Formulation of Gradient and Hessian Terms of the Distortion-Dilation Term

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1. Introduction

The distortion-dilation functional of an n-dimensional (i.e., 2D or 3D) mesh to minimize is:

$$\boxed{I_h(\boldsymbol{R}) = \sum_{c=1}^{N\text{cells}} \int_{\hat{\Omega}_c} E_\theta(S_c(\boldsymbol{R}))d\boldsymbol{\xi}}\,, \tag{1}$$

where:

- $\boldsymbol{R} \in \mathcal{R}^{n \times N_{\text{nodes}}}$ is a vector containing the node locations of the mesh in the physical domain
- $S(\boldsymbol{R})$ is the Jacobian of the mapping from the physical cell to the reference cell. The dependence of this mapping on the node locations $\boldsymbol{R}$ is made explicit.
- $\boldsymbol{\xi}$ denotes the multidimensional reference coordinates.
- $E_\theta(S(\boldsymbol{R}))$ is the distortion-dilation function.

The distortion-dilation function is given by

$$\boxed{E_\theta(S(\boldsymbol{R})) = (1-\theta)\beta(S(\boldsymbol{R})) + \theta\mu(S(\boldsymbol{R}))}\,, \tag{2}$$

where θ is a weight between zero and one, and β and μ are measures of element distortion and dilation, given by:

$$\boxed{\beta(S(\boldsymbol{R})) = \frac{\left(\frac{1}{n}\text{tr}(S^T S(\boldsymbol{R}))\right)^{\frac{n}{2}}}{\chi_\epsilon(|S(\boldsymbol{R})|)}} \tag{3}$$

and

$$\mu(S(\boldsymbol{R})) = \frac{v + \frac{|S(\boldsymbol{R})|^2}{v}}{2\chi_\epsilon(|S(\boldsymbol{R})|}, \tag{4}$$

where n is the dimension of the mesh, $|S|$ denotes the determinant of S, and v is the arithmetic average value of the element-averaged $|S|$. The function $\chi_\epsilon(|S|)$ is used in place of $|S|$ such that the metrics are well-defined for degenerate and folded elements:

$$\chi_\epsilon(|S|) = \frac{1}{2}\left(|S| + \sqrt{\epsilon^2 + |S|^2}\right), \tag{5}$$

where ϵ is a small number that prevents χ_ϵ from being zero. For brevity, $\chi_\epsilon(|S|$ and it's first ($\chi'_\epsilon(|S|)$) and second ($\chi''_\epsilon(|S|)$) derivatives with respect to $\det(S)$ will be abbreviated by χ_ϵ, χ'_ϵ, and χ''_ϵ, respectively. These functions will never take parameters other than $\det(S)$.

2. Minimization Proceedure

We utilize Newton's method to solve the following minimization problem:

$$\boldsymbol{R}_{\text{smooth}} = \arg\min_{\boldsymbol{R}} I_h(\boldsymbol{R})\,. \tag{6}$$

At the minimum of I_h, the gradient of I_h with respect to the components of $\boldsymbol{R}$ will be zero:

$$\nabla_{\boldsymbol{R}} I_h(\boldsymbol{R})|_{\boldsymbol{R}_{\text{smooth}}} = \boldsymbol{0}\,. \tag{7}$$

Newton's method can be used to find $\boldsymbol{R}_{\text{smooth}}$. The update iteration $k+1$ is:

$$\boldsymbol{R}^{k+1} = \boldsymbol{R}^k - H^{-1}(I_h(\boldsymbol{R}^k))\nabla_{\boldsymbol{R}} I_h(\boldsymbol{R}^k)\,. \tag{8}$$

where $H(I_h)$ denotes the Jacobian of the gradient of I_h (i.e., the Hessian):

$$H(I_h) = \nabla_{\boldsymbol{R}}\nabla_{\boldsymbol{R}} I_h\,. \tag{9}$$

It is clear that in order to use Newton's method, we must first write down expressions for the gradient and Hessian of I_h.

