Technical Supplement to "Isotropic ARAP energy using Cauchy-Green invariants"

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This document provides the derivations for the 3D, 2D and 1D polynomial expressions that we use to rewrite the ARAP energy in terms of the Cauchy-Green invariants. We also provide the derivations and closed-form expressions for the eigenvectors of the 1D ARAP energy for a fast and concise implementation of implicit time integration using Newton solvers.

CCS Concepts: • **Computing methodologies** → **Mesh geometry models**.

Additional Key Words and Phrases: Second-order methods, geometry optimization, ARAP, Cauchy-Green invariants, corotational methods

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1 INTRODUCTION

The following descriptions assume a d-dimensional finite element ($d = 1, 2$ or 3) embedded in three-dimensional space. Each such element is imbued with a deformation gradient tensor $\mathbf{F} \in \mathbb{R}^{3\times \mathrm{d}}$ with which we compute the Cauchy-Green (CG) tensor as $\mathbf{C} = \mathbf{F}^\top \mathbf{F} \in \mathbb{R}^{\mathrm{d}\times \mathrm{d}}$.

The deformation gradient can be decomposed and analysed in several ways for the purpose of measuring strain, and distilling matrix/tensor properties which we use to derive the polynomials.

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One method is polar factorisation $\mathbf{F} = \mathbf{R}\mathbf{S}$ yielding a unitary rotation $\mathbf{R} \in \mathbb{R}^{3\times \mathrm{d}}$, and a stretch $\mathbf{S} \in \mathbb{R}^{\mathrm{d}\times \mathrm{d}}$ which is symmetric with real eigenvalues. This polar factorisation is also related to the singular value decomposition (SVD) $\mathbf{F} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$, where $\mathbf{U}$ and $\mathbf{V}$ are rotation factors, and $\mathbf{\Sigma}$ is a diagonal matrix of singular values σ_i. Moreover, the columns of $\mathbf{V}$ are the eigenvectors of $\mathbf{F}$ which also define the diagonalisable stretch $\mathbf{S} = \mathbf{V}\mathbf{\Sigma}\mathbf{V}^\top$, and the corresponding rotation factor may also be defined as $\mathbf{R} = \mathbf{V}\mathbf{U}^\top$ from this SVD.

With this view, the CG invariants may be written as

$$I_C = \mathrm{tr}(\mathbf{C}) = \sum_i^d \sigma_i^2, \tag{1}$$

$$II_C = \|\mathbf{C}\|_\mathrm{F}^2 = \sum_i^d \sigma_i^4, \tag{2}$$

$$III_C = \det(\mathbf{C}) = \prod_{i=1}^d \sigma_i^2, \tag{3}$$

which we use to derive the polynomial(s) necessary to rewrite corotational energies.

2 POLYNOMIAL FOR THE 3D ENERGY

In this section, we summarise the derivation of the quartic polynomial which we use to rewrite the 3D ARAP energy in terms of the CG invariants and show that the trace term is a root. Let us revisit the trace term:

$$\mathrm{tr}\left(\mathbf{F}^\top \mathbf{R}\right) = \sigma_1 + \sigma_2 + \sigma_3, \tag{4}$$

which is a sum of the three singular values σ_i of $\mathbf{F} \in \mathbb{R}^{3\times 3}$. The invariants in 3D are

$$\begin{aligned} I_C &= \sigma_1^2 + \sigma_2^2 + \sigma_3^2 \\ II_C^* &= \frac{1}{2}\left(I_C^2 - II_C\right) = (\sigma_1\sigma_2)^2 + (\sigma_1\sigma_3)^2 + (\sigma_2\sigma_3)^2 \\ III_C &= (\sigma_1\sigma_2\sigma_3)^2, \end{aligned} \tag{5}$$

which we'll use to rewrite the energy.

