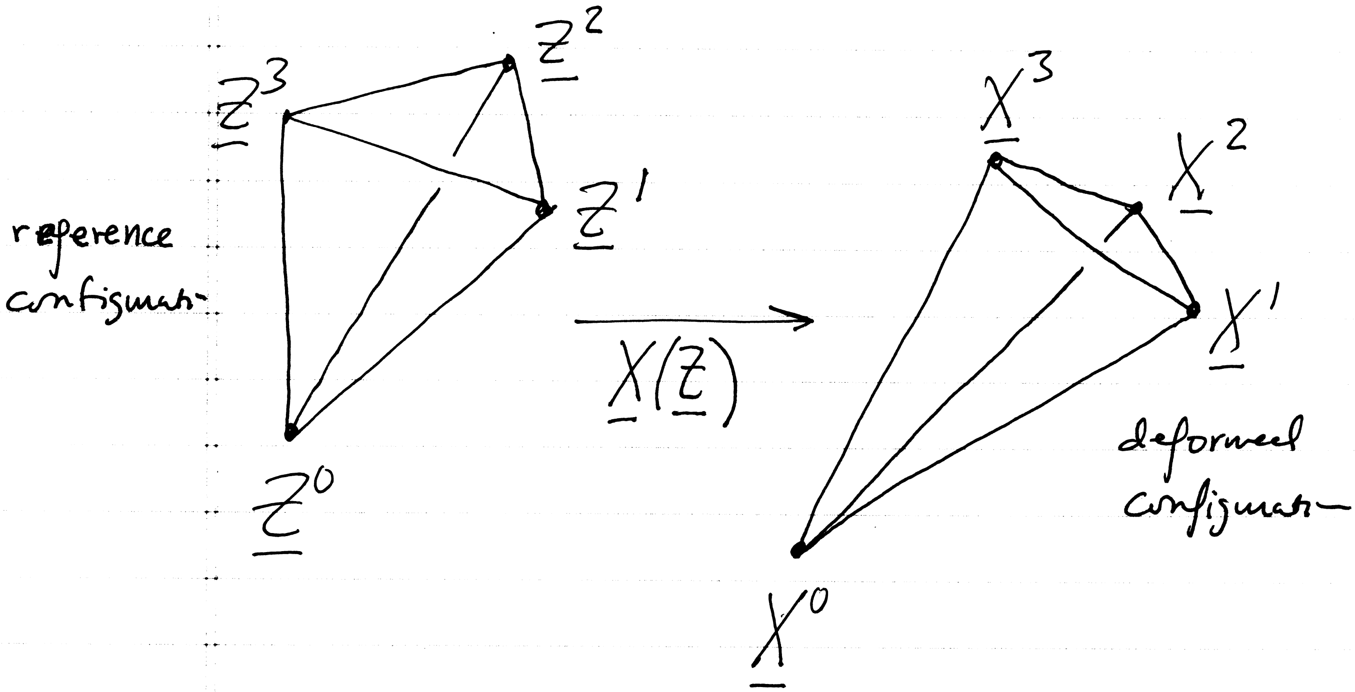
are equally spaced along a straight line, but there is nothing in that energy function to control the spacing, i.e., to resist stretch or compression. For this reason it is often combined with the energy function of Example #1, above to produce a fiber which resists stretch, compression and bending:

$$E(\underline{X}_1 \cdots \underline{X}_N) = \frac{K_s}{2} \sum_{k=1}^{N-1} \left( \frac{|\underline{X}_{k+1} - \underline{X}_k|}{\Delta\xi} - 1 \right)^2 \Delta\xi$$

$$+ \frac{K_b}{2} \sum_{k=2}^{N-1} \left| \frac{\underline{X}_{k+1} + \underline{X}_{k-1} - 2\underline{X}_k}{(\Delta\xi)^2} \right|^2 \Delta\xi$$

The stretching term keeps $|\underline{X}_{k+1} - \underline{X}_k|$ close to $\Delta\xi$, while the bending term resists curvature.

3) Finite element representation of a general 3D elastic medium




$$X_\alpha - X_\alpha^0 = \sum_{\beta=1}^{3} A_{\alpha\beta}(Z_\beta - Z_\beta^0)$$

where the $A_{\alpha\beta}$ are determined by

$$X_\alpha^1 - X_\alpha^0 = \sum_{\beta=1}^{3} A_{\alpha\beta}(Z_\beta^1 - Z_\beta^0)$$

$$X_\alpha^2 - X_\alpha^0 = \sum_{\beta=1}^{3} A_{\alpha\beta}(Z_\beta^2 - Z_\beta^0)$$

$$X_\alpha^3 - X_\alpha^0 = \sum_{\beta=1}^{3} A_{\alpha\beta}(Z_\beta^3 - Z_\beta^0)$$

For each $\alpha = 1, 2,$ or $3$, we have 3 equations in the 3 unknowns $A_{\alpha 1}, A_{\alpha 2}, A_{\alpha 3}$.

