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Finite element description of a general hyperelastic 3D material

The state of an elastic material at any particular time is described by a map from a <u>reference configuration</u>, in which we use Cartesian coordinates $\underline{z} = (z_1, z_2, z_3)$ to a <u>current configuration</u>, in which we use Cartesian coordinates $\underline{x} = (x_1, x_2, x_3)$. Let $\underline{x}(\underline{z})$ denote the position at the present time of the material point that had the location $\underline{z}$ in the reference configuration.

The 3×3 matrix $\partial \underline{x} / \partial \underline{z}$ with elements

(1) $$\left(\frac{\partial \underline{x}}{\partial \underline{z}}\right)_{\alpha\beta} = \frac{\partial x_\alpha}{\partial z_\beta} \quad , \quad \alpha, \beta = 1, 2, 3$$

plays a fundamental role in the theory. If the material is incompressible, $\partial \underline{x} / \partial \underline{z}$ satisfies

(2) $$\det\left(\frac{\partial \underline{x}}{\partial \underline{z}}\right) = 1$$

In the context of the IB method, however, we do not need to deal with this constraint explicitly, since it will be enforced in Eulerian form, that is, by imposing the constraint $\nabla \cdot \underline{u} = 0$ on the velocity field in which the elastic material is moving.

If the material is <u>hyperelastic</u>, it is characterized by an energy density $\mathcal{E}(\partial \underline{X}/\partial \underline{Z})$. Note that this is a density with respect to volume in the reference configuration, and since $\partial \underline{X}/\partial \underline{Z}$ is a function of $\underline{Z}$, it is expressed in reference-configuration coordinates.

It is a remarkable fact that $\mathcal{E}$ depends only on the <u>first</u> derivatives of $\underline{x}(\underline{z})$. This is not an approximation coming from truncation of a Taylor series; we are concerned here with nonlinear elasticity, and the deformations we are considering are not assumed to be small. What the restriction to first derivatives expresses is the scale invariance of 3D elasticity. The first derivatives $\partial x_\alpha / \partial z_\beta$ are dimensionless and therefore scale invariant, but the second derivatives, for example, have units of inverse length, and all higher derivatives have units of inverse length to some higher power. Thus, higher derivatives than the first can only appear in the energy if there are some parameters of the problem with units involving length. Those parameters might be geometric, as in the case of a beam, the energy of which is proportional to the square of the curvature, and the relevant length is the thickness of the beam. This length appears in the problem when we reduce the 3D description to an approximate 1D description by integration over the cross section of the beam. Such lower-dimensional models are called <u>elastica</u>, and they do have higher derivatives than the first in their energy functions. Higher derivatives can also come into the energy functions of 3D materials if the material is being described on a scale close to that of the microstructure, so that scale invariance is not applicale.

In general, the energy density $\mathcal{E}$ may have explicit dependence on position and time, so that it is of the form $\mathcal{E}(\partial \underline{x}/\partial \underline{z}; \underline{z}, t)$. Explicit position dependence makes the material <u>inhomogeneous</u> and explicit time dependence makes the material <u>active</u>. We ignore these complications here.

It should also be mentioned that there are some restrictions on the form of $\mathcal{E}(\partial \underline{x}/\partial \underline{z})$ that are related to rotation:

For any 3×3 matrix R that satisfies
$R^T = R^{-1}$ and $\det(R) = +1$,
we require, for all $\partial \underline{x}/\partial \underline{z}$, that

(3) $$\mathcal{E}\left(R \frac{\partial \underline{x}}{\partial \underline{z}}\right) = \mathcal{E}\left(\frac{\partial \underline{x}}{\partial \underline{z}}\right)$$

for any material, and

(4) $$\mathcal{E}\left(\frac{\partial \underline{x}}{\partial \underline{z}} R\right) = \mathcal{E}\left(\frac{\partial \underline{x}}{\partial \underline{z}}\right)$$

if the material is isotropic. The difference between (3) and (4) is that the rotation R is applied to the deformed state of the material in (3) and to the reference configuration in (4).

