Anisotropic Elasticity for Inversion-Safety and Element Rehabilitation (Supplement)

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1 MATRIX AND TENSOR NOTATION

We closely follow the tensor notation of Smith et al. [2019]. Generalized n-th order tensor notations are available (e.g. Einstein notation), but we are only dealing with 3$^{\text{rd}}$- and 4$^{\text{th}}$-order tensors, so we have found it useful to use a notation that is specialized to these orders. For readability, we will be presenting the 2D versions of tensors and matrices, as the 3D versions can become quite large.

1.1 3$^{\text{rd}}$-order Tensors

Many tensor conventions and interpretations are available [Kolda and Bader 2009; Simmonds 2012], but we specifically choose to view 3$^{\text{rd}}$order tensors as a *vector of matrices*. The key tensor that arises of this form is $\frac{\partial \mathbf{F}}{\partial \mathbf{u}}$, i.e. the gradient of the deformation gradient with respect to displacement. In 2D, this tensor is $\frac{\partial \mathbf{F}}{\partial \mathbf{u}} \in \Re^{2\times2\times6}$,

$$\frac{\partial \mathbf{F}}{\partial \mathbf{u}} = \left[\left[\frac{\partial \mathbf{F}}{\partial \mathbf{u}_0} \right] \quad \left[\frac{\partial \mathbf{F}}{\partial \mathbf{u}_1} \right] \quad \left[\frac{\partial \mathbf{F}}{\partial \mathbf{u}_2} \right] \dots \left[\frac{\partial \mathbf{F}}{\partial \mathbf{u}_5} \right], \right] \tag{1}$$

where each individual $\frac{\partial \mathbf{F}}{\partial \mathbf{u}_i} \in \Re^{2\times2}$. This specific tensor arises when we convert a PK1 into the force vector for a triangle element:

$$\mathbf{f}_{\text{orce}} = \frac{\partial \mathbf{F}}{\partial \mathbf{u}}^T : \mathbf{P}(\mathbf{F}). \tag{2}$$

Here, the double contraction (:) denotes a generalized dot product,

$$\mathbf{A} : \mathbf{B} = \sum_{i=0}^{n} \sum_{j=0}^{n} \mathbf{A}_{ij} \mathbf{B}_{ij}, \tag{3}$$

$$\begin{bmatrix} a & c \\ b & d \end{bmatrix} : \begin{bmatrix} e & g \\ f & h \end{bmatrix} = ae + bf + cg + dh, \tag{4}$$

$$\begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix} : \begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix} = (1 + 4 + 9 + 16) = 30, \tag{5}$$

but an indexing convention needs to be defined when the tensor orders are mismatched. We use the following ordering to contract 3$^{\text{rd}}$- and 2$^{\text{nd}}$-order tensors:

$$\frac{\partial \mathbf{F}}{\partial \mathbf{u}}^T : \mathbf{P}(\mathbf{F}) = \left[\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix} \dots \begin{bmatrix} 6 & 6 \\ 6 & 6 \end{bmatrix} \right]^T : \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 4 \\ 8 \\ 12 \\ 16 \\ 20 \\ 24 \end{bmatrix}. \tag{6}$$

Notably, while the overall vector is transposed, each individual $\frac{\partial \mathbf{F}}{\partial \mathbf{u}_i}$ is not.

1.2 4$^{\text{th}}$-order Tensors

4$^{\text{th}}$-order tensors arise when we take the Hessian of a strain energy, $\frac{\partial^2 \Psi(\mathbf{F})}{\partial \mathbf{F}^2}$, though it can sometimes be helpful to phrase it as the gradient of the PK1 $\frac{\partial \mathbf{P}(\mathbf{F})}{\partial \mathbf{F}}$, i.e. the matrix-valued-gradient ($\mathbf{F} \in \Re^{2\times2}$) of a matrix ($\mathbf{P}(\mathbf{F}) \in \Re^{2\times2}$). From this perspective, it is natural to interpret this tensor as a *matrix of matrices*:

$$\frac{\partial \mathbf{P}(\mathbf{F})}{\partial \mathbf{F}} = \begin{bmatrix} \left[\frac{\partial \mathbf{P}(\mathbf{F})}{\partial \mathbf{F}_{00}} \right] & \left[\frac{\partial \mathbf{P}(\mathbf{F})}{\partial \mathbf{F}_{01}} \right] \\ \left[\frac{\partial \mathbf{P}(\mathbf{F})}{\partial \mathbf{F}_{10}} \right] & \left[\frac{\partial \mathbf{P}(\mathbf{F})}{\partial \mathbf{F}_{11}} \right] \end{bmatrix}, \tag{7}$$

A double contraction convention must then be established, and we use the following:

$$\frac{\partial \mathbf{P}(\mathbf{F})}{\partial \mathbf{F}} : \mathbf{X} = \begin{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} & \begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix} \\ \begin{bmatrix} 3 & 3 \\ 3 & 3 \end{bmatrix} & \begin{bmatrix} 4 & 4 \\ 4 & 4 \end{bmatrix} \end{bmatrix} : \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 4 & 8 \\ 12 & 16 \end{bmatrix}. \tag{8}$$

The notion of an *eigenmatrix* is now well-defined, $\mathbb{A} : \mathbf{X} = \lambda \mathbf{X}$, where $\mathbb{A} \in \Re^{2\times2\times2\times2}$ and $\lambda \in \Re$ is the corresponding eigenvalue.

