Majorants de distances aux classes de symétrie

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INTRODUCTION

Even if some analytical attempts exist (Vianello, 1997, Stahn et al, 2020), the distance to an elasticity symmetry class problem (Gazis et al, 1963) is often

- solved numerically, following Arts et al (1991, 1993) and François et al (1995, 1996, 1998),
- using the parameterization by a rotation *g*:

$$d(\mathbf{E}_0,[G]) := \min_{\mathbf{E} \in \overline{\Sigma}_{[G]}} \|\mathbf{E}_0 - \mathbf{E}\| = \min_{g \in \mathrm{SO}(3)} \|\mathbf{E}_0 - g \star \mathbf{R}_G(g^t \star \mathbf{E}_0)\|$$

- *G* is a symmetry group (\mathbb{Z}_2 , \mathbb{D}_2 , \mathbb{D}_3 , \mathbb{D}_4 , \mathbb{O} , O(2), SO(3), Forte-Vianello, 1996),
- \mathbf{R}_G is the Reynolds (group averaging) operator.

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- solved numerically, following Arts et al (1991, 1993) and François et al (1995, 1996, 1998),
- using the parameterization rotation g / normal form A (Dellinger, 2005):

$$d(\mathbf{E}_0, [G]) := \min_{\mathbf{E} \in \overline{\Sigma}_{[G]}} \|\mathbf{E}_0 - \mathbf{E}\| = \min_{g, \mathbf{A}} \|\mathbf{E}_0 - g \star \mathbf{A}\|$$

- G is a symmetry group $(\mathbb{Z}_2, \mathbb{D}_2, \mathbb{D}_3, \mathbb{D}_4, \mathbb{O}, O(2), SO(3), Forte-Vianello, 1996),$
- \mathbf{R}_G is the Reynolds (group averaging) operator.

UPPER BOUNDS ESTIMATES RATHER THAN DISTANCES

For 3D elasticity, upper bounds estimates of the distance to a symmetry stratum have been formulated

- by Gazis, Tadjbakhsh and Toupin (1963) for cubic symmetry,
- by Klimeš (2018) for transverse isotropy,
- and by Stahn, Müller and Bertram (2020) for all symmetry classes, using a second-order harmonic component (a covariant) of the elasticity tensor introduced by Backus (1970). This covariant is assumed to carry the likely symmetry coordinate system of E₀.

All second-order covariants of an exactly cubic elasticity tensor are isotropic. Therefore, for a material expected to be cubic, a methodology based on second-order covariants is probably meaningless.

OUTLINE

- Geometry of the elasticity tensor
- 2 Literature on upper bounds estimates of the distance to a symmetry class
- 3 Symmetry coordinate system of a close to be cubic or orthotropic tensor
- Reduction to an eigenvalue problem
- 5 Upper bounds estimates of the distance to cubic elasticity
- 6 Upper bounds estimates of the distance to orthotropy

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SYMMETRY GROUPS, SYMMETRY CLASSES

Given an elasticity tensor E in

Geometry of E

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$$\mathbb{E} \mathrm{la} = \mathbb{S}^2(\mathbb{S}^2(\mathbb{R}^3)) = \left\{ \mathbf{E} \in \otimes^4 \mathbb{R}^3, \ E_{iikl} = E_{iikl} = E_{iilk} = E_{klii} \right\},\,$$

its symmetry group $G_{\rm E}$ is defined as the set of all rotations g such that

$$g \star \mathbf{E} = \mathbf{E}$$
.

Given $\overline{\mathbf{E}} = r \star \mathbf{E}$ deduced from \mathbf{E} by a rotation r, then its symmetry group $G_{\overline{\mathbf{E}}}$ is conjugate to $G_{\mathbf{E}}$, meaning that

$$G_{\overline{\mathbf{E}}} = rG_{\mathbf{E}}r^{-1} = \left\{ rg\,r^{-1}, g \in G_{\mathbf{E}} \right\}.$$

What is meaningful is the conjugacy class $[G_E]$, which is the set of all subgroups which are conjugate to G_E . Such a set is called a symmetry class. Examples: $[\mathbb{O}] = \text{cubic symmetry}$, $[\mathbb{D}_2] = \text{orthotropy}$.

SYMMETRY STRATA AND REPRESENTATIVE GROUPS

For each symmetry class [G], it is therefore useful to provide an explicit representative subgroup G in this class.

Example: orthotropy $[\mathbb{D}_2]$, $\mathbb{D}_2 = \{e, \mathbf{r}(\boldsymbol{e}_1, \pi), \mathbf{r}(\boldsymbol{e}_2, \pi), \mathbf{r}(\boldsymbol{e}_3, \pi)\}$, $|\mathbb{D}_2| = 4$.

The set of $\mathbf{E} \in \mathbb{E}$ la with $G_{\mathbf{E}}$ conjugate to representative subgroup G is the symmetry stratum $\Sigma_{[G]}$ associated to the symmetry class [G].

Examples: $\Sigma_{[\mathbb{O}]} = \text{cubic stratum}, \Sigma_{[\mathbb{D}_2]} = \text{orthotropic stratum}.$

NORMAL FORM

An elasticity tensor \mathbf{E} in the symmetry stratum $\Sigma_{[G]}$ may have exactly as symmetry group the canonical representative group G,

$$g \star \mathbf{E} = \mathbf{E}, \quad \forall g \in G.$$

In that case, we say that **E** is in its normal form (expressed in its natural basis).

Example

When $G = \mathbb{O}$, elasticity tensors in cubic normal form are written as

$$[\mathbf{E}] = \begin{pmatrix} E_{1111} & E_{1122} & E_{1122} & 0 & 0 & 0 \\ E_{1122} & E_{1111} & E_{1122} & 0 & 0 & 0 \\ E_{1122} & E_{1122} & E_{1111} & 0 & 0 & 0 \\ 0 & 0 & 0 & 2E_{1212} & 0 & 0 \\ 0 & 0 & 0 & 0 & 2E_{1212} & 0 \\ 0 & 0 & 0 & 0 & 0 & 2E_{1212} \end{pmatrix},$$

in Kelvin matrix representation.

