Supplementary Technical Document

1 Isotropic stress derivatives in terms of singular values

When specifying a constitutive model energy density Ψ in terms of singular values σ_i, it is convenient to compute the first Piola-Kirchoff stress tensor $\mathbf{P} = \frac{\partial \Psi}{\partial \mathbf{F}}$ and its derivatives $\mathbf{M} = \frac{\partial \mathbf{P}}{\partial \mathbf{F}}$ directly in terms of $\frac{\partial \Psi}{\partial \sigma_i}$ and $\frac{\partial^2 \Psi}{\partial \sigma_i \partial \sigma_j}$. To do this we parameterized $\mathbf{F}$ in terms of the singular values using the singular value decomposition $\mathbf{F} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$. Let $K = \{\sigma_1, \sigma_2, \sigma_3, u_1, u_2, u_3, v_1, v_2, v_3\}$ be the degrees of freedom parameterizing $\mathbf{U}$, $\mathbf{\Sigma}$, and $\mathbf{V}$. We parameterize the rotations using Rodrigues' rotation formula, though any parameterization that is well-behaved around the identity would suffice. Let $C_{i\alpha} = \frac{\partial F_i}{\partial K_\alpha}$, where Latin characters (i, j) are used to represent the degrees of freedom of $\mathbf{F}$ (flattened into a 9-vector) and Greek letters (α, β, γ) are used to represent the degrees of freedom parameterizing the singular value decomposition. Then, $C_{i\alpha}$ is the Jacobian matrix (in terms of K) for the change of variables. Let $D_{\alpha j}$ be the inverse of the Jacobian (also in terms of K), so that $C_{i\alpha}D_{\alpha j} = \delta_{ij}$. Let Ψ be the energy in terms of the degrees of freedom of $\mathbf{F}$ and $\hat{\Psi}$ be the energy in terms of the degrees of freedom K. Using commas to indicate partial differentiation,

$$
\begin{aligned}
\Psi_{,i}C_{i,\alpha} &= \hat{\Psi}_{,\alpha} \\
\left(\Psi_{,i}C_{i,\alpha}\right)_{,\beta} &= \hat{\Psi}_{,\alpha\beta} \\
\Psi_{,ij}C_{i,\alpha}C_{j,\beta} + \Psi_{,i}C_{i,\alpha\beta} &= \hat{\Psi}_{,\alpha\beta} \\
C_{i,\alpha}D_{\alpha j} &= \delta_{ij} \\
\Psi_{,i} &= \hat{\Psi}_{,\alpha}D_{\alpha i} \\
\Psi_{,ij}C_{i,\alpha}D_{\alpha k}C_{j,\beta} &= \hat{\Psi}_{,\alpha\beta}D_{\alpha k} - \Psi_{,i}C_{i,\alpha\beta}D_{\alpha k} \\
\Psi_{,kj}C_{j,\beta} &= \hat{\Psi}_{,\alpha\beta}D_{\alpha k} - \Psi_{,i}C_{i,\alpha\beta}D_{\alpha k} \\
\Psi_{,ij} &= \hat{\Psi}_{,\alpha\beta}D_{\alpha i}D_{\beta j} - \hat{\Psi}_{,\gamma}D_{\gamma k}C_{k,\alpha\beta}D_{\alpha i}D_{\beta j}
\end{aligned}
$$

The Piola-Kirchoff stress tensor $\Psi_{,i}$ in diagonal space can be computed as $\Psi_{,i}(\mathbf{F}(K))\big|_{\mathbf{U}=\mathbf{V}=\mathbf{I}}$. It is a diagonal matrix whose diagonals are $\frac{\partial \hat{\Psi}}{\partial \sigma_i}$ and corresponds to $\hat{\mathbf{P}}(\boldsymbol{\sigma})$ from Section 2 of [1]. The stress derivatives in diagonal space are similarly given by $\Psi_{,ij}(\mathbf{F}(K))\big|_{\mathbf{U}=\mathbf{V}=\mathbf{I}}$. This corresponds to the $\frac{\partial \mathbf{P}}{\partial \mathbf{F}}(\mathbf{\Sigma})$ from Section 2 of [1]. When this computation is performed, one finds that the 9×9 matrix can be permuted into a block diagonal matrix with diagonal blocks $\mathbf{A}^{3\times3}$, $\mathbf{B}_{12}^{2\times2}$, $\mathbf{B}_{13}^{2\times2}$, $\mathbf{B}_{23}^{2\times2}$.

$$
\mathbf{A} = \begin{pmatrix} M_{1111} & M_{1122} & M_{1133} \\ M_{2211} & M_{2222} & M_{2233} \\ M_{3311} & M_{3322} & M_{3333} \end{pmatrix} = \begin{pmatrix} \hat{\Psi}_{,\sigma_1\sigma_1} & \hat{\Psi}_{,\sigma_1\sigma_2} & \hat{\Psi}_{,\sigma_1\sigma_3} \\ \hat{\Psi}_{,\sigma_2\sigma_1} & \hat{\Psi}_{,\sigma_2\sigma_2} & \hat{\Psi}_{,\sigma_2\sigma_3} \\ \hat{\Psi}_{,\sigma_3\sigma_1} & \hat{\Psi}_{,\sigma_3\sigma_2} & \hat{\Psi}_{,\sigma_3\sigma_3} \end{pmatrix}
$$

and

$$
\mathbf{B}_{ij} = \begin{pmatrix} M_{ijij} & M_{ijji} \\ M_{jiij} & M_{jiji} \end{pmatrix} = \frac{1}{\sigma_i^2 - \sigma_j^2} \begin{pmatrix} \sigma_i\hat{\Psi}_{,\sigma_i} - \sigma_j\hat{\Psi}_{,\sigma_j} & \sigma_j\hat{\Psi}_{,\sigma_i} - \sigma_i\hat{\Psi}_{,\sigma_j} \\ \sigma_j\hat{\Psi}_{,\sigma_i} - \sigma_i\hat{\Psi}_{,\sigma_j} & \sigma_i\hat{\Psi}_{,\sigma_i} - \sigma_j\hat{\Psi}_{,\sigma_j} \end{pmatrix}
$$

for $(ij) \in \{(12), (13), (23)\}$.