We derive of the quartic polynomial (see Eq. (21) in the paper) by starting from Eq. (4) and squaring both sides to obtain:

$$\begin{aligned} \mathrm{tr}\left(\mathbf{F}^\top \mathbf{R}\right)^2 &= \left(\sum_{i=1}^3 \sigma_i\right)^2 \\ &= \underbrace{\left(\sum_{i=1}^3 \sigma_i^2\right)}_{I_C} + 2\left(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_1\sigma_3\right). \end{aligned} \tag{6}$$

The first invariant I_C appears immediately on the right-hand-side (RHS) but the second term is not reducible to any invariant which is crucial for rewriting the energy and evaluating the necessary derivatives. We resolve this by further rearranging and once more squaring both sides to get

$$\begin{aligned}\left(\mathrm{tr}\,(\mathbf{F}^\top\mathbf{R})^2 - I_C\right)^2 &= 4\left(\sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_1\sigma_3\right)^2\\ &= 4\left[(\sigma_1\sigma_2)^2+(\sigma_2\sigma_3)^2+(\sigma_1\sigma_3)^2\right]+\\ &\quad 8(\sigma_1^2\sigma_2\sigma_3+\sigma_1\sigma_2^2\sigma_3+\sigma_1\sigma_2\sigma_3^2)\\ &= 4II_C^* + 8\sigma_1\sigma_2\sigma_3\sum_{i=1}^{3}\sigma_i\\ &= 4II_C^* + 8\sqrt{III_C}\,\mathrm{tr}\,(\mathbf{F}^\top\mathbf{R}),\end{aligned} \tag{7}$$

which, after manipulation, yields the following

$$t^4 - 2I_Ct^2 - 8Jt + I_C^2 - 4II_C^* = 0, \tag{8}$$

as the quartic polynomial with which we rewrite the ARAP energy, where $t := \mathrm{tr}\,(\mathbf{F}^\top\mathbf{R})$, and J is directly used in place of $\sqrt{III_C}$ for brevity and practical convenience.

2.1 The trace term is a root

To find the roots of the Eq. (8), one popular method is the Ferrari's method. The Ferrari's method to solve Eq. (8) can be summarized as follows,

$$\begin{aligned}\alpha &= -2I_C,\\ \beta &= -8J,\\ \gamma &= I_C^2 - 4II_C^*,\end{aligned}$$

if $\beta = 0$ (*i.e.* element has zero volume) then, the four roots are

$$x = \pm_s\sqrt{\frac{-\alpha \pm_t \sqrt{\alpha^2-4\gamma}}{2}}. \tag{9}$$

Otherwise, continue with

$$\begin{aligned}P &= -\frac{\alpha^2}{12} - \gamma,\\ Q &= -\frac{\alpha^3}{108} + \frac{\alpha\gamma}{3} - \frac{\beta^2}{8},\\ L &= -\frac{Q}{2} + \sqrt{\frac{Q^2}{4}+\frac{P^3}{27}},\\ Z &= \sqrt[3]{L},\\ y &= -\frac{5}{6}\alpha + \begin{cases} -\sqrt[3]{Q}, & Z = 0\\ Z - \dfrac{P}{3Z}, & Z \neq 0\end{cases},\\ W &= \sqrt{\alpha+2y},\\ x &= \frac{\pm_s W \pm_t \sqrt{-(3\alpha+2y\pm_s\frac{2\beta}{W})}}{2}.\end{aligned} \tag{10}$$

The two symbols $\pm_s$ must have the same sign, the symbol $\pm_t$ is independent to $\pm_s$. To get the four roots, we compute x for $\pm_s.\pm_t = +,+$ and for $+,-$; and for $-,+$ and for $-,-$. Finally these four roots of the polynomial can be reduced to the following form

$$\begin{aligned}x_1 &= \sigma_x - \sigma_y - \sigma_z,\\ x_2 &= \sigma_y - \sigma_x - \sigma_z,\\ x_3 &= \sigma_z - \sigma_y - \sigma_x,\\ x_4 &= \sigma_x + \sigma_y + \sigma_z,\end{aligned} \tag{11}$$

where x_4 is the trace term we need, and its expression is Eq. (10) with $+_s, +_t$.

3 POLYNOMIAL FOR THE 2D ENERGY

The CG invariants of the deformation gradient $\mathbf{F} \in \mathbb{R}^{3\times 2}$ from a 2D element are[1]

$$I_C = \sigma_1^2 + \sigma_2^2, \tag{12}$$

$$II_C = \sigma_1^4 + \sigma_2^4, \tag{13}$$

$$III_C = (\sigma_1\sigma_2)^2. \tag{14}$$

The trace term will reduce to

$$\mathrm{tr}\,(\mathbf{F}^\top\mathbf{R}) = \mathrm{tr}\,(\mathbf{S}) = \sigma_1 + \sigma_2, \tag{15}$$