3. Matrix Calculus Identities

Some matrix calculus identities are important in this work. In this context, S is a square matrix. The derivative of a scalar-valued function $f(S)$ with respect to S is a matrix with the k, l entry given by

$$\left(\frac{\partial f(S)}{\partial S}\right)_{kl} = \frac{\partial f(S)}{\partial S_{kl}}\,. \tag{10}$$

The following identities hold for the matrix derivatives of $f(S) = |S|$ and $f(S) = \mathrm{tr}(S^T S)$:

$$\boxed{\frac{\partial |S|}{\partial S} = |S| S^{-T}}\,, \tag{11}$$

$$\boxed{\frac{\partial \mathrm{tr}(S^T S)}{\partial S} = 2S}\,. \tag{12}$$

The derivative of a matrix-valued function $F(S)$ with respect to S is a fourth-order tensor with the i, j, k, ℓ entry given by

$$\left(\frac{\partial F(S)}{\partial S}\right)_{ijk\ell} = \frac{\partial F(S)_{ij}}{\partial S_{k\ell}}\,. \tag{13}$$

The following identity holds for the matrix derivative of S^{-T} with respect to S:

$$\boxed{\left(\frac{\partial S^{-T}}{\partial S}\right)_{ijk\ell} = -S^{-1}_{li} S^{-1}_{jk}}\,. \tag{14}$$

4. Gradient of $\boldsymbol{I_h}$

The gradient of I_h is given by

$$\begin{aligned} \nabla_{\boldsymbol{R}} I_h(\boldsymbol{R}) &= \sum_{c=1}^{N\text{cells}} \int_{\hat{\Omega}_c} \nabla_{\boldsymbol{R}} E_\theta(S_c(\boldsymbol{R})) d\boldsymbol{\xi} \\ &= \sum_{c=1}^{N\text{cells}} \int_{\hat{\Omega}_c} \left((1-\theta)\nabla_{\boldsymbol{R}} \beta(S_c(\boldsymbol{R})) + \theta \nabla_{\boldsymbol{R}} \mu(S_c(\boldsymbol{R}))\right) d\boldsymbol{\xi}\,. \end{aligned} \tag{15}$$

It follows that we need to compute $\nabla_{\boldsymbol{R}} \beta$ and $\nabla_{\boldsymbol{R}} \mu$.

4.1. $\nabla_{\boldsymbol{R}}\beta$

By definition,

$$\nabla_{\boldsymbol{R}}\beta(\boldsymbol{R}) = \nabla_{\boldsymbol{R}} \frac{\left(\frac{1}{n}\mathrm{tr}(S^T S(\boldsymbol{R}))\right)^{\frac{n}{2}}}{\chi_\epsilon(|S(\boldsymbol{R})|)} \,. \tag{16}$$

Denoting the gradient with respect to $\boldsymbol{R}$ (i.e., $\nabla_{\boldsymbol{R}}$) by $\partial/\partial\boldsymbol{R}$, and employing chain rule,

$$\begin{aligned} \nabla_{\boldsymbol{R}}\beta(\boldsymbol{R}) &= \frac{\partial}{\partial\boldsymbol{R}}\beta(\boldsymbol{R}) \\ &= \frac{\partial\beta(\boldsymbol{R})}{\partial S}\frac{\partial S}{\partial\boldsymbol{R}} \,, \end{aligned} \tag{17}$$

or element-wise,

$$\begin{aligned} \nabla_{\boldsymbol{R}_\ell}\beta(\boldsymbol{R}) &= \frac{\partial}{\partial\boldsymbol{R}_\ell}\beta(\boldsymbol{R}) \\ &= \sum_a\sum_b \frac{\partial\beta(\boldsymbol{R})}{\partial S_{ab}}\frac{\partial S_{ab}}{\partial\boldsymbol{R}_\ell} \,. \end{aligned} \tag{18}$$

First, we will compute the term $\partial S/\partial\boldsymbol{R}$. In libMesh, the Jacobian matrix within cell c, $S(\boldsymbol{R}_c)$, has the following representation:

$$S(\boldsymbol{R}_c) = \sum_{m=1}^{N_{\mathrm{nodes},c}} \boldsymbol{R}_{c,m}(\nabla_{\boldsymbol{\xi}}\phi_m(\boldsymbol{\xi}))^T \,, \tag{19}$$

where $\boldsymbol{R}_{c,m} \in \mathcal{R}^n$ are the physical coordinates of the m-th node in cell c and ϕ_m is the spatial basis function for the m-th node. Note that this Jacobian matrix is of shape (n, n). The expression for element i, j is:

$$S(\boldsymbol{R}_c)_{ij} = \sum_{m=1}^{N_{\mathrm{nodes},c}} R_{c,m,i}\partial_{\xi_j}\phi_m(\boldsymbol{\xi}) \,, \tag{20}$$

where $R_{c,m,i}$ denotes the coordinate in the i-th dimension of node $\boldsymbol{R}_{c,m}$ and ∂_{ξ_j} denotes the j-th component of the gradient operator $\nabla_{\boldsymbol{\xi}}$. Using this definition, we see that

$$\boxed{\frac{\partial S(\boldsymbol{R}_c)_{i,j}}{\partial R_{c,m,k}} = \delta_{ik}\partial_{\xi_j}\phi_m(\boldsymbol{\xi})} \,. \tag{21}$$

Because Eq. (21) holds for $i, j \in [0, n)$ and $k \in [0, n \times N_{\text{nodes}})$, $\partial S/\partial \boldsymbol{R}$ is a third-order tensor (i.e., the derivative of a matrix with respect to a vector).

Next, we will compute the $\partial\beta/\partial S$ term. Note that in all derivations, we use product + chain rules as opposed to quotient rule because quotient rule sucks. Quotient rule is fake math invented by Big Mathematics so they had extra material to put in textbooks and sell them for more. On top of that, anyone who prefers to use quotient rule instead of writing $1/\chi_\epsilon = \chi_\epsilon^{-1}$ is obviously delusional and should not be trusted. Also note that we utilized the identities from Section 3 when using chain rule.

$$\begin{aligned}\frac{\partial\beta}{\partial S} &= \frac{\partial}{\partial S}\frac{\left(\frac{1}{n}\text{tr}(S^TS)\right)^{\frac{n}{2}}}{\chi_\epsilon} \\ &= \frac{\frac{n}{2}\left(\frac{1}{n}\text{tr}(S^TS)\right)^{\frac{n}{2}-1}\frac{1}{n}2S}{\chi_\epsilon} - \frac{\left(\frac{1}{n}\text{tr}(S^TS)\right)^{\frac{n}{2}}}{\chi_\epsilon^2}\frac{\partial\chi_\epsilon(|S|)}{\partial S} \\ &= \boxed{\left(\frac{\left(\frac{1}{n}\text{tr}(S^TS)\right)^{\frac{n}{2}-1}}{\chi_\epsilon}\right)S - \left(\frac{\left(\frac{1}{n}\text{tr}(S^TS)\right)^{\frac{n}{2}}}{\chi_\epsilon^2}\chi_\epsilon'|S|\right)S^{-T}},\end{aligned} \tag{22}$$

where we have used

$$\boxed{\frac{\partial\chi_\epsilon}{\partial S} = \underbrace{\frac{1}{2}\left(1 + \frac{|S|}{\sqrt{\epsilon^2 + |S|^2}}\right)}_{\chi_\epsilon'}|S|S^{-T}}. \tag{23}$$

The results of Eqs. (21) and (22) can be substituted into Eq. (17) and Eq. (18) to obtain $\nabla_{\boldsymbol{R}}\beta(\boldsymbol{R})$ in terms of S and ϕ_l. Note that Eq. (21) is a rank 3 tensor of dimension $(n, n, n \times N_{\text{nodes}})$ and Eq. (22) is a matrix of dimension (n, n):

$$\nabla_{\boldsymbol{R}}\beta(\boldsymbol{R}) = \underbrace{\frac{\partial\beta(\boldsymbol{R})}{\partial S}}_{(n,n)}\underbrace{\frac{\partial S}{\partial\boldsymbol{R}}}_{(n,n,n\times N_{\text{nodes}})} \tag{24}$$

The expected result for the gradient of a scalar function is a vector, which can be obtained by first multiplying common dimensions together and then summing over them to obtain a vector of length $n \times N_{\text{nodes}}$. Using Einstein notation, the ℓ-th entry of this vector is given by

$$\boxed{(\nabla_{\boldsymbol{R}}\beta)_\ell = \left(\frac{\partial\beta}{\partial S}\right)_{ab}\left(\frac{\partial S}{\partial\boldsymbol{R}}\right)_{ab\ell}}. \tag{25}$$

This result is in agreement with Eq. (18).