The division by $\sigma_i^2 - \sigma_j^2$ is problematic when two singular values are nearly equal or when two singular values nearly sum to zero. The latter is possible with a convention for permitting negative singular values.

Expanding $\mathbf{B}_{ij}$ in terms of partial fractions yields the useful decomposition

$$\mathbf{B}_{ij} = \frac{1}{2}\frac{\hat{\Psi}_{,\sigma_i} - \hat{\Psi}_{,\sigma_j}}{\sigma_i - \sigma_j}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix} + \frac{1}{2}\frac{\hat{\Psi}_{,\sigma_i} + \hat{\Psi}_{,\sigma_j}}{\sigma_i + \sigma_j}\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}.$$

Note that if $\hat{\Psi}$ is invariant under permutation of the singular values, then $\hat{\Psi}_{,\sigma_i} \to \hat{\Psi}_{,\sigma_j}$ as $\sigma_i \to \sigma_j$. Thus, the first term can normally be computed robustly for an isotropic model if implemented carefully. The other fraction has deeper implications. This term can be computed robustly if $\hat{\Psi}_{,\sigma_i} + \hat{\Psi}_{,\sigma_j} \to 0$ as $\sigma_i + \sigma_j \to 0$. This property is unfavorable, as it means the constitutive model will have difficulty recovering from many inverted configurations. This corresponds to the kink described in Section 3.1 of [1]. Since we are specifically interested in models with robust behavior under inversion, this term will necessarily be unbounded under some circumstances. We address this by clamping the magnitude of the denominator to not be smaller than 10^{-6} before division to bound the derivatives.

2 C^1 model

In this section, we construct the energy density and its derivatives for the C^1 extrapolation model. We begin by presenting the model in 3D. This model has four regions, depending on how many singular values are below the cutoff $\sigma_i = a$. If all of the singular values are above this threshold, then the energy is just the base model Ψ. Next, assume one singular value crosses this threshold ($\sigma_3 < a$), and let $\Delta\sigma_3 = \sigma_3 - a < 0$. Let

$$\phi = \Psi|_q \qquad g_i = \left.\frac{\partial\Psi}{\partial\sigma_i}\right|_q \qquad H_{ij} = \left.\frac{\partial^2\Psi}{\partial\sigma_i\partial\sigma_j}\right|_q \qquad T_{ijk} = \left.\frac{\partial^3\Psi}{\partial\sigma_i\partial\sigma_j\partial\sigma_k}\right|_q \qquad A_{ijkl} = \left.\frac{\partial^4\Psi}{\partial\sigma_i\partial\sigma_j\partial\sigma_k\partial\sigma_l}\right|_q.$$

Then we extrapolate the energy across the threshold, add a quadratic term, and compute the derivatives

$$\hat{\Psi} = \phi + g_3\Delta\sigma_3 + k\Delta\sigma_3^2 \qquad \frac{\partial\hat{\Psi}}{\partial\sigma_1} = g_1 + H_{13}\Delta\sigma_3 \qquad \frac{\partial\hat{\Psi}}{\partial\sigma_3} = g_3 + 2k\Delta\sigma_3$$

$$\frac{\partial^2\hat{\Psi}}{\partial\sigma_1^2} = H_{11} + T_{113}\Delta\sigma_3 \qquad \frac{\partial^2\hat{\Psi}}{\partial\sigma_3^2} = 2k \qquad \frac{\partial^2\hat{\Psi}}{\partial\sigma_1\partial\sigma_2} = H_{12} + H_{12}\Delta\sigma_3 \qquad \frac{\partial^2\hat{\Psi}}{\partial\sigma_1\partial\sigma_3} = H_{13}$$

The remaining terms are obtained by exchanging the indices 1 and 2.

If we instead assume two singular values cross this threshold ($\sigma_2 < a$, $\sigma_3 < a$), and let $\Delta\sigma_2 = \sigma_2 - a < 0$ and $\Delta\sigma_3 = \sigma_3 - a < 0$. Then the extrapolated energy is

$$\hat{\Psi} = \phi + g_2\Delta\sigma_2 + g_3\Delta\sigma_3 + H_{23}\Delta\sigma_2\Delta\sigma_3 + k\Delta\sigma_2^2 + k\Delta\sigma_3^2$$

$$\frac{\partial\hat{\Psi}}{\partial\sigma_1} = g_1 + H_{12}\Delta\sigma_2 + H_{13}\Delta\sigma_3 + T_{123}\Delta\sigma_2\Delta\sigma_3 \qquad \frac{\partial\hat{\Psi}}{\partial\sigma_2} = g_2 + H_{23}\Delta\sigma_3 + 2k\Delta\sigma_2$$

$$\frac{\partial^2\hat{\Psi}}{\partial\sigma_1^2} = H_{11} + T_{112}\Delta\sigma_2 + T_{113}\Delta\sigma_3 + A_{1123}\Delta\sigma_2\Delta\sigma_3 \qquad \frac{\partial^2\hat{\Psi}}{\partial\sigma_2^2} = 2k$$

$$\frac{\partial^2\hat{\Psi}}{\partial\sigma_1\partial\sigma_2} = H_{12} + T_{123}\Delta\sigma_3 \qquad \frac{\partial^2\hat{\Psi}}{\partial\sigma_2\partial\sigma_3} = H_{23}$$

The remaining terms are obtained by exchanging the indices 2 and 3.