1.3 Flattening Convention

Any n-th order tensor can be *flattened* (a.k.a *matricized* or *unfolded*) into a matrix. However, there is no one canonical way to flatten a tensor, i.e. there are three ways to flatten a 3$^{\text{rd}}$-order tensor, so the convention should be selected carefully to preserve the tensor's underlying structure.

Following Golub and Van Loan [2012], we define a flattening convention by defining a vectorization operator "vec". Given a matrix

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$\mathbf{A} = \begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix}$, the flattening occurs in column-wise order:

$$\text{vec}(\mathbf{A}) = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}. \tag{9}$$

A 3$^{\text{rd}}$-order tensor is flattened by vectorizing each column:

$$\mathbb{B} = \left[\begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix} \quad \begin{bmatrix} 5 & 7 \\ 6 & 8 \end{bmatrix} \quad \begin{bmatrix} 9 & 11 \\ 10 & 12 \end{bmatrix} \right] \tag{10}$$

$$= \left[\; [\mathbf{B}_0] \quad [\mathbf{B}_1] \quad [\mathbf{B}_2] \; \right] \tag{11}$$

$$\text{vec}(\mathbb{B}) = \left[\; \text{vec}(\mathbf{B}_0) \; \middle| \; \text{vec}(\mathbf{B}_1) \; \middle| \; \text{vec}(\mathbf{B}_2) \; \right] \tag{12}$$

$$= \begin{bmatrix} 1 & 5 & 9 \\ 2 & 6 & 10 \\ 3 & 7 & 11 \\ 4 & 8 & 12 \end{bmatrix}. \tag{13}$$

And a 4$^{\text{th}}$-order tensor is flattened by first flattening the matrix-of-matrices in column-wise order, and then applying vec to each matrix:

$$\mathbb{C} = \begin{bmatrix} \begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix} & \begin{bmatrix} 9 & 11 \\ 10 & 12 \end{bmatrix} \\ \begin{bmatrix} 5 & 7 \\ 6 & 8 \end{bmatrix} & \begin{bmatrix} 13 & 15 \\ 14 & 16 \end{bmatrix} \end{bmatrix} \tag{14}$$

$$= \begin{bmatrix} [\mathbf{C}_{00}] & [\mathbf{C}_{01}] \\ [\mathbf{C}_{10}] & [\mathbf{C}_{11}] \end{bmatrix} \tag{15}$$

$$\text{vec}(\mathbb{C}) = \left[\; \text{vec}(\mathbf{C}_{00}) \; \middle| \; \text{vec}(\mathbf{C}_{10}) \; \middle| \; \text{vec}(\mathbf{C}_{01}) \; \middle| \; \text{vec}(\mathbf{C}_{11}) \; \right] \tag{16}$$

$$= \begin{bmatrix} 1 & 5 & 9 & 13 \\ 2 & 6 & 10 & 14 \\ 3 & 7 & 11 & 15 \\ 4 & 8 & 12 & 16 \end{bmatrix} \tag{17}$$

2 STRAIN ENERGY TENSORS

2.1 Flattening the Energy Hessian, $\frac{\partial^2 \Psi}{\partial \mathbf{F}^2}$

Assume we have an arbitrary hyperelastic, isotropic strain energy Ψ. In order to use this energy in a Newton-type solver, we need to compute the eigensystem of its Hessian. This could be written in either tensor form, $\frac{\partial^2 \Psi}{\partial \mathbf{F}^2} \in \Re^{2\times2\times2\times2}$, or directly in flattened form, $\frac{\partial^2 \Psi}{\partial \mathbf{f}^2} \in \Re^{4\times4}$, where $\text{vec}(\mathbf{F}) = \mathbf{f}$.

It can often be more concise to write the Hessian in flattened form, $\frac{\partial^2 \Psi}{\partial \mathbf{f}^2} \in \Re^{4\times4}$, because the expression can be written in terms of outer products. This is especially helpful when performing an eigenanalysis, because the vectors that comprise the outer products can turn out to be the actual eigenvectors.