Let $\underline{A}_\alpha$ be the vector with these unknowns as its components. The three equations may then be written

$$X_\alpha^1 - X_\alpha^0 = \underline{A}_\alpha \cdot (\underline{Z}^1 - \underline{Z}^0)$$

$$X_\alpha^2 - X_\alpha^0 = \underline{A}_\alpha \cdot (\underline{Z}^2 - \underline{Z}^0)$$

$$X_\alpha^3 - X_\alpha^0 = \underline{A}_\alpha \cdot (\underline{Z}^3 - \underline{Z}^0)$$

Look for a solution of the form

$$\begin{aligned} \underline{A}_\alpha = {} & \lambda_1 (\underline{Z}^2 - \underline{Z}^0) \times (\underline{Z}^3 - \underline{Z}^0) \\ & + \lambda_2 (\underline{Z}^3 - \underline{Z}^0) \times (\underline{Z}^1 - \underline{Z}^0) \\ & + \lambda_3 (\underline{Z}^1 - \underline{Z}^0) \times (\underline{Z}^2 - \underline{Z}^0) \end{aligned}$$

Then

$$X^1_\alpha - X^0_\alpha = \lambda_1 6V_Z$$

$$X^2_\alpha - X^0_\alpha = \lambda_2 6V_Z$$

$$X^3_\alpha - X^0_\alpha = \lambda_3 6V_Z$$

where

$$V_Z = \frac{1}{6}\left(\left(\underline{Z}^1 - \underline{Z}^0\right) \times \left(\underline{Z}^2 - \underline{Z}^0\right)\right) \cdot \left(\underline{Z}^3 - \underline{Z}^0\right)$$

= volume of tetrahedron in its reference configuration

Thus

$$\underline{A}_\alpha = \frac{1}{6V_Z}\Big[\left(X^1_\alpha - X^0_\alpha\right)\left(\underline{Z}^2 - \underline{Z}^0\right) \times \left(\underline{Z}^3 - \underline{Z}^0\right)$$
$$+ \left(X^2_\alpha - X^0_\alpha\right)\left(\underline{Z}^3 - \underline{Z}^0\right) \times \left(\underline{Z}^1 - \underline{Z}^0\right)$$
$$+ \left(X^3_\alpha - X^0_\alpha\right)\left(\underline{Z}^1 - \underline{Z}^0\right) \times \left(\underline{Z}^2 - \underline{Z}^0\right)\Big]$$

Let the elastic energy density of the material be any function of the $A_{\alpha\beta}$, where "density" means per unit volume in the reference configuration.

Since the $A_{\alpha\beta}$ are constant on the tetrahedron, the total energy of the tetrahedron is simply

$$E = V_Z\, \mathcal{E}(\cdots A_{\alpha'\beta'} \cdots).$$

For any particular $\alpha$, $X^0_\alpha$ appears only in

$$A_{\alpha 1},\ A_{\alpha 2},\ A_{\alpha 3}$$

Therefore

$$\frac{\partial E}{\partial X^0_\alpha} = V_Z \sum_{\beta=1}^{3} \frac{\partial \mathcal{E}}{\partial A_{\alpha\beta}} \frac{\partial A_{\alpha\beta}}{\partial X^0_\alpha}$$

$$= V_Z\, \frac{\partial \mathcal{E}}{\partial \underline{A}_\alpha} \cdot \frac{\partial \underline{A}_\alpha}{\partial X^0_\alpha}$$

where $\partial \mathcal{E}/\partial \underline{A}_\alpha$ is the vector with components

$$\frac{\partial \mathcal{E}}{\partial A_{\alpha 1}},\ \frac{\partial \mathcal{E}}{\partial A_{\alpha 2}},\ \frac{\partial \mathcal{E}}{\partial A_{\alpha 3}}$$

