Derivation of Quasistatics and Landmark Optimization for Muscles
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1 Problem

Given a muscle-driven facial rig $x(\theta)$ we want to be able to solve problems of the form:

$$\text{minimize}_\theta \frac{1}{2}||g^* - g(x(\theta))||_2^2$$

For the sake of simplicity, assume that $x(y) = y$ and that $g^* = x^*$ is a target mesh with the same topology as our facial rig. Thus,

$$\text{minimize}_\theta \frac{1}{2}||x^* - x(\theta)||_2^2 \tag{1}$$

We can solve this problem using the Gauss-Newton method for solving non-linear least squares (NLLQ). At each step t in the optimization, we solve the following least-squares problem given the current state θ_t:

$$\begin{aligned}\frac{\partial x}{\partial \theta}(\theta_t)^T \frac{\partial x}{\partial \theta}(\theta_t)\Delta\theta &= \frac{\partial x}{\partial \theta}(\theta_t)^T (x^* - x(\theta_t)) \\ \theta_{t+1} &= \theta_t + \Delta\theta\end{aligned}$$

Note that the first equation is equivalent to solving the following equation using QR decomposition:

$$\frac{\partial x}{\partial \theta}(\theta_t)\Delta\theta = x^* - x(\theta_t) \tag{2}$$

More details about the Gauss-Newton method and other NLLQ optimization methods can be found in [4].

2 Overview of Muscle-Based Facial Rig Parameters

Our muscle-based facial rig uses quasistatics to compute the vertex positions ($x(\theta)$). To be more consistent with [7], let us separate our parameters into θ_k and θ_a which are the kinematic (jaw/cranium) parameters and muscle activation parameters respectively. Additionally, the vertices can be split into unconstrained vertices $x^U(\theta_k)$ and constrained vertices $x^C(\theta_a, \theta_k)$. The goal of quasistatics is to find the vertex positions at which the net force on all the unconstrained vertices is 0. Thus the quasistatics equation looks like:

$$f(x^C(\theta_a, \theta_k), x^U(\theta_k), \theta_a) = 0 \tag{3}$$

In this section, I will give a brief overview on what effect each parameter has. For additional information on any of these computations, see [7].

2.1 Muscle Activations

Our muscles are linearly activated, that is the force is a linear combination of the elastic material response, passive muscle forces, and active muscle force:

$$f(x^C(\theta_a, \theta_k), x^U(\theta_k), \theta_a) = f_0(x^C, x^U) + \sum_i \theta_{a,i} f_i(x^C, x^U) \tag{4}$$

The reasoning behind the choice of these activations being linear can be found in [11]. Computation of each of these forces will be explained later.

2.2 Cranium Parameters

The cranium is modeled as a rigid frame that affects all the vertices in the face. That is:

$$\hat{x}_i = M_c(\theta_k)x_i + t_c(\theta_k)$$

When computing the Jacobian, there is no assumption that M_c is orthogonal. Instead, additional energy terms are put into the computation to ensure orthogonality. Therefore, 12 of the parameters of θ_k deal with the cranium parameters (9 for M_c, 3 for t_c). It is important to remember that this affine transformation is applied to every node of the facial rig. See [7] for more details.

2.3 Jaw Parameters

Similar to the cranium, the jaw is also modeled as an affine transformation.

$$\hat{x}_i = M_j(\theta_k)x_i + t_j(\theta_k)$$

When computing the Jacobian, there is no assumption that M_j is orthogonal. Instead, additional energy terms are put into the computation to ensure orthogonality. Therefore, 12 of the parameters of θ_k deal with the jaw parameters (9 for M_j, 3 for t_j). Unlike the cranium, this affine transformation is **NOT** applied to every node of the facial rig. See [7] for more details.

3 Quasistatic Derivatives

This problem can be solved using a Newton-Raphson solver and at each step we compute $\frac{\partial f}{\partial x^U}$. The rest of this section will assume we that $\frac{\partial f}{\partial x^U}$ is a known quantity. I will derive it later in this document. When solving quasistatics, given θ_k, θ_a, we want to find the x^U such that the net force is 0. However, in the problem above, we want to find θ_k and θ_a such that the mesh positions match the target positions. We thus need to be able to compute: $\frac{\partial x^C}{\partial \theta_k}$, $\frac{\partial x^U}{\partial \theta_a}$, and $\frac{\partial x^U}{\partial \theta_k}$. Note that $\frac{\partial x^C}{\partial \theta_a} = 0$. The other quantities can be computed using the quasistatic equation. For brevity, the following equations omit the fact that the Jacobians/gradients are evaluated at the current state of θ_a, θ_k, x^C and x^U.

3.1 Computing $\frac{\partial x^U}{\partial \theta_{a,i}}$

$$
\begin{aligned}
\frac{\partial f}{\partial \theta_{a,i}} &= \frac{\partial f}{\partial x^U}\frac{\partial x^U}{\partial \theta_{a,i}} + \frac{\partial f}{\partial \theta_{a,i}} && && (5)\\
-\frac{\partial f}{\partial x^U}\frac{\partial x^U}{\partial \theta_{a,i}} &= \frac{\partial f}{\partial \theta_{a,i}} && \text{This is true since the force and its Jacobian is equal to 0.} && (6)\\
&= f_i(x^C, x^U) && \text{This follows from Equation (4).} && (7)
\end{aligned}
$$

This is a linear system and can easily be solved.

3.2 Computing $\frac{\partial x}{\partial \theta_{k,i}}$ (Cranium)

Note that every vertex of the face gets an affine transformation applied to it due to the cranium transformation. Therefore:

- The internal forces do not change when the cranium transformation changes.
- Every vertex has the same $\frac{\partial x}{\partial \theta_{k,i}}$ regardless of whether it is contrained of unconstrained.

Thus the Jacobian can trivially computed:

$$
\frac{\partial x}{\partial \theta_k} = \frac{\partial M_c}{\partial \theta_k}x + \frac{\partial t_c}{\partial \theta_k}
$$

3.3 Computing $\frac{\partial x^C}{\partial \theta_{k,i}}$ (Jaw)

The Jacobian for the constrained jaw nodes is similar to the cranium nodes:

$$
\frac{\partial x^C}{\partial \theta_k} = \frac{\partial M_j}{\partial \theta_k}x + \frac{\partial t_j}{\partial \theta_k}
$$

3.4 Computing $\frac{\partial x^U}{\partial \theta_{k,i}}$ (Jaw)

The Jacobian for the unconstrained nodes for a jaw deformation differential can be computed as a linear system.

$$
\frac{\partial f}{\partial \theta_{k,i}} = \frac{\partial f}{\partial x^C}\frac{\partial x^C}{\partial \theta_{k,i}} + \frac{\partial f}{\partial x^U}\frac{\partial x^U}{\partial \theta_{k,i}} \tag{8}
$$

$$
-\frac{\partial f}{\partial x^U}\frac{\partial x^U}{\partial \theta_{k,i}} = \frac{\partial f}{\partial x^C}\frac{\partial x^C}{\partial \theta_{k,i}} \tag{9}
$$

Note that $\frac{\partial f}{\partial x^U}$, $\frac{\partial f}{\partial x^C}$, and $\frac{\partial x^C}{\partial \theta_{k,i}}$ are known quantities and we thus have a linear system. $\frac{\partial f}{\partial x^U}$ and $\frac{\partial f}{\partial x^C}$ will be derived later in this document.

4 FVM Force Derivations

In this section, I will go through the derivation of f_0, f_i, $\frac{\partial f}{\partial x^U}$ and $\frac{\partial f}{\partial x^C}$. Note that $\frac{\partial f}{\partial x^U}$ and $\frac{\partial f}{\partial x^C}$ can be computed as a single $\frac{\partial f}{\partial x}$ and the appropriate columns can be selected to get the other derivatives.

4.1 Geometric Calculation of Strain/Deformation Gradient

Assume we are given a tetrahedron with undeformed (material space) vertices $x_{m,1}$, $x_{m,2}$, $x_{m,3}$, $x_{m,4}$ and deformed spatial coordinates $x_{s,1}$, $x_{s,2}$, $x_{s,3}$, $x_{s,4}$. We can construct a matrix of edges for both the undeformed state and the deformed state:

$$D_s = \begin{bmatrix}(x_{s,2} - x_{s,1}) & (x_{s,3} - x_{s,1}) & (x_{s,4} - x_{s,1})\end{bmatrix} \qquad D_m = \begin{bmatrix}(x_{m,2} - x_{m,1}) & (x_{m,3} - x_{m,1}) & (x_{m,4} - x_{m,1})\end{bmatrix}$$

The strain/deformation gradient of a tetrahedron can thus be computed as: $F = D_s D_m^{-1}$.

4.2 Constitutive Model

The constitutive model for muscles can be found in [8] and [9].

$$W(I_1, I_2, \lambda, a_0, \alpha) = F_1(I_1, I_2) + U(J) + F_2(\lambda, \alpha) \tag{10}$$

This function computes the strain energy of the muscle. Some notable variables:

$J = \det(F)$	Relative volume between the deformed state and the undeformed state
$C = J^{-2/3} F^T F$	
$I_1 = \mathrm{Tr}(C)$	Deviatoric isotropic invariant of the strain
$I_2 = \frac{1}{2}((\mathrm{Tr}(C))^2 - \mathrm{Tr}(C^2))$	Deviatoric isotropic invariant of the strain
a_0	Muscle fiber direction
α	Muscle activation
$\lambda = \sqrt{a_0^T C a_0}$	The stretch in the fiber direction. The slack length is at $\lambda = 1$

The various terms in the constitutive model are computed as:

$F_1(I_1, I_2) = AI_1 + BI_2$	A Mooney-Rivlin rubber-like model where A and B are constants.
$U(J) = \frac{1}{2} K \ln(J)^2$	The incompressibility term where K is a constant.
	Note that this definition differs from [8] to try and better match [9]
$F_2(\lambda, \alpha) = \alpha F_{\text{active}}(\lambda) + F_{\text{passive}}(\lambda)$	The passive and active response of the muscle.

Note that $F_{\text{active}}(\lambda)$ and $F_{\text{passive}}(\lambda)$ are pre-defined function curves. These terms are described in more detail in [8].

4.3 First Piola-Kirchoff Stress

The first Piola-Kirchoff stress can be computed as $P(F) = \frac{\partial W}{\partial F}$. For an isotropic constitutive model, $P(F) = UP(\hat{F})V^T$ where $F = U\hat{F}V^T$ using the SVD. Note that $\hat{F}$ is diagonal. An anisotropic constitutive model can also be used in this formulation by replacing the anisotropic direction with a rotated direction. For example, in the muscle constitutive model, $f_m = V^T a_0$. The derivation of the first Piola-Kirchoff stress in this section will assume we are working with $\hat{F}$ and f_m. The Matrix Cookbook [6] was extremely useful in all my derivations.

4.3.1 Mooney-Rivlin Term

The Mooney-Rivlin term is $F_1 = AI_1 + BI_2$. Computation of $\frac{\partial AI_1}{\partial \hat{F}}$:

$$\begin{aligned}
\frac{\partial AI_1}{\partial \hat{F}} &= \frac{\partial AJ^{-2/3}\operatorname{Tr}(\hat{F}^T\hat{F})}{\partial \hat{F}} \\
&= A(\frac{\partial J^{-2/3}}{\partial \hat{F}}\operatorname{Tr}(\hat{F}^T\hat{F}) + \det(\hat{F})^{-2/3}\frac{\partial \operatorname{Tr}(\hat{F}^T\hat{F})}{\partial \hat{F}}) \\
&= A(\frac{\partial \det(\hat{F})^{-2/3}}{\partial \hat{F}}\operatorname{Tr}(\hat{F}^T\hat{F}) + 2\det(\hat{F})^{-2/3}\hat{F}) \\
&= A(-\frac{2}{3}\det(\hat{F})^{-2/3}\hat{F}^{-T}\operatorname{Tr}(\hat{F}^T\hat{F}) + 2\det(\hat{F})^{-2/3}\hat{F}) \\
&= A(-\frac{2}{3}\det(\hat{F})^{-2/3}\operatorname{Tr}(\hat{F}^2)\hat{F}^{-1} + 2\det(\hat{F})^{-2/3}\hat{F}) \\
&= 2A(-\frac{1}{3}\det(\hat{F})^{-2/3}\operatorname{Tr}(\hat{F}^2)\hat{F}^{-1} + \det(\hat{F})^{-2/3}\hat{F})
\end{aligned}$$

