Tensor calculus and anisotropic elasticity for the impatient

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Tensor calculus is introduced to Physics and Mechanical engineering students in 2D and 3D and applied to anisotropic elasticity such as in condensed matter physics approaching the subject from the practical tool aspect point of view. It provides powerful mathematical techniques to tackle many aspects of Vector Calculus, Continuum mechanics, Solid State Physics, Electromagnetism...

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I. INTRODUCTION

Tensor calculus is usually introduced at the graduate/undergraduate level in Special Relativity or General Relativity/Gravitation/Cosmology courses. It has been used by Einstein to tackle the daunting mathematical operations needed in performing many required differential geometry tasks in curved space.

Prior to relativity courses, physics students are typically exposed to Vector calculus [1] in Classical Mechanics, Electromagnetism or in Mathematics for Physicists since they employ, in these courses, vector differential operators like the gradient, divergence, curl, Laplacian...

Tensor calculus provides the students a powerful geometrical extension of Vector calculus to arbitrary dimension and to mathematical objects they were not familiar with to tackle problems in fluids, elasticity, continuum mechanics...

Another field of application of Tensor calculus [2] is Solid State Physics where students become acquainted with geometry of anisotropic materials and recently with mathematics of Topological materials.

It is natural to suppose that a quantitative description of physical phenomena cannot depend on the coordinate system in which they are expressed. The argument may be returned: since physical phenomena are independent of the coordinate system, what are the possible implications on the nature of the quantities describing these phenomena?

Einstein covariance principle (ECP) states that Laws of Physics are same in every Lorentz reference (observer) frame, implying a geometric view of physical laws and calling for the mathematical formulation of any change in a physical quantity under a change of reference frame [3].

The study of implications and the resulting classification of physical quantities constitutes the theory of tensor calculus which was used by Einstein. In this work we introduce some calculation rules used in tensor manipulation and show how the tensors are transformed by change of axis. We apply these results to the elasticity case.

This work is not only useful to Physics and Mechanical engineering students but also to those endeavoring in Fluid and Continuum Mechanics. It is organized as follows: In section 2, we introduce tensor fields and coordinate systems in compliance with ECP and in Section 3 Tensor methods for treating Linear Algebra and Vector Calculus [1, 2] is described. We treat three distinct cases: Cartesian, orthogonal curvilinear and non-orthogonal curvilinear coordinates. Section 4 is dedicated to Tensor extension and contraction of physical quantities and Section 5 is dedicated to Elasticity problems as an application. Section 6 contains a conclusion and perspectives.

Appendix A describes Tensor etymology and its evolution, Appendix B is about covariant derivative needed in curvilinear coordinates and Appendix C discusses Voigt notation heavily used in Elasticity.

II. PHYSICAL FIELDS AND TENSOR FIELDS IN GENERALIZED COORDINATES

Physical fields are function of position in space thus it is imperative to introduce coordinate systems that will allow us to express accurately these fields. A field is a quantity that takes values "instantaneously" at some arbitrary position in space. It is obvious this can't be true according to Feynman and Special Relativity since we know that any change a physical quantity undergoes a signal is needed to transmit the information. As an example, if we have a charge q at a point considered in $\boldsymbol{R}^3$ as the origin $\boldsymbol{r} = 0$ and if we want know the value of the electric field at any point $\boldsymbol{r} \neq 0$, it is necessary that a photon (called "longitudinal") is transmitted from the origin to the point $\boldsymbol{r}$. Since the speed of the photon and of light are finite, a certain time for this information to travel.

Let us contemplate some fields at some point $\boldsymbol{r}$ with different nature such as scalar, vector, tensorial.... Temperature field in a room is a scalar field $T(\boldsymbol{r})$ while the speed within a fluid is a vector field $\boldsymbol{V}(\boldsymbol{r})$. When we consider the electromagnetic field, we have two vector quantities $\boldsymbol{E}(\boldsymbol{r})$ and $\boldsymbol{H}(\boldsymbol{r})$ knowing that the electric field $\boldsymbol{E}(\boldsymbol{r})$ is intrinsically related to the magnetic field $\boldsymbol{H}(\boldsymbol{r})$ via Maxwell's equations. One relevant question that we answer later in subsection IV A is: since $\boldsymbol{E}(\boldsymbol{r})$ $\boldsymbol{H}(\boldsymbol{r})$ fields are intimately related, is it possible to encapsulate them compactly in Maxwell's equations?

A. 2D covariant and contravariant coordinates

ECP being our guide, we start with a general description of coordinates before describing reference (observer) frame transformation. This word is distinct from the covariant adjective that means "form invariant" when it concerns physical laws (pertinent to ECP) or "transforms as standard basis vectors" when it concerns basis vectors. We use this notion in order to describe the different ways of expressing a 2D position vector in a given set of basis vectors $\boldsymbol{e}_1$, $\boldsymbol{e}_2$ (cf fig. 1). Covariance principle has been debated extensively and several workers questioned its validity and pondered about its consequences (see for instance references [4, 5]).

We assume that $\boldsymbol{e}_1$, $\boldsymbol{e}_2$ are normalized ($||\boldsymbol{e}_1|| = ||\boldsymbol{e}_2|| = 1$) and making an angle θ (cf fig. 1).