Finally, if all three singular values cross the threshold ($\sigma_1 < a$, $\sigma_2 < a$, $\sigma_3 < a$), let $\Delta\sigma_1 = \sigma_1 - a < 0$, $\Delta\sigma_2 = \sigma_2 - a < 0$ and $\Delta\sigma_3 = \sigma_3 - a < 0$. Then the extrapolated energy is then

$$\begin{aligned}
\hat{\Psi} &= \phi + g_1\Delta\sigma_1 + g_2\Delta\sigma_2 + g_3\Delta\sigma_3 + H_{12}\Delta\sigma_1\Delta\sigma_2 + H_{13}\Delta\sigma_1\Delta\sigma_3 + H_{23}\Delta\sigma_2\Delta\sigma_3 \\
&\quad + T_{123}\Delta\sigma_1\Delta\sigma_2\Delta\sigma_3 + k\Delta\sigma_1^2 + k\Delta\sigma_2^2 + k\Delta\sigma_3^2 \\
\frac{\partial\hat{\Psi}}{\partial\sigma_1} &= g_1 + H_{12}\Delta\sigma_2 + H_{13}\Delta\sigma_3 + T_{123}\Delta\sigma_2\Delta\sigma_3 + 2k\Delta\sigma_1 \\
\frac{\partial^2\hat{\Psi}}{\partial\sigma_1^2} &= 2k \\
\frac{\partial^2\hat{\Psi}}{\partial\sigma_1\partial\sigma_2} &= H_{12} + T_{123}\Delta\sigma_3
\end{aligned}$$

The remaining derivatives are obtained by cycling the indices.

2.1 Continuity

To see that the model is in fact C^1, we need to show that the energy and first derivatives match at the interfaces between regions. In the case of one singular value right at the extrapolation surface, $\Delta\sigma_3 \to 0$, and

$$\hat{\Psi} = \phi + g_3\Delta\sigma_3 + k\Delta\sigma_3^2 \to \phi \qquad \frac{\partial\hat{\Psi}}{\partial\sigma_1} = g_1 + H_{13}\Delta\sigma_3 \to g_1 \qquad \frac{\partial\hat{\Psi}}{\partial\sigma_3} = g_3 + 2k\Delta\sigma_3 \to g_3.$$

These are just the base model. At the transition from two to one singular values outside the extrapolation surface, $\Delta\sigma_2 \to 0$ and

$$\hat{\Psi} = \phi + g_2\Delta\sigma_2 + g_3\Delta\sigma_3 + H_{23}\Delta\sigma_2\Delta\sigma_3 + k\Delta\sigma_2^2 + k\Delta\sigma_3^2 \to \phi + g_3\Delta\sigma_3 + k\Delta\sigma_3^2$$

$$\frac{\partial\hat{\Psi}}{\partial\sigma_1} = g_1 + H_{12}\Delta\sigma_2 + H_{13}\Delta\sigma_3 + T_{123}\Delta\sigma_2\Delta\sigma_3 \to g_1 + H_{13}\Delta\sigma_3$$

$$\frac{\partial\hat{\Psi}}{\partial\sigma_2} = g_2 + H_{23}\Delta\sigma_3 + 2k\Delta\sigma_2 \to g_2 + H_{23}\Delta\sigma_3 \qquad \frac{\partial\hat{\Psi}}{\partial\sigma_3} = g_3 + H_{23}\Delta\sigma_2 + 2k\Delta\sigma_3 \to g_3 + 2k\Delta\sigma_3$$

These agree with the values obtained when only one singular value was extrapolated. Finally, in the transition from three to two singular values outside the extrapolation surface, $\Delta\sigma_1 \to 0$ and

$$\begin{aligned}
\hat{\Psi} &= \phi + g_1\Delta\sigma_1 + g_2\Delta\sigma_2 + g_3\Delta\sigma_3 + H_{12}\Delta\sigma_1\Delta\sigma_2 + H_{13}\Delta\sigma_1\Delta\sigma_3 + H_{23}\Delta\sigma_2\Delta\sigma_3 \\
&\quad + T_{123}\Delta\sigma_1\Delta\sigma_2\Delta\sigma_3 + k\Delta\sigma_1^2 + k\Delta\sigma_2^2 + k\Delta\sigma_3^2 \\
&\to \phi + g_2\Delta\sigma_2 + g_3\Delta\sigma_3 + H_{23}\Delta\sigma_2\Delta\sigma_3 + k\Delta\sigma_2^2 + k\Delta\sigma_3^2 \\
\frac{\partial\hat{\Psi}}{\partial\sigma_1} &= g_1 + H_{12}\Delta\sigma_2 + H_{13}\Delta\sigma_3 + T_{123}\Delta\sigma_2\Delta\sigma_3 + 2k\Delta\sigma_1 \\
&\to g_1 + H_{12}\Delta\sigma_2 + H_{13}\Delta\sigma_3 + T_{123}\Delta\sigma_2\Delta\sigma_3 \\
\frac{\partial\hat{\Psi}}{\partial\sigma_2} &= g_2 + H_{23}\Delta\sigma_3 + H_{12}\Delta\sigma_1 + T_{123}\Delta\sigma_1\Delta\sigma_3 + 2k\Delta\sigma_2 \\
&\to g_2 + H_{23}\Delta\sigma_3 + 2k\Delta\sigma_2
\end{aligned}$$

These match the expressions obtained for the case where two singular values are beyond the extrapolation surface, so C^1 continuity is established.

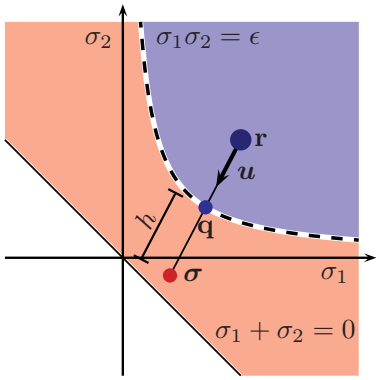

Figure 1: This figures shows some of the quantities used for the C^2 extrapolation.