Computation of $\frac{\partial BI_2}{\partial \hat{F}}$:

$$\begin{aligned}
\frac{\partial \operatorname{Tr}(C)^2}{\partial \hat{F}} &= 2\operatorname{Tr}(C)\frac{\partial \operatorname{Tr}(C)}{\partial \hat{F}} \\
&= 2\det(\hat{F})^{-2/3}\operatorname{Tr}(\hat{F}^T\hat{F})\frac{\partial \det(\hat{F})^{-2/3}\operatorname{Tr}(\hat{F}^T\hat{F})}{\partial \hat{F}} \\
&= 2\det(\hat{F})^{-2/3}\operatorname{Tr}(\hat{F}^T\hat{F})(\frac{\partial \det(\hat{F})^{-2/3}}{\partial \hat{F}}\operatorname{Tr}(\hat{F}^T\hat{F}) + \det(\hat{F})^{-2/3}\frac{\partial \operatorname{Tr}(\hat{F}^T\hat{F})}{\partial \hat{F}}) \\
&= 2\det(\hat{F})^{-2/3}\operatorname{Tr}(\hat{F}^T\hat{F})(\frac{-2}{3}\det(\hat{F})^{-2/3}\operatorname{Tr}(\hat{F}^T\hat{F})\hat{F}^{-1} + 2\det(\hat{F})^{-2/3}\hat{F}) \\
&= \det(\hat{F})^{-2/3}\operatorname{Tr}(\hat{F}^T\hat{F})(\frac{-4}{3}\det(\hat{F})^{-2/3}\operatorname{Tr}(\hat{F}^T\hat{F})\hat{F}^{-1} + 4\det(\hat{F})^{-2/3}\hat{F}) \\
&= \frac{-4}{3}\det(\hat{F})^{-4/3}\operatorname{Tr}(\hat{F}^T\hat{F})^2\hat{F}^{-1} + 4\det(\hat{F})^{-4/3}\operatorname{Tr}(\hat{F}^T\hat{F})\hat{F}
\end{aligned}$$

$$
\begin{aligned}
\frac{\partial \operatorname{Tr}(C^2)}{\partial \hat{F}} &= \frac{\partial \det(\hat{F})^{-4/3} \operatorname{Tr}(\hat{F}^T\hat{F}\hat{F}^T\hat{F})}{\partial \hat{F}} \\
&= \frac{\partial \det(\hat{F})^{-4/3}}{\partial \hat{F}} \operatorname{Tr}((\hat{F}^T\hat{F})^2) + \det(\hat{F})^{-4/3} \frac{\partial \operatorname{Tr}((\hat{F}^T\hat{F})^2)}{\partial \hat{F}} \\
&= \frac{-4}{3} \det(\hat{F})^{-4/3} \hat{F}^{-T} \operatorname{Tr}((\hat{F}^T\hat{F})^2) + \det(\hat{F})^{-4/3} \frac{\partial \operatorname{Tr}((\hat{F}^T\hat{F})^2)}{\partial \hat{F}} \\
&= \frac{-4}{3} \det(\hat{F})^{-4/3} \hat{F}^{-T} \operatorname{Tr}((\hat{F}^T\hat{F})^2) + \det(\hat{F})^{-4/3} 4\hat{F}\hat{F}^T\hat{F} \\
&= \frac{-4}{3} \det(\hat{F})^{-4/3} \operatorname{Tr}(\hat{F}^4)\hat{F}^{-1} + \det(\hat{F})^{-4/3} 4\hat{F}^3
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial BI_2}{\partial \hat{F}} &= \frac{\partial B\frac{1}{2}((\operatorname{Tr}(C))^2 - \operatorname{Tr}(C^2))}{\partial \hat{F}} \\
&= \frac{B}{2}(\frac{\partial \operatorname{Tr}(C)^2}{\partial \hat{F}} - \frac{\partial \operatorname{Tr}(C^2)}{\partial \hat{F}}) \\
&= \frac{B}{2}(\frac{-4}{3} \det(\hat{F})^{-4/3} \operatorname{Tr}(\hat{F}^T\hat{F})^2\hat{F}^{-1} + 4\det(\hat{F})^{-4/3} \operatorname{Tr}(\hat{F}^T\hat{F})\hat{F} - \frac{-4}{3} \det(\hat{F})^{-4/3} \operatorname{Tr}(\hat{F}^4)\hat{F}^{-1} - \det(\hat{F})^{-4/3} 4\hat{F}^3) \\
&= \frac{B}{2}(\frac{-4}{3} \det(\hat{F})^{-4/3}(\operatorname{Tr}(\hat{F}^T\hat{F})^2\hat{F}^{-1} - \operatorname{Tr}(\hat{F}^4)\hat{F}^{-1}) + 4\det(\hat{F})^{-4/3}(\operatorname{Tr}(\hat{F}^T\hat{F})\hat{F} - \hat{F}^3))
\end{aligned}
$$

4.3.2 Incompressibility Term

The incompressibility term is $U(J) = \frac{1}{2}K\ln(J)^2$. Note once again that $J = \det(\hat{F})$ and K is a constant. Then computation of $\frac{\partial U(J)}{\partial \hat{F}}$:

$$
\begin{aligned}
\frac{\partial U(J)}{\partial \hat{F}} &= \frac{1}{2}K\frac{\partial \ln(J)^2}{\partial \hat{F}} \\
&= \frac{1}{2}K\frac{\partial \ln(J)^2}{\partial \ln(J)} \frac{\partial \ln(J)}{\partial J} \frac{\partial J}{\partial \hat{F}} \\
&= K\frac{\ln(J)}{J} \frac{\partial \det(\hat{F})}{\partial \hat{F}} \\
&= K\frac{\ln(J)}{\det(\hat{F})} \det(\hat{F})\hat{F}^{-1} \\
&= K\ln(J)\hat{F}^{-1}
\end{aligned}
$$

4.3.3 Passive/Active Response Terms

The active and passive muscle response is $F_2(\lambda, \alpha) = \alpha F_{\text{active}}(\lambda) + F_{\text{passive}}(\lambda)$. Note once again that $\lambda = \sqrt{a_0^T C a_0} = \sqrt{a_0^T \det(\hat{F})^{-2/3}\hat{F}^T\hat{F}a_0}$. Since we are working in the material space:

$$
\begin{aligned}
\lambda &= \sqrt{f_m^T \det(\hat{F})^{-2/3}\hat{F}^T\hat{F}f_m} \\
&= \det(\hat{F})^{-1/3}\sqrt{f_m^T\hat{F}^T\hat{F}f_m} \\
&= \det(\hat{F})^{-1/3}\sqrt{(\hat{F}f_m)^T\hat{F}f_m}
\end{aligned}
$$

Then computing $\frac{\partial F_2(\lambda,\alpha)}{\partial \hat{F}}$:

$$\begin{aligned}
\frac{\partial F_2(\lambda,\alpha)}{\partial \hat{F}} &= \alpha \frac{\partial F_{\text{active}}}{\partial \hat{F}} + \frac{\partial F_{\text{passive}}}{\partial \hat{F}} \\
&= (\alpha \frac{\partial F_{\text{active}}}{\partial \lambda} + \frac{\partial F_{\text{passive}}}{\partial \lambda}) \frac{\partial \lambda}{\partial \hat{F}}
\end{aligned}$$

Since F_{active} and F_{passive} are pre-defined functions of λ, $(\alpha \frac{\partial F_{\text{active}}}{\partial \lambda} + \frac{\partial F_{\text{passive}}}{\partial \lambda})$ can be easily computed. For now, let us use $T(\alpha,\lambda) = (\alpha \frac{\partial F_{\text{active}}}{\partial \lambda} + \frac{\partial F_{\text{passive}}}{\partial \lambda})/\lambda$ which is the muscle tension/stress. The division by λ is an implementation detail. Then:

$$\frac{\partial F_2(\lambda,\alpha)}{\partial \hat{F}} = T(\alpha,\lambda)\lambda \frac{\partial \lambda}{\partial \hat{F}}$$

Then to compute $\frac{\partial \lambda}{\partial \hat{F}}$:

$$\begin{aligned}
\frac{\partial \lambda}{\partial \hat{F}} &= \frac{\partial (\det(\hat{F})^{-2/3} (\hat{F} f_m)^T \hat{F} f_m)^{1/2}}{\partial \hat{F}} \\
&= \frac{1}{2\lambda} \frac{\partial \det(\hat{F})^{-2/3} (\hat{F} f_m)^T \hat{F} f_m}{\partial \hat{F}} \\
&= \frac{1}{2\lambda} (\frac{\partial \det(\hat{F})^{-2/3}}{\partial \hat{F}} (\hat{F} f_m)^T \hat{F} f_m + \det(\hat{F})^{-2/3} \frac{\partial (\hat{F} f_m)^T \hat{F} f_m}{\partial \hat{F}}) \\
&= \frac{1}{2\lambda} (\frac{-2}{3} \lambda^2 F^{-1} + \det(\hat{F})^{-2/3} 2 \hat{F} f_m f_m^T) \\
&= \frac{1}{\lambda} (\frac{-1}{3} \lambda^2 F^{-1} + \det(\hat{F})^{-2/3} \hat{F} f_m f_m^T) \\
&= \frac{-1}{3} \lambda F^{-1} + \frac{\det(\hat{F})^{-2/3}}{\lambda} \hat{F} f_m f_m^T
\end{aligned}$$

Finally,

$$\begin{aligned}
\frac{\partial F_2(\lambda,\alpha)}{\partial \hat{F}} &= T(\alpha,\lambda)\lambda (\frac{-1}{3} \lambda F^{-1} + \frac{\det(\hat{F})^{-2/3}}{\lambda} \hat{F} f_m f_m^T) \\
&= T(\alpha,\lambda) (\frac{-1}{3} \lambda^2 F^{-1} + \det(\hat{F})^{-2/3} \hat{F} f_m f_m^T)
\end{aligned}$$

WARNING: I will use the above definition of $\frac{\partial F_2(\lambda,\alpha)}{\partial \hat{F}}$ to compute the 1st Piola-Kirchoff tensor in this section to match [9]. However, PhysBAM does not actually use the deviatoric muscle fiber part. That is, $\tilde{\lambda} = \sqrt{f_m^T F^T F f_m}$ (notice the lack of the determinant). Later on, I will use $\tilde{\lambda}$ when computing the force differentials because resembles what is actually happening in the code. That is,

$$\begin{aligned}
\frac{\partial F_2}{\partial F} &= T(\alpha,\tilde{\lambda}) \frac{\partial \tilde{\lambda}}{\partial F} \\
&= T(\alpha,\tilde{\lambda}) \frac{1}{\tilde{\lambda}} \hat{F} f_m f_m^T
\end{aligned}$$

From discussions with Matt Cong, apparently the intention is to use the deviatoric fiber definition but somehow this was not done. Additionally, adding in the deviatoric fiber definition did not seem to change much.

4.3.4 Putting it all Together

We can simplify some of these equations by using variables (note that some variables are redefined):

$$\begin{aligned}
C &= \hat{F}^T\hat{F} = \hat{F}^2 \\
J_c &= \det(\hat{F})^{-1/3} \\
J_{cc} &= J_c^2 \\
I_1 &= \operatorname{Tr}(C) \\
w_1 &= 2J_{cc}A \\
w_2 &= 2J_{cc}^2 B \\
w_{12} &= w_1 + I_1 w_2 \\
p &= K\ln(J) \\
p_f &= \frac{1}{3}(w_{12}\operatorname{Tr}(C) - w_2\operatorname{Tr}(C^2) + T\lambda^2)
\end{aligned}$$

Note that this is from [9] with some important adjustments to make the derivation work properly.

$$\begin{aligned}
\frac{\partial F_1}{\partial F} &= 2A(-\frac{1}{3}\det(\hat{F})^{-2/3}\operatorname{Tr}(\hat{F}^2)\hat{F}^{-1} + \det(\hat{F})^{-2/3}\hat{F}) + B\frac{\partial I_2}{\partial F} \\
&= 2A(-\frac{1}{3}J_{cc}\operatorname{Tr}(\hat{F}^2)\hat{F}^{-1} + J_{cc}\hat{F}) + B\frac{\partial I_2}{\partial F} \\
&= 2A(-\frac{1}{3}\operatorname{Tr}(J_{cc}\hat{F}^2)\hat{F}^{-1} + J_{cc}\hat{F}) + B\frac{\partial I_2}{\partial F} \\
&= 2A(-\frac{1}{3}I_1\hat{F}^{-1} + J_{cc}\hat{F}) + B\frac{\partial I_2}{\partial F} \\
&= -\frac{2A}{3}I_1\hat{F}^{-1} + 2AJ_{cc}\hat{F} + \frac{B}{2}(\frac{-4}{3}\det(\hat{F})^{-4/3}(\operatorname{Tr}(\hat{F}^T\hat{F})^2\hat{F}^{-1} - \operatorname{Tr}(\hat{F}^4)\hat{F}^{-1}) + 4\det(\hat{F})^{-4/3}(\operatorname{Tr}(\hat{F}^T\hat{F})\hat{F} - \hat{F}^3)) \\
&= -\frac{2A}{3}I_1\hat{F}^{-1} + 2AJ_{cc}\hat{F} + \frac{B}{2}(\frac{-4}{3}J_{cc}^2(\operatorname{Tr}(C)^2\hat{F}^{-1} - \operatorname{Tr}(C^2)\hat{F}^{-1}) + 4J_{cc}^2(\operatorname{Tr}(C)\hat{F} - \hat{F}^3)) \\
&= -\frac{2A}{3}I_1\hat{F}^{-1} + 2AJ_{cc}\hat{F} + \frac{-2B}{3}J_{cc}^2(\operatorname{Tr}(C)^2\hat{F}^{-1} - \operatorname{Tr}(C^2)\hat{F}^{-1}) + 2BJ_{cc}^2(\operatorname{Tr}(C)\hat{F} - \hat{F}^3) \\
&= -\frac{2A}{3}I_1\hat{F}^{-1} + 2AJ_{cc}\hat{F} + \frac{-2B}{3}J_{cc}^2(\operatorname{Tr}(C)^2 - \operatorname{Tr}(C^2))\hat{F}^{-1} + 2BJ_{cc}^2(\operatorname{Tr}(C)\hat{F} - \hat{F}^3) \\
&= -\frac{2A}{3}I_1\hat{F}^{-1} + 2AJ_{cc}\hat{F} + \frac{-2B}{3}J_{cc}^2(\operatorname{Tr}(C)^2 - \operatorname{Tr}(C^2))\hat{F}^{-1} + 2BJ_{cc}^2\operatorname{Tr}(C)\hat{F} - 2BJ_{cc}^2\hat{F}^3 \\
&= -\frac{2A}{3}I_1\hat{F}^{-1} + 2AJ_{cc}\hat{F} + \frac{-2B}{3}J_{cc}^2(\operatorname{Tr}(C)^2 - \operatorname{Tr}(C^2))\hat{F}^{-1} + 2BJ_{cc}I_1\hat{F} - 2BJ_{cc}^2\hat{F}^3 \\
&= (2AJ_{cc} + 2BJ_{cc}I_1)\hat{F} + (-\frac{2A}{3}I_1 + \frac{-2B}{3}J_{cc}^2(\operatorname{Tr}(C)^2 - \operatorname{Tr}(C^2)))\hat{F}^{-1} + (-2BJ_{cc}^2\hat{F}^3) \\
&= (w_1 + w_2 I_1)\hat{F} - \frac{1}{3}(2AJ_{cc}\operatorname{Tr}(C) + 2BJ_{cc}^2\operatorname{Tr}(C)^2 - 2BJ_{cc}^2\operatorname{Tr}(C^2))\hat{F}^{-1} - w_2\hat{F}^3 \\
&= w_{12}\hat{F} - \frac{1}{3}((2AJ_{cc} + 2BJ_{cc}^2\operatorname{Tr}(C))\operatorname{Tr}(C) - 2BJ_{cc}^2\operatorname{Tr}(C^2))\hat{F}^{-1} - \frac{w_2}{2}\hat{F}^3 \\
&= w_{12}\hat{F} - \frac{1}{3}(w_{12}\operatorname{Tr}(C) - w_2\operatorname{Tr}(C^2))\hat{F}^{-1} - w_2\hat{F}^3
\end{aligned}$$