From our previous formula for $\underline{A}_\alpha$, it is easy to evaluate

$$\frac{\partial \underline{A}_\alpha}{\partial X^0_\alpha} = -\frac{1}{6V_Z}\Big[\left(\underline{Z}^2-\underline{Z}^0\right)\times\left(\underline{Z}^3-\underline{Z}^0\right)$$

$$+\left(\underline{Z}^3-\underline{Z}^0\right)\times\left(\underline{Z}^1-\underline{Z}^0\right)$$

$$+\left(\underline{Z}^1-\underline{Z}^0\right)\times\left(\underline{Z}^2-\underline{Z}^0\right)\Big]$$

$$= -\frac{1}{6V_Z}\Big[\left(\underline{Z}^1\times\underline{Z}^2\right)+\left(\underline{Z}^2\times\underline{Z}^3\right)+\left(\underline{Z}^3\times\underline{Z}^1\right)\Big]$$

Therefore

$$-\frac{\partial E}{\partial X^0_\alpha} = \frac{1}{6}\frac{\partial \mathcal{E}}{\partial \underline{A}_\alpha}\cdot\Big[\left(\underline{Z}^1\times\underline{Z}^2\right)+\left(\underline{Z}^2\times\underline{Z}^3\right)+\left(\underline{Z}^3\times\underline{Z}^1\right)\Big]$$

With multiple tetrahedra, the force on any node is the sum of the contributions from all tetrahedra that touch that node.

Example: Linear Elasticity

Strain: $e_{\mu\nu} = \frac{1}{2}\left(A_{\mu\nu} + A_{\nu\mu}\right) - \delta_{\mu\nu}$

elasticity tensor: $C_{\kappa\lambda\mu\nu}$

$$\mathcal{E} = \frac{1}{2} C_{\kappa\lambda\mu\nu}\, e_{\kappa\lambda}\, e_{\mu\nu} \qquad \left(\begin{matrix}\text{summation}\\ \text{convention}\end{matrix}\right)$$

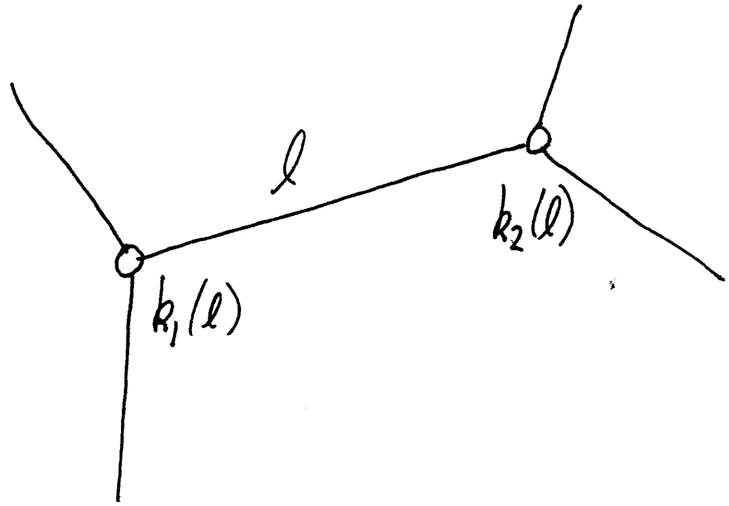
$$\frac{\partial \mathcal{E}}{\partial A_{\alpha\beta}} = \frac{1}{2} C_{\kappa\lambda\mu\nu}\, 2\, \frac{\partial e_{\kappa\lambda}}{\partial A_{\alpha\beta}}\, e_{\mu\nu}$$

$$= \frac{1}{2} C_{\kappa\lambda\mu\nu}\, 2\, \frac{1}{2}\left(\delta_{\kappa\alpha}\delta_{\lambda\beta} + \delta_{\kappa\beta}\delta_{\lambda\alpha}\right) e_{\mu\nu}$$

$$= \frac{1}{2}\left(C_{\alpha\beta\mu\nu} + C_{\beta\alpha\mu\nu}\right) e_{\mu\nu}$$

$$= C_{\alpha\beta\mu\nu}\, e_{\mu\nu}$$

4) Arbitrary network of possibly nonlinear springs




$k_1(l)$, $k_2(l)$ = indices of nodes joined by link $l$ (in either order)

Here it is natural to work directly with force, not force density

Also there is no benefit to starting from an energy formulation

Let

$T_l(\ ) =$ tension in link $l$ as a function of its length

$L_l = |\underline{X}_{k_2(l)} - \underline{X}_{k_1(l)}| =$ length of link $l$

$$\underline{\tau}_l = \frac{\underline{X}_{k_2(l)} - \underline{X}_{k_1(l)}}{L_l}$$