which is now a sum of the two singular values of $\mathbf{F}$ in 2D. Squaring of Eq. (15) gives

$$(\sigma_1+\sigma_2)^2 = \sigma_1^2 + \sigma_2^2 + 2\sigma_1\sigma_2, \tag{16}$$

where, after substituting the CG invariants, we get

$$\mathrm{tr}\,(\mathbf{F}^\top\mathbf{R})^2 = \begin{cases} I_C + 2\sqrt{III_C}, & \det(\mathbf{F}) \geq 0,\\ I_C - 2\sqrt{III_C}, & \det(\mathbf{F}) < 0,\end{cases} \tag{17}$$

as the polynomial expression(s) with which to rewrite an energy. This 2D case is dependent on the first I_C and third III_C invariants, where the case-by-case (or piecewise) continuity of Eq. (17) is due to the fact that III_C discards the sign information from the singular values because it is evaluated from $\mathbf{C}$.

Once more, the trace term (*cf.* Eq. (15)) is a root of the polynomial expression(s) in Eq. (17). To show this, we bring to focus the expression for the case where $\det(\mathbf{F}) \geq 0$ and let $t := \mathrm{tr}\,(\mathbf{F}^\top\mathbf{R})$ to then rewrite the Eq. (17) as

$$t^2 = I_C + 2\sqrt{III_C} \quad \text{or,} \quad t^2 - I_C - 2\sqrt{III_C} = 0. \tag{18}$$

Since Eq. (18) is quadratic, the two roots are found using the classic form

$$x = \frac{-b \pm \sqrt{b^2-4ac}}{2a}, \tag{19}$$

which, upon substituting Eq. (12) and Eq. (14) into Eq. (18), will give

$$x_1 = -\sigma_1 - \sigma_2, \quad \text{and,} \quad x_2 = \sigma_1 + \sigma_2, \tag{20}$$

where x_2 is the trace.

The condition $\det(\mathbf{F}) \geq 0$ is always true for any non-square deformation gradient $\mathbf{F} \in \mathbb{R}^{n\times d}$ where $n > d$ since there are insufficient degrees of freedom to induce inversion *i.e.* inverting a d-dimensional element in n-dimensional space can always be represented as a rotation in n-dimensional space. This means we can always use the polynomial corresponding to the condition $\det(\mathbf{F}) \geq 0$ when working with a non-square deformation gradient because the respective element cannot ever be inverted by definition.

[1] These definitions are also valid for 2D elements embedded in 2D space with $\mathbf{F} \in \mathbb{R}^{2\times 2}$

3.1 Root function derivatives

We summarise the derivatives of the root expression (which we call f) corresponding to the trace in this section.

Following the same approach as in §4 of the paper, the first-order derivatives are given by

$$\frac{\partial f}{\partial I_C} = \frac{1}{2f}, \quad \frac{\partial f}{\partial II_C} = 0, \quad \frac{\partial f}{\partial III_C} = \frac{1}{2f\sqrt{III_C}}, \tag{21}$$

and the second-order derivatives follow by

$$\begin{aligned}
&\frac{\partial^2 f}{\partial I_C^2} = \frac{-\left(\frac{\partial f}{\partial I_C}\right)^2}{f}, \quad \frac{\partial^2 f}{\partial I_C \partial II_C} = 0, \quad \frac{\partial^2 f}{\partial I_C \partial III_C} = \frac{-\frac{\partial f}{\partial I_C}\frac{\partial f}{\partial III_C}}{f} \\
&\frac{\partial^2 f}{\partial II_C \partial I_C} = 0, \quad \frac{\partial^2 f}{\partial II_C^2} = 0, \quad \frac{\partial^2 f}{\partial II_C \partial III_C} = 0 \\
&\frac{\partial^2 f}{\partial III_C \partial I_C} = \frac{-\frac{\partial f}{\partial III_C}\frac{\partial f}{\partial I_C}}{f}, \quad \frac{\partial^2 f}{\partial III_C \partial II_C} = 0, \\
&\frac{\partial^2 f}{\partial III_C^2} = \frac{-2\left(\frac{\partial f}{\partial III_C}\right)^2 - \frac{1}{2III_C^{\frac{3}{2}}}}{2f}.
\end{aligned} \tag{22}$$