ELASTICITY TENSORS FIXED BY A GROUP G

The set of tensors E which are fixed by a group G (not necessarily a representative symmetry group), i.e. such as

$$g \star \mathbf{E} = \mathbf{E}, \quad \forall g \in G,$$

is called the fixed point set of G and denoted by $\mathbb{F}ix(G)$. It is a linear subspace of the vector space $\mathbb{E}la$ of elasticity tensors.

Example $(G = r\mathbb{O}r^{-1} \text{ with } r = \mathbf{r}(\boldsymbol{e}_1, \frac{\pi}{3}))$

Geometry of E

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Literature

 \mathbb{F} ix $(G) \subset \overline{\Sigma}_{[\mathbb{O}]}$ is the subvector space of elasticity tensors of the form

$$E_{3333} = \frac{1}{4}(E_{1111} + 3E_{1122} + 6E_{1212}), \quad E_{1133} = \frac{1}{4}(3E_{1111} + E_{1122} - 6E_{1212}), \quad E_{1112} = \frac{1}{4}\sqrt{3}(E_{1111} - E_{1122} - 2E_{1212}).$$

ORTHOGONAL PROJECTION ON \mathbb{F} ix(G)

The orthogonal projection on the vector space $\mathbb{F}ix(G)$ is uniquely defined. It can be expressed as the averaging

$$\mathbf{R}_{G}(\mathbf{E}) = \frac{1}{|G|} \sum_{g \in G} g \star \mathbf{E},$$

 \mathbf{R}_G is called the Reynolds operator associated with the finite group G.

The cardinal of
$$G = r\mathbb{D}_2 r^{-1}$$
 is $|G| = |\mathbb{D}_2| = 4$.
The cardinal of $G = r\mathbb{O}r^{-1}$ is $|G| = |\mathbb{O}| = 24$.

HARMONIC DECOMPOSITION

The second-order dilatation and Voigt tensors are defined as

$$\mathbf{d} := \operatorname{tr}_{12} \mathbf{E}, \quad \mathbf{v} := \operatorname{tr}_{13} \mathbf{E} \quad (i.e., d_{ij} = E_{kkij}, v_{ij} = E_{kikj}),$$

Harmonic decomposition of E (Backus, 1970, Cowin, 1989, Baerheim, 1993):

$$\mathbf{E} = (\lambda, \mu, \mathbf{d}', \mathbf{v}', \mathbf{H}) \in \mathbb{H}^0 \oplus \mathbb{H}^0 \oplus \mathbb{H}^2 \oplus \mathbb{H}^2 \oplus \mathbb{H}^4$$

where $\lambda = \frac{1}{15}(2\operatorname{tr}\mathbf{d} - \operatorname{tr}\mathbf{v})$, $\mu = \frac{1}{30}(3\operatorname{tr}\mathbf{v} - \operatorname{tr}\mathbf{d})$ and $(\mathbf{a}\odot\mathbf{b} = (\mathbf{a}\otimes\mathbf{b})^s$ being the symmetrized tensor product)

$$\mathbf{H} = \mathbf{E}^{s} - (2\mu + \lambda)\mathbf{1}\odot\mathbf{1} - \frac{2}{7}\mathbf{1}\odot(\mathbf{d}' + 2\mathbf{v}')$$

Remark

Geometry of E

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When the Euclidean norm $\|\mathbf{E}\| = \sqrt{\mathbf{E} :: \mathbf{E}} = \sqrt{E_{ijkl}E_{ijkl}}$, is used, one gets

$$\|\mathbf{E}\|^2 = 3\left(3\lambda^2 + 4\lambda\mu + 8\mu^2\right) + \frac{2}{21}\|\mathbf{d}' + 2\mathbf{v}'\|^2 + \frac{4}{3}\|\mathbf{d}' - \mathbf{v}'\|^2 + \|\mathbf{H}\|^2.$$

INVARIANTS /COVARIANTS OF THE ELASTICITY TENSOR

• The quantities

Geometry of E

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$$\lambda = \lambda(\mathbf{E}), \quad \mu = \mu(\mathbf{E}), \quad \mathbf{d}' = \mathbf{d}'(\mathbf{E}), \quad \mathbf{v}' = \mathbf{v}'(\mathbf{E}), \quad \mathbf{H} = \mathbf{H}(\mathbf{E}),$$
 are covariants $\mathbf{C}(\mathbf{E})$ of \mathbf{E} (of degree one and resp. order 0, 0, 2, 2 and 4).

- The scalars λ and μ are linear invariants of **E**.
- $\mathbf{d}'(\mathbf{E})$, $\mathbf{v}'(\mathbf{E})$ and $\mathbf{H} = \mathbf{H}(\mathbf{E})$ are linear covariants of \mathbf{E} .

Covariants of a tensor **E** satisfy the rule, $\forall r \in SO(3)$,

$$\mathbf{C}(r \star \mathbf{E}) = r \star \mathbf{C}(\mathbf{E}), \qquad \Big(I(r \star \mathbf{E}) = I(\mathbf{E}) \text{ for invariants } I(\mathbf{E})\Big).$$

A covariant C(E) of E inherits the symmetry of E: C(E) has at least the symmetry of E,

$$G_{\mathbf{E}} \subset G_{\mathbf{C}(\mathbf{E})}$$
.

POLYNOMIAL COVARIANTS

• There exist polynomial covariants of higher degree, for example (Boehler et al, 1994)

$$\mathbf{d}_2(\mathbf{H}) := \mathbf{H} : \mathbf{H}, \qquad (i.e., (\mathbf{d}_2)_{ij} = H_{ipqr}H_{pqrj}),$$

- The algebra of (totally symmetric) polynomial covariants of the elasticity tensor has been defined by Olive et al (2021).
- A minimal integrity basis for the invariant algebra of $\mathbf{H} \in \mathbb{H}^4$ has been derived in (Boehler et al, 2021) (it is of cardinal 9).
- A minimal integrity basis for the invariant algebra of **E** has been derived in (Auffray et al, 2021) and (Olive et al, 2021) (it is of cardinal 294).
- A minimal integrity basis for the covariant algebra of $\mathbf{H} \in \mathbb{H}^4$ has been derived in (Olive et al, 2021) (it is of cardinal 70).