Conversely, it can be helpful to write the eigensystems of the Hessian in terms of eigenmatrices. Given the eigenvalues λ_i and eigenmatrices $\mathbf{Q}_i$ of a strain energy, it is straightforward to convert this form back into a flattened Hessian:

$$\frac{\partial^2 \Psi}{\partial \mathbf{f}^2} = \sum_{i=0}^{3} \lambda_i \, \text{vec}(\mathbf{Q}_i) \, \text{vec}(\mathbf{Q}_i)^T. \tag{18}$$

When a Hessian needs to be projected to positive semi-definiteness inside a Newton solver, if simple expressions are available for the $(\mathbf{Q}_i, \lambda_i)$ eigenpairs, then then projection can be realized by merely clamping any negative λ_i to zero.

2.2 Analytic Eigenpairs from Smith et al. [2019]

Simple, closed-form expressions for the $(\mathbf{Q}_i, \lambda_i)$ eigenpairs are the primary findings of Smith et al. [2019]. We summarize the relevant details here.

We denote the 4$^{\text{th}}$-order Hessian $\frac{\partial^2 \Psi}{\partial \mathbf{F}^2} = \mathbb{H}$ and its flattened version as $\text{vec}\left(\frac{\partial^2 \Psi}{\partial \mathbf{F}^2}\right) = \frac{\partial^2 \Psi}{\partial \mathbf{f}^2} = \mathbf{H}$. If $\mathbf{Q}$ is an eigenmatrix of $\mathbb{H}$, then $\text{vec}(\mathbf{Q}) = \mathbf{q}$ is an eigenvector of $\mathbf{H}$. This is important because *the SVD of the eigenmatrix* $\mathbf{Q}$ *can reveal simple structures that are impossible to discover by inspecting the corresponding eigenvector* $\mathbf{q}$.

In particular, let us take the SVD of the deformation gradient $\mathbf{F}$:

$$\mathbf{F} = \mathbf{U}\Sigma\mathbf{V}^T. \tag{19}$$

Smith et al. [2019] defined the following twist ($\mathbf{T}$) and flip ($\mathbf{L}$) matrices in 2D:

$$\mathbf{T} = \frac{1}{\sqrt{2}} \mathbf{U} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \mathbf{V}^T \tag{20}$$

$$\mathbf{L} = \frac{1}{\sqrt{2}} \mathbf{U} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \mathbf{V}^T. \tag{21}$$

Here, the $\mathbf{U}$ and $\mathbf{V}$ are the exact same rotations as those from the SVD of $\mathbf{F}$. Smith et al. [2019] showed that $\mathbf{T}$ and $\mathbf{L}$ are *always* two of the four eigenmatrices in *all* isotropic, hyperelastic energies. An automatic process was also proposed for obtaining closed-form expressions for their corresponding eigenvalues, and it was also shown that simple expressions could often be found for the other two eigenmatrices in 2D.

A similar result was found in 3D, where six of the nine eigenmatrices always have the following closed form:

$$\mathbf{T}_1 = \frac{1}{\sqrt{2}} \mathbf{U} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \mathbf{V}^T \tag{22}$$

$$\mathbf{L}_1 = \frac{1}{\sqrt{2}} \mathbf{U} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \mathbf{V}^T \tag{23}$$

$$\mathbf{T}_2 = \frac{1}{\sqrt{2}}\mathbf{U}\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}\mathbf{V}^T \tag{24}$$

$$\mathbf{L}_2 = \frac{1}{\sqrt{2}}\mathbf{U}\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}\mathbf{V}^T \tag{25}$$

$$\mathbf{T}_3 = \frac{1}{\sqrt{2}}\mathbf{U}\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}\mathbf{V}^T \tag{26}$$

$$\mathbf{L}_3 = \frac{1}{\sqrt{2}}\mathbf{U}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}\mathbf{V}^T. \tag{27}$$

We make use of these eigenmatrices in our current work.

3 THE CHANGE-OF-BASIS TENSOR $\frac{\partial \mathbf{F}_{\text{iso}}}{\partial \mathbf{u}}$

3.1 The Original Tensor

The original, isotropic change-of-basis matrix $\frac{\partial \mathbf{F}}{\partial \mathbf{u}}$ can be written as $\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}} \cdot \mathbf{D}_m^{-1}$, and the entries of the $\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}} \in \Re^{3\times3\times12}$ 3rd-order tensor can be written:

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_0} = \begin{bmatrix} -1 & -1 & -1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_1} = \begin{bmatrix} 0 & 0 & 0 \\ -1 & -1 & -1 \\ 0 & 0 & 0 \end{bmatrix} \tag{28}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_2} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \end{bmatrix} \quad \frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_3} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{29}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_4} = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_5} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \tag{30}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_6} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_7} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{31}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_8} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \quad \frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_9} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{32}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_{10}} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \quad \frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_{11}} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{33}$$

While the tensor is verbose, it clearly has a simple structure.