4.2. $\nabla_{\boldsymbol{R}}\mu$

By definition,

$$\nabla_{\boldsymbol{R}}\mu(\boldsymbol{R}) = \nabla_{\boldsymbol{R}} \frac{v + \frac{|S(\boldsymbol{R})|^2}{v}}{2\chi_\epsilon(|S(\boldsymbol{R})|)} . \tag{26}$$

Using chain rule in the same manner as the previous section,

$$\begin{aligned} \nabla_{\boldsymbol{R}}\mu(\boldsymbol{R}) &= \frac{\partial}{\partial \boldsymbol{R}}\mu(\boldsymbol{R}) \\ &= \frac{\partial \mu(\boldsymbol{R})}{\partial S}\frac{\partial S}{\partial \boldsymbol{R}} . \end{aligned} \tag{27}$$

The $\partial S/\partial \boldsymbol{R}$ term is given by Eq. (21). Using product rule and the Section 3 identities for chain rule,

$$\begin{aligned} \frac{\partial \mu}{\partial S} &= \frac{\partial}{\partial S}\left(\frac{v + \frac{|S|^2}{v}}{2\chi_\epsilon}\right) \\ &= \left(\frac{|S|^2}{v\chi_\epsilon}\right) S^{-T} - \left[\frac{v + \frac{|S|^2}{v}}{2\chi_\epsilon^2}\right]\frac{\partial \chi_\epsilon}{\partial S} \\ &= \left(\frac{|S|^2}{v\chi_\epsilon}\right) S^{-T} - \left(\left[\frac{v + \frac{|S|^2}{v}}{2\chi_\epsilon^2}\right]\chi_\epsilon'|S|\right) S^{-T} \\ &= \frac{|S|}{\chi_\epsilon}\left(\frac{|S|}{v} - \left[\frac{v + \frac{|S|^2}{v}}{2\chi_\epsilon}\right]\chi_\epsilon'\right) S^{-T} \\ &= \boxed{\underbrace{\frac{1}{2v\chi_\epsilon}\left(-\chi_\epsilon'|S|^3 + 2\chi_\epsilon|S|^2 - v^2\chi_\epsilon'|S|\right)}_{:=\alpha(S)} S^{-T}} , \end{aligned} \tag{28}$$

where χ_ϵ' is given by Eq. (23). The results of Eqs. (21) and (28) can be substituted into Eq. (27) to obtain $\nabla_{\boldsymbol{R}}\mu(\boldsymbol{R})$ in terms of S and ϕ_l. Note that Eq. (21) is a rank 3 tensor of dimension $(n, n, n \times N_{\text{nodes}})$ and Eq. (22) is a matrix of dimension (n, n):

$$\nabla_{\boldsymbol{R}}\mu(\boldsymbol{R}) = \underbrace{\frac{\partial \mu(\boldsymbol{R})}{\partial S}}_{(n,n)} \underbrace{\frac{\partial S}{\partial \boldsymbol{R}}}_{(n,n,n\times N_{\text{nodes}})} . \tag{29}$$

The expected result for the gradient of a scalar function is a vector, which can be obtained by first multiplying common dimensions together and then summing over them to obtain a vector of length $n \times N_{\text{nodes}}$. Using Einstein notation, the ℓ-th entry of this vector is given by

$$\boxed{(\nabla_{\boldsymbol{R}}\mu)_\ell = \left(\frac{\partial \mu}{\partial S}\right)_{ab}\left(\frac{\partial S}{\partial \boldsymbol{R}}\right)_{ab\ell}}\,. \tag{30}$$

5. Hessian of I_h

The Hessian of I_h is given by

$$\begin{aligned} H(I_h(\boldsymbol{R})) &= \sum_{c=1}^{N\text{cells}} \int_{\hat{\Omega}_c} H(E_\theta(S_c(\boldsymbol{R})))d\boldsymbol{\xi} \\ &= \sum_{c=1}^{N\text{cells}} \int_{\hat{\Omega}_c} \left((1-\theta)H(\beta(S_c(\boldsymbol{R}))) + \theta H(\mu(S_c(\boldsymbol{R})))\right) d\boldsymbol{\xi}\,. \end{aligned} \tag{31}$$

Computing the Hessian of I_h entails the computation of the Jacobian of the gradient of I_h, or loosely speaking,

$$H(I_h) = \nabla_{\boldsymbol{R}}\nabla_{\boldsymbol{R}} I_h\,. \tag{32}$$

We computed the gradient of I_h ($\nabla_{\boldsymbol{R}} I_h$) in the previous section. To compute the Hessian, we simply need to take the Jacobian of those results.