For an example of an energy density function that satisfies (3) but not (4), let

$$\mathcal{E}\left(\frac{\partial \underline{X}}{\partial \underline{z}}\right) = \frac{1}{2} C \sum_{\alpha=1}^{3} \left(\frac{\partial X_\alpha}{\partial z_1}\right)^2 \tag{5}$$

Then

$$\mathcal{E}\left(R \frac{\partial \underline{X}}{\partial \underline{z}}\right) = \frac{1}{2} C \sum_{\alpha=1}^{3} \left(\sum_{\beta=1}^{3} R_{\alpha\beta} \frac{\partial X_\beta}{\partial z_1}\right)^2 \tag{6}$$

$$= \frac{1}{2} C \sum_{\alpha=1}^{3} \sum_{\beta,\beta'=1}^{3} R_{\alpha\beta} R_{\alpha\beta'} \frac{\partial X_\beta}{\partial z_1} \frac{\partial X_{\beta'}}{\partial z_1}$$

$$= \frac{1}{2} C \sum_{\beta=1}^{3} \left(\frac{\partial X_\beta}{\partial z_1}\right)^2 = \mathcal{E}\left(\frac{\partial \underline{X}}{\partial \underline{z}}\right)$$

But

(7) $$\mathcal{E}\left(\frac{\partial \underline{X}}{\partial \underline{Z}} R\right) = \frac{1}{2} G \sum_{\alpha=1}^{3} \left(\sum_{\beta=1}^{3} \frac{\partial X_\alpha}{\partial Z_\beta} R_{\beta 1} \right)^2$$

$$= \frac{1}{2} G \sum_{\alpha=1}^{3} \sum_{\beta,\beta'=1}^{3} \frac{\partial X_\alpha}{\partial Z_\beta} \frac{\partial X_\alpha}{\partial Z_{\beta'}} R_{\beta 1} R_{\beta' 1}$$

To see that this cannot agree with (5) for all $\partial \underline{X}/\partial \underline{Z}$ and for all orthogonal R with $\det(R) = 1$, consider the special case

(8) $$\frac{\partial X_\alpha}{\partial Z_\beta} = \lambda_\alpha \delta_{\alpha\beta}$$

Then (5) becomes

(9) $$\mathcal{E}\left(\frac{\partial \underline{x}}{\partial \underline{z}}\right) = \frac{1}{2} C \lambda_1^2$$

but (7) becomes

(10) $$\mathcal{E}\left(\frac{\partial \underline{x}}{\partial \underline{z}} R\right) = \frac{1}{2} C \sum_{\alpha=1}^{3} \lambda_\alpha^2 R_{\alpha 1}^2$$

The only way that (9) & (10) can agree for all choices of $\lambda_1, \lambda_2, \lambda_3$ is if

(11) $$R_{11} = \pm 1, \quad R_{21} = 0, \quad R_{31} = 0$$

but there certainly exist orthogonal 3x3 matrices with determinant equal to +1 that do not satisfy these conditions. This shows that (4) is not satisfied by the energy density (5).

Now we are ready to consider a finite element discretization of a material described by an elastic energy density $\mathcal{E}(\partial \underline{x} / \partial \underline{z})$.

We use a tetrahedral mesh with the following property (in which we regard the tetrahedra as closed sets, so that each tetrahedron includes its boundary):
If any two distinct tetrahedra have a non-empty intersection, that intersection is exactly one of the following:

i) A single point that is a vertex of both tetrahedra, or

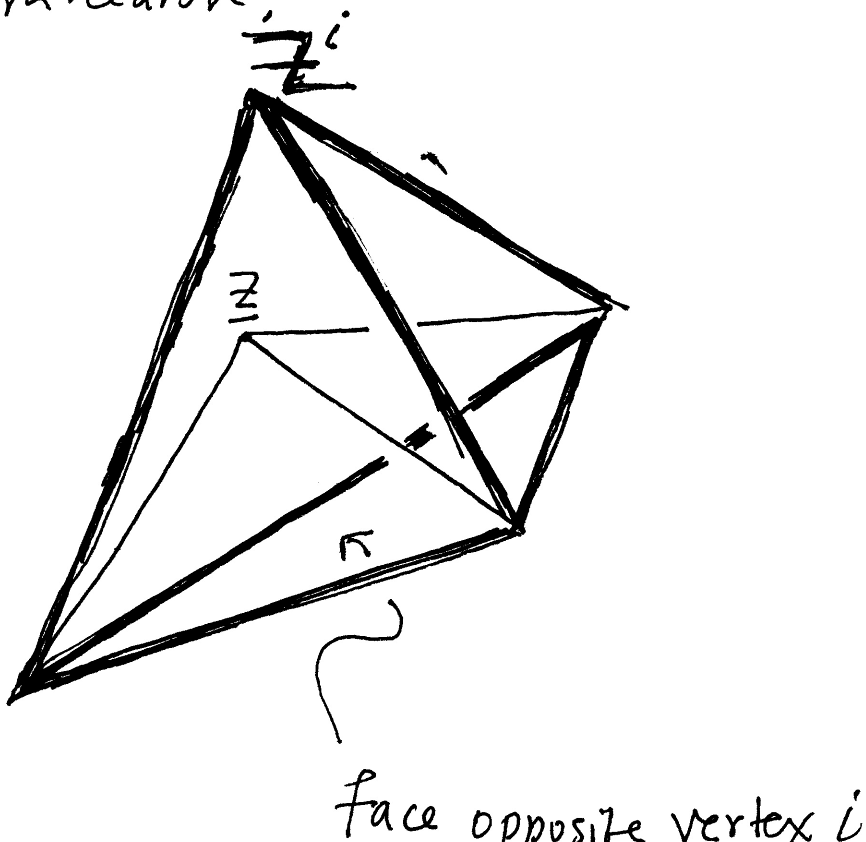
ii) A line segment that is a complete edge in both tetrahedra, or

iii) A triangle (including its interior) that is a complete face of both tetrahedra.

Now consider a deformation of the material that is continuous overall, and piecewise linear, i.e., linear on each tetrahedron. Such a deformation is determined by giving the positions of the vertices of the tetrahedra, before and after the deformation.

Now consider any one tetrahedron with vertices indexed by $i=1,2,3,4$.
Let the position of vertex i in the reference configuration of the tetrahedron be denoted $\underline{Z}^i$, and let the position of that vertex in the deformed configuration be denoted $\underline{X}^i$. Let V be the volume of the reference tetrahedron, and for any point $\underline{Z}$ of the reference tetrahedron, let $V^i(\underline{Z})$ be the volume of the sub-tetrahedron of the reference tetrahedron with $\underline{Z}$ as one vertex, and with the other three

vertices being those of the face that is <u>opposite</u> to vertex i in the reference tetrahedron,



For any point $\underline{z}$ in the reference tetrahedron, let

(12) $$\underline{x}(\underline{z}) = \sum_{i=1}^{4} \underline{X}^i \, \frac{V^i(\underline{z})}{V}$$

In components

(13) $$x_\alpha(\underline{z}) = \sum_{i=1}^{4} X_\alpha^i \frac{V^i(\underline{z})}{V}, \quad \alpha = 1,2,3$$

Since the volume of a tetrahedron is 1/3 the area of its base time the height, it is easy to see that

(14) $$\nabla_{\underline{z}} V^i = \frac{1}{3} \underline{A}^i$$

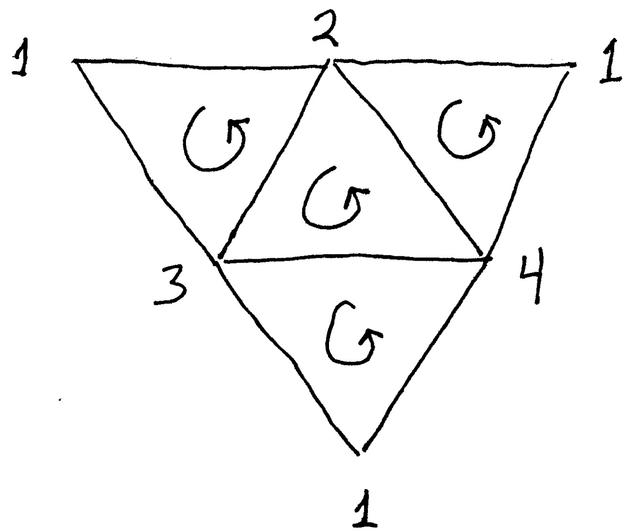
where $\underline{A}^i$ is the <u>area vector</u> of the face of the reference tetrahedron that is opposite to vertex i. By definition, the magnitude of $\underline{A}^i$ is the area of the face opposite vertex i, and the direction of $\underline{A}^i$ is normal to that face pointing inward. Let (j, k, l) be the indices of the vertices of the face that is opposite to vertex i, in counterclockwise order as seen from vertex i. Then