3.2 The Rehabilitated Tensor

The rehabilitated $\frac{\partial \mathbf{F}_{\text{iso}}}{\partial \mathbf{u}} = \frac{\partial \mathbf{D}_{s,\text{iso}}}{\partial \mathbf{u}} \cdot \mathbf{D}_{s,\text{iso}}^{-1}$ tensor has a more complex form, because $\mathbf{D}_{s,\text{iso}}$ is more complicated. The tensor is:

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_0} = \begin{bmatrix} -1 & -\bar{b}_0 - \bar{b}_2 & -1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & & 0 \\ 0 & \|\bar{\mathbf{e}}_{\max}\| \frac{\partial \mathbf{n}}{\partial \mathbf{u}_0} & 0 \\ 0 & & 0 \end{bmatrix} \tag{34}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_1} = \begin{bmatrix} 0 & 0 & 0 \\ -1 & -\bar{b}_0 - \bar{b}_2 & -1 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & & 0 \\ 0 & \|\bar{\mathbf{e}}_{\max}\| \frac{\partial \mathbf{n}}{\partial \mathbf{u}_1} & 0 \\ 0 & & 0 \end{bmatrix} \tag{35}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_2} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -1 & -\bar{b}_0 - \bar{b}_2 & -1 \end{bmatrix} + \begin{bmatrix} 0 & & 0 \\ 0 & \|\bar{\mathbf{e}}_{\max}\| \frac{\partial \mathbf{n}}{\partial \mathbf{u}_2} & 0 \\ 0 & & 0 \end{bmatrix} \tag{36}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_3} = \begin{bmatrix} 1 & \bar{b}_0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & & 0 \\ 0 & \|\bar{\mathbf{e}}_{\max}\| \frac{\partial \mathbf{n}}{\partial \mathbf{u}_3} & 0 \\ 0 & & 0 \end{bmatrix} \tag{37}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_4} = \begin{bmatrix} 0 & 0 & 0 \\ 1 & \bar{b}_0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & & 0 \\ 0 & \|\bar{\mathbf{e}}_{\max}\| \frac{\partial \mathbf{n}}{\partial \mathbf{u}_4} & 0 \\ 0 & & 0 \end{bmatrix} \tag{38}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_5} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & \bar{b}_0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & & 0 \\ 0 & \|\bar{\mathbf{e}}_{\max}\| \frac{\partial \mathbf{n}}{\partial \mathbf{u}_5} & 0 \\ 0 & & 0 \end{bmatrix} \tag{39}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_6} = \frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_7} = \frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_8} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{40}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_9} = \begin{bmatrix} 0 & \bar{b}_2 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & & 0 \\ 0 & \|\bar{\mathbf{e}}_{\max}\| \frac{\partial \mathbf{n}}{\partial \mathbf{u}_9} & 0 \\ 0 & & 0 \end{bmatrix} \tag{41}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_{10}} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \bar{b}_2 & 1 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & & 0 \\ 0 & \|\bar{\mathbf{e}}_{\max}\| \frac{\partial \mathbf{n}}{\partial \mathbf{u}_{10}} & 0 \\ 0 & & 0 \end{bmatrix} \tag{42}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_{11}} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & \bar{b}_2 & 1 \end{bmatrix} + \begin{bmatrix} 0 & & 0 \\ 0 & \|\bar{\mathbf{e}}_{\max}\| \frac{\partial \mathbf{n}}{\partial \mathbf{u}_{11}} & 0 \\ 0 & & 0 \end{bmatrix} \tag{43}$$

We must now define the normal derivative, $\frac{\partial \mathbf{n}}{\partial \mathbf{u}_*}$, where the inward-facing normal is,

$$\mathbf{n} = \frac{\mathbf{e}_2 \times \mathbf{e}_0}{\|\mathbf{e}_2 \times \mathbf{e}_0\|} \tag{44}$$

which yields

$$\frac{\partial \mathbf{n}}{\partial \mathbf{u}_*} = \frac{1}{\|\mathbf{e}_2 \times \mathbf{e}_0\|}\frac{\partial \mathbf{e}_2 \times \mathbf{e}_0}{\partial \mathbf{u}_*} - \frac{(\mathbf{e}_2 \times \mathbf{e}_0)^T \frac{\partial \mathbf{e}_2 \times \mathbf{e}_0}{\partial \mathbf{u}_*}}{\left[(\mathbf{e}_2 \times \mathbf{e}_0)^T(\mathbf{e}_2 \times \mathbf{e}_0)\right]^{\frac{3}{2}}}(\mathbf{e}_2 \times \mathbf{e}_0). \tag{45}$$