5.1. $\nabla_{\boldsymbol{R}}\nabla_{\boldsymbol{R}}\beta$

From Section 4.1, we have

$$\begin{aligned} \nabla_{\boldsymbol{R}}\beta(\boldsymbol{R}) &= \frac{\partial \beta(\boldsymbol{R})}{\partial S}\frac{\partial S}{\partial \boldsymbol{R}}\,, \\ \frac{\partial S(\boldsymbol{R}_c)_{i,j}}{\partial R_{c,m,k}} &= \delta_{ik}\partial_{\xi_j}\phi_m(\boldsymbol{\xi})\,, \\ \frac{\partial \beta(\boldsymbol{R})}{\partial S_{k\ell}} &= \left(\frac{\left(\frac{1}{n}\mathrm{tr}(S^TS)\right)^{\frac{n}{2}-1}}{\chi_\epsilon}\right) S_{k\ell} - \left(\frac{\left(\frac{1}{n}\mathrm{tr}(S^TS)\right)^{\frac{n}{2}}}{\chi_\epsilon^2}\chi_\epsilon'|S|\right) S_{k\ell}^{-T}\,. \end{aligned} \tag{33}$$

Applying another derivative with respect to $\boldsymbol{R}$, the Hessian of β is expressed as:

$$
\begin{aligned}
H(\beta(\boldsymbol{R})) &= \frac{\partial}{\partial \boldsymbol{R}} \left(\frac{\partial \beta(\boldsymbol{R})}{\partial S} \frac{\partial S}{\partial \boldsymbol{R}} \right) \\
&= \frac{\partial}{\partial \boldsymbol{R}} \left(\frac{\partial \beta(\boldsymbol{R})}{\partial S} \right) \frac{\partial S}{\partial \boldsymbol{R}} + \frac{\partial \beta(\boldsymbol{R})}{\partial S} \frac{\partial}{\partial \boldsymbol{R}} \left(\frac{\partial S}{\partial \boldsymbol{R}} \right) \\
&= \frac{\partial}{\partial S} \left(\frac{\partial \beta(\boldsymbol{R})}{\partial S} \right) \frac{\partial S}{\partial \boldsymbol{R}} \frac{\partial S}{\partial \boldsymbol{R}} + \frac{\partial \beta(\boldsymbol{R})}{\partial S} \underbrace{\frac{\partial^2 S}{\partial \boldsymbol{R}^2}}_{=0 \text{ by } Eq.\ (21)} \\
&= \frac{\partial^2 \beta(\boldsymbol{R})}{\partial S^2} \frac{\partial S}{\partial \boldsymbol{R}} \frac{\partial S}{\partial \boldsymbol{R}} .
\end{aligned}
\tag{34}
$$

Entry-wise, this is

$$
\begin{aligned}
H(\beta(\boldsymbol{R}))_{\ell p} &= \left(\frac{\partial}{\partial \boldsymbol{R}} \left(\frac{\partial}{\partial \boldsymbol{R}} \beta(\boldsymbol{R}) \right)_{\ell} \right)_{p} \\
&= \frac{\partial}{\partial R_p} \frac{\partial}{\partial R_\ell} \beta(\boldsymbol{R}) \\
&= \frac{\partial}{\partial R_p} \sum_a \sum_b \left(\frac{\partial \beta(\boldsymbol{R})}{\partial S_{ab}} \frac{\partial S_{ab}}{\partial R_\ell} \right) \\
&= \sum_a \sum_b \left[\frac{\partial}{\partial R_p} \left(\frac{\partial \beta(\boldsymbol{R})}{\partial S_{ab}} \right) \frac{\partial S_{ab}}{\partial R_\ell} + \frac{\partial \beta(\boldsymbol{R})}{\partial S_{ab}} \frac{\partial}{\partial R_p} \left(\frac{\partial S_{ab}}{\partial R_\ell} \right) \right] \\
&= \sum_a \sum_b \left[\sum_i \sum_j \frac{\partial}{\partial S_{ij}} \left(\frac{\partial \beta(\boldsymbol{R})}{\partial S_{ab}} \right) \frac{\partial S_{ab}}{\partial R_\ell} \frac{\partial S_{ij}}{\partial R_p} + \frac{\partial \beta(\boldsymbol{R})}{\partial S_{ab}} \underbrace{\frac{\partial^2 S_{ab}}{\partial R_p \partial R_\ell}}_{=0 \text{ by } Eq.\ (21)} \right] \\
&= \sum_a \sum_b \frac{\partial S_{ab}}{\partial R_\ell} \sum_i \sum_j \left(\frac{\partial^2 \beta(\boldsymbol{R})}{\partial S_{ij} \partial S_{ab}} \right) \left(\frac{\partial S_{ij}}{\partial R_p} \right) .
\end{aligned}
\tag{35}
$$