3.2 Inversion awareness for $\mathbf{F} \in \mathbb{R}^{2\times 2}$

Working with a square deformation gradient $\mathbf{F}$ (*e.g.* as in parameterization problems; see also § 2) requires that we account for the case where $\det(\mathbf{F}) < 0$. However, this implies that we evaluate derivatives for the normal and inverted case separately via Eq. (17). A more practical solution is to replace $\sqrt{III_C}$ with J. This means we can work with a single expression where the trace is always the root with which we can evaluate the derivatives (for the energy gradient and Hessian). In this regard, we update Eq. (18) to

$$t^2 - I_C - 2J = 0 \tag{23}$$

which is now agnostic to the sign information of the singular values of $\mathbf{F}$ that indicate whether an element is inverted or not (see §3.4 in the paper). The derivatives that follow can be computed similarly with Eq. (21) and Eq. (22) (*i.e.* deriving w.r.t J instead of III_C).

4 POLYNOMIAL FOR THE 1D ENERGY

We summarise the derivation of the 1D polynomial in this section, which is useful for simulating elastic strands.

Following from Equations 1-3, the invariants of the deformation gradient $\mathbf{F} \in \mathbb{R}^{3\times 1}$ from a 1D element are

$$I_C = \sigma_1^2 \tag{24}$$

$$II_C = \sigma_1^4 = I_C^2 \tag{25}$$

$$III_C = \sigma_1^2 = I_C, \tag{26}$$

where the first and third invariant are equal and the second is their square. The notion of a trace operator will reduce to an expression with one singular value

$$\mathrm{tr}\left(\mathbf{F}^\top \mathbf{R}\right) = \mathrm{tr}\left(\mathbf{S}\right) = \mathrm{tr}\left(\Sigma\right) = \sigma_1, \tag{27}$$

since the stretch factor $\mathbf{S}$ is tensor of order-zero *i.e.* a scalar. A rewriting in terms of the invariants (Equations 1-3) is achieved by squaring

$$\mathrm{tr}\left(\mathbf{F}^\top \mathbf{R}\right)^2 = \sigma_i^2 \equiv I_C, \tag{28}$$

which yields a simple expression with I_C. Using $t \coloneqq \mathrm{tr}\left(\mathbf{F}^\top \mathbf{R}\right)$ and rearranging $t^2 - I_C = 0$, the roots can be found easily $t = \pm\sqrt{I_C}$, which, after substitution, gives

$$x_1 = -\sigma_1, \quad \text{and} \quad x_2 = \sigma_1, \tag{29}$$

where x_2 is the trace.

4.1 Root function derivatives

The derivatives of the root equation corresponding to the trace are likewise needed to evaluate the energy gradients and Hessian. To this end, we let f be the expression for the root evaluating to the trace term *e.g.* x_2 in Eq. (20). The first-order derivatives of this f are

$$\frac{\partial f}{\partial I_C} = \frac{1}{2f}, \quad \frac{\partial f}{\partial II_C} = 0, \quad \frac{\partial f}{\partial III_C} = 0, \tag{30}$$

and the second-order derivatives are of the form

$$\begin{aligned}
&\frac{\partial^2 f}{\partial I_C^2} = \frac{-\left(\frac{\partial f}{\partial I_C}\right)^2}{f}, \quad \frac{\partial^2 f}{\partial I_C \partial II_C} = 0, \quad \frac{\partial^2 f}{\partial I_C \partial III_C} = 0, \\
&\frac{\partial^2 f}{\partial II_C \partial I_C} = 0, \quad \frac{\partial^2 f}{\partial II_C^2} = 0, \quad \frac{\partial^2 f}{\partial II_C \partial III_C} = 0, \\
&\frac{\partial^2 f}{\partial III_C \partial I_C} = 0, \quad \frac{\partial^2 f}{\partial III_C \partial II_C} = 0, \quad \frac{\partial^2 f}{\partial III_C^2} = 0.
\end{aligned} \tag{31}$$

5 ANALYTIC EIGENSYSTEM OF 1D STRAND ENERGY

Here we summarise the process of how we arrive at the analytic eigensystem of the 1D (strand) energy. We follow similar steps as Smith et al. [3] and the experimental procedure outlined by Kim and Eberle [2].