If we can define expressions for $\frac{\partial \mathbf{e}_2 \times \mathbf{e}_0}{\partial \mathbf{u}_*}$, we are done:

$$\frac{\partial \mathbf{e}_2 \times \mathbf{e}_0}{\partial \mathbf{u}_0} = \begin{bmatrix} 0 \\ \mathbf{e}_{0,z} - \mathbf{e}_{2,z} \\ -\mathbf{e}_{0,y} + \mathbf{e}_{2,y} \end{bmatrix} \quad \frac{\partial \mathbf{e}_2 \times \mathbf{e}_0}{\partial \mathbf{u}_1} = \begin{bmatrix} -\mathbf{e}_{0,z} + \mathbf{e}_{2,z} \\ 0 \\ \mathbf{e}_{0,x} - \mathbf{e}_{2,x} \end{bmatrix} \tag{46}$$

$$\frac{\partial \mathbf{e}_2 \times \mathbf{e}_0}{\partial \mathbf{u}_2} = \begin{bmatrix} \mathbf{e}_{0,y} - \mathbf{e}_{2,y} \\ -\mathbf{e}_{0,x} + \mathbf{e}_{2,x} \\ 0 \end{bmatrix} \quad \frac{\partial \mathbf{e}_2 \times \mathbf{e}_0}{\partial \mathbf{u}_3} = \begin{bmatrix} 0 \\ \mathbf{e}_{2,z} \\ -\mathbf{e}_{2,y} \end{bmatrix} \tag{47}$$

$$\frac{\partial \mathbf{e}_2 \times \mathbf{e}_0}{\partial \mathbf{u}_4} = \begin{bmatrix} -\mathbf{e}_{2,z} \\ 0 \\ \mathbf{e}_{2,x} \end{bmatrix} \quad \frac{\partial \mathbf{e}_2 \times \mathbf{e}_0}{\partial \mathbf{u}_5} = \begin{bmatrix} \mathbf{e}_{2,y} \\ -\mathbf{e}_{2,x} \\ 0 \end{bmatrix} \tag{48}$$

$$\frac{\partial \mathbf{e}_2 \times \mathbf{e}_0}{\partial \mathbf{u}_6} = \frac{\partial \mathbf{e}_2 \times \mathbf{e}_0}{\partial \mathbf{u}_7} = \frac{\partial \mathbf{e}_2 \times \mathbf{e}_0}{\partial \mathbf{u}_8} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{49}$$

$$\frac{\partial \mathbf{e}_2 \times \mathbf{e}_0}{\partial \mathbf{u}_9} = \begin{bmatrix} 0 \\ -\mathbf{e}_{0,z} \\ \mathbf{e}_{0,y} \end{bmatrix} \quad \frac{\partial \mathbf{e}_2 \times \mathbf{e}_0}{\partial \mathbf{u}_{10}} = \begin{bmatrix} \mathbf{e}_{0,z} \\ 0 \\ -\mathbf{e}_{0,x} \end{bmatrix} \quad \frac{\partial \mathbf{e}_2 \times \mathbf{e}_0}{\partial \mathbf{u}_{11}} = \begin{bmatrix} -\mathbf{e}_{0,y} \\ \mathbf{e}_{0,x} \\ 0 \end{bmatrix}. \tag{50}$$

Above, $\mathbf{e}_{0,\{x,y,z\}}$ respectively denote the x, y and z components of the $\mathbf{e}_0$ vector.

3.3 Iben [2007] Approximation

The Moore-Penrose pseudo-inverse described by Iben [2007], $\frac{\partial \mathbf{F}}{\partial \mathbf{u}} = \frac{\partial \mathbf{D}_s}{\partial \mathbf{u}} \mathbf{D}_m^{\dagger}$, is equivalent to the $\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}}$:

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_0} = \begin{bmatrix} -1 & 0 & -1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_1} = \begin{bmatrix} 0 & 0 & 0 \\ -1 & 0 & -1 \\ 0 & 0 & 0 \end{bmatrix} \tag{51}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_2} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -1 & 0 & -1 \end{bmatrix} \quad \frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_3} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{52}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_4} = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_5} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \tag{53}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_6} = \frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_7} = \frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_8} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{54}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_9} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_{10}} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \tag{55}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_{11}} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{56}$$

Similar to the rehabilitated tensor, $\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_6}$, $\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_7}$, $\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_8}$ are zeroed out, but the middle columns in $\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_0}$, $\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_1}$, and $\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_2}$ are as well. Interestingly, if we add back the middle columns back to $\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_0}$, $\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_1}$, and $\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_2}$ and apply this simpler tensor in lieu of the one from §3.2, the resulting forces approximate the exact result quite closely. In practice, we found this to be an excellent approximation of the exact tensor.

4 REHABILITATING TWO DEGENERATE DIRECTIONS

Elements with two degenerate directions, e.g. a 3D tetrahedron that has collapsed into a needle, can be addressed using an approach similar to one degenerate direction. Whereas before we assumed that only $\bar{\mathbf{e}}_1$ was degenerate, we now assume that $\bar{\mathbf{e}}_2$ is as well. The $\bar{\mathbf{e}}_0$ is now the only remaining "good" direction.