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Baerheim (1993) has observed that, generically, the trace $\operatorname{tr}_{12} \mathbf{E}^a = \mathbf{1} : \mathbf{E}^a$ of the asymmetric part of **E** (Backus, 1970)

$$\mathbf{E}^a := \mathbf{E} - \mathbf{E}^s, \qquad egin{cases} (\mathbf{E}^s)_{ijkl} = rac{1}{3} \left(E_{ijkl} + E_{ikjl} + E_{iljk}
ight), \ (\mathbf{E}^a)_{ijkl} = rac{1}{3} \left(2E_{ijkl} - E_{ikjl} - E_{iljk}
ight), \end{cases}$$

carries information related to a so-called symmetry coordinate system of E.

• In the case of an orthotropic tensor \mathbf{E} , the trace $\mathbf{1} : \mathbf{E}^a$ is diagonal in the natural orthotropy coordinate system.

The second-order tensor

$$\mathbf{t} := \mathbf{1} : \mathbf{E}^a = \frac{2}{3} \left(\mathbf{d} - \mathbf{v} \right),$$

is in fact a covariant of E. It inherits the symmetry of E, and, generically, $\mathbf{t}(E)$ is orthotropic if E is orthotropic, with

$$G_{\mathbf{E}} = G_{\mathbf{t}(\mathbf{E})}$$
.

LITERATURE UPPER BOUNDS ESTIMATES

The distance of \mathbf{E}_0 to $\Sigma_{[G]}$ is defined by

$$d(\mathbf{E}_0, \Sigma_{[G]}) = \min_{\mathbf{E} \in \Sigma_{[G]}} \|\mathbf{E}_0 - \mathbf{E}\|.$$

Estimates of the distance to a symmetry class are obtained as

$$M(\mathbf{E}_0, \Sigma_{[G]}) = \min_{\mathbf{E} \in \mathcal{S} \subset \Sigma_{[G]}} ||\mathbf{E}_0 - \mathbf{E}||,$$

i.e., as the minimum over a subset S of the considered symmetry stratum.

It satisfies thus

$$d(\mathbf{E}_0, \Sigma_{[G]}) \leq M(\mathbf{E}_0, \Sigma_{[G]}).$$

Examples: Gazis–Tadjbakhsh–Toupin (1963), Vianello (1997), Klimeš (2018), Stahn–Müller–Bertram (2020), Oliver-Leblond et al. (2021)

THE AXIS OF TRANSVERSE ISOTROPY [O(2)]

Klimeš (2016) did observe that for elasticity tensors $\mathbf{E} \in \Sigma_{[O(2)]}$, with transverse isotropy axis \mathbf{n} , one has

$$\left. \frac{d}{d\theta} \right|_{\theta=0} \Big(\mathbf{r}(\mathbf{n},\theta) \star \mathbf{E} - \mathbf{E} \Big) = \rho_4'(\mathbf{n}) \mathbf{E} = 0,$$

so that

$$\mathbf{T}(\mathbf{E}, \mathbf{n}) := \rho_4'(\mathbf{n})\mathbf{E} = 0,$$

$$T_{ijkl}(\mathbf{E},\boldsymbol{n}) = \frac{1}{4}n_m \left(\varepsilon_{min}E_{njkl} + \varepsilon_{mjn}E_{inkl} + \varepsilon_{mkn}E_{ijnl} + \varepsilon_{mln}E_{ijkn}\right),$$

which is linear both in the transverse isotropy direction n and E.

Remark

The vector \mathbf{n} is not a covariant of \mathbf{E} , since all vector covariants of \mathbf{E} vanish when $\mathbf{E} \in \Sigma_{[O(2)]}$ is transversely isotropic.

Klimeš upper bound estimate (transverse isotropy [O(2)])

Klimeš (2018) likely transverse isotropy coordinate system of (raw) \mathbf{E}_0 is such as $\mathbf{e}_3 = \mathbf{n}$ minimizes

$$\min_{\|\boldsymbol{n}\|=1}\|\boldsymbol{T}(\boldsymbol{E}_0,\boldsymbol{n})\|^2.$$

This is a quadratic minimization problem, and its solution is a unit eigenvector n determined analytically.

Once the axis $\langle \mathbf{n} \rangle$ of the transversely isotropic symmetry group G (conjugate to O(2)) is known, an upper bound estimate

$$M(\mathbf{E}_0, \Sigma_{[O(2)]}) = \|\mathbf{E}_0 - \mathbf{R}_G(\mathbf{E}_0)\|.$$

is obtained by standard Reynolds averaging.

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NATURAL COORDINATE SYSTEM OF A CUBIC ELASTICITY TENSOR

It has been shown (Abramian et al, 2020) that an orthotropic solution \mathbf{a}' of the linear equation

$$\operatorname{tr}(\mathbf{H} \times \mathbf{a}) = \operatorname{tr}(\mathbf{H} \times \mathbf{a}') = 0, \qquad \mathbf{H} \times \mathbf{a} := -(\mathbf{a} \cdot \boldsymbol{\varepsilon} \cdot \mathbf{H})^{s}$$

provides the axes of symmetry $\langle \mathbf{e}_i \rangle$ of the cubic harmonic tensor $\mathbf{H} \in \Sigma_{[\mathbb{O}]}$.

LIKELY CUBIC COORDINATE SYSTEM

In the spirit of Klimeš for transverse isotropy, the equation $tr(\mathbf{H} \times \mathbf{a}') = 0$ can be used to determine a likely cubic coordinate system.

Given a raw elasticity tensor

$$\mathbf{E}_0 = (\lambda_0, \mu_0, \mathbf{d}'_0, \mathbf{v}'_0, \mathbf{H}_0),$$

a likely cubic basis $(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$ for \mathbf{E}_0 is the eigenbasis of an orthotropic deviatoric second-order tensor \mathbf{a}' which minimizes

$$\min_{\|\boldsymbol{a}'\|=1}\|\mathrm{tr}(\boldsymbol{H}_0\times\boldsymbol{a}')\|^2, \qquad \boldsymbol{a}'\in\mathbb{H}^2.$$

The function to be minimized can be rewritten as

$$\|\mathrm{tr}(\mathbf{H}_0 \times \mathbf{a}')\|^2 = \frac{9}{200} \|\mathbf{H}_0\|^2 \|\mathbf{a}'\|^2 - \frac{3}{20} \mathbf{a}' : \mathbf{H}_0^2 : \mathbf{a}' + \frac{27}{100} \mathbf{d}_2'(\mathbf{H}_0) : \mathbf{a}'^2,$$

where

Geometry of E

$$\mathbf{H}_0^2 = \mathbf{H}_0 : \mathbf{H}_0 \quad \text{and} \quad \mathbf{d}_{20} = \mathbf{d}_2(\mathbf{H}_0)$$