$$\begin{aligned}
\frac{\partial U}{\partial \hat{F}} &= K\ln(J)\hat{F}^{-1} \\
&= p\hat{F}^{-1}
\end{aligned}$$

$$
\begin{aligned}
\frac{\partial F_2}{\partial \hat{F}} &= T(\alpha,\lambda)(\frac{-1}{3}\lambda^2 F^{-1} + \det(\hat{F})^{-2/3}\hat{F} f_m f_m^T) \\
&= \frac{-1}{3}T(\alpha,\lambda)\lambda^2 F^{-1} + J_{cc}T(\alpha,\lambda)\hat{F} f_m f_m^T
\end{aligned}
$$

$$
\begin{aligned}
P &= \frac{\partial W}{\partial F} && (11)\\
&= \frac{\partial F_1}{\partial F} + \frac{\partial U}{\partial F} + \frac{\partial F_2}{\partial F} && (12)\\
&= w_{12}\hat{F} - \frac{1}{3}(w_{12}\operatorname{Tr}(C) - w_2\operatorname{Tr}(C^2))\hat{F}^{-1} - w_2\hat{F}^3 + p\hat{F}^{-1} + \frac{-1}{3}T(\alpha,\lambda)\lambda^2 F^{-1} + J_{cc}T(\alpha,\lambda)\hat{F} f_m f_m^T && (13)\\
&= w_{12}\hat{F} + (p - \frac{1}{3}(w_{12}\operatorname{Tr}(C) - w_2\operatorname{Tr}(C^2) + T(\alpha,\lambda)\lambda^2))\hat{F}^{-1} - w_2\hat{F}^3 + J_{cc}T(\alpha,\lambda)\hat{F} f_m f_m^T && (14)\\
&= w_{12}\hat{F} - w_2\hat{F}^3 + (p - p_f)\hat{F}^{-1} + J_{cc}T(\alpha,\lambda)\hat{F} f_m f_m^T && (15)
\end{aligned}
$$

This is nearly equivalent to the derivation in [9]. The primary differences are:

- I did not redefine λ to remove the extra $\det(\hat{F})^{-2/3}$. Note however that their derivation of $\frac{\partial \lambda}{\partial \hat{F}}$ contains the extra $\det(\hat{F})^{-2/3}$ – it just does not make it into the stress tensor.
- The $J_{cc}T(\alpha,\lambda)\hat{F} f_m f_m^T$ term is missing a constant multiplier; my initial guess would be an error in their derivation.
- w_1 and w_2 are redefined to be 2 times the constants A and B instead of 4. Their definition is non-standard as $F_1 = AI_1 + BI_2$ is the standard Mooney-Rivlin parameters (using I_1 defined in Section 4.2) and the derivation does not end up with a multiplier of 4...
- Their definition of $I_1 = J_{cc}C$ is insane because 1) I_1 should be a scalar and 2) having $w_{12} = w_1 + I_1 w_2$ where $I_1 = J_{cc}\operatorname{Tr}(C)$ would cause the appearance of $\frac{w_2}{J_{cc}}$ in the derivation which is obviously incorrect.

4.3.5 Without Diagonalized Deformation Gradient Assumption

The above computation of the 1st Piola-Kirchoff stress tensor assumes that the deformation gradient is diagonal. This assumption is fine (and holds) when we want to compute the value of P; however, later on in this document we will need to compute $\frac{\partial P}{\partial F}$ (that is the non-diagonalized deformation gradient). Thus, I will briefly write out the Jacobian of each component of the strain energy with respect to a general deformation gradient.

$$
\begin{aligned}
\frac{\partial AI_1}{\partial F} &= A(-\frac{2}{3}\det(F)^{-2/3}F^{-T}\operatorname{Tr}(F^TF) + 2\det(F)^{-2/3}F) \\
&= 2A\det(F)^{-2/3}(-\frac{1}{3}\operatorname{Tr}(F^TF)F^{-T} + F)
\end{aligned}
$$

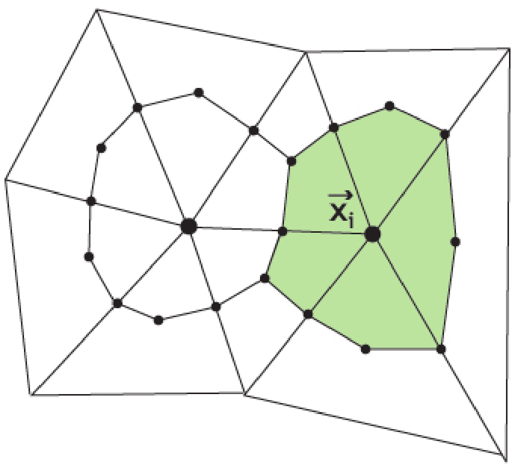
$$
\begin{aligned}
\frac{\partial BI_2}{\partial F} &= \frac{B}{2}(\frac{-4}{3}\det(F)^{-4/3}\operatorname{Tr}(F^TF)^2F^{-T} + 4\det(F)^{-4/3}\operatorname{Tr}(F^TF)F \\
&\quad - \frac{-4}{3}\det(F)^{-4/3}\operatorname{Tr}(F^TFF^TF)F^{-T} - \det(F)^{-4/3}4FF^TF) \\
&= 2B\det(F)^{-4/3}(\frac{-1}{3}\operatorname{Tr}(F^TF)^2F^{-T} + \operatorname{Tr}(F^TF)F + \frac{1}{3}\operatorname{Tr}(F^TFF^TF)F^{-T} - FF^TF) \\
&= 2B\det(F)^{-4/3}(\frac{1}{3}(\operatorname{Tr}(F^TFF^TF) - \operatorname{Tr}(F^TF)^2)F^{-T} + \operatorname{Tr}(F^TF)F - FF^TF)
\end{aligned}
$$

$$\frac{\partial U}{\partial F} = K \ln(J) F^{-T}$$

$$\frac{\partial F_2}{\partial F} = T(\alpha, \lambda)(\frac{-1}{3}\lambda^2 F^{-T} + \det(F)^{-2/3} F f_m f_m^T)$$

4.4 Force Computation

Note that this section borrows heavily from [8]. The *Finite Volume Method* section in that paper is very clear. This reproduction is primarily for my own benefit and may be less clear than the original.



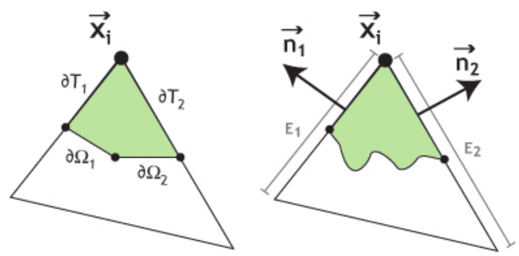


Figure 2: Integration over arbitrary paths in a triange from [8].

Figure 1: FVM integration regions from [8].

At the end of the day, we want to compute the force at each node f_i. The previous 1st Piola-Kirchoff stress tensor was computed for every tetrahedron. We can imagine each vertex as being surrounded by a voronoi region Ω as seen in Figure 1. If we are dealing with 2D triangles instead of 3D tetrahedrons then,

$$\begin{aligned} f_i &= \oint_{\partial\Omega} t dS \\ &= \oint_{\partial\Omega} \sigma n dS \end{aligned}$$

Here, t is the surface traction along the boundary of the region Ω and $\sigma n = t$ is the Cauchy stress. Note that the surface traction vector is the "force vector on a cross-section divided by that cross-section's area" [5]. We can divide this problem into computing a part of the surface integral in each of the separate triangles as shown in Figure 2. Using the divergence theorem ($\iiint_V (\nabla \cdot F) dV = \oiint_S (F \cdot n) dS$, note in our case $\nabla \cdot F$ is 0 because the stress in a tetrahedron is constant),

$$\oint_{\partial\Omega_1} \sigma n dS + \oint_{\partial\Omega_2} \sigma n dS + \oint_{\partial T_1} \sigma n dS + \oint_{\partial T_2} \sigma n dS = 0$$

See Figure 2 for the definition of the various integral limits. However, to compute f_i we only need $\oint_{\partial\Omega_1} \sigma n dS + \oint_{\partial\Omega_2} \sigma n dS$ thus we have:

$$\oint_{\partial\Omega_1} \sigma n dS + \oint_{\partial\Omega_2} \sigma n dS = -\oint_{\partial T_1} \sigma n dS - \oint_{\partial T_2} \sigma n dS$$

This now becomes a much easiest quantity to compute because we can easily determine the areas of T_1 and T_2 (those segments both go from the vertex to the mid-point of the corresponding segment). Thus,

$$\oint_{\partial\Omega_1} \sigma n dS + \oint_{\partial\Omega_2} \sigma n dS = -\frac{1}{2}\sigma(e_1 n_1 + e_2 n_2)$$
$$f_i \mathrel{+}= -\frac{1}{2}\sigma(e_1 n_1 + e_2 n_2)$$

Here, e_1 and e_2 are the edge lengths of the triangle while n_1 and n_2 are the normal vectors of those edges. This can easily be extended into 3D tetrahedrons:

$$f_i \mathrel{+}= -\frac{1}{3}\sigma(a_1 n_1 + a_2 n_2 + a_3 n_3)$$

Now we just have triangle areas instead of segment lengths and triangle normals instead of edge normals. This is written in terms of the Cauchy stress. Instead, we want it written in terms of the 1st Piola-Kirchoff stress tensor (which we already derived). Using known relations between the various stress measures. In the following equation, σ is the Cauchy stress, S is the 2nd Piola-Kirchoff stress, and P is the 1st Piola-Kirchoff stress, F is the deformation gradient, and $J = \det(F)$:

$$\sigma = J^{-1} F S F^T \tag{16}$$
$$P = FS \tag{17}$$
$$f_i \mathrel{+}= -\frac{1}{3} J^{-1} F S F^T (a_1 n_1 + a_2 n_2 + a_3 n_3) \tag{18}$$
$$= -\frac{1}{3} J^{-1} P F^T (a_1 n_1 + a_2 n_2 + a_3 n_3) \tag{19}$$
$$= -\frac{1}{3} P (J^{-1} F^T a_1 n_1 + J^{-1} F^T a_2 n_2 + J^{-1} F^T a_3 n_3) \tag{20}$$
$$= -\frac{1}{3} P (A_1 N_1 + A_2 N_2 + A_3 N_3) \tag{21}$$

Where A_i is the area of the triangle in the undeformed state and N_i is the normal of the triangle in the undeformed state. This follows from the identity $an = JF^{-T}AN$. This can easily be proved. Assume we are given two vectors in material space v_1, v_2. To map them into deformed space we get Fv_1, Fv_2. Note that original area weighted normal of the triangle defined by v_1 and v_2 is $an = v_1 \times v_2$. The new area weighted normal is then:

$$Fv_1 \times Fv_2 = \det(F) F^{-T} (v_1 \times v_2)$$
$$an = JF^{-T} AN$$

We can further simplify this equation by defining a variable $g_i = Pb_i$ where $B_m = \begin{bmatrix} b_1 & b_2 & b_3 \end{bmatrix} = -VD_m^{-T}$ where V is the volume of the tetrahedron in material space [10]. Let us show demonstrate the claim that $b_i = \frac{-1}{3}(A_1N_1 + A_2N_2 + A_3N_3)$. Equivalently, let us show that $D_m^T B_m = VI$. Each row of D_m^T is $d_{m,i} = x_{m,i+1} - x_{m,1}$. We want to compute a dot product with each column of B_m where $b_j = \frac{-1}{3}(A_1N_1 + A_2N_2 + A_3N_3)$ where A_kN_k are the area weighted normals of the faces surrounding $x_{m,j+1}$. The area weighted normals of a tetrahedron sum to 0: $\sum_k A_kN_k = 0$ therefore $b_j = \frac{1}{3}A_4N_4$, the area weighted normal of the face that does not include $x_{m,j+1}$ times 1/3. Thus, each element of $D_m^T B_m$ is a scalar triple product. It is easy to show that when $i = j$, you get the negative volume of the tetrahedron and when $i \neq j$ you get 0 because you get the dot product of a vector with an orthogonal vector. Note that you get the negative volume because A_4N_4 will point in the negative direction of the "height" of the tetrahedron. Then, $f_i + = g_i$. Note that $\sum_{i=0}^{3} g_i = 0$ so $g_0 = -(g_1 + g_2 + g_3)$. We can write the other g_i and b_i in matrix form as G and B then $G = PB_m$.