4.1 Building An Orthogonal Basis

The most significant difference is that the degeneracies now span an arbitrary plane, so must select two directions within the plane. We build a direction orthogonal $\bar{\mathbf{e}}_0$ using a matrix $\mathbf{O}$, i.e. $\mathbf{O}\bar{\mathbf{e}}_0$, where $\mathbf{O}$ can be any of the $\mathbf{T}_x$, $\mathbf{T}_y$ or $\mathbf{T}_z$ twist matrices from the main document. The third direction then follows as the new normal $\bar{\mathbf{n}} = \frac{\mathbf{O}\bar{\mathbf{e}}_0 \times \bar{\mathbf{e}}_0}{\|\mathbf{O}\bar{\mathbf{e}}_0 \times \bar{\mathbf{e}}_0\|}$. We can then construct a new version of $\mathbf{D}_{m,\text{iso}}$:

$$\mathbf{D}_{m,\text{iso}} = \begin{bmatrix} \bar{\mathbf{e}}_0 & \hat{\mathbf{e}}_1 & \hat{\mathbf{e}}_2 \end{bmatrix} \tag{57}$$

$$= \begin{bmatrix} \bar{\mathbf{e}}_0 & \bar{b}_{01}\bar{\mathbf{e}}_0 + \|\bar{\mathbf{e}}_0\|\bar{\mathbf{n}} & \left(\bar{b}_{02}\mathbf{I} + \|\bar{\mathbf{e}}_0\|\mathbf{O}\right)\bar{\mathbf{e}}_0 \end{bmatrix} \tag{58}$$

where $\bar{b}_{01} = \frac{\bar{\mathbf{e}}_1 \cdot \bar{\mathbf{e}}_0}{\|\mathbf{e}_0\|_2^2}$ and $\bar{b}_{02} = \frac{\bar{\mathbf{e}}_2 \cdot \bar{\mathbf{e}}_0}{\|\mathbf{e}_0\|_2^2}$ are the normalized projections onto $\bar{\mathbf{e}}_0$. Under deformation, $\mathbf{n} = \frac{\mathbf{e}_0 \times \mathbf{O}\mathbf{e}_0}{\|\mathbf{e}_0 \times \mathbf{O}\mathbf{e}_0\|}$, and $\mathbf{D}_{s,\text{iso}}$ becomes:

$$\mathbf{D}_{s,\text{iso}} = \begin{bmatrix} \mathbf{e}_0 & \bar{b}_{01}\mathbf{e}_0 + \|\bar{\mathbf{e}}_0\|\mathbf{n} & \left(\bar{b}_{02}\mathbf{I} + \|\bar{\mathbf{e}}_0\|\mathbf{O}\right)\mathbf{e}_0 \end{bmatrix}. \tag{59}$$

4.2 The Change-of-Basis Tensor

A rehabilitated $\frac{\partial \mathbf{D}_{s,\text{iso}}}{\partial \mathbf{u}}$ must now be constructed again for the change-of-basis tensor $\frac{\partial \mathbf{F}_{\text{iso}}}{\partial \mathbf{u}}$. Whereas three matrices, $\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_{6\ldots8}}$, were zeroed out in the case of one degenerate direction, six matrices are zeroed for two degenerate directions: $\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_{6\ldots11}}$. The other six matrices are:

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_0} = \begin{bmatrix} -1 & -\bar{b}_{01} & -\bar{b}_{02} - \|\bar{\mathbf{e}}_0\| \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & & 0 \\ 0 & \|\bar{\mathbf{e}}_0\| \frac{\partial \mathbf{n}}{\partial \mathbf{u}_0} & 0 \\ 0 & & 0 \end{bmatrix} \tag{60}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_1} = \begin{bmatrix} 0 & 0 & 0 \\ -1 & -\bar{b}_{01} & -\bar{b}_{02} - \|\bar{\mathbf{e}}_0\| \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & & 0 \\ 0 & \|\bar{\mathbf{e}}_0\| \frac{\partial \mathbf{n}}{\partial \mathbf{u}_1} & 0 \\ 0 & & 0 \end{bmatrix} \tag{61}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_2} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -1 & -\bar{b}_{01} & -\bar{b}_{02} - \|\bar{\mathbf{e}}_0\| \end{bmatrix} + \begin{bmatrix} 0 & & 0 \\ 0 & \|\bar{\mathbf{e}}_0\| \frac{\partial \mathbf{n}}{\partial \mathbf{u}_2} & 0 \\ 0 & & 0 \end{bmatrix} \tag{62}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_3} = \begin{bmatrix} 1 & \bar{b}_{01} & \bar{b}_{02} + \|\bar{\mathbf{e}}_0\| \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & & 0 \\ 0 & \|\bar{\mathbf{e}}_0\| \frac{\partial \mathbf{n}}{\partial \mathbf{u}_3} & 0 \\ 0 & & 0 \end{bmatrix} \tag{63}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_4} = \begin{bmatrix} 0 & 0 & 0 \\ 1 & \bar{b}_{01} & \bar{b}_{02} + \|\bar{\mathbf{e}}_0\| \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & & 0 \\ 0 & \|\bar{\mathbf{e}}_0\| \frac{\partial \mathbf{n}}{\partial \mathbf{u}_4} & 0 \\ 0 & & 0 \end{bmatrix} \tag{64}$$