Remark

Since $\mathbf{d}_2'(\mathbf{H}_0) = 0$ when \mathbf{H}_0 is cubic (Olive et al., 2021), another likely cubic coordinate system is obtained using the alternative minimization problem,

$$\min_{\|\mathbf{b}'\|=1} \left(\frac{9}{200} \|\mathbf{H}_0\|^2 \|\mathbf{b}'\|^2 - \frac{3}{20} \mathbf{b}' : \mathbf{H}_0^2 : \mathbf{b}' \right), \qquad \mathbf{b}' \in \mathbb{H}^2.$$

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a' SOLUTION OF A QUADRATIC MINIMIZATION PROBLEM

We recast the quadratic form $\|\operatorname{tr}(\mathbf{H} \times \mathbf{a})\|^2$ as $\langle A_{\mathbf{H}} \mathbf{a}', \mathbf{a}' \rangle$, where

$$\mathbf{A_H} = \frac{9}{200}\|\mathbf{H}\|^2\mathbf{J} - \frac{3}{20}\mathbf{H}^2 + \frac{27}{200}\mathbf{J}: \left(\mathbf{1} \ \overline{\underline{\otimes}} \ \mathbf{d}_2' + \mathbf{d}_2' \ \overline{\underline{\otimes}} \ \mathbf{1}\right): \mathbf{J},$$

with

$$d_2'(H)=(H\,\dot{\cdot}\,H)',\qquad J:=I-\frac{1}{3}\mathbf{1}\otimes\mathbf{1}.$$

The minimization problem

$$\min_{\|\boldsymbol{a}'\|=1} \langle A_{\boldsymbol{H}} \big|_{\mathbb{H}^2} \, \boldsymbol{a}', \boldsymbol{a}' \rangle, \qquad \boldsymbol{a}' \in \mathbb{H}^2,$$

defines a likely cubic basis (e_i) (as the eigenbasis of \mathbf{a}' solution).

SOLUTION \mathbf{a}' AS AN EIGENVECTOR OF $A_{\mathbf{H}}$

- One has $A_H : 1 = 0$.
- In practice, it is not necessary to calculate $A_{\mathbf{H}}|_{\mathbb{H}^2}$. We need only to calculate the eigenvalues of $A_{\mathbf{H}}$ (in Kelvin matrix representation) and consider its smallest positive eigenvalue λ_{min} .
- An eigenvector $\mathbf{a} = \mathbf{a}'$ for $\lambda_{min} > 0$ is thus a candidate to provide our likely cubic/orthotropic normal basis.
- To fully solve the problem, the deviatoric second-order tensor **a**' has to be orthotropic, not transversely isotropic. This turns out to be generic.

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A CUBIC HARMONIC FOURTH-ORDER TENSOR FROM AN ORTHOTROPIC SECOND ORDER TENSOR **a**

Let **a** be an orthotropic second order tensor,

$$\mathbf{a}^2 \times \mathbf{a} := -(\mathbf{a}^2 \cdot \boldsymbol{\varepsilon} \cdot \mathbf{a})^s \in \mathbb{H}^3,$$

and $(\cdot)'$ denote the leading harmonic part.

Then

$$\frac{\left(\left(\boldsymbol{a}^2\times\boldsymbol{a}\right)\cdot\left(\boldsymbol{a}^2\times\boldsymbol{a}\right)\right)'}{\|\boldsymbol{a}^2\times\boldsymbol{a}\|^2}\in\mathbb{H}^4,$$

is cubic of axes the eigenvectors of a.

In the eigenbasis of **a**, we get the Kelvin matrix representations,

and

$$\left[\frac{\left(\left(\mathbf{a}^2\times\mathbf{a}\right)\cdot\left(\mathbf{a}^2\times\mathbf{a}\right)\right)'}{\|\mathbf{a}^2\times\mathbf{a}\|^2}\right]\propto\begin{pmatrix} -2 & 1 & 1 & 0 & 0 & 0\\ 1 & -2 & 1 & 0 & 0 & 0\\ 1 & 1 & -2 & 0 & 0 & 0\\ 0 & 0 & 0 & 2 & 0 & 0\\ 0 & 0 & 0 & 0 & 2 & 0\\ 0 & 0 & 0 & 0 & 0 & 2 \end{pmatrix}.$$

A CUBIC HARMONIC FOURTH-ORDER PROJECTOR $\mathbf{C_a}$

We define

$$\boldsymbol{C_a} := \sqrt{\frac{15}{2}} \; \frac{\left(\left(\boldsymbol{a}^2 \times \boldsymbol{a}\right) \cdot \left(\boldsymbol{a}^2 \times \boldsymbol{a}\right)\right)'}{\|\boldsymbol{a}^2 \times \boldsymbol{a}\|^2}, \qquad \|\boldsymbol{C_a}\| = 1,$$

of cubic symmetry group $G_{\mathbf{C_a}} \in [\mathbb{O}]$.

• Let \mathbf{H}_0 be a given harmonic tensor. Its orthogonal projection on the fixed point set $\mathbb{F}ix(G_{\mathbf{C}_a})$ is

$$\mathbf{H} = \mathbf{R}_{G_{\mathbf{C}_{\mathbf{a}}}}(\mathbf{H}_0) = (\mathbf{C}_{\mathbf{a}} :: \mathbf{H}_0) \, \mathbf{C}_{\mathbf{a}} \in \mathbb{H}^4.$$

• Let $\mathbf{E}_0 = (\lambda_0, \mu_0, \mathbf{d}'_0, \mathbf{v}'_0, \mathbf{H}_0)$ be a given elasticity tensor. Its orthogonal projection on the fixed point set $\mathbb{F}ix(G_{\mathbf{C}_a})$ is

$$\mathbf{E} = \mathbf{R}_{G_{\mathbf{C_a}}}(\mathbf{E}_0) = (\lambda_0, \mu_0, 0, 0, \mathbf{R}_{G_{\mathbf{C_a}}}(\mathbf{H}_0)) \in \mathbb{E}$$
la.