4.5 Force Differential

Once again note that the goal of quasistatics is to find the state where the sum of forces on each node is equal to 0 (as seen in Equation 3). We solve this non-linear system of equations using a Newton-Raphson iterative solver. At each iteration you solve a linear system:

$$-\frac{\partial f}{\partial x}(x)\Delta x = f(x) \tag{22}$$

This is standard Newton-Raphson and more details can be found in [4]. We can alternatively formulate this linear system using the strain energy W.

$$\frac{\partial^2 W}{\partial x^2}(x)\Delta x = -\frac{\partial W}{\partial x}(x)$$

This equation relies on Equation 21 as each force is the negative sum of a constant times the 1st Piola-Kirchoff stress tensor. Furthermore the 1st Piola-Kirchoff stress tensor can be written as $P = \frac{\partial W}{\partial F}$. Finally, we can get P as a function of x: $P = \frac{\partial W}{\partial F}\frac{\partial F}{\partial x} = \frac{\partial W}{\partial x}$. Note that $\frac{\partial^2 W}{\partial x^2}(x) = -\frac{\partial f}{\partial x}(x)$. These equations come from [10]. At the end of the day we want to be able to compute the change in force given a change in positions using a first-order Taylor expansion (how excite):

$$\delta f = \frac{\partial f}{\partial x}(x)\delta x$$

Let us monetarily refocus and go back to examining a single tetrahedron as the forces on each node are merely a sum of the forces from the tets. The deformation gradient is $F = D_s D_m^{-1} = U\hat{F}V^T$. Put another way, $\hat{F} = U^T D_s D_m^{-1} V$. We then want to use $\hat{F}$ to compute $P(\hat{F})$. $P(\hat{F})$ will then be used to compute the force on each node: $g_i = UP(\hat{F})V^T b_i$. Or back in matrix form: $G = UP(\hat{F})V^T B_m$. In the end we want to compute the Jacobian $\frac{\partial f}{\partial x}$ which we can easily compute if we can compute the differential δG given a δF. From [10], $\delta G = \delta P B_m = U\{\frac{\partial P(\hat{F})}{\partial F} : U^T \delta F V\}V^T B_m$ where $\delta P = \frac{\partial P(\hat{F})}{\partial F} : U^T \delta F V$.

First, let us compute δF given a change in positions δx. Note once again that $F = D_s D_m^{-1}$ so $\delta F = \delta D_s D_m^{-1}$. Plugging this into the equation for δP gets $\delta P = \frac{\partial P(\hat{F})}{\partial F} : U^T \delta D_s D_m^{-1} V$. Note that δD_s is trivial to compute.

$$D_s = \begin{bmatrix}(x_{s,2} - x_{s,1}) & (x_{s,3} - x_{s,1}) & (x_{s,4} - x_{s,1})\end{bmatrix}$$

Note that we only compute the forces on x_2 (g_2), x_3 (g_3), x_4 (g_4), and compute the force at x_1 using $g_1 = -(g_2 + g_3 + g_4)$. We can compute each dimension and each vertex separately so that when computing the force differential for vertex i, dimension j, then δD_s is a matrix of zeros with only $(\delta D_s)_{ji} = 1$.

Now, let us derive the $3 \times 3 \times 3 \times 3$ tensor $\frac{\partial P(\hat{F})}{\partial F}$. We know that $\frac{\partial P}{\partial F}$ is a 4th rank tensor.

$$\frac{\partial P}{\partial F} = \begin{bmatrix} \frac{\partial P}{\partial F_{11}} & \cdots & \frac{\partial P}{\partial F_{13}} \\ \vdots & \ddots & \vdots \\ \frac{\partial P}{\partial F_{31}} & \cdots & \frac{\partial P}{\partial F_{33}} \end{bmatrix}$$

For simplicity, let us ignore the extra rotations for now (U^T and V). Then to compute δP given a differential δF:

$$\delta P = \frac{\partial P}{\partial F} : \delta F$$

Written in tensor notation:

$$(\delta P)_{kl} = \left(\frac{\partial P}{\partial F}\right)_{ijkl} (\delta F)_{kl} \tag{23}$$

Note that the fourth order tensor $\frac{\partial P}{\partial F}$ can be re-written as a 9×9 matrix [10]. Then δF becomes a vector $\delta \tilde{F}$:

$$\delta \tilde{F} = \begin{bmatrix} F_{11} \\ F_{22} \\ F_{33} \\ F_{12} \\ F_{21} \\ F_{13} \\ F_{31} \\ F_{23} \\ F_{32} \end{bmatrix}$$

P also becomes a vector $\tilde{P}$:

$$\delta \tilde{P} = \begin{bmatrix} P_{11} \\ P_{22} \\ P_{33} \\ P_{12} \\ P_{21} \\ P_{13} \\ P_{31} \\ P_{23} \\ P_{32} \end{bmatrix}$$

From Equation 23 we can see that $P_{11} = \left(\frac{\partial P}{\partial F}\right)_{11kl} (\delta F)_{kl}$. This can be-rewritten using the vector form of $\delta F - \delta \tilde{F}$.

$$P_{11} = m_{11} \cdot \delta \tilde{F}$$

We thus need to find the vector m_{11} so that $m_{11} \cdot \delta \tilde{F} = \left(\frac{\partial P}{\partial F}\right)_{11kl} (\delta F)_{kl}$. This vector can easily be extracted from Equation 23:

$$m_{11} = \begin{bmatrix} \frac{\partial P}{\partial F_{11}}_{1,1} \\ \frac{\partial P}{\partial F_{22}}_{1,1} \\ \frac{\partial P}{\partial F_{33}}_{1,1} \\ \frac{\partial P}{\partial F_{12}}_{1,1} \\ \frac{\partial P}{\partial F_{21}}_{1,1} \\ \frac{\partial P}{\partial F_{13}}_{1,1} \\ \frac{\partial P}{\partial F_{31}}_{1,1} \\ \frac{\partial P}{\partial F_{23}}_{1,1} \\ \frac{\partial P}{\partial F_{32}}_{1,1} \end{bmatrix}$$

In other words, we take the element at row 1, column 1 in each of the Jacobians that make up $\frac{\partial P}{\partial F}$. Thus, more generally:

$$m_{ij} = \begin{bmatrix} \frac{\partial P}{\partial F_{11}}_{i,j} \\ \frac{\partial P}{\partial F_{22}}_{i,j} \\ \frac{\partial P}{\partial F_{33}}_{i,j} \\ \frac{\partial P}{\partial F_{12}}_{i,j} \\ \frac{\partial P}{\partial F_{21}}_{i,j} \\ \frac{\partial P}{\partial F_{13}}_{i,j} \\ \frac{\partial P}{\partial F_{31}}_{i,j} \\ \frac{\partial P}{\partial F_{23}}_{i,j} \\ \frac{\partial P}{\partial F_{32}}_{i,j} \end{bmatrix}$$

Then the 9×9 matrix form of $\frac{\partial P}{\partial F}$ takes the form

$$M = \begin{bmatrix} m_{11}^T \\ m_{22}^T \\ m_{33}^T \\ m_{12}^T \\ m_{21}^T \\ m_{13}^T \\ m_{31}^T \\ m_{23}^T \\ m_{32}^T \end{bmatrix}$$

The goal of this section is to show that M is block diagonal with form:

$$M = \begin{bmatrix} A & & & \\ & B_{12} & & \\ & & B_{13} & \\ & & & B_{23} \end{bmatrix}$$

for isotropic materials. Here, A is a 3×3 matrix while B_{ij} are 2×2 matrices. Then, I will show how to compute M for the anistropic part of the constitutive model as well. In the rest of these sections I will use the notation L^{ij} which is a single-entry matrix with a 1 at (i, j) and 0 everywhere else. Additionally, I will show that

$$A = \begin{bmatrix} \alpha_{11} + \beta_{11} + \gamma_{11} & \gamma_{12} & \gamma_{13} \\ \gamma_{12} & \alpha_{22} + \beta_{22} + \gamma_{22} & \gamma_{23} \\ \gamma_{13} & {}_{23} & \alpha_{33} + \beta_{33} + \gamma_{33} \end{bmatrix}$$

and

$$B_{ij} = \begin{bmatrix} \alpha_{ij} & \beta_{ij} \\ \beta_{ij} & \alpha_{ij} \end{bmatrix}$$

Note that in the notation of [10], $\gamma = F_{\text{base}} \eta F_{\text{base}}^T$ where η is another symmetric 3×3 matrix and

$$F_{\text{base}} = \begin{bmatrix} \hat{F}_{11} & \hat{F}_{11}^3 & \hat{F}_{11}^{-1} \\ \hat{F}_{22} & \hat{F}_{22}^3 & \hat{F}_{22}^{-1} \\ \hat{F}_{33} & \hat{F}_{33}^3 & \hat{F}_{33}^{-1} \end{bmatrix}$$

If you do not care much for the derivation of these matrices, skip to Section 4.5.1.4 for a summary of the values of each element. Finally, note that the final $\frac{\partial P}{\partial F}$ is the summation of the isotropic and anisotropic part.

4.5.1 Isotropic Materials

The isotropic part of the strain energy in Equation 10 is:

$$W_{\text{isotropic}} = AI_1 + BI_2 + U(J)$$

Now, we want to compute $\frac{\partial P_{\text{isotropic}}}{\partial F_{ij}}$. Note that we need to differentiate the 1st Piola Kirchoff stress tensor without the diagonal deformation gradient assumption (see Section 4.3.5):

$$P_{\text{isotropic}} = \frac{\partial AI_1}{\partial F} + \frac{\partial BI_2}{\partial F} + \frac{\partial U}{\partial F}$$

Let us rename these sections to $P_1 = \frac{\partial AI_1}{\partial F}$, $P_2 = \frac{\partial BI_2}{\partial F}$, and $P_3 = \frac{\partial U}{\partial F}$. Now we want to compute $\frac{\partial P_1}{\partial F_{ij}}(\hat{F})$,$\frac{\partial P_2}{\partial F_{ij}}(\hat{F})$, $\frac{\partial P_3}{\partial F_{ij}}(\hat{F})$ (fun). Note that $\hat{F} = \begin{bmatrix} \sigma_1 & & \\ & \sigma_2 & \\ & & \sigma_3 \end{bmatrix}$ (a diagonal matrix).

4.5.1.1 Incompressibility

$$\begin{aligned} \frac{\partial P_3}{\partial F_{ij}}(\hat{F}) &= \frac{\partial K \ln(J) F^{-T}}{\partial F_{ij}} \\ &= K(\frac{\partial \ln(J)}{\partial F_{ij}} \hat{F}^{-1} + \ln(J) \frac{\partial F^{-T}}{\partial F_{ij}}) \\ &= K \left(\text{Tr}(\hat{F}^{-1} \frac{\partial F}{\partial F_{ij}}) \hat{F}^{-1} + \ln(J) \begin{bmatrix} \frac{\partial F_{11}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{21}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{31}^{-1}}{\partial F_{ij}}(\hat{F}) \\ \frac{\partial F_{12}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{22}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{32}^{-1}}{\partial F_{ij}}(\hat{F}) \\ \frac{\partial F_{13}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{23}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{33}^{-1}}{\partial F_{ij}}(\hat{F}) \end{bmatrix} \right) \end{aligned}$$

Examining the first part,

$$K\,\mathrm{Tr}(\hat{F}^{-1}\frac{\partial F}{\partial F_{ij}})\hat{F}^{-1}$$

Note that $\frac{\partial F}{\partial F_{ij}}$ is the matrix L^{ij}. Then $\hat{F}^{-1}L^{ij}$ will place $\frac{1}{\sigma_i}$ at (i,j). That is: $\hat{F}^{-1}L^{ij} = \frac{L^{ij}}{\sigma_i}$. Note that $\mathrm{Tr}(\frac{L^{ij}}{\sigma_i}) \neq 0$ only when $i = j$. Therefore, this term will only be relevant when $F_{ij} \in \{F_{11}, F_{22}, F_{33}\}$ and thus will only be relevant to the first three columns of M. Notice that $K\,\mathrm{Tr}(\hat{F}^{-1}\frac{\partial F}{\partial F_{ij}})\hat{F}^{-1} = K\,\mathrm{Tr}(\frac{L^{ij}}{\sigma_i})\hat{F}^{-1}$ is a non-zero diagonal matrix when $F_{ij} \in \{F_{11}, F_{22}, F_{33}\}$. The fact that it is diagonal means that it will only affect the first three rows of M. Putting both conditions together means that it will only affect the matrix A (a perfect candidate for putting into γ). However, we need to determine what effect it has on η. When this term is non-zero:

$$K\,\mathrm{Tr}(\frac{L^{ij}}{\sigma_i})\hat{F}^{-1} = \begin{bmatrix} K\sigma_i^{-1}\sigma_1^{-1} & & \\ & K\sigma_i^{-1}\sigma_2^{-1} & \\ & & K\sigma_i^{-1}\sigma_3^{-1} \end{bmatrix}$$