$$(15) \qquad \underline{A}^i = \frac{1}{2}\left(\underline{\underline{Z}}^j - \underline{\underline{Z}}^l\right) \times \left(\underline{\underline{Z}}^k - \underline{\underline{Z}}^l\right)$$

$$= \frac{1}{2}\left(\left(\underline{\underline{Z}}^j \times \underline{\underline{Z}}^k\right) + \left(\underline{\underline{Z}}^k \times \underline{\underline{Z}}^l\right) + \left(\underline{\underline{Z}}^l \times \underline{\underline{Z}}^j\right)\right)$$

Note that this is a sum over the directed edges of the face opposite vertex i, with the direction being counterclockwise as seen from inside the tetrahedron.

If the tetrahedron is numbered so that vertices $(2,3,4)$ appear in counterclockwise order as seen from vertex 1, then equation (15) is correct if (i,j,k,l) is any <u>even</u> permutation of $(1,2,3,4)$. To see that this is the case, we can cut along edges involving vertex 1 and then unfold the tetrahedron so that its faces lie in a plane with their inner sides facing up, as in the following diagram:



Then the four vertices, and their opposite faces with vertices in counterclockwise order can be listed as

1	2	3	4
2	1	4	3
3	4	1	2
4	3	2	1

In the above list of permutations, each permutation is obtained from the previous one by making exactly two interchanges, so all of them are even permutations of (1,2,3,4).

Of course, for each face we are also free to make any <u>cyclic</u> permutation of the indices of its vertices, but for any <u>three</u> objects, the cyclic permutations coincide with the even permutations, so any such cyclic permutation of the last three indices will still leave us with an even permutation of (1,2,3,4).

Every edge of a tetrahedron belongs to exactly two faces, and the above assignment of direction to an edge gives each edge the opposite direction in each of the two faces to which it belongs. For this reason, an immediate consequence of equation (15) is that

(16) $$\sum_{i=1}^{4} \underline{A}^i = 0$$

From (13) & (14)

(17) $$\frac{\partial x_\alpha}{\partial z_\beta} = \frac{1}{3V} \sum_{i=1}^{4} X_\alpha^i A_\beta^i$$

Since this is independent of $\underline{z}$, the functions $x_\alpha(\underline{z})$ defined by (13) are linear. Also, it is easy to see from the geometric definition of $V^i(\underline{z})$ that

(18) $$V^i(\underline{Z}^j) = \delta_{ij} V$$

and it therefore follows from (13) that

(19) $$x_\alpha(\underline{Z}^j) = X_\alpha^j \qquad j = 1 \ldots 4; \; \alpha = 1,2,3$$

Thus $x_\alpha(\underline{z})$ as given by (13) is the linear interpolant of $(X_\alpha^1 \cdots X_\alpha^4)$ over the reference tetrahedron.