$$\frac{\partial \mathbf{D}_s}{\partial \mathbf{u}_5} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & \bar{b}_{01} & \bar{b}_{02} + \|\bar{\mathbf{e}}_0\| \end{bmatrix} + \begin{bmatrix} 0 & & 0 \\ 0 & \|\bar{\mathbf{e}}_0\| \frac{\partial \mathbf{n}}{\partial \mathbf{u}_5} & 0 \\ 0 & & 0 \end{bmatrix} \tag{65}$$

We must again compute a normal derivative for this case, which takes the form:

$$\frac{\partial \mathbf{n}}{\partial \mathbf{u}_*} = \frac{1}{\|\mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0\|}\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_*} - \frac{(\mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0)^T \frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_*}}{\left[(\mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0)^T(\mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0)\right]^{\frac{3}{2}}}(\mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0). \tag{66}$$

We could then define $\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_*}$, but more useful expressions are obtained for specific $\mathbf{O}$. When $\mathbf{O} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$, the vectors are:

$$\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_0} = -\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_3} = \begin{bmatrix} -\mathbf{e}_{0,z} \\ 0 \\ 2\mathbf{e}_{0,x} \end{bmatrix} \tag{67}$$

$$\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_1} = -\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_4} = \begin{bmatrix} 0 \\ -\mathbf{e}_{0,z} \\ 2\mathbf{e}_{0,y} \end{bmatrix} \tag{68}$$

$$\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_2} = -\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_5} = \begin{bmatrix} -\mathbf{e}_{0,x} \\ -\mathbf{e}_{0,y} \\ 0 \end{bmatrix} \tag{69}$$

For $\mathbf{O} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$, they are:

$$\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_0} = -\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_3} = \begin{bmatrix} 0 \\ -\mathbf{e}_{0,y} \\ -\mathbf{e}_{0,z} \end{bmatrix} \tag{70}$$

$$\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_1} = -\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_4} = \begin{bmatrix} 2\mathbf{e}_{0,y} \\ -\mathbf{e}_{0,x} \\ 0 \end{bmatrix} \tag{71}$$

$$\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_2} = -\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_5} = \begin{bmatrix} 2\mathbf{e}_{0,z} \\ 0 \\ -\mathbf{e}_{0,x} \end{bmatrix} \tag{72}$$

Finally, when $\mathbf{O} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}$:

$$\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_0} = -\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_3} = \begin{bmatrix} -\mathbf{e}_{0,y} \\ 2\mathbf{e}_{0,x} \\ 0 \end{bmatrix} \tag{73}$$

$$\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_1} = -\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_4} = \begin{bmatrix} -\mathbf{e}_{0,x} \\ 0 \\ -\mathbf{e}_{0,z} \end{bmatrix} \tag{74}$$

$$\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_2} = -\frac{\partial \mathbf{O}\mathbf{e}_0 \times \mathbf{e}_0}{\partial \mathbf{u}_5} = \begin{bmatrix} 0 \\ 2\mathbf{e}_{0,z} \\ -\mathbf{e}_{0,y} \end{bmatrix} \tag{75}$$