We can see we want to do:

$$\gamma += \begin{bmatrix} K\sigma_1^{-1}\sigma_1^{-1} & K\sigma_1^{-1}\sigma_2^{-1} & K\sigma_1^{-1}\sigma_3^{-1} \\ K\sigma_2^{-1}\sigma_1^{-1} & K\sigma_2^{-1}\sigma_2^{-1} & K\sigma_2^{-1}\sigma_3^{-1} \\ K\sigma_3^{-1}\sigma_1^{-1} & K\sigma_3^{-1}\sigma_2^{-1} & K\sigma_3^{-1}\sigma_3^{-1} \end{bmatrix} \tag{24}$$

We can get an equivalent result by doing:

$$\eta_{33} += K \tag{25}$$

Examining the second part,

$$K\ln(J)\begin{bmatrix} \frac{\partial F^{-1}_{11}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F^{-1}_{21}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F^{-1}_{31}}{\partial F_{ij}}(\hat{F}) \\ \frac{\partial F^{-1}_{12}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F^{-1}_{22}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F^{-1}_{32}}{\partial F_{ij}}(\hat{F}) \\ \frac{\partial F^{-1}_{13}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F^{-1}_{23}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F^{-1}_{33}}{\partial F_{ij}}(\hat{F}) \end{bmatrix}$$

Note that $\frac{\partial F^{-1}_{kl}}{\partial F_{ij}}(\hat{F}) = -(\hat{F}^{-1})_{ki}(\hat{F}^{-1})_{jl}$. Since $\hat{F}$ is diagonal, $\frac{\partial F^{-1}_{kl}}{\partial F_{ij}}(\hat{F}) \neq 0$ only when $k = i$ and $j = l$. Note that given a F_{ij}, there is only one element where $\frac{\partial F^{-1}_{kl}}{\partial F_{ij}}(\hat{F}) \neq 0$. That is, $\frac{\partial F^{-1}_{ij}}{\partial F_{ij}}(\hat{F}) = -(\hat{F}^{-1})_{ii}(\hat{F}^{-1})_{jj}$. In terms of the earlier notation, we can say that:

$$\beta_{ij} -= \frac{K\ln(J)}{\sigma_i\sigma_j} \tag{26}$$

If you work out the locations of the non-zero elements you will see why it belongs in β and not in α.

4.5.1.2 Mooney-Rivlin AI_1

$$\begin{aligned}
\frac{\partial P_1}{\partial F_{ij}}(\hat{F}) &= \frac{\partial 2A \det(F)^{-2/3}(-\frac{1}{3}\operatorname{Tr}(F^TF)F^{-T} + F)}{\partial F_{ij}} \\
&= 2A\frac{\partial \det(F)^{-2/3}(-\frac{1}{3}\operatorname{Tr}(F^TF)F^{-T} + F)}{\partial F_{ij}} \\
&= 2A\left(\frac{\partial \det(F)^{-2/3}}{\partial F_{ij}}(-\frac{1}{3}\operatorname{Tr}(F^TF)F^{-T} + F) + \det F^{-2/3}\frac{\partial(-\frac{1}{3}\operatorname{Tr}(F^TF)F^{-T} + F)}{\partial F_{ij}}\right) \\
&= 2A\left(\frac{\partial \det(F)^{-2/3}}{\partial F_{ij}}(-\frac{1}{3}\operatorname{Tr}(F^TF)F^{-T} + F) + \det F^{-2/3}\left(-\frac{\partial\frac{1}{3}\operatorname{Tr}(F^TF)F^{-T}}{\partial F_{ij}} + \frac{\partial F}{\partial F_{ij}}\right)\right)
\end{aligned}$$

Let us break this into multiple parts so we only deal with a single Jacobian at a time (3 in particular):

$$\begin{aligned}
M_{1,\mathrm{MR1}} &= 2A\frac{\partial \det(F)^{-2/3}}{\partial F_{ij}}(-\frac{1}{3}\operatorname{Tr}(F^TF)F^{-T} + F) \\
M_{1,\mathrm{MR2}} &= -2A\det F^{-2/3}\frac{\partial\frac{1}{3}\operatorname{Tr}(F^TF)F^{-T}}{\partial F_{ij}} \\
M_{1,\mathrm{MR3}} &= 2A\det F^{-2/3}\frac{\partial F}{\partial F_{ij}}
\end{aligned}$$

4.5.1.2.1 Computing $M_{1,\mathbf{MR1}}$

$$M_{1,\mathrm{MR1}} = 2A\frac{\partial \det(F)^{-2/3}}{\partial F_{ij}}(-\frac{1}{3}\operatorname{Tr}(F^TF)F^{-T} + F)$$

The crux of this equation lies in computing the derivative $\frac{\partial \det(F)^{-2/3}}{\partial F_{ij}}$:

$$\begin{aligned}
\frac{\partial \det(F)^{-2/3}}{\partial F_{ij}}(\hat{F} &= \frac{-2}{3}\det(\hat{F})^{-5/3}\frac{\partial \det(F)}{\partial F_{ij}} \\
&= \frac{-2}{3}\det(\hat{F})^{-5/3}\det(\hat{F})\operatorname{Tr}(\hat{F}^{-1}\frac{\partial F}{\partial F_{ij}}) \\
&= \frac{-2}{3}\det(\hat{F})^{-2/3}\operatorname{Tr}(\hat{F}^{-1}L^{ij})
\end{aligned}$$

Note that $\hat{F}$ is diagonal. Additionally, note that $\operatorname{Tr}(\hat{F}^{-1}L^{ij}) \neq 0$ only when $i = j$. When it is non-zero, $\operatorname{Tr}(\hat{F}^{-1}L^{ij}) = \sigma_i^{-1}$ much like in the incompressibility term. Therefore, this term only affects the first three columns of M and thus must be a part of γ.

Next, let us look at $-\frac{1}{3}\operatorname{Tr}(F^TF)F^{-T} + F$. Note that we are always passing in a diagonal $\hat{F}$ and thus the equation can be rewritten: $-\frac{1}{3}\operatorname{Tr}(\hat{F}^2)\hat{F}^{-1} + \hat{F}$. This is once again a diagonal matrix. Thus when the trace is non-zero we get:

$$\gamma+ = \begin{bmatrix}
\frac{-2}{3}J_{cc}\sigma_1^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_1^{-1} + \sigma_1) & \frac{-2}{3}J_{cc}\sigma_2^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_1^{-1} + \sigma_1) & \frac{-2}{3}J_{cc}\sigma_3^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_1^{-1} + \sigma_1) \\
\frac{-2}{3}J_{cc}\sigma_1^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_2^{-1} + \sigma_2) & \frac{-2}{3}J_{cc}\sigma_2^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_2^{-1} + \sigma_2) & \frac{-2}{3}J_{cc}\sigma_3^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_2^{-1} + \sigma_2) \\
\frac{-2}{3}J_{cc}\sigma_1^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_3^{-1} + \sigma_3) & \frac{-2}{3}J_{cc}\sigma_2^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_3^{-1} + \sigma_3) & \frac{-2}{3}J_{cc}\sigma_3^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_3^{-1} + \sigma_3)
\end{bmatrix}$$

Once again, this needs to be expressed in terms of η. We need to find some η such that $F_{base}\eta F_{base}^T$ equals the above matrix. For simplicity, let us split the above matrix into two parts: The second (and simpler) part is:

$$\begin{bmatrix} \sigma_1^{-1}(\sigma_1) & \sigma_2^{-1}(\sigma_1) & \sigma_3^{-1}(\sigma_1) \\ \sigma_1^{-1}(\sigma_2) & \sigma_2^{-1}(\sigma_2) & \sigma_3^{-1}(\sigma_2) \\ \sigma_1^{-1}(\sigma_3) & \sigma_2^{-1}(\sigma_3) & \sigma_3^{-1}(\sigma_3) \end{bmatrix}$$

This matrix can be accomplished by $\eta_{13} += 1$. This can easily be verified:

$$\begin{aligned} F_{base}\eta F_{base}^T &= \begin{bmatrix} \hat{F}_{11} & \hat{F}_{11}^3 & \hat{F}_{11}^{-1} \\ \hat{F}_{22} & \hat{F}_{22}^3 & \hat{F}_{22}^{-1} \\ \hat{F}_{33} & \hat{F}_{33}^3 & \hat{F}_{33}^{-1} \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} \hat{F}_{11} & \hat{F}_{11}^3 & \hat{F}_{11}^{-1} \\ \hat{F}_{22} & \hat{F}_{22}^3 & \hat{F}_{22}^{-1} \\ \hat{F}_{33} & \hat{F}_{33}^3 & \hat{F}_{33}^{-1} \end{bmatrix}^T \\ &= \begin{bmatrix} \hat{F}_{11} & \hat{F}_{11}^3 & \hat{F}_{11}^{-1} \\ \hat{F}_{22} & \hat{F}_{22}^3 & \hat{F}_{22}^{-1} \\ \hat{F}_{33} & \hat{F}_{33}^3 & \hat{F}_{33}^{-1} \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ F_{11} & F_{22} & F_{33} \end{bmatrix} \\ &= \begin{bmatrix} \sigma_1^{-1}(\sigma_1) & \sigma_2^{-1}(\sigma_1) & \sigma_3^{-1}(\sigma_1) \\ \sigma_1^{-1}(\sigma_2) & \sigma_2^{-1}(\sigma_2) & \sigma_3^{-1}(\sigma_2) \\ \sigma_1^{-1}(\sigma_3) & \sigma_2^{-1}(\sigma_3) & \sigma_3^{-1}(\sigma_3) \end{bmatrix} \end{aligned}$$

Thus, taking into account the constant multipliers results in

$$\eta_{13} += \frac{-4}{3} A J_{cc} \tag{27}$$

The first part is:

$$\begin{bmatrix} \sigma_1^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_1^{-1}) & \sigma_1^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_2^{-1}) & \sigma_1^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_3^{-1}) \\ \sigma_2^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_1^{-1}) & \sigma_2^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_2^{-1}) & \sigma_2^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_3^{-1}) \\ \sigma_3^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_1^{-1}) & \sigma_3^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_2^{-1}) & \sigma_3^{-1}(\frac{-1}{3}\operatorname{Tr}(C)\sigma_3^{-1}) \end{bmatrix}$$

Although this looks complex, this matrix is a similar structure to Equation 24. Therefore we can also get a similar addition to η_{33}:

$$\eta_{33} += \frac{4}{9} A J_{cc} \operatorname{Tr}(C) \tag{28}$$

4.5.1.2.2 Computing $M_{1,\mathbf{MR2}}$

$$\begin{aligned} M_{1,\mathrm{MR2}} &= -2A \det F^{-2/3} \frac{\partial \frac{1}{3}\operatorname{Tr}(F^T F) F^{-T}}{\partial F_{ij}} \\ &= \frac{-2}{3} A J_{cc} \frac{\partial \operatorname{Tr}(F^T F) F^{-T}}{\partial F_{ij}} \end{aligned}$$

We can compute the derivative using the product rule:

$$\frac{\partial \operatorname{Tr}(F^T F) F^{-T}}{\partial F_{ij}} = \frac{\partial \operatorname{Tr}(F^T F)}{\partial F_{ij}} F^{-T} + \operatorname{Tr}(F^T F) \frac{\partial F^{-T}}{\partial F_{ij}}$$

Once again, for simplicity, let us break this into two parts. The first part being:

$$\frac{\partial\,\mathrm{Tr}(F^T F)}{\partial F_{ij}} F^{-T}$$

Note that $\mathrm{Tr}(F^T F) = ||F||_F^2 = \sum_i \sum_j F_{ij}^2$ (the squared Frobenius norm). Therefore:

$$\frac{\partial\,\mathrm{Tr}(F^T F)}{\partial F_{ij}} = 2F_{ij}$$

However, given that we evaluate $\frac{\partial P}{\partial F}$ at a diagonal $\hat{F}$, $2F_{ij}$ is only non-zero when $i = j$. Therefore, this term is only relevant in the first three columns of M and is thus a γ term. Thus, the total γ change from this part of $M_{1,\mathrm{MR2}}$ would be:

$$\gamma \mathrel{+}= \frac{-4}{3} A J_{cc} \begin{bmatrix} \sigma_1\sigma_1^{-1} & \sigma_2\sigma_1^{-1} & \sigma_3\sigma_1^{-1} \\ \sigma_1\sigma_2^{-1} & \sigma_2\sigma_2^{-1} & \sigma_3\sigma_2^{-1} \\ \sigma_1\sigma_3^{-1} & \sigma_2\sigma_3^{-1} & \sigma_3\sigma_3^{-1} \end{bmatrix}$$

This comes from a change in η as follows:

$$\eta_{31} {+} = \frac{-4}{3} A J_{cc} \tag{29}$$

The second part being:

$$\mathrm{Tr}(F^T F) \frac{\partial F^{-T}}{\partial F_{ij}}$$

Once again, we come upon the Jacobian of F^{-T}:

$$\frac{\partial F^{-T}}{\partial F_{ij}} = \begin{bmatrix} \frac{\partial F_{11}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{21}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{31}^{-1}}{\partial F_{ij}}(\hat{F}) \\ \frac{\partial F_{12}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{22}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{32}^{-1}}{\partial F_{ij}}(\hat{F}) \\ \frac{\partial F_{13}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{23}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{33}^{-1}}{\partial F_{ij}}(\hat{F}) \end{bmatrix}$$