The term $\partial S / \partial \boldsymbol{R}$ is given by Eq. (21). The term $\partial^2 \beta / \partial S^2$ is given by differentiating Eq. (22) with respect to S. Using the identities from Section

3,

$$
\begin{aligned}
\frac{\partial^2 \beta(\boldsymbol{R})}{\partial S_{ab} \partial S_{ij}} &= \frac{\partial}{\partial S_{ab}} \left[\left(\frac{\left(\frac{1}{n}\operatorname{tr}(S^T S)\right)^{\frac{n}{2}-1}}{\chi_\epsilon} \right) S_{ij} - \left(\frac{\left(\frac{1}{n}\operatorname{tr}(S^T S)\right)^{\frac{n}{2}}}{\chi_\epsilon^2} \chi'_\epsilon |S| \right) S_{ij}^{-T} \right] \\
&= \frac{1}{\chi_\epsilon} \left[\frac{n-2}{2} \left(\frac{1}{n}\operatorname{tr}(S^T S) \right)^{\frac{n}{2}-2} \frac{2 S_{ab}}{n} S_{ij} + \left(\frac{1}{n}\operatorname{tr}(S^T S) \right)^{\frac{n}{2}-1} I_{ia} I_{jb} \right] \\
&- \frac{1}{\chi_\epsilon^2} \left(\frac{1}{n}\operatorname{tr}(S^T S) \right)^{\frac{n}{2}-1} \chi'_\epsilon |S| S_{ab}^{-T} S_{ij} \\
&- \frac{1}{\chi_\epsilon^2} \left[\frac{n}{2} \left(\frac{1}{n}\operatorname{tr}(S^T S) \right)^{\frac{n}{2}-1} \frac{2 S_{ab}}{n} \chi'_\epsilon |S| S_{ij}^{-T} \right. \\
&+ \left(\frac{1}{n}\operatorname{tr}(S^T S) \right)^{\frac{n}{2}} \chi''_\epsilon |S|^2 S_{ab}^{-T} S_{ij}^{-T} \\
&+ \left. \left(\frac{1}{n}\operatorname{tr}(S^T S) \right)^{\frac{n}{2}} \chi'_\epsilon |S| S_{ab}^{-T} S_{ij}^{-T} \right] \\
&+ \frac{2}{\chi_\epsilon^3} \left[\left(\frac{1}{n}\operatorname{tr}(S^T S) \right)^{\frac{n}{2}} \chi'_\epsilon |S| S_{ab}^{-T} \chi'_\epsilon |S| S_{ij}^{-T} \right] \\
&+ \left(\frac{\left(\frac{1}{n}\operatorname{tr}(S^T S)\right)^{\frac{n}{2}}}{\chi_\epsilon^2} \chi'_\epsilon |S| \right) S_{bi}^{-1} S_{ja}^{-1} \\
&\boxed{\displaystyle = \left[\left(\frac{1}{n}\operatorname{tr}(S^T S) \right)^{\frac{n}{2}-1} \frac{1}{\chi_\epsilon} \right] I_{ia} I_{jb} + \left[\frac{n-2}{n \chi_\epsilon} \left(\frac{1}{n}\operatorname{tr}(S^T S) \right)^{\frac{n}{2}-2} \right] S_{ab} S_{ij}} \\
&\boxed{\displaystyle - \left[\left(\frac{1}{n}\operatorname{tr}(S^T S) \right)^{\frac{n}{2}-1} \frac{\chi'_\epsilon |S|}{\chi_\epsilon^2} \right] S_{ba}^{-1} S_{ij} - \left[\left(\frac{1}{n}\operatorname{tr}(S^T S) \right)^{\frac{n}{2}-1} \frac{\chi'_\epsilon |S|}{\chi_\epsilon^2} \right] S_{ab} S_{ji}^{-1}} \\
&\boxed{\displaystyle + \left(\frac{1}{n}\operatorname{tr}(S^T S) \right)^{\frac{n}{2}} \left(\frac{|S|}{\chi_\epsilon^2} \right) \left[\frac{2 {\chi'_\epsilon}^2 |S|}{\chi_\epsilon} - \chi''_\epsilon |S| - \chi'_\epsilon \right] S_{ba}^{-1} S_{ji}^{-1}} \\
&\boxed{\displaystyle - \left(\frac{\left(\frac{1}{n}\operatorname{tr}(S^T S)\right)^{\frac{n}{2}}}{\chi_\epsilon^2} \chi'_\epsilon |S| \right) S_{bi}^{-1} S_{ja}^{-1}} .
\end{aligned}
\tag{36}
$$