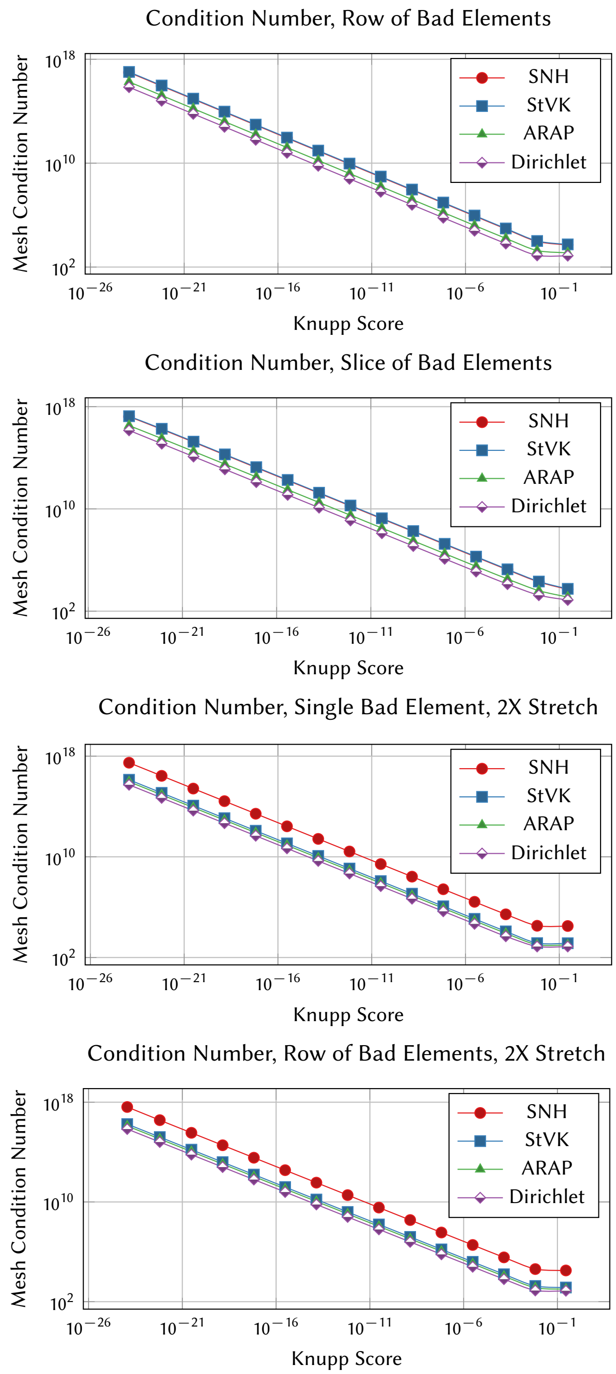

Fig. 1. We ruin the Knupp score of a varying number of tets in a mesh, both at rest, and when the mesh has been stretched by a factor of 2X, so that the configuration is far from equilibrium. The condition number of a mesh degrades at the same exponential rate under all these scenarios.

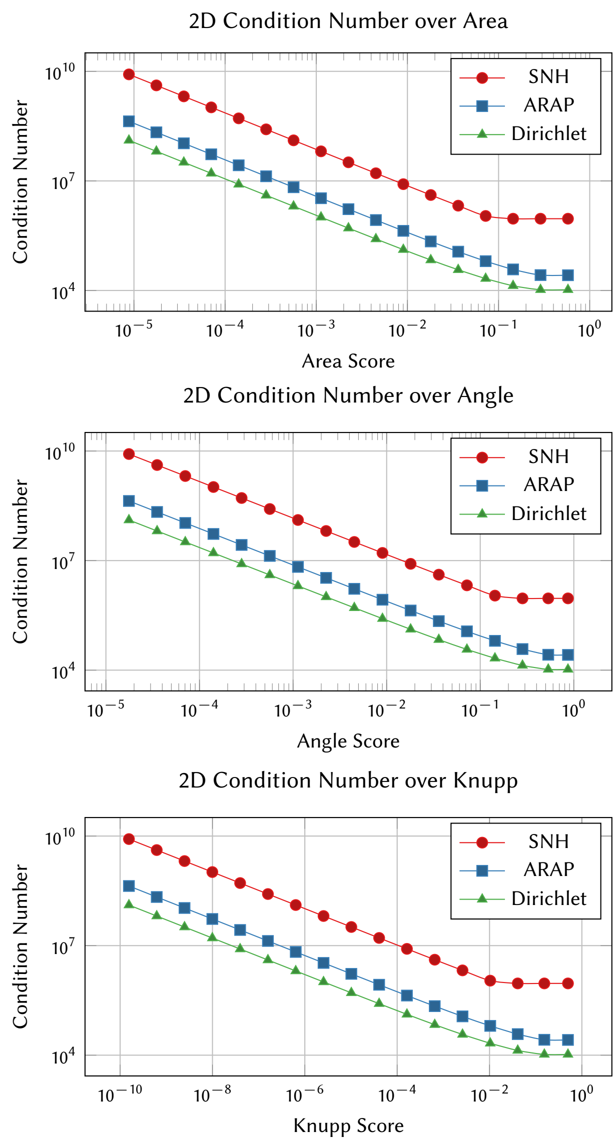

Fig. 2. The exponential trends appear in 2D, regardless of the quality measure. Area, angle, and Knupp scores were used, and the trend persists.

5 MESH CONDITION NUMBER UNDER ALTERNATIVE SCENARIOS

We progressively ruined the conditioning of a mesh by flattening a single tet, a row of tets, and a slab of tets in Figure 1. We ran the test at the rest state of the mesh, and after the mesh had been scaled by a factor of 2 in the x direction. While the translations of the plots change, the trend remains exactly the same.

The exponential decay of the condition number appears to be relatively insensitive to both the mesh dimensionality and the quality measure. We flattened a single triangle in a 2D mesh in the same manner as the 3D case, and plotted the trend of the condition number using the Knupp score, as well as the area term and angle term in isolation (Fig. 2). Again, the trend appears the same.

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