= unit vector along link $l$ from $k_1(l)$ to $k_2(l)$

$$\underline{F}_k = \sum_l T_l(L_l)\,\underline{\tau}_l\left(\delta_{k,k_1(l)} - \delta_{k,k_2(l)}\right)$$

= force on node $k$

Matlab code:

```
F = zeros(kmax, 3)
for l = 1:lmax
    DX = X(k2(l),:) - X(k1(l),:)
    L = sqrt(sum(DX.^2))
    Flmk = (T(L,l)/L) * DX
    F(k1(l),:) = F(k1(l),:) + Flmk
    F(k2(l),:) = F(k2(l),:) - Flmk
end
```

<u>Warning</u>

In the foregoing, everything up to the lines that update F could have been vectorized, but those two lines cannot. The difficulty is that more than one link can touch a node, and we need to <u>sum</u> all of those link forces (with the correct sign) to get the force on the node.

To see what goes wrong, suppose we have vectorized the computation of Flink so that it is an array with dimensions lmax × 3 that contains the link force vectors. Then we could try to write

$$F(k1,:) = F(k1,:) + Flink$$
$$F(k2,:) = F(k2,:) - Flink$$

but this will give <u>incorrect results</u>. Since each line will only be executed once, and since F was initialized to zero, the first line is equivalent to

$$F(k1,:) = Flink$$

For any value of k that appears more than once in the list k1, only the link numbered last that touches node k will be recorded in F, and the other link forces will be lost. No sum will be performed.

Example: Nearly rigid body in fluid

Construct a network that would be rigid if made of constant-length links, and then make each link be a spring with sufficiently large stiffness

Example (Lisa Fauci):

Body that swims by undergoing a prescribed deformation. Let the desired deformation be given as $\underline{\xi} \to \underline{\eta}(\underline{\xi}, t)$.

Construct a rigid network of springs as above, but let the rest length of the spring in link $\ell$ depend on time as follows:

$$L_\ell^0(t) = \left| \underline{\eta}(\underline{\xi}_{k_2(\ell)}, t) - \underline{\eta}(\underline{\xi}_{k_1(\ell)}, t) \right|$$

This will make the network deform in the prescribed manner, but note that global displacements and rotations that may be in $\underline{\eta}$ are discarded, as they should be. The deformation is prescribed, but the motion of the swimmer is not.

5) Target Points

Sometimes, we want to tie a structure down to fixed points in space, e.g., to study flow past a body, as in traditional fluid mechanics. This can be done in an extremely simple way:

$$E = \frac{K}{2} \sum_{k=1}^{N} \left| \underline{X}_k - \underline{Z}_k \right|^2 (\Delta \underline{Z})_k$$

where the $\underline{Z}_k$ are the fixed, given locations that we call <u>target points</u>, and where the $\underline{X}_k$ are the usual immersed boundary points that interact with the fluid. The numbers $(\Delta \underline{Z})_k$ represent the measures that we associate with the target points. They are only provided so that the above expression approximates an integral, which may be a volume, area, or line integral depending on the application. As usual, we derive

$$\underline{F}_k (\Delta \underline{Z})_k = -\frac{\partial E}{\partial \underline{X}_k} = -K(\underline{X}_k - \underline{Z}_k) \Delta \underline{Z}_k$$

$$\underline{F}_k = -K(\underline{X}_k - \underline{Z}_k)$$

The force described by $\underline{F}_k$ provides a feedback mechanism that keeps $\underline{X}_k$ close to $\underline{Z}_k$.

Note that the above energy function $E(\underline{X}_1 \cdots \underline{X}_N)$ is not invariant under translations and rotations, since the $\underline{Z}_k$ are fixed. Therefore, we typically have

$$\sum_{k=1}^{N} \underline{F}_k(\Delta \underline{Z}_k) \neq 0$$

$$\sum_{k=1}^{N} \left(\underline{X}_k \times \underline{F}_k\right)\left(\Delta \underline{Z}_k\right) \neq 0$$

Recall that these quantities are preserved during structure-fluid interaction by the immersed boundary method. In flow past a body, they are important output quantities, since they are equal to minus the total force (which may be further resolved into lift and drag) and minus the total torque that are applied by the fluid to the body. Note that these quantities are being evaluated without any consideration of the fluid stress tensor at the surface of the body.

In most applications of target points, the constant $K$ has no physical meaning and we are interested in the limit $K \to \infty$. In this limit $\underline{X}_k \to \underline{Z}_k$, and $\underline{F}_k \to$ the force that is needed to hold the immersed body or boundary in place. Thus $K$ plays the role of a <u>penalty parameter</u>.