where

$$\boxed{\chi_\epsilon'' = \frac{1}{2}\left(\frac{1}{\sqrt{\epsilon^2+|S|^2}} - \frac{|S|^2}{(\epsilon^2+|S|^2)^{3/2}}\right)}\,. \tag{37}$$

5.2. $\nabla_{\boldsymbol{R}}\nabla_{\boldsymbol{R}}\mu$

From Section 4.2, we have

$$\begin{aligned}
\nabla_{\boldsymbol{R}}\mu(\boldsymbol{R}) &= \frac{\partial \mu(\boldsymbol{R})}{\partial S}\frac{\partial S}{\partial \boldsymbol{R}}\,,\\
\frac{\partial S(\boldsymbol{R}_c)_{i,j}}{\partial R_{c,m,k}} &= \delta_{ik}\partial_{\xi_j}\phi_m(\boldsymbol{\xi})\,,\\
\frac{\partial \mu(\boldsymbol{R})}{\partial S} &= \alpha(S)S^{-T}\,,\\
\alpha(S) &= \frac{1}{2v\chi_\epsilon}\left(-\chi_\epsilon'|S|^3 + 2\chi_\epsilon|S|^2 - v^2\chi_\epsilon'|S|\right)\,.
\end{aligned} \tag{38}$$

Applying another derivative with respect to $\boldsymbol{R}$, the Hessian of μ is expressed as:

$$\begin{aligned}
H(\mu(\boldsymbol{R})) &= \frac{\partial}{\partial \boldsymbol{R}}\left(\frac{\partial \mu(\boldsymbol{R})}{\partial S}\frac{\partial S}{\partial \boldsymbol{R}}\right)\\
&= \frac{\partial}{\partial \boldsymbol{R}}\left(\frac{\partial \mu(\boldsymbol{R})}{\partial S}\right)\frac{\partial S}{\partial \boldsymbol{R}} + \frac{\partial \mu(\boldsymbol{R})}{\partial S}\frac{\partial}{\partial \boldsymbol{R}}\left(\frac{\partial S}{\partial \boldsymbol{R}}\right)\\
&= \frac{\partial}{\partial S}\left(\frac{\partial \mu(\boldsymbol{R})}{\partial S}\right)\frac{\partial S}{\partial \boldsymbol{R}}\frac{\partial S}{\partial \boldsymbol{R}} + \frac{\partial \mu(\boldsymbol{R})}{\partial S}\underbrace{\frac{\partial^2 S}{\partial \boldsymbol{R}^2}}_{=0 \text{ by } Eq.\ (21)}\\
&= \frac{\partial^2 \mu(\boldsymbol{R})}{\partial S^2}\frac{\partial S}{\partial \boldsymbol{R}}\frac{\partial S}{\partial \boldsymbol{R}}\,.
\end{aligned} \tag{39}$$