Let us express the components of some arbitrary 2D vector $\boldsymbol{r}$: $\boldsymbol{r} = x^1\boldsymbol{e}_1 + x^2\boldsymbol{e}_2$ where x^i are the ordinary components (contravariant). Geometrically, the covariant components x_i are obtained by perpendicular projection on to the standard basis axes (cf fig. 1).
Thus $x_i = \boldsymbol{r} \cdot \boldsymbol{e}_i, i = 1, 2$. Substituting $\boldsymbol{r}$ in the latter yields: $x_i = (x^1\boldsymbol{e}_1 + x^2\boldsymbol{e}_2) \cdot \boldsymbol{e}_i$, i.e: $x_1 = (x^1\boldsymbol{e}_1 + x^2\boldsymbol{e}_2) \cdot \boldsymbol{e}_1 = x^1 + x^2\boldsymbol{e}_2 \cdot \boldsymbol{e}_1 = x^1 + x^2 \cos\theta$, $x_2 = (x^1\boldsymbol{e}_1 + x^2\boldsymbol{e}_2) \cdot \boldsymbol{e}_2 = x^2 + x^1\boldsymbol{e}_2 \cdot \boldsymbol{e}_1 = x^1 \cos\theta + x^2$

Assuming a symmetry principle between covariance and contravariance, let us rewrite $\boldsymbol{r} = \sum_i x_i\boldsymbol{e}^i$ (cf fig. 1).

Taking the scalar product with $\boldsymbol{e}_j$ yields: $\boldsymbol{e}_j \cdot \boldsymbol{r} = \sum_i x_i\boldsymbol{e}_j \cdot \boldsymbol{e}^i$. Assuming the covariant coordinate x_j is the projection of $\boldsymbol{r}$ over $\boldsymbol{e}_j$ we get: $x_j = \boldsymbol{e}_j \cdot \boldsymbol{r} = \sum_i x_i\boldsymbol{e}_j \cdot \boldsymbol{e}^i$ then the scalar product $\boldsymbol{e}_j \cdot \boldsymbol{e}^i = \delta^i_j$ the Kronecker symbol written in a

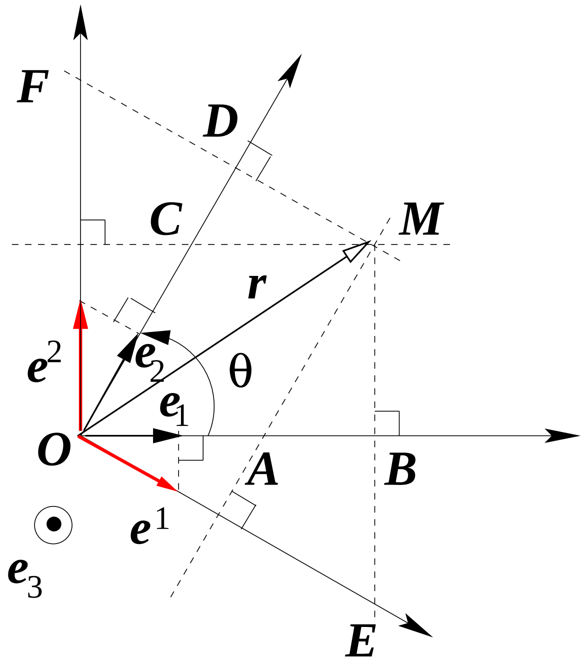

FIG. 1: (Color on-line) 2D Covariant and contravariant coordinates of $\boldsymbol{r} = \boldsymbol{OM}$ in the "standard basis" made of covariant vectors $(\boldsymbol{e}_1, \boldsymbol{e}_2)$. Ordinary (contravariant) coordinates: $\boldsymbol{OA} = x^1$ and $\boldsymbol{OC} = x^2$ are made of projections parallel to basis axes whereas covariant coordinates $\boldsymbol{OB} = x_1$ and $\boldsymbol{OD} = x_2$ are made from perpendicular projections. $\boldsymbol{e}_3$ is a unit vector perpendicular to the $(\boldsymbol{e}_1, \boldsymbol{e}_2)$ plane. Contravariant basis vectors $\boldsymbol{e}^1, \boldsymbol{e}^2$ (in red) are such that $\boldsymbol{e}_1 \perp \boldsymbol{e}^2$ and $\boldsymbol{e}_2 \perp \boldsymbol{e}^1$. Note that $\boldsymbol{e}_1$ is the projection of $\boldsymbol{e}^1$ while $\boldsymbol{e}_2$ is the projection of $\boldsymbol{e}^2$.

mixed fashion but meaning same as generally known i.e. $\delta^i_j = 0$ if $i \neq j$ and $\delta^i_j = 1$ if $i = j$.

Thus, the contravariant basis is orthogonal to the covariant and is termed dual basis in Mathematics or Reciprocal basis in Crystallography [6].

We can express this mathematically by introducing a $\boldsymbol{e}_3$ unit vector perpendicular to the $\boldsymbol{e}_1, \boldsymbol{e}_2$ plane. An explicit expression of the contravariant basis vectors can be derived by exploiting the reciprocal of the standard basis formula [6]:

$$\boldsymbol{e}^1 = \frac{\boldsymbol{e}_2 \times \boldsymbol{e}_3}{(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)}, \boldsymbol{e}^2 = \frac{\boldsymbol{e}_3 \times \boldsymbol{e}_1}{(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)} \tag{1}$$

The triple product $(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3) = \sin\theta$ confirming the geometrical construct in fig. 1 that $\boldsymbol{e}_1$ is the projection of $\boldsymbol{e}^1$ and $\boldsymbol{e}_2$ is the projection of $\boldsymbol{e}^2$ with the values of the norms $||\boldsymbol{e}^1|| = ||\boldsymbol{e}^2|| = 1/\sin\theta$.