This term can thus be treated similarly to Equation 26. That is:

$$\beta_{ij} \mathrel{+}= \frac{\frac{2}{3} A J_{cc}\,\mathrm{Tr}(\hat{F}^T F)}{\sigma_i \sigma_j} \tag{30}$$

4.5.1.2.3 Computing $M_{1,\mathrm{MR3}}$

$$M_{1,\mathrm{MR3}} = 2A \det F^{-2/3} \frac{\partial F}{\partial F_{ij}}$$

This one is fairly simple since $\frac{\partial F}{\partial F_{ij}} = L^{ij}$ – a result I have used previously. This indicates that the resulting matrix only has one non-zero element and it resides at element (i, j). This means that this term gets added to the diagonal of M and is thus accounted for in the α terms. Note that this contribution is the same across the entire diagonal. Therefore:

$$\alpha_{ij} \mathrel{+}= 2AJ_{cc} \tag{31}$$

4.5.1.3 Mooney-Rivlin BI_2

$$\begin{aligned}
\frac{\partial P_2}{\partial F_{ij}} &= \frac{\partial 2B\det(F)^{-4/3}(\frac{1}{3}(\mathrm{Tr}(F^TFF^TF) - \mathrm{Tr}(F^TF)^2)F^{-T} + \mathrm{Tr}(F^TF)F - FF^TF)}{\partial F_{ij}} \\
&= 2B\frac{\partial \det(F)^{-4/3}(\frac{1}{3}(\mathrm{Tr}(F^TFF^TF) - \mathrm{Tr}(F^TF)^2)F^{-T} + \mathrm{Tr}(F^TF)F - FF^TF)}{\partial F_{ij}} \\
&= 2B(\frac{\partial \det(F)^{-4/3}}{\partial F_{ij}}(\frac{1}{3}(\mathrm{Tr}(F^TFF^TF) - \mathrm{Tr}(F^TF)^2)F^{-T} + \mathrm{Tr}(F^TF)F - FF^TF) \\
&+ \det(F)^{-4/3}\frac{\partial(\frac{1}{3}(\mathrm{Tr}(F^TFF^TF) - \mathrm{Tr}(F^TF)^2)F^{-T} + \mathrm{Tr}(F^TF)F - FF^TF)}{\partial F_{ij}}) \\
&= 2B(\frac{\partial \det(F)^{-4/3}}{\partial F_{ij}}(\frac{1}{3}(\mathrm{Tr}(F^TFF^TF) - \mathrm{Tr}(F^TF)^2)F^{-T} + \mathrm{Tr}(F^TF)F - FF^TF) \\
&+ \det(F)^{-4/3}((\frac{1}{3}\frac{\partial \mathrm{Tr}(F^TFF^TF)F^{-T}}{\partial F_{ij}} - \frac{1}{3}\frac{\partial \mathrm{Tr}(F^TF)^2F^{-T}}{\partial F_{ij}} + \frac{\partial \mathrm{Tr}(F^TF)F}{\partial F_{ij}} - \frac{\partial FF^TF}{\partial F_{ij}})))
\end{aligned}$$

Although long, ultimately, this equation is made up of multiple smaller parts that are much easier to compute. Much like I did for the other Mooney-Rivlin term, let us take this equation and break it into smaller parts where each part corresponds to a single derivative/Jacobian computation.

$$\begin{aligned}
M_{2,\mathrm{MR1}} &= 2B(\frac{\partial \det(F)^{-4/3}}{\partial F_{ij}}(\frac{1}{3}(\mathrm{Tr}(F^TFF^TF) - \mathrm{Tr}(F^TF)^2)F^{-T} + \mathrm{Tr}(F^TF)F - FF^TF) \\
M_{2,\mathrm{MR2}} &= \frac{2B\det(F)^{-4/3}}{3}\frac{\partial \mathrm{Tr}(F^TFF^TF)F^{-T}}{\partial F_{ij}} \\
M_{2,\mathrm{MR3}} &= -\frac{2B\det(F)^{-4/3}}{3}\frac{\partial \mathrm{Tr}(F^TF)^2F^{-T}}{\partial F_{ij}} \\
M_{2,\mathrm{MR4}} &= 2B\det(F)^{-4/3}\frac{\partial \mathrm{Tr}(F^TF)F}{\partial F_{ij}} \\
M_{2,\mathrm{MR5}} &= -2B\det(F)^{-4/3}\frac{\partial FF^TF}{\partial F_{ij}}
\end{aligned}$$

4.5.1.3.1 Computing $M_{2,\mathbf{MR1}}$

$$M_{2,\mathrm{MR1}} = 2B(\frac{\partial \det(F)^{-4/3}}{\partial F_{ij}}(\frac{1}{3}(\mathrm{Tr}(F^TFF^TF) - \mathrm{Tr}(F^TF)^2)F^{-T} + \mathrm{Tr}(F^TF)F - FF^TF)$$

Much like what has already been derived for Equation 27,

$$\frac{\partial \det(F)^{-4/3}}{\partial F_{ij}} = \frac{-4}{3}\det(\hat{F})^{-4/3}\,\mathrm{Tr}(\hat{F}^{-1}L^{ij})$$

Once again note that $\mathrm{Tr}(\hat{F}^{-1}L^{ij}) \neq 0$ only when $i = j$. Therefore, this term contributes to γ. In that case, $\mathrm{Tr}(\hat{F}^{-1}L^{ij}) = \sigma_i^{-1}$. We can simplify the rest of the equation by using the fact that we know the incoming matrix is diagonal:

$$\frac{1}{3}(\mathrm{Tr}(F^TFF^TF) - \mathrm{Tr}(F^TF)^2)F^{-T} + \mathrm{Tr}(F^TF)F - FF^TF = \frac{1}{3}(\mathrm{Tr}(\hat{F}^4) - \mathrm{Tr}(\hat{F}^2)^2)\hat{F}^{-1} + \mathrm{Tr}(\hat{F}^2)\hat{F} - \hat{F}^3$$

Again, let us examine the 4 matrices separately.

The first matrix:

$$\frac{-8B}{9}\det(\hat{F})^{-4/3}\,\mathrm{Tr}(\hat{F}^{-1}L^{ij})\,\mathrm{Tr}(\hat{F}^4)\hat{F}^{-1}$$

The contribution to γ will then be:

$$\gamma \mathrel{+}= \frac{-8B}{9}J_{cc}^2\,\mathrm{Tr}(C^2)\begin{bmatrix}\sigma_1^{-1}\sigma_1^{-1} & \sigma_2^{-1}\sigma_1^{-1} & \sigma_3^{-1}\sigma_1^{-1}\\ \sigma_1^{-1}\sigma_2^{-1} & \sigma_2^{-1}\sigma_2^{-1} & \sigma_3^{-1}\sigma_2^{-1}\\ \sigma_1^{-1}\sigma_3^{-1} & \sigma_2^{-1}\sigma_3^{-1} & \sigma_3^{-1}\sigma_3^{-1}\end{bmatrix}$$

The contribution to η is thus simply:

$$\eta_{33} \mathrel{-}= \frac{8B}{9}J_{cc}^2\,\mathrm{Tr}(C^2) \tag{32}$$

The second matrix:

$$\frac{8B}{9}\det(\hat{F})^{-4/3}\,\mathrm{Tr}(\hat{F}^{-1}L^{ij})\,\mathrm{Tr}(\hat{F}^2)^2\hat{F}^{-1}$$

Similar to the above matrix, the contribution to γ is:

$$\gamma \mathrel{+}= \frac{8B}{9}J_{cc}^2\,\mathrm{Tr}(C)^2\begin{bmatrix}\sigma_1^{-1}\sigma_1^{-1} & \sigma_2^{-1}\sigma_1^{-1} & \sigma_3^{-1}\sigma_1^{-1}\\ \sigma_1^{-1}\sigma_2^{-1} & \sigma_2^{-1}\sigma_2^{-1} & \sigma_3^{-1}\sigma_2^{-1}\\ \sigma_1^{-1}\sigma_3^{-1} & \sigma_2^{-1}\sigma_3^{-1} & \sigma_3^{-1}\sigma_3^{-1}\end{bmatrix}$$

Which makes the contribution to η easy:

$$\eta_{33} \mathrel{+}= \frac{8B}{9}J_{cc}^2\,\mathrm{Tr}(C)^2 \tag{33}$$

The third matrix:

$$\frac{-8B}{3}\det(\hat{F})^{-4/3}\,\mathrm{Tr}(\hat{F}^{-1}L^{ij})\,\mathrm{Tr}(\hat{F}^2)\hat{F}$$

Nothing fancy here, the γ contribution is:

$$\gamma \mathrel{-}= \frac{8B}{9}J_{cc}^2\,\mathrm{Tr}(C)\begin{bmatrix}\sigma_1^{-1}\sigma_1 & \sigma_2^{-1}\sigma_1 & \sigma_3^{-1}\sigma_1\\ \sigma_1^{-1}\sigma_2 & \sigma_2^{-1}\sigma_2 & \sigma_3^{-1}\sigma_2\\ \sigma_1^{-1}\sigma_3 & \sigma_2^{-1}\sigma_3 & \sigma_3^{-1}\sigma_3\end{bmatrix}$$

The η contribution is thus:

$$\eta_{13} -= \frac{8B}{9} J_{cc}^2 \operatorname{Tr}(C) \tag{34}$$

The last matrix:

$$\frac{8B}{3} \det(\hat{F})^{-4/3} \operatorname{Tr}(\hat{F}^{-1} L^{ij}) \hat{F}^3$$

This translates into:

$$\gamma += \frac{8B}{3} J_{cc}^2 \begin{bmatrix} \sigma_1^{-1}\sigma_1^3 & \sigma_2^{-1}\sigma_1^3 & \sigma_3^{-1}\sigma_1^3 \\ \sigma_1^{-1}\sigma_2^3 & \sigma_2^{-1}\sigma_2^3 & \sigma_3^{-1}\sigma_2^3 \\ \sigma_1^{-1}\sigma_3^3 & \sigma_2^{-1}\sigma_3^3 & \sigma_3^{-1}\sigma_3^3 \end{bmatrix}$$

Which again translates into:

$$\eta_{23} += \frac{8B}{3} J_{cc}^2 \tag{35}$$

4.5.1.3.2 Computing $M_{2,\mathbf{MR2}}$

$$M_{2,\mathrm{MR2}} = \frac{2B \det(F)^{-4/3}}{3} \frac{\partial \operatorname{Tr}(F^T F F^T F) F^{-T}}{\partial F_{ij}}$$

Here the Jacobian is:

$$\frac{\partial \operatorname{Tr}(F^T F F^T F) F^{-T}}{\partial F_{ij}} = \frac{\partial \operatorname{Tr}(F^T F F^T F)}{\partial F_{ij}} F^{-T} + \operatorname{Tr}(F^T F F^T F) \frac{\partial F^{-T}}{\partial F_{ij}}$$

Let us examine both parts separately. The first matrix:

$$\frac{2B \det(F)^{-4/3}}{3} \frac{\partial \operatorname{Tr}(F^T F F^T F)}{\partial F_{ij}} F^{-T}$$

The derivative here can be computed:

$$\begin{aligned} \frac{\partial \operatorname{Tr}(F^T F F^T F)}{\partial F_{ij}} &= \frac{\partial ||F^T F||_F^2}{\partial F_{ij}} \\ &= \frac{\partial \sum_k \sum_l ((F^T F)_{kl})^2}{\partial F_{ij}} \\ &= \sum_k \sum_l \frac{\partial ((F^T F)_{kl})^2}{\partial F_{ij}} \\ &= \sum_k \sum_l \left(2(F^T F)_{kl} \frac{\partial (F^T F)_{kl}}{\partial F_{ij}} \right) \end{aligned}$$

Let us rewrite the matrix F as $F = \begin{bmatrix} f_1 & f_2 & f_3 \end{bmatrix}$ where f_i is the ith column of F. Then, $((F^T F)_{kl})^2 = (f_k^T f_l)^2$. Note that $\frac{\partial (f_k^T f_l)}{\partial F_{ij}} \neq 0$ only when $k = j$ or $l = j$. Furthermore note that $f_k^T f_l = \sum_r F_{rk} F_{rl}$ so

$\frac{\partial(f_k^T f_l)}{\partial F_{ij}} = \sum_r \frac{\partial F_{rk} F_{rl}}{\partial F_{ij}}$. And $\frac{\partial F_{rk} F_{rl}}{\partial F_{ij}} \neq 0$ only when $r = i$. Therefore the conditions for a non-zero derivative is ($k = j$ OR $l = j$) AND ($r = i$). Which brings us to the conclusion that:

$$\begin{aligned}
\sum_k \sum_l \left(2(F^T F)_{kl} \frac{\partial (F^T F)_{kl}}{\partial F_{ij}} \right) &= \sum_k \sum_l \left(2 f_k^T f_l \frac{\partial f_k^T f_l}{\partial F_{ij}} \right) \\
&= \sum_k \sum_l \left(2 f_k^T f_l \sum_r \frac{\partial F_{rk} F_{rl}}{\partial F_{ij}} \right) \\
&= \sum_k \sum_l f_k^T f_l \sum_r \left(2 \frac{\partial F_{rk} F_{rl}}{\partial F_{ij}} \right) \\
&= 2 \sum_k \sum_l f_k^T f_l \sum_r \left((\delta_{kj} + \delta_{lj}) \delta_{ri} \frac{\partial F_{rk} F_{rl}}{\partial F_{ij}} \right) \\
&= 2 \sum_k \sum_l f_k^T f_l \left((\delta_{kj} + \delta_{lj}) \frac{\partial F_{ik} F_{il}}{\partial F_{ij}} \right) \\
&= 2 \sum_k \sum_l f_k^T f_l \left(\delta_{kj} \frac{\partial F_{ik} F_{il}}{\partial F_{ij}} + \delta_{lj} \frac{\partial F_{ik} F_{il}}{\partial F_{ij}} \right) \\
&= 2 \left(\sum_l \left(f_j^T f_l F_{il} \right) + \sum_k \left(f_k^T f_j F_{ik} \right) \right)
\end{aligned}$$