The rewritten 1D energy

$$\begin{aligned}
\Psi_{1D} &= I_C - 2\mathrm{tr}(\mathbf{R}^\top \mathbf{F}) + 1, \\
&= I_C - 2\left(\mathcal{P}(t)|_{t=f} = 0\right) + 1, \\
&\equiv I_C - 2\sqrt{I_C} + 1,
\end{aligned} \tag{32}$$

has a PK1 of the form

$$\mathbf{P}(\mathbf{F}) = \frac{\partial \Psi_{1D}}{\partial \mathbf{F}} = \frac{\Psi_{1D}}{\partial I_C}\frac{\partial I_C}{\partial \mathbf{F}}. \tag{33}$$

The corresponding Hessian (a 2nd-order tensor *e.g.* $\in \mathbb{R}^{3\times 3}$) is given by

$$\begin{aligned}
\frac{\partial \mathbf{P}(\mathbf{F})}{\partial \mathbf{F}} &= \frac{\partial^2 \Psi_{1D}}{\partial I_C^2}\mathbb{G}_{I_C} \otimes \mathbb{G}_{I_C} + \frac{\partial \Psi_{1D}}{\partial I_C}\mathbb{H}_{I_C}, \\
&\equiv \frac{\partial^2 \Psi_{1D}}{\partial I_C^2}\mathbf{g}_{I_C}\mathbf{g}_{I_C}^\top + \frac{\partial \Psi_{1D}}{\partial I_C}\mathbf{H}_{I_C},
\end{aligned} \tag{34}$$

where $\mathbf{g}_{I_C} = \mathrm{vec}\left(\mathbb{G}_{I_C}\right)$ is the vectorised gradient and $\mathbf{H}_{I_C} = \mathrm{vec}\left(\mathbb{H}_{I_C}\right)$ the correspondingly vectorised Hessian. Their definitions are given as follows

$$\mathbf{g}_{I_C} = 2\mathbf{F} \tag{35}$$

$$\mathbf{H}_{I_C} = 2\mathbf{I}_{3\times 3} \tag{36}$$

The eigenvalues and the eigenvectors of Eq. (34) are provided as follows:

$$\lambda_0 = 1, \qquad Q_0 = \mathbf{U}\mathbf{T}_x\mathbf{V}^\top, \tag{37}$$

$$\lambda_1 = 1 - \frac{1}{\sigma_1}, \qquad Q_1 = \mathbf{U}\mathbf{T}_y\mathbf{V}^\top, \tag{38}$$

$$\lambda_2 = 1 - \frac{1}{\sigma_1}, \qquad Q_2 = \mathbf{U}\mathbf{T}_z\mathbf{V}^\top. \tag{39}$$

Moreover, the new 'twist' tensors are given by

$$\mathbf{T}_x = \begin{bmatrix}1\\0\\0\end{bmatrix}, \quad \mathbf{T}_y = \begin{bmatrix}0\\1\\0\end{bmatrix}, \quad \mathbf{T}_z = \begin{bmatrix}0\\0\\1\end{bmatrix}, \tag{40}$$

which we determine by following Smith et al. [3] using trial-and-error experimentation as described by Kim and Eberle [2].

Rotation factors $\mathbf{U}$ and $\mathbf{V}$ of our non-square deformation gradient $\mathbf{F} \in \mathbb{R}^{3\times1}$ are determined by first observing that $\mathbf{V} \in \mathbb{R}^{1\times1}$ is an orthonormal order-zero tensor (scalar) by definition (*i.e.* from $\mathbf{F} = \mathbf{U}\Sigma\mathbf{V}^\top$). That is, $\mathbf{V} = 1$ always holds. Following from our proof in Appendix C of the main paper, the rotation part of $\mathbf{F}$ can be constructed as

$$\mathbf{R} = \mathbf{U}\begin{bmatrix}\mathbf{V}^\top\\0\\0\end{bmatrix} = \mathbf{U}\begin{bmatrix}1\\0\\0\end{bmatrix}, \tag{41}$$

which implies that the first column of $\mathbf{U} \in \mathbb{R}^{3\times3}$ is $\mathbf{R} \in \mathbb{R}^{3\times1}$ computed using Eq. (35) in the main paper. The remaining two columns of $\mathbf{U}$ are arbitrarily and can be chosen as any two vectors that are of unit length $\in \mathbb{R}^{3\times1}$ and forming an orthonormal 3D basis with this $\mathbf{R}$ *e.g.* using Householder orthogonalisation like Frisvad [1].

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