Let us rewrite the position vector as $\boldsymbol{r} = x^i \boldsymbol{e}_i$ with Einstein summation rule stating that whenever we have an index appearing twice as covariant and contravariant, a summation over it is implied.

Using laws relating covariant and contravariant components, we define a "metric matrix" g_{ij} in the following way $g_{ij} = \begin{pmatrix} 1 & \cos\theta \\ \cos\theta & 1 \end{pmatrix}, i = 1, 2$. g_{ij} allows us to go between covariant and contravariant coordinates since: $x_i = g_{ij} x^j$. g_{ij} makes the indices "move" down implying by symmetry the existence of another contravariant metric matrix g^{ij} that makes the indices "move" up. Note that $g_{ij} = \boldsymbol{e}_i \cdot \boldsymbol{e}_j$ (respectively $g^{ij} = \boldsymbol{e}^i \cdot \boldsymbol{e}^j$) relates two vectors $\boldsymbol{e}_i$ and $\boldsymbol{e}_j$ (resp. $\boldsymbol{e}^i$ and $\boldsymbol{e}^j$) and if the standard basis $\boldsymbol{e}_i$ is orthonormal ($\theta = \pi/2$), $g_{ij} = \delta_{ij}$ the 2D unit matrix and $x^i = x_i$ making covariant and contravariant coordinates same. Evaluating g^{ij} from the scalar products of $\boldsymbol{e}^i, \boldsymbol{e}^j$ using the previous definitions 1 and fig 1 yields: $[g^{ij}] = \frac{1}{\sin^2\theta} \begin{pmatrix} 1 & -\cos\theta \\ -\cos\theta & 1 \end{pmatrix}, i = 1, 2$.

$[g_{ij}]$ and $[g^{ij}]$ are inverse of one another as consequence of their respective definitions. We provide an alternate proof based on their determinants: $det[g_{ij}] = \sin^2\theta = (\boldsymbol{e}_1 \times \boldsymbol{e}_2)^2$ and $det[g^{ij}] = (\boldsymbol{e}^1 \times \boldsymbol{e}^2)^2$ moreover $(\boldsymbol{e}_1 \times \boldsymbol{e}_2) \parallel \boldsymbol{e}_3$ and $(\boldsymbol{e}^1 \times \boldsymbol{e}^2) \parallel \boldsymbol{e}_3$. Thus $(\boldsymbol{e}_1 \times \boldsymbol{e}_2)^2 (\boldsymbol{e}^1 \times \boldsymbol{e}^2)^2 = [(\boldsymbol{e}_1 \times \boldsymbol{e}_2) \cdot (\boldsymbol{e}^1 \times \boldsymbol{e}^2)]^2$ yielding $det[g_{ij}] det[g^{ij}] = [(\boldsymbol{e}_1 \times \boldsymbol{e}_2) \cdot (\boldsymbol{e}^1 \times \boldsymbol{e}^2)]^2$.

Using the dot product of two cross products [7]:

$$(\boldsymbol{a} \times \boldsymbol{b}) \cdot (\boldsymbol{c} \times \boldsymbol{d}) = \begin{vmatrix} \boldsymbol{a} \cdot \boldsymbol{c} & \boldsymbol{a} \cdot \boldsymbol{d} \\ \boldsymbol{b} \cdot \boldsymbol{c} & \boldsymbol{b} \cdot \boldsymbol{d} \end{vmatrix} \tag{2}$$

we get:

$$(\boldsymbol{e}_1 \times \boldsymbol{e}_2) \cdot (\boldsymbol{e}^1 \times \boldsymbol{e}^2) = \begin{vmatrix} \boldsymbol{e}_1 \cdot \boldsymbol{e}^1 & \boldsymbol{e}_1 \cdot \boldsymbol{e}^2 \\ \boldsymbol{e}_2 \cdot \boldsymbol{e}^1 & \boldsymbol{e}_2 \cdot \boldsymbol{e}^2 \end{vmatrix} = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \tag{3}$$

proving once again that $[g_{ij}]$ and $[g^{ij}]$ are inverse of one another.

We prove further below that $[g_{ij}]$ and $[g^{ij}]$ are rank-2 tensors allowing to write compactly index lowering $x_i = g_{ij}x^j$ and lifting $x^i = g^{ij}x_j$ operations.