Now we can further simplify this equation by using the assumption that the passed in matrix $\hat{F}$ is diagonal in which case $F_{ij} = 0$ when $i \neq j$. So:

$$\begin{aligned}
2 \left(\sum_l \left(f_j^T f_l F_{il} \right) + \sum_k \left(f_k^T f_j F_{ik} \right) \right) &= 2 \left(f_j^T f_i F_{ii} + f_i^T f_j F_{ii} \right) \\
&= 4 f_i^T f_j F_{ii} \\
&= 4 \sigma_i^3 \qquad \text{Note that the previous equation is non-zero only when } i = j.
\end{aligned}$$

Thus we have the following matrix when $i = j$:

$$\frac{2B \det(F)^{-4/3}}{3} \frac{\partial \operatorname{Tr}(F^T F F^T F)}{\partial F_{ij}} F^{-T} = \frac{8 B J_{cc}^2 \sigma_i^3}{3} F^{-T}$$

Thus, only the first three columns of M are affected and thus we get a contribution to γ.

$$\gamma \mathrel{+}= \frac{8 B J_{cc}^2}{3} \begin{bmatrix} \sigma_1^3 \sigma_1^{-1} & \sigma_2^3 \sigma_1^{-1} & \sigma_3^3 \sigma_1^{-1} \\ \sigma_1^3 \sigma_2^{-1} & \sigma_2^3 \sigma_2^{-1} & \sigma_3^3 \sigma_2^{-1} \\ \sigma_1^3 \sigma_3^{-1} & \sigma_2^3 \sigma_3^{-1} & \sigma_3^3 \sigma_3^{-1} \end{bmatrix}$$

This results in a change in η:

$$\eta_{32} \mathrel{+}= \frac{8 B J_{cc}^2}{3} \tag{36}$$

The second matrix once again contains the matrix $\frac{\partial F^{-T}}{\partial F_{ij}}$:

$$\frac{2B \det(F)^{-4/3}}{3} \operatorname{Tr}(F^T F F^T F) \frac{\partial F^{-T}}{\partial F_{ij}} = \frac{2B \det(F)^{-4/3}}{3} \operatorname{Tr}(F^T F F^T F) \begin{bmatrix} \frac{\partial F_{11}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{21}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{31}^{-1}}{\partial F_{ij}}(\hat{F}) \\ \frac{\partial F_{12}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{22}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{32}^{-1}}{\partial F_{ij}}(\hat{F}) \\ \frac{\partial F_{13}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{23}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{33}^{-1}}{\partial F_{ij}}(\hat{F}) \end{bmatrix}$$

Just like before, let us treat it like Equation 26 and Equation 30. That is:

$$\beta_{ij} \mathrel{-}= \frac{\frac{2}{3} B J_{cc}^2 \operatorname{Tr}(C^2)}{\sigma_i \sigma_j} \tag{37}$$

4.5.1.3.3 Computing $M_{2,\mathrm{MR3}}$

$$\begin{aligned} M_{2,\mathrm{MR3}} &= -\frac{2B \det(F)^{-4/3}}{3} \frac{\partial \operatorname{Tr}(F^T F)^2 F^{-T}}{\partial F_{ij}} \\ &= -\frac{2BJ_{cc}^2}{3} \frac{\partial \operatorname{Tr}(F^T F)^2 F^{-T}}{\partial F_{ij}} \end{aligned}$$

The Jacobian here can be split into two parts (again...):

$$\frac{\partial \operatorname{Tr}(F^T F)^2 F^{-T}}{\partial F_{ij}} = \frac{\partial \operatorname{Tr}(F^T F)^2}{\partial F_{ij}} F^{-T} + \operatorname{Tr}(F^T F)^2 \frac{\partial F^{-T}}{\partial F_{ij}}$$

The first matrix being:

$$-\frac{2BJ_{cc}^2}{3} \frac{\partial \operatorname{Tr}(F^T F)^2}{\partial F_{ij}} F^{-T} = -\frac{4BJ_{cc}^2 \operatorname{Tr}(F^T F)}{3} \frac{\partial \operatorname{Tr}(F^T F)}{\partial F_{ij}} F^{-T}$$

Note from before that:

$$\frac{\partial \operatorname{Tr}(F^T F)}{\partial F_{ij}} = 2F_{ij}$$

and that F_{ij} is non-zero only when $i = j$. Thus,

$$-\frac{8BJ_{cc}^2 \operatorname{Tr}(F^T F)}{3} F_{ij} F^{-T}$$

This term is only relevant in the first columns of M and is thus a γ term.

$$\gamma \mathrel{-}= -\frac{8BJ_{cc}^2 \operatorname{Tr}(F^T F)}{3} \begin{bmatrix} \sigma_1\sigma_1^{-1} & \sigma_2\sigma_1^{-1} & \sigma_3\sigma_1^{-1} \\ \sigma_1\sigma_2^{-1} & \sigma_2\sigma_2^{-1} & \sigma_3\sigma_2^{-1} \\ \sigma_1\sigma_3^{-1} & \sigma_2\sigma_3^{-1} & \sigma_3\sigma_3^{-1} \end{bmatrix}$$

Thus the η contribution is:

$$\eta_{31} \mathrel{-}= \frac{8BJ_{cc}^2 \operatorname{Tr}(F^T F)}{3} \tag{38}$$

The second matrix being:

$$-\frac{2BJ_{cc}^2}{3} \operatorname{Tr}(F^T F)^2 \frac{\partial F^{-T}}{\partial F_{ij}} = -\frac{2BJ_{cc}^2}{3} \operatorname{Tr}(F^T F)^2 \begin{bmatrix} \frac{\partial F_{11}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{21}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{31}^{-1}}{\partial F_{ij}}(\hat{F}) \\ \frac{\partial F_{12}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{22}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{32}^{-1}}{\partial F_{ij}}(\hat{F}) \\ \frac{\partial F_{13}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{23}^{-1}}{\partial F_{ij}}(\hat{F}) & \frac{\partial F_{33}^{-1}}{\partial F_{ij}}(\hat{F}) \end{bmatrix}$$

Thus we know that it is a β term:

$$\beta_{ij} \mathrel{+}= \frac{\frac{2BJ_{cc}^2}{3} \operatorname{Tr}(F^T F)^2}{\sigma_i \sigma_j} \tag{39}$$

4.5.1.3.4 Computing $M_{2,\mathbf{MR4}}$

$$M_{2,\mathrm{MR4}} = 2B\det(F)^{-4/3}\frac{\partial\,\mathrm{Tr}(F^TF)F}{\partial F_{ij}}$$

The derivative can be split into two parts:

$$\begin{aligned}\frac{\partial\,\mathrm{Tr}(F^TF)F}{\partial F_{ij}} &= \frac{\partial\,\mathrm{Tr}(F^TF)}{\partial F_{ij}}F + \mathrm{Tr}(F^TF)\frac{\partial F}{\partial F_{ij}} \\ &= 2F_{ij}F + \mathrm{Tr}(F^TF)L^{ij} && \text{Note that } F_{ij} = 0 \text{ when } i \neq j.\end{aligned}$$

The first part:

$$4BJ_{cc}^2 F_{ij}\hat{F}$$

This is a contribution to γ:

$$\gamma \mathrel{+}= 4BJ_{cc}^2\begin{bmatrix}\sigma_1\sigma_1 & \sigma_1\sigma_2 & \sigma_1\sigma_3\\ \sigma_2\sigma_1 & \sigma_2\sigma_2 & \sigma_2\sigma_3\\ \sigma_3\sigma_1 & \sigma_3\sigma_2 & \sigma_3\sigma_3\end{bmatrix}$$

The corresponding contribution to η:

$$\eta_{11} \mathrel{+}= 4BJ_{cc}^2 \tag{40}$$

The second part:

$$2BJ_{cc}^2\,\mathrm{Tr}(F^TF)L^{ij}$$

Similar to Equation 31, this term gets added across the diagonal of M and thus gets added to α.

$$\alpha_{ij} \mathrel{+}= 2BJ_{cc}^2\,\mathrm{Tr}(F^TF) \tag{41}$$

4.5.1.3.5 Computing $M_{2,\mathbf{MR5}}$

$$M_{2,\mathrm{MR5}} = -2B\det(F)^{-4/3}\frac{\partial FF^TF}{\partial F_{ij}}$$

Once again, let us split up the derivative using the product rule:

$$\begin{aligned}\frac{\partial FF^TF}{\partial F_{ij}} &= \frac{\partial F}{\partial F_{ij}}F^TF + F\frac{\partial F^TF}{\partial F_{ij}} \\ &= \frac{\partial F}{\partial F_{ij}}F^TF + F\left(\frac{\partial F^T}{\partial F_{ij}}F + F^T\frac{\partial F}{\partial F_{ij}}\right) \\ &= \frac{\partial F}{\partial F_{ij}}F^TF + F\frac{\partial F^T}{\partial F_{ij}}F + FF^T\frac{\partial F}{\partial F_{ij}} \\ &= L^{ij}F^TF + FL^{ji}F + FF^TL^{ij}\end{aligned}$$

In all of these parts, they will take advantage of the fact that $L^{ij} = 1$ only when $i = j$ and the fact that we pass in a diagonal $\hat{F}$.

First part:

$$-2BJ_{cc}^2 L^{ij} F^T F = -2BJ_{cc}^2 L^{ij} \hat{F}^2$$

This one has familiar form where the scalar is applied along the diagonal of M and thus:

$$\alpha_{ij} \mathrel{-}= 2BJ_{cc}^2 \sigma_j^2 \tag{42}$$

Second part:

$$-2BJ_{cc}^2 F L^{ji} F$$

This one is slightly more complex. First, $L^{ji}F$ selects σ_i and puts it at (j,i). Next, $F(\sigma_i L^{ji})$ selects σ_j and multiplies it by σ_i and puts it at (j,i). Ultimately we get a term that looks like $\sigma_i \sigma_j L^{ji}$. This is thus a perfect β term:

$$\beta_{ij} \mathrel{-}= 2BJ_{cc}^2 \sigma_i \sigma_j \tag{43}$$

Third part:

$$-2BJ_{cc}^2 F F^T L^{ij} = -2BJ_{cc}^2 \hat{F}^2 L^{ij}$$

This one has familiar form where the scalar is applied along the diagonal of M and thus:

$$\alpha_{ij} \mathrel{-}= 2BJ_{cc}^2 \sigma_i^2 \tag{44}$$

4.5.1.4 Summary Putting it all together, we have 3 symmetric 3×3 matrices α, β, η. Finally, $\gamma = F_{\text{base}} \eta F_{\text{base}}^T$ which is also symmetric since η is symmetric.

4.5.1.4.1 Equations for the α matrix

$$\begin{aligned}\alpha_{ij} \mathrel{+}&= 2AJ_{cc} + 2BJ_{cc}^2 \operatorname{Tr}(F^T F) - 2BJ_{cc}^2 \sigma_j^2 - 2BJ_{cc}^2 \sigma_i^2 \\ &= 2J_{cc}(A + BJ_{cc}^2(\operatorname{Tr}(\hat{F}^T \hat{F}) - \sigma_j^2 - \sigma_i^2))\end{aligned}$$

Sourced from equations: 31, 41, 42, 44

4.5.1.4.2 Equations for the β matrix

$$\begin{aligned}\beta_{ij} \mathrel{+}&= \frac{-K\ln(J)}{\sigma_i\sigma_j} + \frac{\frac{2}{3}AJ_{cc}\operatorname{Tr}(\hat{F}^T\hat{F})}{\sigma_i\sigma_j} - \frac{\frac{2}{3}BJ_{cc}^2\operatorname{Tr}(C^2)}{\sigma_i\sigma_j} + \frac{\frac{2BJ_{cc}^2}{3}\operatorname{Tr}(F^TF)^2}{\sigma_i\sigma_j} - 2BJ_{cc}^2\sigma_i\sigma_j \\ &= \frac{\frac{2}{3}AJ_{cc}\operatorname{Tr}(C) - \frac{2}{3}BJ_{cc}^2\operatorname{Tr}(C^2) + \frac{2}{3}BJ_{cc}^2\operatorname{Tr}(C)^2 - K\ln(J)}{\sigma_i\sigma_j} - 2BJ_{cc}^2\sigma_i\sigma_j \\ &= \frac{\frac{2}{3}J_{cc}(A\operatorname{Tr}(C) - BJ_{cc}\operatorname{Tr}(C^2) + BJ_{cc}\operatorname{Tr}(C)^2) - K\ln(J)}{\sigma_i\sigma_j} - 2BJ_{cc}^2\sigma_i\sigma_j \\ &= \frac{\frac{2}{3}J_{cc}(A\operatorname{Tr}(C) + BJ_{cc}(\operatorname{Tr}(C)^2 - \operatorname{Tr}(C^2))) - K\ln(J)}{\sigma_i\sigma_j} - 2BJ_{cc}^2\sigma_i\sigma_j\end{aligned}$$

Sourced from equations: 26, 30, 37, 39, 43.