APPLICATION TO CUBIC UPPER BOUNDS ESTIMATES

For any orthotropic second-order tensor a, we get a cubic tensor

$$\mathbf{E} = 2\mu_0 \mathbf{I} + \lambda_0 \mathbf{1} \otimes \mathbf{1} + (\mathbf{C_a} :: \mathbf{H_0}) \mathbf{C_a} \in \Sigma_{[\mathbb{O}]},$$

and define an upper bound estimate of $d(\mathbf{E}_0, [\mathbb{O}])$, as

$$\Delta_{\mathbf{a}}(\mathbf{E}_0, [\mathbb{O}]) = \|\mathbf{E}_0 - \mathbf{E}\|.$$

The Stahn et al (2020) cubic upper bound estimate is then simply recovered as

$$M(\mathbf{E}_0, [\mathbb{O}]) = \Delta_{\mathbf{t}_0}(\mathbf{E}_0, [\mathbb{O}]),$$

by setting

$$\mathbf{a} = \mathbf{t}_0 = \frac{2}{3} \left(\mathbf{d}_0 - \mathbf{v}_0 \right).$$

EXAMPLES

Let us compare the upper bounds estimates

$$\Delta_{\boldsymbol{a}}(E_0,[\mathbb{O}])$$

to the distance to cubic symmetry $d(\mathbf{E}_0, [\mathbb{O}])$, for the four different choices:

- $\mathbf{a} = \mathbf{t}_0$ (choice made by Stahn et al (2020)),
- $\mathbf{a} = \mathbf{d}_{20}$ (choice made by Antonelli et al (2021)),
- $\mathbf{a} = \mathbf{a}'$, obtained by the minimization of $\|\operatorname{tr}(\mathbf{H}_0 \times \mathbf{a}')\|^2 = \mathbf{a}' : \mathbf{A}_{\mathbf{H}_0}|_{\mathbb{H}^2} : \mathbf{a}'.$
- ullet ${f a}={f b}',$ obtained by the minimization of ${f b}':{f B}_{{f H}_0}ig|_{{\mathbb H}^2}:{f b}'.$

A better upper bound estimate of $d(\mathbf{E}_0, [\mathbb{O}])$

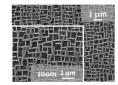
$$\Delta_{opt}(E_0,[\mathbb{O}]) = \min\left(\Delta_{\boldsymbol{t}_0}(E_0,[\mathbb{O}]),\Delta_{\boldsymbol{d}_2}(E_0,[\mathbb{O}]),\Delta_{\boldsymbol{a}'}(E_0,[\mathbb{O}]),\Delta_{\boldsymbol{b}'}(E_0,[\mathbb{O}])\right)$$

EXAMPLE OF NI-BASED SUPERALLOY

Consider the elasticity tensor (in Kelvin representation)

$$[\mathbf{E}_0] = \begin{pmatrix} 243 & 136 & 135 & 22\sqrt{2} & 52\sqrt{2} & -17\sqrt{2} \\ 136 & 239 & 137 & -28\sqrt{2} & 11\sqrt{2} & 16\sqrt{2} \\ 135 & 137 & 233 & 29\sqrt{2} & -49\sqrt{2} & 3\sqrt{2} \\ 22\sqrt{2} & -28\sqrt{2} & 29\sqrt{2} & 133\cdot2 & -10\cdot2 & -4\cdot2 \\ 52\sqrt{2} & 11\sqrt{2} & -49\sqrt{2} & -10\cdot2 & 119\cdot2 & -2\cdot2 \\ -17\sqrt{2} & 16\sqrt{2} & 3\sqrt{2} & -4\cdot2 & -2\cdot2 & 130\cdot2 \end{pmatrix} \ GPa,$$

measured by François–Geymonat–Berthaud (1998) for a single crystal Ni-based superalloy with a so-called cubic γ/γ' microstructure (Fig. after Mattiello, 2018):



$d(\mathbf{E}_0, [\mathbb{O}]) \mid$	$M=\Delta_{\mathbf{t}_0}$	$\Delta_{\mathbf{d}_{20}}$	$\Delta_{\mathbf{a}'}$	$\Delta_{\mathbf{b'}}$	$\Delta_{ m opt} = \Delta_{{f b}'}$
74.13 Estimate (GPa):	241.7	238.6	114.9	97.8	97.8
0.1039 ¹ Relative estimate:	0.3388	0.3344	0.1610	0.1371	0.1371

Table: Comparison of upper bounds estimates of the distance to cubic elasticity $d(\mathbf{E}_0, [\mathbb{O}])$ for Ni-based single crystal superalloy.

The material considered has a cubic Ni-based microstructure. All the 2nd-order covariants of a cubic elasticity tensor are —close to be— isotropic. They do not carry information about the cubic coordinate system.

Geometry of E

¹François et al (1998).

BEST ESTIMATE

The cubic elasticity tensor corresponding to

$$\Delta_{\mathbf{b'}}(\mathbf{E}_0, [\mathbb{O}]) \approx 97.8 \text{ GPa}, \qquad \frac{\Delta_{\mathbf{b'}}(\mathbf{E}_0, [\mathbb{O}])}{\|\mathbf{E}_0\|} \approx 0.1371,$$

is (in Kelvin representation, in the basis in which is expressed $[E_0]$, in GPa)

$$[\mathbf{E}] = \left(\begin{array}{cccccc} 238.76 & 146.72 & 124.86 & 1.18\sqrt{2} & 42.46\sqrt{2} & -0.41\sqrt{2} \\ 146.72 & 219.91 & 143.71 & -17.89\sqrt{2} & -0.71\sqrt{2} & -3.66\sqrt{2} \\ 124.86 & 143.71 & 241.76 & 16.72\sqrt{2} & -41.75\sqrt{2} & 4.07\sqrt{2} \\ 1.18\sqrt{2} & -17.89\sqrt{2} & 16.72\sqrt{2} & 135.04 \cdot 2 & 4.07 \cdot 2 & -0.71 \cdot 2 \\ 42.46\sqrt{2} & -0.71\sqrt{2} & -41.75\sqrt{2} & 4.07 \cdot 2 & 116.19 \cdot 2 & 1.18 \cdot 2 \\ -0.41\sqrt{2} & -3.66\sqrt{2} & 4.07\sqrt{2} & -0.71 \cdot 2 & 1.18 \cdot 2 & 138.05 \cdot 2 \end{array} \right).$$