B. 3D Covariant and contravariant curvilinear coordinates

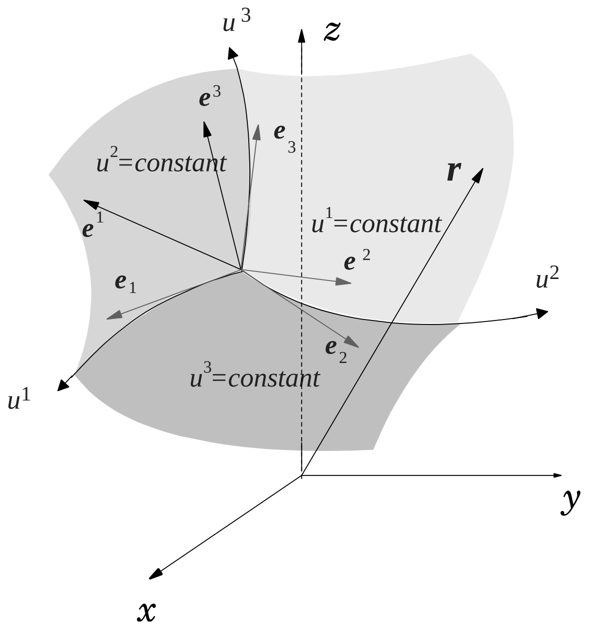

FIG. 2: 3D covariant and contravariant curvilinear coordinates: contravariant vectors are perpendicular to $u^i(x, y, z) = constant$ surfaces whereas covariant basis vectors $\boldsymbol{e}_i$ are tangent to u^i curves that are intersections of u^i surfaces. Position vector $\boldsymbol{r} = (x, y, z)$ can be expressed with u^i coordinates as $\boldsymbol{r}(u^1, u^2, u^3)$.

3D Cartesian orthonormal coordinates (x, y, z) are not appropriate to use in physical problems with special symmetry. It is beneficial to move to curvilinear coordinates $\{x, y, z\} \to \{u^1, u^2, u^3\}$ defined by extending the previous 2D case to contravariant basis vectors $\boldsymbol{e}^i$ perpendicular to $u^i(x, y, z) = constant$ surface as displayed in fig. 2 whereas covariant basis vectors $\boldsymbol{e}_i$ are tangent to u^i curves lying at the intersection between respective u^i surfaces.

Defining $\boldsymbol{e}_i = \frac{\partial \boldsymbol{r}}{\partial u^i}$ and $\boldsymbol{e}^i = \boldsymbol{\nabla} u^i = (\frac{\partial u^i}{\partial x}, \frac{\partial u^i}{\partial y}, \frac{\partial u^i}{\partial z})$, where the operator $\boldsymbol{\nabla} = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})$, it is possible to show that their properties are similar to the 2D case and that many results obtained previously can be extended to the 3D case.

Extending the previous 2D case to 3D, we write explicit expressions of the contravariant basis vectors versus the covariant one $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ as [6]:

$$\boldsymbol{e}^1 = \frac{\boldsymbol{e}_2 \times \boldsymbol{e}_3}{(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)}, \boldsymbol{e}^2 = \frac{\boldsymbol{e}_3 \times \boldsymbol{e}_1}{(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)}, \boldsymbol{e}^3 = \frac{\boldsymbol{e}_1 \times \boldsymbol{e}_2}{(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)} \tag{4}$$

The orthogonality relations $\boldsymbol{e}^i \cdot \boldsymbol{e}_j = 0, i \neq j$ can be proven directly from the line-element $d\boldsymbol{r}$ obtained from Taylor expanding the position vector $\boldsymbol{r}(u^1, u^2, u^3)$ in the u^i basis as:

$$d\boldsymbol{r} = \left(\frac{\partial \boldsymbol{r}}{\partial u^i}\right) du^i \tag{5}$$

Taking the dot product with $\boldsymbol{e}^j = \boldsymbol{\nabla} u^j$ yields $\boldsymbol{\nabla} u^j \cdot d\boldsymbol{r} = \boldsymbol{\nabla} u^j \cdot \left(\frac{\partial \boldsymbol{r}}{\partial u^i}\right) du^i$ and using the gradient definition $\boldsymbol{\nabla} u^j \cdot d\boldsymbol{r} \equiv du^j$, we conclude $\boldsymbol{e}^i \cdot \boldsymbol{e}_j = 0, i \neq j$.

Similarly to the 2D case, a covariant "metric matrix" g_{ij} can be defined from: $g_{ij} = \boldsymbol{e}_i \cdot \boldsymbol{e}_j, i,j = 1,2,3$ as well as a contravariant one $g^{ij} = \boldsymbol{e}^i \cdot \boldsymbol{e}^j, i,j = 1,2,3$ with the properties of raising/lowering indices $x^i = g^{ij}x_j, x_i = g_{ij}x^j$ and mutual orthogonality which translates into $[g_{ij}][g^{ij}] = \mathbb{1}$ and indicially as: $g_{ik}g^{kj} = \delta_i^j$.

Note that $ds^2 = dx^2 + dy^2 + dz^2$ in a Cartesian orthonormal frame $\{x, y, z\}$ with $g_{ij} = g^{ij} = \delta_{ij}$. In a frame characterized by cylindrical coordinates $\{\rho, \phi, z\}$ the line-element squared is given by: $ds^2 = d\rho^2 + \rho^2 d\phi^2 + dz^2$. Using the correspondence $\{1,2,3\} \to \{\rho, \phi, z\}$, the metric matrix components are: $g_{11} = 1, g_{22} = \rho^2, g_{33} = 1, g_{ij} = 0 \quad \text{if} \quad i \neq j, \quad i,j = 1,2,3$. In spherical coordinates $\{r, \theta, \phi\}$ the line-element squared is given by: $ds^2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2\theta d\phi^2$. Using the correspondence $\{r, \theta, \phi\} \to \{1,2,3\}$, the metric matrix components are: $g_{11} = 1, g_{22} = r^2, g_{33} = r^2\sin^2\theta, g_{ij} = 0 \quad \text{if} \quad i \neq j, \quad i,j = 1,2,3$.