4.5.1.4.3 Equations for the η matrix

$$\begin{aligned}
\eta_{11} &= 4BJ_{cc}^2 \\
\eta_{13} &= \frac{-4}{3}AJ_{cc} - \frac{8B}{9}J_{cc}^2\operatorname{Tr}(C) \\
&= \frac{-J_{cc}}{3}\left(4A + 8BJ_{cc}\operatorname{Tr}(C)\right) \\
\eta_{31} &= \frac{-4}{3}AJ_{cc} - \frac{8BJ_{cc}^2\operatorname{Tr}(F^TF)}{3} \\
&= \frac{-J_{cc}}{3}\left(4A + 8BJ_{cc}\operatorname{Tr}(C)\right) \\
\eta_{23} &= \frac{8B}{3}J_{cc}^2 \\
\eta_{32} &= \frac{8B}{3}J_{cc}^2 \\
\eta_{33} &= K + \frac{4}{9}AJ_{cc}\operatorname{Tr}(C) - \frac{8B}{9}J_{cc}^2\operatorname{Tr}(C^2) + \frac{8B}{9}J_{cc}^2\operatorname{Tr}(C)^2 \\
&= \frac{J_{cc}}{9}(4A\operatorname{Tr}(C) - 8BJ_{cc}\operatorname{Tr}(C^2) + 8BJ_{cc}Tr(C)^2) + K \\
&= \frac{J_{cc}}{9}(4A\operatorname{Tr}(C) + 8BJ_{cc}(Tr(C)^2 - \operatorname{Tr}(C^2))) + K
\end{aligned}$$

η_{11} sourced from equation(s): 40.

η_{13} sourced from equation(s): 27, 34.

η_{31} sourced from equation(s): 29, 38.

η_{23} sourced from equation(s): 35.

η_{32} sourced from equation(s): 36.

η_{33} sourced from equation(s): 25, 28, 32, 33.

Notice that η is a symmetric matrix.

4.5.2 Anisotropic Materials

Now, let us compete the contribution to $\frac{\partial P}{\partial F}$ from the anistropic material. As a reminder, I will be using the alternative definition of the anisotropic model where:

$$\begin{aligned}
P_4 &= \frac{\partial F_2}{\partial F} \\
&= T(\alpha, \tilde{\lambda})\frac{1}{\tilde{\lambda}}\hat{F}f_m f_m^T
\end{aligned}$$

where $\tilde{\lambda} = \sqrt{f_m\hat{F}^T\hat{F}f_m}$ where $f_m = V^Ta_0$. In this section, we want to be able to compute the differential δP_4 from δF (computing the whole $\frac{\partial P_4}{\partial F}$ like the isotropic part is unnecessary). For the duration of this section, I will switch back to using $\lambda = \tilde{\lambda}$. Then,

$$\begin{aligned}
\delta P_4 &= \delta(T(\alpha, \lambda)\frac{1}{\lambda}\hat{F}f_m f_m^T) \\
&= \delta(T(\alpha, \lambda)\frac{1}{\lambda})\hat{F}f_m f_m^T + T(\alpha, \lambda)\frac{1}{\lambda}\delta\hat{F}f_m f_m^T
\end{aligned}$$

$$
\begin{aligned}
\delta(T(\alpha,\lambda)\frac{1}{\lambda}) &= \delta T(\alpha,\lambda)\lambda^{-1} + T(\alpha,\lambda)\delta\lambda^{-1} \\
&= T'(\alpha,\lambda)\lambda^{-1}\delta\lambda - \frac{T(\alpha,\lambda)}{\lambda^2}\delta\lambda && \text{Note that } \delta\lambda^{-1} = -\lambda^{-1}\delta\lambda\lambda^{-1} \\
\delta\lambda &= \frac{1}{\lambda}(\hat{F}f_m)^T\delta\hat{F}f_m \\
&= \frac{1}{\lambda}(\delta\hat{F}f_m)^T\hat{F}f_m
\end{aligned}
$$

Let us define some helper variables: $c_1 = T(\alpha,\lambda)/\lambda$ and $c_2 = (T'(\alpha,\lambda) - c_1)/\lambda^2$. Then,

$$
\delta P_4 = \left(c_1\delta\hat{F}f_m + c_2\left((\delta\hat{F}f_m)^T\hat{F}f_m\right)\hat{F}f_m\right)\otimes f_m \tag{45}
$$

5 Practical Optimization

This section will briefly go over the various optimization techniques used to solve the quasistatics/landmark optimization problem. I will not attempt to be comprehensive and go over things like convergence, running time, performance, etc. I will briefly explain the algorithm and explain how the pieces we computed above fit into them.

5.1 Newton-Raphson

The Newton-Raphson iterative algorithm solves the problem:

$$
f(x) = 0
$$

It solves the problem by taking the first-order Taylor approximation of $f(x)$:

$$
f(x+\Delta x) \approx f(x) + \frac{\partial f}{\partial x}(x)\Delta x
$$

We thus want to find where $f(x+\Delta x) = 0$. In the above 1st order approximation, this happens when:

$$
\frac{\partial f}{\partial x}(x)\Delta x = -f(x)
$$

This is a linear system and there are multiple ways to solve it. Using a QR factorization would give you the least squares solution and at that point becomes equivalent to the Gauss-Newton method described in Section 5.3. In PhysBAM, when doing quasistatics for the muscles, we opt to use the conjugate gradient method as we know/force the Jacobian $\frac{\partial f}{\partial x}$ to be symmetric positive definite (SPD). The conjugate gradient (CG) method for solving linear systems will be described in 5.2.

5.2 Conjugate Gradient

The CG method is used to solve linear problems of the form:

$$Ax = b$$

where A is SPD. Furthermore, CG is a Krylov subspace method and thus we only need a way to compute Ax and do not need to compute A explicitly [1]. A derivation of the CG method can be found in [1] or [2]. Below is a reproduction of the algorithm found in [2]:

Algorithm 1 CG for Linear Systems

$x_0 =$ initial guess
$r_0 = b - Ax_0$
$s_0 = r_0$
for $k = 0, 1, 2, ...$ **do**
  $\alpha_k = \frac{r_k^T r_k}{s_k^T A s_k}$
  $x_{k+1} = x_k + \alpha_k s_k$
  $r_{k+1} = r_k - \alpha_k A s_k$
  $\beta_{k+1} = \frac{r_{k+1}^T r_{k+1}}{r_k^T r_k}$
  $s_{k+1} = r_{k+1} + \beta_{k+1} s_k$
end for

Note that PhysBAM uses a preconditioned conjugate gradient (PCG) method which introduces a preconditioning matrix into the algorithm. More details about PCG can also be found in [2].

5.3 Gauss-Newton

As mentioned in Section 5.1, the Gauss-Newton method is the equivalent of the Newton-Raphson method when solving a non-linear least squares (NLLQ) problem. Assume we are given the problem:

$$\text{minimize}_x \quad \frac{1}{2}||f(x)||_2^2$$

Once again, use the 1st-order Taylor expansion of $f(x)$ to get:

$$f(x + \Delta x) \approx f(x) + \frac{\partial f}{\partial x}(x)\Delta x$$

Then,

$$\text{minimize}_{\Delta x} \quad \frac{1}{2}||f(x) + \frac{\partial f}{\partial x}(x)\Delta x||_2^2$$

Note that $||f(x) + \frac{\partial f}{\partial x}(x)\Delta x||_2^2 = (f(x) + \frac{\partial f}{\partial x}(x)\Delta x)^T(f(x) + \frac{\partial f}{\partial x}(x)\Delta x)$. If you expand this out you get: $\frac{1}{2}f(x)^T f(x) + (\frac{\partial f}{\partial x}(x)\Delta x)^T f(x) + \frac{1}{2}(\Delta x)^T(\frac{\partial f}{\partial x}(x))^T \frac{\partial f}{\partial x}(x)\Delta x$. Take the Jacobian with respect to Δx and set to 0 to get:

$$\frac{\partial f}{\partial x}^T f(x) + (\frac{\partial f}{\partial x}(x))^T \frac{\partial f}{\partial x}(x)\Delta x = 0$$
$$(\frac{\partial f}{\partial x}(x))^T \frac{\partial f}{\partial x}(x)\Delta x = -\frac{\partial f}{\partial x}^T f(x)$$

Notice the similarity to the Newton-Raphson equation hence why Gauss-Newton is equivalent to Newton-Raphson where you use an orthogonal transformation to solve the linear system.

5.4 Diagonalization

The following explanation can also be found in [3]. At the crux of these equation is the deformation gradient F and the 1st Piola-Kirchoff stress is a function of F: $P(F)$. Note however, that rigid rotations of the object/deformation gradient should not affect the physics of the object and thus $P(UF) = UP(F)$. Additionally, an isotropic material is also invariant under rotations in material space and thus $P(FV^T) = P(F)V^T$. This is a rotation of material space because $d_s = Fd_m$ (notation from [8]: d_s is a vector in deformed space, d_m is a vector in material space). Thus post-multiplying the rotation V^T to F results in $d_s = FV^T d_m$ which is a rotation in material space. Thus we can compute the 1st Piola Kirchoff stress tensor using a diagonal matrix $\hat{F}$ by using the SVD: $P(U\hat{F}V^T) = UP(\hat{F})V^T$. This makes the computation easier. Note that in the case of an anistropic model like the muscle constitutive model, one can simply rotate the anistropic direction by V^T to be able to use the diagonal $\hat{F}$ when computing P.

5.5 Inverted Element Handling

According to [10], one can handle inverted elements by thresholding the elements of the diagonal $\hat{F}$ to be ≥ 0. Note that this forces $\hat{F}$ to also be positive semi-definite.

5.6 Positive Definiteness

Note that the ultimate goal is to be able to use a CG solver to solve the linear system in Equation 22. However, this requires $-\frac{\partial f}{\partial x}(x)$ to always be SPD (symmetric, positive-definite) and not just positive-definite near local minima. That is: $\delta x^T(-\frac{\partial f}{\partial x})\delta x > 0 \implies \delta x^T \delta f < 0$. If turns out that for this equation to be true, we only need $\frac{\partial P}{\partial F}$ to be positive definite. The original derivation for this result can be found in [10] but is reproduced (a little more explicitly) below:

$$
\begin{aligned}
\delta x^T \delta f &= \sum_{i=1}^{4} \delta x_i^T f_i \\
&= \sum_{i=2}^{4} \delta x_i^T f_i - x_1^T \sum_{i=2}^{4} \delta f_i && \text{Remember that the sum of forces from a tetrahedron to its nodes sums to 0.} \\
&= \sum_{i=2}^{4} \delta x_i^T \delta g_i - \delta x_1^T \sum_{i=2}^{4} \delta g_i && \text{This comes from the fact that } f_i = g_i \text{ and thus } \delta f_i = \delta g_i. \\
&= \sum_{i=2}^{4} (\delta x_i - \delta x_1)^T \delta g_i \\
&= \delta D_s : \delta G \\
&= \mathrm{Tr}(\delta D_s^T \delta G) \\
&= \mathrm{Tr}(\delta D_s^T \delta P B_m) \\
&= \mathrm{Tr}(\delta D_s^T \delta P(-V D_m^{-T})) && \text{Uses the identity found in [10] and Section 4.4.} \\
&= -V\,\mathrm{Tr}(\delta D_s^T \delta P D_m^{-T}) \\
&= -V\,\mathrm{Tr}(D_m^{-T} \delta D_s^T \delta P) && \text{Using the identity that } \mathrm{Tr}(ABC) = \mathrm{Tr}(CAB) \\
&= -V\,\mathrm{Tr}((\delta F)^T \delta P) \\
&= -V(\delta F : \delta P)
\end{aligned}
$$

Thus, $\delta x^T \delta f < 0$ if $\delta F : \delta P > 0$. This equates to $\delta F : \frac{\partial P}{\partial F} : \delta F > 0$. Therefore, if $\frac{\partial P}{\partial F}$ is SPD (it may be easier to think of this matrix in its flattened M form) then $-\frac{\partial f}{\partial x}(x)$ will be SPD as well.

In Section 4.5, we computed the matrix M which is the block diagonal form of $\frac{\partial P}{\partial F}$. If $\frac{\partial P}{\partial F}$ is positive definite, then so must the A and B_{ij} matrices. We can enforce the SPD nature of this matrix by clamping negative eigenvalues to 0. See [10] for why clamping to 0 is probably sufficient even though it technically only guarantees semi-definiteness.

We also want to make sure $\delta F : \delta P_4 > 0$ for the anisotropic material. IS THIS NOT POSSIBLE? ASK MATTHEW? CODE SAYS TO FORCE TENSION DERIVATIVE TO BE POSITIVE. CAN'T PROVE.

5.7 Collisions

Collisions are handled as an external penalty force. This means that $f(x) = f_{\text{muscles}}(x) + f_{\text{collision}}(x)$. This penalty force is just a force that of some strength ϵ that pushes a particle back towards the surface. This force is further scaled by the depth of the particle inside the collision body. The details are not important to this document.

6 References

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