3 C^2 model

This section provides a detailed derivation of the energy density and its derivatives for the C^2 model described in [1].

In this section, index notation is used for conciseness and clarity. We follow the convention that letters $(i, j, k, \ldots)$ are used for indices with the Einstein summation assumed. In a few places, this convention does not fit will. For those cases, we use Greek letters $(\alpha, \beta, \gamma, \ldots)$ for the index to indicate that summation over that index is never implied. Indices that occur after a comma are differentiated. Thus, $\Psi_{,i} = \frac{\partial \Psi}{\partial \sigma_i}$ and $u_{i,jk} = \frac{\partial^2 u_i}{\partial \sigma_j \sigma_k}$. Summation limits are not stated and should go up to the dimension (that is, 2 or 3). The derivation that follows is valid in any dimension, except where noted.

The base energy Ψ is the be extended to the extrapolated energy $\hat{\Psi}$ at the point $\boldsymbol{\sigma}$ by extrapolating along the line to the rest configuration $\boldsymbol{r}$ ($r_i = 1$ for all i). The direction of the line is $u_i = m(\sigma_i - r_i)$, with $m = \|\boldsymbol{\sigma} - \boldsymbol{r}\|^{-1}$. This line intersects the contour $J = a$ at $q_i = r_i + (\sigma_i - r_i)s$. The distance along this line from the contour to $\boldsymbol{\sigma}$ is then $h = (\sigma_i - q_i)u_i$. The extrapolated energy is $\hat{\Psi} = \phi + h g_j u_j + \frac{1}{2} h^2 H_{lj} u_l u_j$, where $\phi = \Psi\big|_q$, $g_i = \Psi_{,i}\big|_q$, and $H_{ij} = \Psi_{,ij}\big|_q$. The scalar s is given by the polynomial equation $a = \prod_\alpha (r_\alpha + (\sigma_\alpha - r_\alpha)s)$.

The differentiation of $\hat{\Psi}$ at first may seem like an impossible task, particularly in terms of debugging. We compute the extrapolated energy in many small intermediate steps, and then we differentiate each of those steps along the way to construct the extrapolated energy derivatives. This breaks the task down into many simpler quantities, which simplifies the implementation. This has the added advantage that the derivatives of each intermediate quantity can be checked numerically, which drastically simplifies the debugging process. See section 4 for suggestions on testing derivatives numerically.

3.1 Simple quantities

First, we start with a few simple quantities. The quantity $\delta_{ij} = 1$ if $i = j$, and $\delta_{ij} = 0$ otherwise. The scalar m is the reciprocal of the distance between $\boldsymbol{r}$ and $\boldsymbol{\sigma}$, which is a convenient intermediate in computing u_i,

the direction along with extrapolation occurs.

$$\begin{aligned}
\sigma_{i,j} &= \delta_{ij} \\
\delta_{ij,k} &= 0 \\
r_{i,j} &= 0 \\
m &= \|\boldsymbol{\sigma} - \boldsymbol{r}\|^{-1} \\
m_{,i} &= -(\sigma_i - r_i)m^3 \\
m_{,ij} &= -\delta_{ij}m^3 + 3(\sigma_i - r_i)(\sigma_j - r_j)m^5 \\
u_i &= m(\sigma_i - r_i) \\
u_{i,k} &= m_{,k}(\sigma_i - r_i) + m\delta_{ik} \\
u_{i,kj} &= m_{,kj}(\sigma_i - r_i) + (m_{,k}\delta_{ij} + m_{,j}\delta_{ik})
\end{aligned}$$

These quantities do not depend on anything else. Throughout this derivation, we will group pairs of terms in Hessians that are symmetric as we have done in the expression for $u_{i,kj}$ with $(m_{,k}\delta_{ij} + m_{,j}\delta_{ik})$. In practice, one of these terms should be computed and then transposed to obtain the other.

3.2 Point on extrapolation surface

Next, we define $\boldsymbol{q}$ as the location where extrapolation begins. It is the location on the segment connecting the rest configuration $\boldsymbol{r}$ and the current configuration $\boldsymbol{\sigma}$ that intersects the extrapolation surface. The energy density will be extrapolated along the segment from $\boldsymbol{q}$ to $\boldsymbol{\sigma}$. The length of this segment is denoted h.

$$\begin{aligned}
q_i &= r_i + (\sigma_i - r_i)s \\
q_{i,j} &= \delta_{ij}s + (\sigma_i - r_i)s_{,j} \\
q_{i,jk} &= (\delta_{ij}s_{,k} + \delta_{ik}s_{,j}) + (\sigma_i - r_i)s_{,jk} \\
h &= (\sigma_i - q_i)u_i \\
h_{,j} &= (\delta_{ij} - q_{i,j})u_i + (\sigma_i - q_i)u_{i,j} \\
h_{,jk} &= -q_{i,jk}u_i + ((\delta_{ij} - q_{i,j})u_{i,k} + (\delta_{ik} - q_{i,k})u_{i,j}) + (\sigma_i - q_i)u_{i,jk}
\end{aligned}$$

Note that these quantities depend on an interpolation fraction s (with $0 < s < 1$) and its derivatives, which we compute next.

3.3 Interpolation fraction

The interpolating fraction is constrained to lie on the extrapolation surface given by $\prod_\alpha q_\alpha = a$ for some constant $0 < a < 1$. This leads to the equation

$$a = \prod_\alpha q_\alpha = \prod_\alpha (r_\alpha + (\sigma_\alpha - r_\alpha)s).$$

This is a cubic equation in the scalar variable s. Note that when $s = 0$

$$\prod_\alpha (r_\alpha + (\sigma_\alpha - r_\alpha)s) - a = \prod_\alpha r_\alpha - a = 1 - a > 0,$$

and at $s = 1$

$$\prod_\alpha (r_\alpha + (\sigma_\alpha - r_\alpha)s) - a = \prod_\alpha \sigma_\alpha - a = J < 0.$$

Thus, we are guaranteed that there will exist a solution s to the cubic in the interval $(0, 1)$. We compute this intersection using the bisection method since it is efficient and robust.