In general (non-orthogonal) curvilinear coordinates, the line-element squared is given by $ds^2 = d\boldsymbol{r} \cdot d\boldsymbol{r} = g_{ij}du^i du^j = g^{ij}du_i du_j$ yielding non-diagonal "metric matrices".

C. Einstein covariance principle and tensor transformation

Another aspect of ECP is that a physical quantity when it undergoes a change of reference frame transforms in a fashion revealing its true nature. Thus, it suffices to study the mathematics of reference frame change in order to understand the underlying nature of any physical quantity.

Using the classical (contravariant) coordinates of a vector x^i in a reference frame $\mathcal{R}$, we call its transform $\bar{x}^i$ in the new reference $\bar{\mathcal{R}}$. Note that x^i can be considered as a function of $\bar{x}^j$ the new coordinates and mathematically express it as $x^i = x^i(\bar{x}^j)$.

Performing a Taylor expansion in n dimensions allow us to find a small displacement as:

$$dx^i = \sum_{j=1}^{n} \frac{\partial x^i}{\partial \bar{x}^j} d\bar{x}^j \tag{6}$$

It is expressed with Einstein summation rule as:

$$dx^i = \frac{\partial x^i}{\partial \bar{x}^j} d\bar{x}^j \tag{7}$$

This shows that we have a "Jacobian" factor of the style $\frac{\partial x^i}{\partial \bar{x}^j}$ which expresses the laws of transformation.

If we start from a scalar field (such as temperature or electric scalar potential), we obviously have:

$$\phi(x^i) = \bar{\phi}(\bar{x}^j) \tag{8}$$

meaning that for a scalar field, there is no "Jacobian" factor while that for a vector field like x^i, we have only one factor. Generalizing, we might say a "Jacobian" factor indicates the rank of the tensor.

Let us take the derivatives of the two members of the equation 8 using the compound derivative since we can consider $x^i = x^i(\bar{x}^j)$ just like $\bar{x}^j = \bar{x}^j(x^i)$:

$$\frac{\partial \phi}{\partial x^i} = \frac{\partial \bar{\phi}}{\partial \bar{x}^j} \frac{\partial \bar{x}^j}{\partial x^i} \tag{9}$$

We infer an "inverse Jacobian" factor $\frac{\partial \bar{x}^j}{\partial x^i}$ appears in the gradient transformation. We conclude that there are two possibilities during a coordinate transformation: a "direct Jacobian" $\frac{\partial x^i}{\partial \bar{x}^j}$ is present in the contravariant case whereas an "inverse Jacobian" $\frac{\partial \bar{x}^j}{\partial x^i}$ appears in the covariant case. Thus $\frac{\partial x^i}{\partial \bar{x}^j} \frac{\partial \bar{x}^j}{\partial x^k} = \delta_k^i$.

For a scalar field (rank-0) there is no Jacobian factor, whereas for a vector field (rank-1) there is a single factor and so on.

It is important to note that for rank-2 tensors, we have a matrix representation by letting its coefficients depend on position $\boldsymbol{r}$. However one should recall that a matrix and a tensor are different mathematical objects.

We summarize below the various transformations of a rank-1 and rank-2 tensors:

- Transformation law for a contravariant field:

$$A^i = \frac{\partial x^i}{\partial \bar{x}^j} \bar{A}^j \tag{10}$$

- Transformation law for a covariant field:

$$A_i = \frac{\partial \bar{x}^j}{\partial x^i} \bar{A}_j \tag{11}$$

- Transformation law for a twice contravariant tensor:

$$A^{ij} = \frac{\partial x^i}{\partial \bar{x}^k} \frac{\partial x^j}{\partial \bar{x}^l} \bar{A}^{kl} \tag{12}$$

- Transformation law for a twice covariant tensor:

$$A_{ij} = \frac{\partial \bar{x}^k}{\partial x^i} \frac{\partial \bar{x}^l}{\partial x^j} \bar{A}_{kl} \tag{13}$$

- Transformation law for a mixed singly covariant, singly contravariant tensor:

$$A_i^k = \frac{\partial \bar{x}^m}{\partial x^i} \frac{\partial x^k}{\partial \bar{x}^l} \bar{A}_m^l \tag{14}$$

D. Tensor construction

After reckoning the 2D metric matrix is built from two basis vectors, a mechanical question arises concerning the pressure involving also two vectors (force and area). Thus, what is the underlying nature of the pressure field?

In fact, pressure is a tensor field of rank-2 since it connects two vector fields as described in the elasticity section V. Essentially, there are several methods to build a tensor:

- From association of several vector (rank-1) components:
  The "metric tensor" we called previously "metric matrix" is obtained from a scalar product operation between two vectors (rank-1 tensors): $g_{ij} = \boldsymbol{e}_i \cdot \boldsymbol{e}_j$ or $g^{ij} = \boldsymbol{e}^i \cdot \boldsymbol{e}^j$, which are both rank-2 tensors. Since ds^2 the squared line-element is a scalar, it can be expressed invariantly in two different coordinate systems $\{x^i\} \to \{\bar{x}^i\}$ where the set $\{x^i\}$ is orthonormal and $\{\bar{x}^i\}$ is not. $ds^2 = \delta_{ij} dx^i dx^j = g_{ij} d\bar{x}^i d\bar{x}^j$. Performing a change of reference frame gives: $dx^i = \frac{\partial x^i}{\partial \bar{x}^j} d\bar{x}^j$. Thus $ds^2 = \delta_{ij} dx^i dx^j = \delta_{ij} \frac{\partial x^i}{\partial \bar{x}^k} d\bar{x}^k \frac{\partial x^j}{\partial \bar{x}^l} d\bar{x}^l = g_{kl} d\bar{x}^k d\bar{x}^l$. Covariant metric tensor components are given by: $g_{kl} = \delta_{ij} \frac{\partial x^i}{\partial \bar{x}^k} \frac{\partial x^j}{\partial \bar{x}^l}$ where coordinates $\bar{x}^i$ are e.g. curvilinear. The contravariant metric tensor $g^{ij} = \boldsymbol{e}^i \cdot \boldsymbol{e}^j$ is the inverse of the covariant g_{ij} as proven previously in subsection II B. Another proof is that $\boldsymbol{e}^i$ being the dual (contravariant, reciprocal) basis, the two "matrices" are inverse of one another [6].

- From direct multiplication of vector components (outer product):
  As an example, take two vector fields A^i and B^j and make the component product by component to obtain a tensor of rank-2: $T^{ij} = A^i B^j$ which can be formally written like $T = \boldsymbol{A} \otimes \boldsymbol{B}$. This is of course generalizable to any dimension. For example with three vector fields $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}$ on can do: $T = \boldsymbol{A} \otimes \boldsymbol{B} \otimes \boldsymbol{C}$ so $T^{ijk} = A^i B^j C^k$ (cf fig. 3). This implies that a tensor of rank- r is constructed from vector fields in D dimensions, we have D^r components.

- From spatial derivation [9] of a scalar field:
  The gradient of a scalar field $\phi(\boldsymbol{r})$ is in fact a means to transform a rank-0 field into a vector field (rank-1): $[\boldsymbol{grad\phi}]_i = \frac{\partial \phi}{\partial x^i}$. Note however that the gradient behaves as a **covariant** vector field (It is shown further below that there are contravariant and covariant varieties of the gradient). As a consequence, derivation (respectively integration) of another tensor field allow to change the rank by 1 (resp. -1).

- From contraction of another tensor:
  Contraction is an operation consisting of equating two indices (say $i = j$) in a tensorial expression and summing over (say i). One example is the scalar product of two covariant vectors: $\boldsymbol{a} \cdot \boldsymbol{b} = a_i b_i$ that transforms a rank-2 tensor $a_i b_j$ after a contraction into a scalar (rank-0). Another example drawn from linear algebra is to apply a matrix M with coefficients M_{ij} to a vector $\boldsymbol{a} = (a_1, a_2, a_3)$ resulting into another vector $\boldsymbol{b}$ such that $\boldsymbol{b} = M\boldsymbol{a}$, meaning indicially $b_i = \sum_{j=1}^{3} M_{ij} a_j$. Using Einstein summation rule, we write $b_i = M_{ij} a_j$ which in fact might be viewed as a contraction $(j = k)$ from a rank-3 tensor $M_{ij} a_k$ to a (rank-1) vector b_i. Rephrasing in Tensor language writes: Suppose $T_{i_1, i_2, i_3,, i_m}$ transforms as a tensor of rank- m then $T_{j,j,i_3,,i_m}$ transforms as a tensor of rank- $(m-2)$. This operation corresponds to a general contraction of a tensor.

- By combining all previous operations

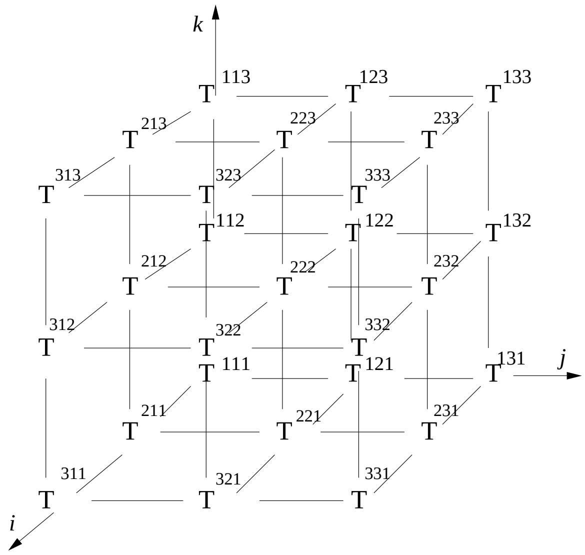

FIG. 3: Pictorial representation of tensor components $T^{ijk} = A^i B^j C^k, i, j, k = 1, 2, 3$ at nodes of a 3D lattice. Adapted from ref. [8]

III. VECTOR ALGEBRA AND CALCULUS WITH TENSORS

A. Linear algebra with tensors in Cartesian coordinates

In Cartesian (Affine) coordinates, the basis vectors are same independent of position. Moreover we do not make any distinction, in this paragraph between contravariant and covariant components since basis vectors are also orthonormal $\boldsymbol{e}_i \cdot \boldsymbol{e}_j = \delta_{ij}$. This implies the Kroenecker symbol [10] is in fact a rank-2 tensor built from the scalar product of two vectors.