Note the ease of representing <u>arbitrary geometry</u> with target points. All we have to do is lay out the points so they model the geometry. Since the points all act individually, there is no topological structure at all — just an array of points that may be numbered arbitrarily.

In fact, there is no need for the target points to stay at fixed locations. To model bodies that move in a prescribed manner, just replace $\underline{Z}_k$ in the foregoing by $\underline{Z}_k(t)$, which are given functions of time.

As a further generalization, we consider target points which carry <u>additional mass</u> (in excess of the mass that is present anyway because there is fluid everywhere in an immersed boundary computation).

Instead of moving in a prescribed manner, these target points move according to Newton's equation of motion (including the effect of gravity).

Let $M_k(\Delta \underline{Z})_k$ be the additional mass associated with the target point whose index is $k$, so that $M_k$ is the density of the additional mass with respect to the measure $(\Delta \underline{Z})_k$.

The equation of motion of the target point is

$$M_k \cancel{(\Delta \underline{Z})_k} \frac{d^2 \underline{Z}_k}{dt^2} = +K(\underline{X}_k - \underline{Z}_k)\cancel{(\Delta \underline{Z})_k}$$

$$- g M_k \cancel{(\Delta \underline{Z})_k}\, \underline{e}_3$$

where $\underline{e}_3$ is a unit vector pointing "up", i.e., against gravity.

In this way, we get the penalty immersed boundary (pIB) method for immersed boundaries with mass (Yongsam Kim), the spatially discretized formulation of which is as follows:

$$\rho\left(\frac{d\underline{u}}{dt} + S(\underline{u})\underline{u}\right) + \underline{D}p = \mu L\underline{u} + \underline{f} - \rho g \underline{e}_3$$

$$\underline{D}\cdot\underline{u} = 0$$

$$\underline{f}(\underline{x},t) = \sum_{k=1}^{N}\left(-K(\underline{X}_k - \underline{Z}_k)(\Delta Z)_k - \frac{\partial E_0}{\partial \underline{X}_k}(\underline{X}_1 \cdots \underline{X}_N)\right)\delta_h(\underline{x} - \underline{X}_k(t))$$

$$\frac{d\underline{X}_k}{dt} = \sum_{\underline{x}\in g_h} \underline{u}(\underline{x},t)\,\delta_h(\underline{x} - \underline{X}_k(t))\,h^d$$

$$M_k \frac{d^2 \underline{Z}_k}{dt^2} = K(\underline{X}_k - \underline{Z}_k) - M_k g \underline{e}_3$$

where $E_0(\underline{X}_1 \cdots \underline{X}_N)$ describes an elastic interaction unrelated to the penalty springs.

If we formally take the limit $K \to \infty$ in the above formulation of the pIB method, we get

$$\underline{Z}_k \longrightarrow \underline{X}_k$$

$$K(\underline{X}_k - \underline{Z}_k) \to M_k\left(\frac{d^2 \underline{X}_k}{dt^2} + g\,\underline{e}_3\right)$$

and hence the limiting system:

$$\rho\left(\frac{d\underline{u}}{dt} + S(\underline{u})\underline{u}\right) + \underline{D}p = \mu L \underline{u} + \underline{f} - \rho g \underline{e}_3$$

$$\underline{D} \cdot \underline{u} = 0$$

$$f(\underline{x},t) = \sum_{k=1}^{N}\left(-M_k(\Delta \underline{Z})_k\left(\frac{d^2\underline{X}_k}{dt^2} + g\underline{e}_3\right) - \frac{\partial E_0}{\partial \underline{X}_k}(\underline{X}_1 \cdots \underline{X}_N)\right)\delta_h(\underline{x} - \underline{X}_k(t))$$

$$\frac{d\underline{X}_k}{dt} = \sum_{\underline{x} \in g_h} \underline{u}(\underline{x},t)\,\delta_h(\underline{x} - \underline{X}_k(t))\,h^d$$

In comparison to the above limiting equations, the advantage of the pIB method is that it avoids the explicit computation of the D'Alembert force

$$-M_k (\Delta \underline{z})_k \frac{d^2 \underline{X}_k}{dt^2}$$

which can lead to stability problems once time has been discretized as well.

As a special case of the pIB method, note that we may completely drop the elastic interaction given by $E_0(\underline{X}_1 \cdots \underline{X}_N)$,

and then we get a method for adding mass to a fluid for the purpose of doing two-fluid, multifluid, or stratified fluid problems.