Entry-wise, this is

$$
\begin{aligned}
H(\mu(\boldsymbol{R}))_{\ell p} &= \left(\frac{\partial}{\partial \boldsymbol{R}}\left(\frac{\partial}{\partial \boldsymbol{R}}\mu(\boldsymbol{R})\right)_{\ell}\right)_{p} \\
&= \frac{\partial}{\partial R_p}\frac{\partial}{\partial R_\ell}\mu(\boldsymbol{R}) \\
&= \frac{\partial}{\partial R_p}\sum_a\sum_b\left(\frac{\partial \mu(\boldsymbol{R})}{\partial S_{ab}}\frac{\partial S_{ab}}{\partial R_\ell}\right) \\
&= \sum_a\sum_b\left[\frac{\partial}{\partial R_p}\left(\frac{\partial \mu(\boldsymbol{R})}{\partial S_{ab}}\right)\frac{\partial S_{ab}}{\partial R_\ell} + \frac{\partial \mu(\boldsymbol{R})}{\partial S_{ab}}\frac{\partial}{\partial R_p}\left(\frac{\partial S_{ab}}{\partial R_\ell}\right)\right] \\
&= \sum_a\sum_b\left[\sum_i\sum_j\frac{\partial}{\partial S_{ij}}\left(\frac{\partial \mu(\boldsymbol{R})}{\partial S_{ab}}\right)\frac{\partial S_{ab}}{\partial R_\ell}\frac{\partial S_{ij}}{\partial R_p} + \frac{\partial \mu(\boldsymbol{R})}{\partial S_{ab}}\underbrace{\frac{\partial^2 S_{ab}}{\partial R_p \partial R_\ell}}_{=0 \text{ by } Eq.\ (21)}\right] \\
&= \sum_a\sum_b\frac{\partial S_{ab}}{\partial R_\ell}\sum_i\sum_j\left(\frac{\partial^2 \mu(\boldsymbol{R})}{\partial S_{ij}\partial S_{ab}}\right)\left(\frac{\partial S_{ij}}{\partial R_p}\right).
\end{aligned}
\tag{40}
$$

The term $\partial S/\partial \boldsymbol{R}$ is given by Eq. (21). The term $\partial^2\mu/\partial S^2$ is given by differentiating Eq. (28) with respect to S. Using the identities from Section

3,

$$
\begin{aligned}
\frac{\partial^2 \mu(\boldsymbol{R})}{\partial S_{ab} \partial S_{ij}} &= \frac{\partial}{\partial S_{ab}} \alpha(S) S_{ij}^{-T} \\
&= \left(\frac{\partial}{\partial S_{ab}} \alpha(S) \right) S_{ij}^{-T} + \alpha(S) \frac{\partial}{\partial S_{ab}} S_{ij}^{-T} \\
&= \frac{\partial}{\partial S_{ab}} \left(\frac{1}{2v\chi_\epsilon} \left(-\chi_\epsilon' |S|^3 + 2\chi_\epsilon |S|^2 - v^2 \chi_\epsilon' |S| \right) \right) S_{ij}^{-T} + \alpha(S) S_{bi}^{-1} S_{ja}^{-1} \\
&= \Bigg(-\frac{2\alpha(S)\chi_\epsilon' |S| S_{ab}^{-T}}{\chi_\epsilon} + \frac{1}{2v\chi_\epsilon^2} \big(-\chi_\epsilon'' |S|^4 S_{ab}^{-T} - 3\chi_\epsilon' |S|^3 S_{ab}^{-T} + 2\chi_\epsilon' |S|^3 S_{ab}^{-T} \\
&\quad + 4\chi_\epsilon |S|^2 S_{ab}^{-T} - v^2 \chi_\epsilon' |S| S_{ab}^{-T} - v^2 |S|^2 \chi_\epsilon'' S_{ab}^{-T} \big) \Bigg) S_{ij}^{-T} + \alpha(S) S_{bi}^{-1} S_{ja}^{-1} \\
&\boxed{= \frac{|S|}{2v\chi_\epsilon^2} \Big(-4v\alpha(S)\chi_\epsilon \chi_\epsilon' - \chi_\epsilon'' |S|^3 - \chi_\epsilon' |S|^2 + 4\chi_\epsilon |S| - v^2 \left(\chi_\epsilon' + |S| \chi_\epsilon'' \right) \Big) S_{ba}^{-1} S_{ji}^{-1}} \\
&\boxed{+ \alpha(S) S_{bi}^{-1} S_{ja}^{-1}} .
\end{aligned}
\tag{41}
$$