EXAMPLE OF A CLOSE TO BE ORTHOTROPIC MATERIAL

Consider now the elasticity tensor studied in (Stahn et al, 2020),

$$[\mathbf{E}_0] = \left(\begin{array}{cccccc} 9.35 & 5.81 & -0.20 & 5.1 & 4.06 & -2.51 \\ 5.81 & 11.09 & 2.67 & -0.83 & -3.92 & 2.79 \\ -0.20 & 2.67 & 11.01 & -0.1 & -2.95 & 0.57 \\ 5.1 & -0.83 & -0.1 & 8.13 & -1.16 & 0.8 \\ 4.06 & -3.92 & -2.95 & -1.16 & 7.94 & 2.01 \\ -2.51 & 2.79 & 0.57 & 0.8 & 2.01 & 8.13 \end{array} \right).$$

$d(\mathbf{E}_0, [\mathbb{O}]) \mid$	$M=\Delta_{\mathbf{t}_0}$	$\Delta_{\mathbf{d}_{20}}$	$\Delta_{\mathbf{a}'}$	$\Delta_{\mathbf{b}'}$	$\Delta_{ m opt} = \Delta_{{f a}'}$
11.4551 Estimate:	11.4573	11.4552	11.4551	14.3961	11.4551
0.409081 Relat. estim.:	0.409162	0.409086	0.409083	0.514110	0.409083

Table: Comparison of upper bounds estimates of the distance to cubic elasticity $d(\mathbf{E}_0, [\mathbb{O}])$ for an academic elasticity tensor.

EXAMPLE OF VOSGES SANDSTONE

Considering the elasticity tensor identified by François (1995) using the ultrasonic measurement of Arts (1993) on a Vosges sandstone specimen (in GPa),

$$[\mathbf{E}_0] = \left(\begin{array}{cccccc} 12.2 & -2.2 & 1.9 & 0.9\sqrt{2} & 0.8\sqrt{2} & -0.5\sqrt{2} \\ -2.2 & 13. & 2.9 & 0.2\sqrt{2} & -0.3\sqrt{2} & 0.4\sqrt{2} \\ 1.9 & 2.9 & 13.9 & 0 & 0 & 0.1\sqrt{2} \\ 0.9\sqrt{2} & 0.2\sqrt{2} & 0 & 4.\cdot 2 & 1.2\cdot 2 & 0 \\ 0.8\sqrt{2} & -0.3\sqrt{2} & 0 & 1.2\cdot 2 & 5.4\cdot 2 & 0 \\ -0.5\sqrt{2} & 0.4\sqrt{2} & 0.1\sqrt{2} & 0 & 0 & 5.4\cdot 2 \end{array} \right).$$

$d(\mathbf{E}_0, [\mathbb{O}])$		$M=\Delta_{\mathbf{t}_0}$	$\Delta_{\mathbf{d}_{20}}$	$\Delta_{\mathbf{a}'}$	$\Delta_{\mathbf{b'}}$	$\Delta_{ m opt} = \Delta_{f t_0}$
6.49	Estimate (GPa):	7.809	7.818	7.848	7.621	7.809
0.2212	Relative estimate:	0.2660	0.2664	0.2674	0.2596	0.2660

Table: Comparison of upper bounds estimates of the distance to cubic elasticity $d(\mathbf{E}_0, [\mathbb{O}])$ for Vosges sandstone.

²François (1995).

OUTLINE

- Geometry of the elasticity tensor
- 2 Literature on upper bounds estimates of the distance to a symmetry class
- 3 Symmetry coordinate system of a close to be cubic or orthotropic tensor
- 4 Reduction to an eigenvalue problem
- 5 Upper bounds estimates of the distance to cubic elasticity
- 6 Upper bounds estimates of the distance to orthotropy

UPPER BOUNDS ESTIMATES OF THE DISTANCE TO ORTHOTROPY

We consider still a given (measured) elasticity tensor \mathbf{E}_0 , triclinic, with harmonic decomposition

$$\mathbf{E}_0 = (\lambda_0, \mu_0, \mathbf{d}'_0, \mathbf{v}'_0, \mathbf{H}_0).$$

- Determine as previously an orthotropic second order tensor that carries the likely cubic/orthotropic coordinate system, say **a**.
- An orthotropic elasticity tensor **E** that allows to define an upper bound estimate

$$\Delta_{\mathbf{a}}(\mathbf{E}_0, [\mathbb{D}_2]) = \|\mathbf{E}_0 - \mathbf{E}\|$$

of the distance $d(\mathbf{E}_0, [\mathbb{D}_2])$ to orthotropy is now

$$\mathbf{E} = \mathbf{R}_{\textit{\textbf{G}}_{\mathbf{a}}}(\mathbf{E}_0) = (\lambda_0, \mu_0, \mathbf{R}_{\textit{\textbf{G}}_{\mathbf{a}}}(\mathbf{d}_0'), \mathbf{R}_{\textit{\textbf{G}}_{\mathbf{a}}}(\mathbf{v}_0'), \mathbf{R}_{\textit{\textbf{G}}_{\mathbf{a}}}(\mathbf{H}_0)) \in \Sigma_{[\mathbb{D}_2]},$$

with $G_{\mathbf{a}} \subset [\mathbb{D}_2]$.

EXAMPLE OF NI-BASED SUPERALLOY

$d(\mathbf{E}_0,[\mathbb{D}_2])$		$M=\Delta_{\mathbf{t}_0'}$	$\Delta_{\mathbf{d}_{20}'}$	$\Delta_{\mathbf{a}'}$	$\Delta_{\mathbf{b'}}$	$\Delta_{ m opt} = \Delta_{{f b}'}$
57.8	Estimate (GPa):	216.1	210.9	109.8	90.3	90.3
0.081^{3}	Relative estimate:	0.3029	0.2943	0.1539	0.1266	0.1266

Table: Comparison of upper bounds estimates of the distance to orthotropic elasticity $d(\mathbf{E}_0, [\mathbb{D}_2])$ for Ni-based single crystal superalloy.