Let us introduce rank-3 Levi-Civita antisymmetric tensor: $\epsilon_{ijk} = \boldsymbol{e}_i \cdot (\boldsymbol{e}_j \times \boldsymbol{e}_k) = (\boldsymbol{e}_i, \boldsymbol{e}_j, \boldsymbol{e}_k), i, j, k = 1..3$ with the following properties: $\epsilon_{ijk} = 0$ for $i = j, j = k, i = k$ whereas $\epsilon_{ijk} = \pm 1$ depending on whether i, j, k is an even or odd permutation of 1,2,3.

Levi-Civita ϵ_{ijk} is in fact a pseudo-tensor [11], since built from a triple-product of vectors (rank-1 tensors). The product of two Levi-Civita tensors is found from a Linear Algebra theorem stating that the determinant of the product of two triple products is the determinant of scalar products: $\epsilon_{ijk}\epsilon_{lmn} = (\boldsymbol{e}_i, \boldsymbol{e}_j, \boldsymbol{e}_k)(\boldsymbol{e}_l, \boldsymbol{e}_m, \boldsymbol{e}_n)$.

Since a triple product is a determinant we use $det(A)det(B) = det(AB)$, thus:

$$\epsilon_{ijk}\epsilon_{lmn} = \begin{vmatrix} \boldsymbol{e}_i \cdot \boldsymbol{e}_l & \boldsymbol{e}_i \cdot \boldsymbol{e}_m & \boldsymbol{e}_i \cdot \boldsymbol{e}_n \\ \boldsymbol{e}_j \cdot \boldsymbol{e}_l & \boldsymbol{e}_j \cdot \boldsymbol{e}_m & \boldsymbol{e}_j \cdot \boldsymbol{e}_n \\ \boldsymbol{e}_k \cdot \boldsymbol{e}_l & \boldsymbol{e}_k \cdot \boldsymbol{e}_m & \boldsymbol{e}_k \cdot \boldsymbol{e}_n \end{vmatrix} = \begin{vmatrix} \delta_{il} & \delta_{im} & \delta_{in} \\ \delta_{jl} & \delta_{jm} & \delta_{jn} \\ \delta_{kl} & \delta_{km} & \delta_{kn} \end{vmatrix}$$

The contraction of two Levi-Civita product:

$$\epsilon_{ijk}\epsilon_{klm} = \begin{vmatrix} \delta_{il} & \delta_{im} \\ \delta_{jl} & \delta_{jm} \end{vmatrix} = \delta_{il}\delta_{jm} - \delta_{jl}\delta_{im}$$

Using the former identity yields $\epsilon_{ijk}\epsilon_{ijl} = 2\delta_{kl}$. Contracting over all indices yields: $\epsilon_{ijk}\epsilon_{ijk} = 2\delta_{kk} = 6$

Let us apply to the scalar product, vector product and double vector product.

- Scalar product:
  Given two vectors $\boldsymbol{A} = A_i\boldsymbol{e}_i$ and $\boldsymbol{B} = B_i\boldsymbol{e}_i$, we write: $\boldsymbol{A} \cdot \boldsymbol{B} = A_i\boldsymbol{e}_i \cdot B_j\boldsymbol{e}_j = A_iB_j\boldsymbol{e}_i \cdot \boldsymbol{e}_j = A_iB_j\delta_{ij} = A_iB_i$

- Vector product:
  $\boldsymbol{A} \times \boldsymbol{B} = A_i\boldsymbol{e}_i \times B_j\boldsymbol{e}_j = A_iB_j\boldsymbol{e}_i \times \boldsymbol{e}_j$. Taking the scalar product with a basis vector: $(\boldsymbol{A} \times \boldsymbol{B}) \cdot \boldsymbol{e}_k = A_iB_j(\boldsymbol{e}_i \times \boldsymbol{e}_j) \cdot \boldsymbol{e}_k = (\boldsymbol{e}_i, \boldsymbol{e}_j, \boldsymbol{e}_k)A_iB_j = \epsilon_{ijk}A_iB_j$

- Double vector product:
  $\boldsymbol{A} \times (\boldsymbol{B} \times \boldsymbol{C})$. Taking the i-th component we get: $\epsilon_{ijk}A_j(\boldsymbol{B} \times \boldsymbol{C})_k = \epsilon_{ijk}A_j\epsilon_{klm}B_lC_m$
  This yields: $(\delta_{il}\delta_{jm} - \delta_{jl}\delta_{im})A_jB_lC_m = A_jB_iC_j - A_jB_jC_i = (\boldsymbol{A} \cdot \boldsymbol{C})B_i - (\boldsymbol{A} \cdot \boldsymbol{B})C_i$
  Thus: $\boldsymbol{A} \times (\boldsymbol{B} \times \boldsymbol{C}) = (\boldsymbol{A} \cdot \boldsymbol{C})\boldsymbol{B} - (\boldsymbol{A} \cdot \boldsymbol{B})\boldsymbol{C}$

B. Differential vector calculus with tensors in Cartesian coordinates

Differential vector calculus is based on the use of the nabla vector operator $\boldsymbol{\nabla}$ yielding the gradient, divergence, curl and Laplacian. In (Affine) Cartesian coordinates, we do not make any distinction between contravariant and covariant components ($A^i = A_i$) since we have $\boldsymbol{e}_i \cdot \boldsymbol{e}_j = \delta_{ij}$. Moreover, the $\boldsymbol{e}_i$ are independent of coordinates giving: $\boldsymbol{\nabla} = \boldsymbol{e}_i \frac{\partial}{\partial x_i} = \boldsymbol{e}_i \partial_i = \partial_i \boldsymbol{e}_i$.