To compute the derivatives, we use implicit differentiation. We introduce two intermediate scalars ζ and ξ (with no particular physical interpretation) to simplify these computations.

$$\begin{aligned}
\zeta &= \sum_\alpha \frac{\sigma_\alpha - r_\alpha}{q_\alpha} \\
\zeta_{,\beta} &= \frac{1}{q_\beta} - \sum_\alpha \frac{\sigma_\alpha - r_\alpha}{q_\alpha^2} q_{\alpha,\beta} \\
\zeta_{,\beta\gamma} &= -\left(\frac{q_{\beta,\gamma}}{q_\beta^2} + \frac{q_{\gamma,\beta}}{q_\gamma^2} \right) + 2 \sum_\alpha \frac{\sigma_\alpha - r_\alpha}{q_\alpha^3} q_{\alpha,\beta} q_{\alpha,\gamma} - \sum_\alpha \frac{\sigma_\alpha - r_\alpha}{q_\alpha^2} q_{\alpha,ik} \\
\xi &= \zeta^{-1} \\
\xi_{,k} &= -\xi^2 \zeta_{,k} \\
\xi_{,ki} &= 2\xi^3 \zeta_{,k} \zeta_{,i} - \xi^2 \zeta_{,ki}
\end{aligned}$$

Now, we can proceed with the differentiation of s.

$$\begin{aligned}
0 &= \sum_\alpha \frac{\delta_{\alpha k} s + (\sigma_\alpha - r_\alpha) s_{,k}}{r_\alpha + (\sigma_\alpha - r_\alpha) s} \\
s_{,\beta} &= -s \left(\sum_\alpha \frac{\sigma_\alpha - r_\alpha}{r_\alpha + (\sigma_\alpha - r_\alpha) s} \right)^{-1} \sum_\alpha \frac{\delta_{\alpha\beta}}{r_\alpha + (\sigma_\alpha - r_\alpha) s} \\
&= -\frac{s}{q_\beta} \left(\sum_\alpha \frac{\sigma_\alpha - r_\alpha}{q_\alpha} \right)^{-1} \\
&= -\frac{s\xi}{q_\beta} \\
s_{,\beta\gamma} &= -\frac{s_{,\gamma}\xi}{q_\beta} - \frac{s\xi_{,\gamma}}{q_\beta} + \frac{s\xi q_{\beta,\gamma}}{q_\beta^2} \\
&= \frac{s\xi^2}{q_\beta q_\gamma} - \frac{s\xi_{,\gamma}}{q_\beta} + \frac{s\xi q_{\beta,\gamma}}{q_\beta^2}
\end{aligned}$$

All the quantities introduced so far can now be computed. The expression for $s_{,\beta\gamma}$ can be shown to be symmetric.

3.4 Base model

The base model and its first four derivatives are required on the extrapolation surface to compute the stress derivatives. These quantities are all evaluated at the point q_i.

$$\begin{aligned}
\phi &= \Psi\big|_q \\
g_i &= \Psi_{,i}\big|_q \\
H_{ij} &= \Psi_{,ij}\big|_q \\
T_{ijk} &= \Psi_{,ijk}\big|_q \\
A_{ijkl} &= \Psi_{,ijkl}\big|_q
\end{aligned}$$

These quantities are symmetric in all of their indices. We will also use some of the derivatives of these quantities. Note that the point q_i is constrained to the extrapolation surface, so the derivatives of these will

depend on the derivatives of q_i.

$$\begin{aligned}
\phi_{,i} &= g_k q_{k,i} \\
\phi_{,ij} &= g_{k,j} q_{k,i} + g_k q_{k,ij} \\
g_{k,i} &= H_{km} q_{m,i} \\
g_{k,ij} &= T_{kmn} q_{m,i} q_{n,j} + H_{km} q_{m,ij} \\
H_{kl,i} &= T_{klm} q_{m,i} \\
H_{kl,ij} &= A_{klmn} q_{m,i} q_{n,j} + T_{klm} q_{m,ij}
\end{aligned}$$

3.5 Extrapolated energy

We now have all of the quantities we need to compute $\hat{\Psi}$ and its derivatives. The scalars $g_k u_k$ and $H_{kl} u_k u_l$ are required for interpolation, and we differentiate them separately first.

$$\begin{aligned}
b &= g_k u_k \\
b_{,i} &= g_{k,i} u_k + g_k u_{k,i} \\
b_{,ij} &= g_{k,ij} u_k + (g_{k,i} u_{k,j} + g_{k,j} u_{k,i}) + g_k u_{k,ij} \\
c &= H_{kl} u_k u_l \\
c_{,i} &= H_{kl,i} u_k u_l + 2 H_{kl} u_{k,i} u_l \\
c_{,ij} &= H_{kl,ij} u_k u_l + (2 H_{kl,i} u_{k,j} u_l + 2 H_{kl,j} u_{k,i} u_l) + 2 H_{kl} u_{k,ij} u_l + 2 H_{kl} u_{k,i} u_{l,j} \\
d &= T_{klj} u_k u_l u_j
\end{aligned}$$

Finally, we compute the extrapolated energy and its derivatives.

$$\begin{aligned}
\hat{\Psi} &= \phi + hb + \frac{1}{2} h^2 c \\
\hat{\Psi}_{,i} &= \phi_{,i} + h_{,i} b + h b_{,i} + h h_{,i} c + \frac{1}{2} h^2 c_{,i} \\
\hat{\Psi}_{,ik} &= \phi_{,ik} + h_{,ik} b + (h_{,i} b_{,k} + h_{,k} b_{,i}) + h b_{,ik} + h_{,k} h_{,i} c + h h_{,ik} c + (h h_{,i} c_{,k} + h h_{,k} c_{,i}) + \frac{1}{2} h^2 c_{,ik}
\end{aligned}$$