EXAMPLE OF A CLOSE TO BE ORTHOTROPIC MATERIAL

	$M=\Delta_{\mathbf{t}_0'}$	$\Delta_{\mathbf{d}_{20}'}$	$\Delta_{\mathbf{a}'}$	$\Delta_{\mathbf{b}'}$	$\Delta_{\mathrm{opt}} = \Delta_{\mathbf{t}_0'}$
Estimate:	0.491	0.651	0.653	6.714	0.491
Relative estimate:	0.0175	0.02325	0.0233	0.2398	0.01753

Table: Comparison of upper bounds estimates of the distance to orthotropic elasticity $d(\mathbf{E}_0, [\mathbb{D}_2])$ for an academic elasticity tensor.

EXAMPLE OF VOSGES SANDSTONE

$d(\mathbf{E}_0, [\mathbb{D}_2])$		$M = \Delta_{\mathbf{t}_0'}$	$\Delta_{\mathbf{d}_{20}'}$	$\Delta_{\mathbf{a}'}$	$\Delta_{\mathbf{b'}}$	$\Delta_{\mathrm{opt}} = \Delta_{\mathbf{t}_0'}$
2.64	Estimate (GPa):	4.3756	4.5587	4.8292	4.5584	4.3756
0.090^4	Relative estimate:	0.14907	0.15531	0.16453	0.15530	0.14907

Table: Comparison of upper bounds estimates of the distance to orthotropic elasticity $d(\mathbf{E}_0, [\mathbb{D}_2])$ for Vosges sandstone.

CLOSURE

- We have addressed the problem of an accurate analytical estimation of the distance of a raw elasticity tensor \mathbf{E}_0 either to cubic symmetry or to orthotropy.
- Key point: the use of a second-order tensor **a** (not necessarily a covariant of E_0), which carries the likely symmetry coordinate system.
- Such tensors are obtained as the solution of a quadratic minimization problem (reducing to an eigenvalue problem).
- We have improved the upper bound estimates of the distance of \mathbf{E}_0 to the cubic or orthotropic symmetry.
- We have provided intrinsic projection formulas (on $\mathbb{F}ix(G)$, both in the cubic case and in the orthotropic —not presented— case).
- The optimal tensor \mathbf{E} , used to define an upper bound estimate as $\|\mathbf{E}_0 \mathbf{E}\|$, is determined a priori. This allows to consider readily other norms than the Euclidean norm.

Log-Euclidean upper bounds estimates

For a given tensor E_0 , once an elasticity tensor E either cubic ($E \in \Sigma_{[\mathbb{O}]}$) or orthotropic ($\mathbf{E} \in \Sigma_{[\mathbb{D}_2]}$) has been computed according to the symmetry group of a second-order tensor, say a, one can easily calculate the upper bounds estimates $\Delta_{\mathbf{a}}(\mathbf{E}_0, \Sigma_{[G]})$ for any norm.

Since an elasticity tensor has to be positive definite, one can consider the Log-Euclidean norm (Arsigny et al, 2005, Moakher and Norris, 2006),

$$\|\mathbf{E}\|_{L} := \|\ln(\mathbf{E})\| = \|\ln([\mathbf{E}])\|_{\mathbb{R}^{6}},$$

which has the property of invariance by inversion.

For this norm, the upper bounds estimates of the distance

$$d(\mathbf{E}_0, \Sigma_{[G]}) = \min_{\Sigma_{[G]}} ||\mathbf{E}_0 - \mathbf{E}||_L,$$

can then be expressed as

$$\Delta_{\mathbf{a}}(\mathbf{E}_0, \Sigma_{[G]}) := \|\mathbf{E}_0 - \mathbf{E}\|_L = \|\ln(\mathbf{E}_0) - \ln(\mathbf{E})\|.$$

EXAMPLES WITH LOG-EUCLIDEAN NORM (CUBIC SYMMETRY)

	$\Delta_{\mathbf{t}_0}$	$\Delta_{\mathbf{d}_{20}}$	$\Delta_{\mathbf{a}'}$	$\Delta_{\mathbf{b'}}$	$\Delta_{ m opt}$
Relative Euclidean estimate:	0.3388	0.3344	0.1610	0.1371	0.1371
Relative Log-Euclidean estimate:	0.1365	0.1353	0.0616	0.0516	0.0516

Table: Comparison of cubic upper bounds estimates for Ni-based single crystal superalloy.

	$\Delta_{\mathbf{t}_0}$	$\Delta_{\mathbf{d}_{20}}$	$\Delta_{\mathbf{a}'}$	$\Delta_{\mathbf{b}'}$	$\Delta_{ m opt}$
Relative Euclidean estimate:	0.2660	0.2664	0.2674	0.2596	0.2596
Relative Log-Euclidean estimate:	0.1261	0.1276	0.1274	0.1256	0.1256

Table: Comparison of cubic upper bounds estimates for Vosges sandstone.

EXAMPLES WITH LOG-EUCLIDEAN NORM (ORTHOTROPY)

	$\Delta_{\mathbf{t}_0'}$	$\Delta_{\mathbf{d}_{20}'}$	$\Delta_{\mathbf{a}'}$	$\Delta_{\mathbf{b}'}$	Δ_{opt}
Relative Euclidean estimate:	0.3029	0.2943	0.1539	0.1266	0.1266
Relative Log-Euclidean estimate:	0.1221	0.1160	0.0529	0.0392	0.0392

Table: Comparison of orthotropic upper bounds estimates for Ni-based single crystal superalloy.

	$\Delta_{\mathbf{t}_0'}$	$\Delta_{\mathbf{d}_{20}'}$	$\Delta_{\mathbf{a}'}$	$\Delta_{\mathbf{b}'}$	$\Delta_{ m opt}$
Relative Euclidean estimate:	0.14907	0.15531	0.16453	0.15530	
Relative Log-Euclidean estimate:	0.0685	0.0728	0.0749	0.0786	

Table: Comparison of orthotropic upper bounds estimates for Vosges sandstone.

The symmetry classes, their number, and their partial ordering are strongly dependent on the tensor type.

There are two symmetry classes for a vector v:

- [SO(2)] (axial symmetry, if $\mathbf{v} \neq 0$)
- and [SO(3)] (isotropy, if $\mathbf{v} = 0$).