Now that we have an expression for $\partial x_\alpha / \partial z_\beta$, we can easily evaluate the elastic energy of the deformed tetrahedron. Since $\partial \underline{x} / \partial \underline{z}$ is independent of $\underline{z}$, $\mathcal{E}(\partial \underline{x} / \partial \underline{z})$ is also independent of $\underline{z}$, and the integral of $\mathcal{E}(\partial \underline{x} / \partial \underline{z})$ over the reference tetrahedron is simply

(20) $$E = V \mathcal{E}(\partial \underline{x} / \partial \underline{z})$$

$$= V \mathcal{E}\left(\cdots \frac{1}{3V} \sum_{i=1}^{4} X_\alpha^i A_\beta^i \cdots\right)$$

The dots here indicate that $\mathcal{E}$ actually has 9 arguments, and these are obtained by setting $\alpha = 1,2,3$ and $\beta = 1,2,3$

To obtain the force on node i from equation (20), we just need to evaluate

$$F_\alpha^i = -\frac{\partial E}{\partial X_\alpha^i} \tag{21}$$

This is easy to do because V is the volume of the tetrahedron in its <u>reference</u> configuration, and the coefficients A_β^i likewise depend only on the <u>reference</u> configuration of the tetrahedron. Thus, V and the numbers A_β^i may be treated as constants when differentiating with respect to X_α^i.

Although it is straightforward to write out an explicit formula for F_α^i based on (20) & (21), that formula is complicated because it involves all nine first derivatives of the function $\mathcal{E}$ with respect to its arguments, so we will not do that here.* Instead, we consider the special case of an incompressible neo-Hookean material, the elastic energy density of which is given by

(22) $$\mathcal{E} = \frac{1}{2} G \sum_{\alpha,\beta=1}^{3} \left(\frac{\partial X_\alpha}{\partial Z_\beta}\right)^2$$

* Not that bad, see Appendix B

Substituting (17) into (22), we get

(23) $$\mathcal{E} = \frac{1}{2}\,\frac{C}{9V^2}\sum_{i,j=1}^{4}\sum_{\alpha,\beta=1}^{3} X^i_\alpha X^j_\alpha A^i_\beta A^j_\beta$$

Then, since $E = V\mathcal{E}$, we have

(24) $$E = \frac{1}{2}\sum_{\alpha=1}^{3}\sum_{i,j=1}^{4} X^i_\alpha S_{ij} X^j_\alpha$$

where

(25) $$S_{ij} = \frac{C}{9V}\sum_{\beta=1}^{3} A^i_\beta A^j_\beta$$

Note that the numbers S_{ij} depend only on the reference configuration of the tetrahedron; they do not change as the tetrahedron deforms.

It follows from (24) that

(26) $$F_\alpha^i = -\frac{\partial E}{\partial X_\alpha^i} = -\sum_{j=1}^{4} S_{ij} X_\alpha^j$$

Thus, each tetrahedron has a time-independent stiffness matrix S with elements given by (25). This matrix can be applied componentwise to the coordinates of the vertices of the tetrahedron to get minus the corresponding components of the elastic forces on the vertices.

Note that $\underline{F}^i$ as given by (26) is a <u>force</u>, not a force density. It is therefore spread to the Eulerian grid of an IB computation as

(27) $$\underline{F}^i \delta_h(\underline{x} - \underline{X}^i)$$

without any quadrature weight being assigned to the node $\underline{X}^i$.

In an actual IB computation, there will, of course, be multiple tetrahedra, and a simple (but somewhat inefficient) way to proceed is to assign an index k to each tetrahedron and then an an index $i = 1,2,3,4$ to each node within the tetrahedron, so that each node of the tetrahedral mesh has a double index (k, i), and the same node gets as many such double indices as the number of tetrahedra in which it appears. In this notation, the force-spreading operation can be written very simply as

$$\underline{f}(\underline{x}, t) = \sum_k \sum_{i=1}^{4} \underline{F}^{k,i}(t)\, \delta_h(\underline{x} - \underline{X}^{k,i}(t)) \tag{28}$$

The computation of $\underline{F}^{k,i}$ involves only the configuration of tetrahedron k, and we do not even need to know which node in tetrahedron k may happen to be the same as a node in some other tetrahedron. Also, when the nodes are moved, the velocity interpolation formula

$$\frac{d\underline{X}^{k,i}}{dt} = \sum_{\underline{x} \in g_h} \underline{u}(\underline{x},t)\, \delta_h\left(\underline{x}-\underline{X}^{k,i}(t)\right) h^3 \tag{29}$$

ensures that any two nodes that coincide at $t=0$ will coincide forever, and this property of the IB method remains true despite temporal discretization of (29).