3.6 Robustness

The formula for $\frac{\partial P_{ij}}{\partial F_{km}}$ requires that terms of the form

$$\frac{\hat{\Psi}_{,i} - \hat{\Psi}_{,t}}{\sigma_i - \sigma_t}$$

be computed robustly. To work out a robust way to do this, it will be very convenient to introduce some new notation. We take the index $[it]$ to indicate quantities like

$$B_{[it]} = \frac{B_i - B_t}{\sigma_i - \sigma_t} \qquad C_{k,[it]} = \frac{C_{k,i} - B_{k,t}}{\sigma_i - \sigma_t}$$

where it is assumed that $i \neq t$. We are after the quantity $\hat{\Psi}_{,[it]}$. We will also reuse notation slightly. Since $r_i = 1$, we will use it for this purpose even when the usage is unrelated to the rest configuration. With this,

we can say $\sigma_{[it]} = r_i r_t$ and $r_{[it]} = 0$. Note that $hm + s = 1$ and $B_k \delta_{k[it]} = B_{[it]}$.

$$
\begin{aligned}
u_{[it]} &= m(\sigma_{[it]} - r_{[it]}) = m r_i r_t \\
m_{,[it]} &= -(\sigma_{[it]} - r_{[it]}) m^3 = -m^3 r_i r_t \\
u_{j,[it]} &= m^{-1} m_{,[it]} u_j + m \delta_{j[it]} \\
&= -m^2 u_j r_i r_t + m \delta_{j[it]} \\
q_{[it]} &= r_{[it]} + (\sigma_{[it]} - r_{[it]}) s = s r_i r_t \\
s_{,[it]} &= \frac{s_{,i} - s_{,s}}{\sigma_i - \sigma_t} \\
&= -s\xi \frac{q_i^{-1} - q_t^{-1}}{\sigma_i - \sigma_t} \\
&= -s\xi q_i^{-1} q_t^{-1} \frac{q_t - q_i}{\sigma_i - \sigma_t} \\
&= s\xi q_i^{-1} q_t^{-1} q_{[it]} \\
&= s^2 \xi q_i^{-1} q_t^{-1} \\
q_{m,[it]} &= \delta_{m[it]} s + (\sigma_m - r_m) s_{,[it]} \\
&= \delta_{m[it]} s + m^{-1} u_m s_{,[it]} \\
h_{,[it]} &= u_{[it]} - q_{k,[it]} u_k + (\sigma_k - q_k) u_{k,[it]} \\
&= m r_i r_t - s u_{[it]} - m^{-1} u_k s_{,[it]} u_k + h u_k (m^{-1} m_{,[it]} u_k + m \delta_{k[it]}) \\
&= m r_i r_t + (hm - s) u_{[it]} - m^{-1} s_{,[it]} + h u_k m^{-1} m_{,[it]} u_k \\
&= (hm - s + 1) m r_i r_t - m^{-1} s_{,[it]} - h m^2 r_i r_t \\
&= h m^2 r_i r_t - m^{-1} s_{,[it]} \\
\phi_{,[it]} &= g_k q_{k,[it]} \\
&= g_{[it]} s + m^{-1} b s_{,[it]} \\
g_{j,[it]} &= H_{jm} q_{m,[it]} \\
&= H_{j[it]} s + m^{-1} H_{jm} u_m s_{,[it]} \\
H_{kl,[it]} &= T_{klm} q_{m,[it]} \\
&= s T_{kl[it]} + m^{-1} T_{klm} u_m s_{,[it]} \\
b_{,[it]} &= g_{k,[it]} u_k + g_k u_{k,[it]} \\
&= H_{k[it]} s u_k + m^{-1} H_{km} u_m s_{,[it]} u_k - g_k m^2 u_k r_i r_t + g_k m \delta_{k[it]} \\
&= H_{k[it]} s u_k + m^{-1} c s_{,[it]} - b m^2 r_i r_t + m g_{[it]} \\
c_{,[it]} &= H_{kl,[it]} u_k u_l + 2 H_{kl} u_{k,[it]} u_l \\
&= s T_{kl[it]} u_k u_l + m^{-1} d s_{,[it]} - 2 H_{kl} m u_k r_i r_t u_l + 2 H_{kl} m \delta_{k[it]} u_l \\
&= s T_{kl[it]} u_k u_l + m^{-1} d s_{,[it]} - 2 c m r_i r_t + 2 H_{k[it]} m u_k
\end{aligned}
$$

Finally, we can assemble the desired quantity $\hat{\Psi}_{,[it]}$.