There are three symmetry classes for a symmetric second-order tensor \mathbf{a} (and for a deviatoric tensor \mathbf{a}'):

- $[\mathbb{D}_2]$ (orthotropy, if **a** has three distinct eigenvalues),
- \bullet [O(2)] (transverse isotropy, if **a** has two distinct eigenvalues),
- and [SO(3)] (isotropy, if $\mathbf{a}' = 0$);

The symmetry classes for an harmonic (totally symmetric and traceless) fourth-order tensor **H** are the same eight symmetry classes as those of an elasticity tensor (Ihrig and Golubitsky, 1984, Forte and Vianello, 1996): $[1], [\mathbb{Z}_2], [\mathbb{D}_2], [\mathbb{D}_3], [\mathbb{D}_4], [\mathbb{O}], [O(2)]$ and [SO(3)] (isotropy, $\mathbf{H} = 0$).

GEOMETRIC CONSEQUENCES

- \bullet the vector covariants $\mathbf{v}(\mathbf{E})$ of a monoclinic elasticity tensor \mathbf{E} are all collinear,
- tetragonal, trigonal, cubic, transversely isotropic or isotropic, all vanish:

$$\mathbf{v}(\mathbf{E}) = 0 \quad \forall \mathbf{E} \in \Sigma_{[\mathbb{D}_2]} \cup \Sigma_{[\mathbb{D}_3]} \cup \Sigma_{[\mathbb{D}_4]} \cup \Sigma_{[\mathbb{O}]} \cup \Sigma_{[\mathrm{O}(2)]} \cup \Sigma_{[\mathrm{SO}(3)]},$$

- \bullet the second-order covariants $\mathbf{c}(\mathbf{E})$ of an elasticity tensor either cubic or isotropic are all isotropic,
- lacktriangledown the second-order covariants $\mathbf{c}(\mathbf{E})$ of an elasticity tensor \mathbf{E} either tetragonal, trigonal or transversely isotropic, of axis $\langle n \rangle$, are all at least transversely isotropic of axis $\langle n \rangle$,
- \bullet the second-order covariants $\mathbf{c}(\mathbf{E})$ of an orthotropic elasticity tensor \mathbf{E} are all at least orthotropic (and all of them commute with each other).
- \bullet the second-order covariants $\mathbf{c}(\mathbf{E})$ of a triclinic elasticity tensor \mathbf{E} are all at least orthotropic (but the natural basis may differ from one covariant to another). ◆□ → ◆□ → ◆□ → ◆□ → □

Remark

Geometry of E

Any other second-order covariant $\mathbf{c}(\mathbf{E}_0)$ of the elasticity tensor \mathbf{E}_0 can be added to the list $\{\mathbf{t}_0, \mathbf{d}_{20}, \mathbf{a}', \mathbf{b}'\}$, such as

EXPLICIT HARMONIC DECOMPOSITION

Geometry of E

The explicit harmonic decomposition of E is (Backus, 1970, Spencer, 1970)

$$\mathbf{E} = 2\mu \mathbf{I} + \lambda \mathbf{1} \otimes \mathbf{1} + \frac{2}{7} \mathbf{1} \odot (\mathbf{d}' + 2\mathbf{v}') + 2 \mathbf{1} \otimes_{(2,2)} (\mathbf{d}' - \mathbf{v}') + \mathbf{H},$$

which can also be written as (Cowin, 1989, Baerheim, 1993)

$$\mathbf{E} = 2\mu \mathbf{I} + \lambda \mathbf{1} \otimes \mathbf{1}$$

$$+ \frac{1}{7} \left(\mathbf{1} \otimes (5\mathbf{d}' - 4\mathbf{v}') + (5\mathbf{d}' - 4\mathbf{v}') \otimes \mathbf{1} \right)$$

$$+ 2\mathbf{1} \overline{\otimes} (6\mathbf{v}' - 4\mathbf{d}') + 2(6\mathbf{v}' - 4\mathbf{d}') \overline{\otimes} \mathbf{1}$$

$$+ \mathbf{H}.$$

where $\otimes_{(2,2)}$ is the Young-symmetrized tensor product,

$$\mathbf{a} \otimes_{(2,2)} \mathbf{b} = \frac{1}{3} (\mathbf{a} \otimes \mathbf{b} + \mathbf{b} \otimes \mathbf{a} - \mathbf{a} \overline{\otimes} \mathbf{b} - \mathbf{b} \overline{\otimes} \mathbf{a}),$$

$$(\mathbf{a} \ \overline{\otimes} \ \mathbf{b})_{ijkl} := \frac{1}{2} (a_{ik}b_{jl} + a_{il}b_{jk}), \qquad I_{ijkl} = (\mathbf{1} \ \overline{\otimes} \ \mathbf{1})_{ijkl} = \frac{1}{2} (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}).$$

The normal form $\mathbf{E}_{\mathbb{O}}$ of the cubic estimate \mathbf{E} is obtained directly, as

$$[\mathbf{E}] = \begin{pmatrix} (\mathbf{E})_{1111} & (\mathbf{E})_{1122} & (\mathbf{E})_{1122} & 0 & 0 & 0 \\ (\mathbf{E})_{1122} & (\mathbf{E})_{1111} & (\mathbf{E})_{1122} & 0 & 0 & 0 \\ (\mathbf{E})_{1122} & (\mathbf{E})_{1122} & (\mathbf{E})_{1111} & 0 & 0 & 0 \\ 0 & 0 & 0 & 2(\mathbf{E})_{1212} & 0 & 0 \\ 0 & 0 & 0 & 0 & 2(\mathbf{E})_{1212} & 0 \\ 0 & 0 & 0 & 0 & 0 & 2(\mathbf{E})_{1212} \end{pmatrix},$$

in Kelvin matrix representation, with

$$\begin{split} &(\mathbf{E}_{\mathbb{O}})_{1111} = 2\mu_0 + \lambda_0 - \frac{2}{\sqrt{30}}\mathbf{C_a} :: \mathbf{H}_0, \\ &(\mathbf{E}_{\mathbb{O}})_{1122} = \lambda_0 + \frac{1}{\sqrt{30}}\mathbf{C_a} :: \mathbf{H}_0, \\ &(\mathbf{E}_{\mathbb{O}})_{1212} = \mu_0 + \frac{1}{\sqrt{30}}\mathbf{C_a} :: \mathbf{H}_0. \end{split}$$