Appendix A: Minimization of the neo-Hookean elastic energy density over incompressible deformations

Let A be an $n \times n$ matrix with $\det(A) = 1$. We claim that

$$\sum_{i,j=1}^{n} A_{ij}^2 \geq n$$

with equality only if A is orthogonal

Proof:

First, recall that

$$\sum_{i,j=1}^{n} A_{ij}^2 = \mathrm{trace}(A^T A)$$

The matrix $A^T A$ is symmetric; it is

obviously non-negative, since $x^T A^T A x = \|Ax\|^2 \geq 0$; and it is non-singular, since $\det(A^T A) = (\det(A))^2 = 1$. It follows that $A^T A$ has real <u>positive</u> eigenvalues, which we write as $\lambda_1 \cdots \lambda_n$. (If an eigenvalue has multiplicity m, it is simply listed m times.) Then

$$\prod_{i=1}^{n} \lambda_i = 1$$

$$\sum_{i=1}^{n} \lambda_i = \operatorname{trace}(A^T A)$$

Since all of the λ_i are positive, we may set $\lambda_i = e^{\mu_i}$, and then

$$\sum_{i=1}^{n} \mu_i = 0$$

$$\sum_{i=1}^{n} e^{\mu_i} = \text{trace}(A^T A)$$

But

$$e^{\mu} \geq 1 + \mu$$

with equality only if $\mu = 0$, since e^{μ} is strictly convex and the graph of $1+\mu$ is the tangent line to the graph of e^{μ} at $\mu = 0$. Therefore

$$\text{trace}(A^T A) \geq \sum_{i=1}^{n} (1 + \mu_i) = n$$

with equality only if $\mu_i = 0$ for all i, that is, if $\lambda_i = 1$ for all i. But the only matrix with all of its eigenvalues equal to 1 is the identity matrix.

Thus, we have shown that

$$\det(A) = 1 \Rightarrow$$

$$\text{trace}(A^T A) \geq n$$

with equality only if $A^T A = I$

Applying this to our situation in which $\partial \underline{X} / \partial \underline{z}$ is 3×3, we have

$$\det(\partial \underline{X} / \partial \underline{z}) = 1 \Rightarrow$$

$$\sum_{\alpha,\beta=1}^{3} \left(\frac{\partial X_\alpha}{\partial z_\beta} \right)^2 \geq 3$$

with equality only if $\partial \underline{X} / \partial \underline{z}$ is a rotation.

(Reflections are <u>not allowed</u>, since $\partial \underline{X} / \partial \underline{z}$ has to be continuously connected to the identity.) It makes sense that rotations are the class of matrices that minimize the elastic energy density, since rotations do not actually deform the elastic material at all.

Appendix B

Here we write out the general formula for F_α^i, see equations (20) & (21). Note that for any particular i, α, the variable X_α^i only appears in 3 of the 9 arguments of $\mathcal{E}$, namely $\partial X_\alpha / \partial z_\beta$ for $\beta = 1, 2, 3$. Also, in the sum over vertices, X_α^i only appears in the term for vertex i. It follows that

$$F_\alpha^i = -\frac{1}{3} \sum_{\beta=1}^{3} \mathcal{E}_{\alpha\beta} \left(\cdots \frac{1}{3V} \sum_{j=1}^{4} X_{\alpha'}^j A_{\beta'}^j \cdots \right) A_\beta^i$$

Here $\mathcal{E}_{\alpha\beta}$ denotes the derivative of $\mathcal{E}$ with

respect to its (α,β) argument.
In the special case of neo-Hookean material

$$\mathcal{E}_{\alpha\beta} = G\,\frac{\partial x_\alpha}{\partial z_\beta}$$

$$= \frac{G}{3V}\sum_{j=1}^{4} X_\alpha^j A_\beta^j$$

and therefore

$$F_\alpha^i = -\frac{G}{9V}\sum_{j=1}^{4}\sum_{\beta=1}^{3} A_\beta^i A_\beta^j X_\alpha^j$$

This is the same as equations (25-26), so all is well.