$$\begin{aligned}
h_{,[it]}b + hb_{,[it]} &= -m^{-1}s_{,[it]}b + hm^2 r_i r_t b + hH_{k[it]}su_k + hm^{-1}cs_{,[it]} - hbm^2 r_i r_t + hmg_{[it]} \\
&= m^{-1}(hc-b)s_{,[it]} + hsH_{k[it]}u_k + hmg_{[it]} \\
hh_{,[it]}c + \frac{1}{2}h^2 c_{,[it]} &= -hcm^{-1}s_{,[it]} + h^2 cm^2 r_i r_t + \frac{1}{2}h^2 sT_{kl[it]}u_k u_l + \frac{1}{2}h^2 m^{-1}ds_{,[it]} - h^2 cmr_i r_t + h^2 H_{k[it]}mu_k \\
&= \frac{1}{2}m^{-1}h(hd-2c)s_{,[it]} + \frac{1}{2}h^2 sT_{kl[it]}u_k u_l + h^2 H_{k[it]}mu_k \\
\hat{\Psi}_{,[it]} &= \phi_{,[it]} + h_{,[it]}b + hb_{,[it]} + hh_{,[it]}c + \frac{1}{2}h^2 c_{,[it]} \\
&= \phi_{,[it]} + m^{-1}(hc-b)s_{,[it]} + hsH_{k[it]}u_k + hmg_{[it]} + \frac{1}{2}m^{-1}h(hd-2c)s_{,[it]} \\
&\quad + \frac{1}{2}h^2 sT_{kl[it]}u_k u_l + h^2 H_{k[it]}mu_k \\
&= \phi_{,[it]} + \frac{1}{2}m^{-1}\big(h^2 d - 2b\big)s_{,[it]} + hH_{k[it]}u_k + hmg_{[it]} + \frac{1}{2}h^2 sT_{kl[it]}u_k u_l \\
&= g_{[it]}s + m^{-1}bs_{,[it]} + \frac{1}{2}m^{-1}\big(h^2 d - 2b\big)s_{,[it]} + hH_{k[it]}u_k + hmg_{[it]} + \frac{1}{2}h^2 sT_{kl[it]}u_k u_l \\
&= g_{[it]} + hH_{k[it]}u_k + \frac{1}{2}h^2 sT_{kl[it]}u_k u_l + \frac{1}{2}m^{-1}h^2 ds_{,[it]}
\end{aligned}$$

This formula is elegant, but unfortunately $H_{k[it]}$ and $T_{kl[it]}$ cannot be computed robustly.

The solution to this problem is to compute $hH_{k[it]}u_k$ and $T_{kl[it]}u_k u_l$, since they can be computed robustly. Consider the computation of $hH_{k[12]}u_k$ (the others can be obtained by cycling indices).

$$\begin{aligned}
H_{[12]j}u_j &= H_{[12]1}u_1 + H_{[12]2}u_2 + H_{[12]3}u_3 \\
&= \frac{H_{11}u_1 - H_{12}u_1 + H_{12}u_2 - H_{22}u_2}{\sigma_1 - \sigma_2} + H_{[12]3}u_3 \\
&= \frac{H_{11}u_1 - H_{11}u_2}{\sigma_1 - \sigma_2} + \frac{H_{11}u_2 - H_{22}u_2}{\sigma_1 - \sigma_2} - \frac{H_{12}u_1 - H_{12}u_2}{\sigma_1 - \sigma_2} + H_{[12]3}u_3 \\
&= H_{11}u_{[12]} + H_{[11,22]}u_2 - H_{12}u_{[12]} + H_{[12]3}u_3
\end{aligned}$$

where we have introduced the new notation

$$H_{[11,22]} = \frac{H_{11} - H_{22}}{\sigma_1 - \sigma_2}.$$

The resulting terms can each be computed robustly. Note that expanding in this way allows us to isolate the base model $(H_{11}, H_{12}, H_{[12]3}, H_{[11,22]})$ from the details of the extrapolation $(u_2, u_3, u_{[12]})$.

Similarly, we can compute $T_{jk[12]}u_j u_k$ robustly

$$\begin{aligned}
T_{jk[12]}u_j u_k &= T_{33[12]}u_3 u_3 + T_{31[12]}u_3 u_1 + T_{32[12]}u_3 u_2 + T_{13[12]}u_3 u_1 + T_{11[12]}u_1 u_1 + T_{12[12]}u_1 u_2 \\
&\quad + T_{23[12]}u_3 u_2 + T_{21[12]}u_2 u_1 + T_{22[12]}u_2 u_2 \\
&= T_{33[12]}u_3 u_3 + 2T_{12[12]}u_1 u_2 + 2T_{31[12]}u_3 u_1 + 2T_{32[12]}u_3 u_2 + T_{11[12]}u_1 u_1 + T_{22[12]}u_2 u_2 \\
&= T_{33[12]}u_3 u_3 + 2T_{12[12]}u_1 u_2 + 2u_3(T_{311}u_{[12]} + T_{3[11,22]}u_2 - T_{312}u_{[12]}) \\
&\quad + (T_{[111,222]} - T_{12[12]})u_1^2 + (T_{222} - T_{122})\frac{u_1^2 - u_2^2}{\sigma_1 - \sigma_2} \\
&= T_{33[12]}u_3 u_3 + 2T_{12[12]}u_1 u_2 + 2u_3(T_{311}u_{[12]} + T_{3[11,22]}u_2 - T_{312}u_{[12]}) \\
&\quad + (T_{[111,222]} - T_{12[12]})u_1^2 + m^2(T_{222} - T_{122})(\sigma_1 + \sigma_2 - 2)
\end{aligned}$$

where we have introduced the new notation

$$T_{3[11,22]} = \frac{T_{311} - T_{322}}{\sigma_1 - \sigma_2} \qquad T_{[111,222]} = \frac{T_{111} - T_{222}}{\sigma_1 - \sigma_2}.$$

As before, these quantities can be computed robustly, and the base model is isolated from the details of the extrapolation. The 2D formulas for $H_{[12]j}u_j$ and $T_{jk[12]}u_ju_k$ are obtained by discarding all terms containing the index 3.

3.7 Continuity

To establish C^2 continuity for this model, we need to establish that $\hat{\Psi} = \phi$, $\hat{\Psi}_{,i} = g_i$, and $\hat{\Psi}_{,ik} = H_{ik}$ at the extrapolation surface. At this surface, $s = 1$ and $h = 0$. With these,

$$\begin{aligned}
q_i &= r_i + (\sigma_i - r_i)s \\
q_i &= \sigma_i \\
q_{i,j} &= \delta_{ij}s + (\sigma_i - r_i)s_{,j} \\
&= \delta_{ij} + m^{-1}u_i s_{,j} \\
\delta_{ij} - q_{i,j} &= -m^{-1}u_i s_{,j} \\
h_{,j} &= (\delta_{ij} - q_{i,j})u_i + (\sigma_i - q_i)u_{i,j} \\
&= -m^{-1}s_{,j} \\
h_{,jk} &= -q_{i,jk}u_i + ((\delta_{ij} - q_{i,j})u_{i,k} + (\delta_{ik} - q_{i,k})u_{i,j}) + (\sigma_i - q_i)u_{i,jk} \\
&= -q_{i,jk}u_i \\
g_{k,i} &= H_{km}q_{m,i} \\
&= H_{ki} + m^{-1}H_{km}u_m s_{,i} \\
g_{k,ij} &= T_{kmn}q_{m,i}q_{n,j} + H_{km}q_{m,ij} \\
&= T_{kmn}q_{m,i}q_{n,j} + H_{km}q_{m,ij} \\
b_{,i} &= g_{k,i}u_k + g_k u_{k,i} \\
&= H_{ki}u_k + m^{-1}H_{km}u_m s_{,i}u_k + m_{,i}(\sigma_k - r_k)g_k + mg_i \\
&= H_{ki}u_k + m^{-1}cs_{,i} + m_{,i}m^{-1}b + mg_i \\
&= H_{ki}u_k + m^{-1}cs_{,i} + (g_i - u_i b)m
\end{aligned}$$

With these, C^1 is established readily

$$\begin{aligned}
\hat{\Psi} &= \phi + hb + \frac{1}{2}h^2 c \\
&= \phi \\
\hat{\Psi}_{,i} &= \phi_{,i} + h_{,i}b + hb_{,i} + hh_{,i}c + \frac{1}{2}h^2 c_{,i} \\
&= \phi_{,i} + h_{,i}b \\
&= g_k q_{k,i} - m^{-1}s_{,i}b \\
&= g_i + g_k u_k m^{-1}s_{,i} - m^{-1}s_{,i}b \\
&= g_i
\end{aligned}$$

Finally, C^2 can be established with a bit of work.

$$\begin{aligned}
\hat{\Psi}_{,ik} &= \phi_{,ik} + h_{,ik}b + (h_{,i}b_{,k} + h_{,k}b_{,i}) + hb_{,ik} + h_{,k}h_{,i}c + hh_{,ik}c + (hh_{,i}c_{,k} + hh_{,k}c_{,i}) + \frac{1}{2}h^2c_{,ik} \\
&= \phi_{,ik} + h_{,ik}b + (h_{,i}b_{,k} + h_{,k}b_{,i}) + h_{,k}h_{,i}c \\
&= g_{j,k}q_{j,i} + g_jq_{j,ik} - q_{j,ik}u_jb + (h_{,i}b_{,k} + h_{,k}b_{,i}) + h_{,k}h_{,i}c \\
&= g_{j,k}q_{j,i} + (g_j - u_jb)q_{j,ik} + (h_{,i}b_{,k} + h_{,k}b_{,i}) + h_{,k}h_{,i}c \\
&= g_{j,k}q_{j,i} + (g_j - u_jb)(\delta_{ji}s_{,k} + \delta_{jk}s_{,i} + m^{-1}u_js_{,ik}) + (h_{,i}b_{,k} + h_{,k}b_{,i}) + h_{,k}h_{,i}c \\
&= g_{j,k}q_{j,i} + (g_i - u_ib)s_{,k} + (g_k - u_kb)s_{,i} + (h_{,i}b_{,k} + h_{,k}b_{,i}) + h_{,k}h_{,i}c \\
&= g_{j,k}q_{j,i} + (b_{,i} - (g_i - u_ib)m)h_{,k} + (b_{,k} - (g_k - u_kb)m)h_{,i} + h_{,k}h_{,i}c \\
&= g_{j,k}q_{j,i} + (H_{ji}u_j + m^{-1}cs_{,i})h_{,k} + (H_{jk}u_j + m^{-1}cs_{,k})h_{,i} + h_{,k}h_{,i}c \\
&= g_{j,k}q_{j,i} - ch_{,i}h_{,k} + H_{ji}u_jh_{,k} + H_{jk}u_jh_{,i} \\
&= g_{i,k} - g_{j,k}u_jh_{,i} - ch_{,i}h_{,k} + H_{ji}u_jh_{,k} + H_{jk}u_jh_{,i} \\
&= H_{ik} + m^{-1}H_{im}u_ms_{,k} - H_{jk}u_jh_{,i} - m^{-1}H_{jm}u_ms_{,k}u_jh_{,i} - ch_{,i}h_{,k} + H_{ji}u_jh_{,k} + H_{jk}u_jh_{,i} \\
&= H_{ik} - m^{-1}H_{jm}u_ms_{,k}u_jh_{,i} - ch_{,i}h_{,k} \\
&= H_{ik}
\end{aligned}$$

This establishes C^2 continuity for this model.

4 Note on testing derivatives numerically

We suggest above that the derivatives can be tested numerically. Here, we present a simple yet effective way to do this. Choose a small random perturbation $\delta\mathbf{x}$. Suppose we have a scalar f and its derivative ∇f evaluated at $\mathbf{x}$ and $\delta\mathbf{x}$. Then,

$$f(\mathbf{x} + \delta\mathbf{x}) - f(\mathbf{x}) - \frac{1}{2}(\nabla f(\mathbf{x} + \delta\mathbf{x}) + \nabla f(\mathbf{x})) \cdot \delta\mathbf{x} = O(\|\delta\mathbf{x}\|^3).$$

This test compares a second order accurate central difference approximation against a second order average, which makes the test much less ambiguous. When the test fails, the error will generally only be of order $O(\|\delta\mathbf{x}\|)$. If the quantities being tested are on the order of one, then it is most effective to choose $\|\delta\mathbf{x}\|^3$ to be around floating point precision. If f were instead a vector quantity, then the error quantity computed on the left hand side would be a vector, which should be nearly zero. Second order derivatives are tested against first order derivatives.

References

[1] I. Anonymous. Energetically consistent invertible elasticity. 2012.