- Scalar field gradient:
  Given a scalar field $\phi(\boldsymbol{r})$, the i-th component of the gradient is $[\boldsymbol{grad}\phi(\boldsymbol{r})]_i = \boldsymbol{\nabla}_i \phi(\boldsymbol{r}) = \frac{\partial \phi(\boldsymbol{r})}{\partial x_i} = \partial_i \phi$.
- Vector field gradient:
  For a vector field $\boldsymbol{A}(\boldsymbol{r})$, the i-th component of the gradient of j-th component of $\boldsymbol{A}$ is $[\boldsymbol{\nabla}(\boldsymbol{A})_j]_i = \boldsymbol{\nabla}_i A_j = \partial_i A_j$
- Vector field divergence:
  Given a vector field $\boldsymbol{A}(\boldsymbol{r})$, its divergence is: $\boldsymbol{\nabla} \cdot \boldsymbol{A}(\boldsymbol{r}) = \boldsymbol{e}_i \partial_i \cdot A_j \boldsymbol{e}_j = \partial_i A_j \boldsymbol{e}_i \cdot \boldsymbol{e}_j = \partial_i A_j \delta_{ij} = \partial_i A_i$.
- Vector field curl:
  Given a vector field $\boldsymbol{A}(\boldsymbol{r})$, its curl is: $\boldsymbol{\nabla} \times \boldsymbol{A}(\boldsymbol{r}) = \boldsymbol{e}_i \partial_i \times A_j \boldsymbol{e}_j = \partial_i A_j (\boldsymbol{e}_i \times \boldsymbol{e}_j)$. The i-th component is $[\boldsymbol{curl}\boldsymbol{A}]_i = \epsilon_{ijk} \partial_j A_k$.
- Scalar field Laplacian:
  The Laplacian of a scalar field $\phi(\boldsymbol{r})$ is $\Delta\phi(\boldsymbol{r}) = \boldsymbol{\nabla} \cdot \boldsymbol{\nabla}\phi(\boldsymbol{r}) = \partial_i \partial_i \phi$.
- Curl divergence:
  $div\ \boldsymbol{curl}\boldsymbol{A}(\boldsymbol{r}) = \partial_i \epsilon_{ijk} \partial_j A_k = \epsilon_{ijk} \partial_i \partial_j A_k = 0$.
  This stems from the fact a contraction of two tensors with one symmetric ($\partial_i \partial_j$) [12] and the other antisymmetric ϵ_{ijk} gives zero.
- Gradient curl:
  $[\boldsymbol{curl}\ \boldsymbol{grad}\phi(\boldsymbol{r})]_i = \epsilon_{ijk} \partial_j \partial_k \phi = 0$.
  This originates as before from the contraction of a symmetric ($\partial_j \partial_k$) and antisymmetric ϵ_{ijk} tensors.
- curl of curl:

$$\begin{aligned} [\boldsymbol{curl}\ \boldsymbol{curl}\boldsymbol{A}(\boldsymbol{r})]_i = \epsilon_{ijk} \partial_j [\boldsymbol{curl}\boldsymbol{A}(\boldsymbol{r})]_k &= \\ \epsilon_{ijk} \partial_j \epsilon_{klm} \partial_l A_m = \epsilon_{ijk} \epsilon_{klm} \partial_j \partial_l A_m &= \\ (\delta_{il}\delta_{jm} - \delta_{jl}\delta_{im}) \partial_j \partial_l A_m = \partial_i \partial_m A_m - \partial_j \partial_j A_i &= \\ \partial_i (div\boldsymbol{A}) - [\Delta \boldsymbol{A}]_i & \end{aligned} \tag{15}$$

  We end up with: $\boldsymbol{curl}\ \boldsymbol{curl}\boldsymbol{A} = \boldsymbol{grad}(div\boldsymbol{A}) - \Delta\boldsymbol{A}$
- Vector field Laplacian:
  In case of a vector field $\boldsymbol{A}(\boldsymbol{r})$ we apply the Laplacian operator on every component: $[\Delta\boldsymbol{A}]_i = \partial_j \partial_j A_i$. Note that this is not true for curvilinear coordinates case as seen further below.

C. Differential operators in orthogonal curvilinear coordinates

The gradient of a scalar field $\phi(\boldsymbol{r}(u^i))$ is evaluated by comparing its differential $d\phi = \frac{\partial \phi}{\partial u^i} du^i$ to the corresponding gradient expression $d\phi = \boldsymbol{grad}\phi \cdot d\boldsymbol{r}$. The line-element expression: $d\boldsymbol{r} = h_i \boldsymbol{e}_i du^i$ uses h_i coefficients that are scale factors [13] rendering $\boldsymbol{e}_i$ normalized. An important difference between this case and the Cartesian is that $\boldsymbol{e}_i$ depend on coordinates u^j. Moreover any vector is expressed with the scale factors as: $\boldsymbol{A} = h_i A^i \boldsymbol{e}_i$.

The $\boldsymbol{\nabla}$ operator in orthogonal curvilinear coordinates is defined by: $\boldsymbol{\nabla} = \boldsymbol{e}_i \frac{\partial}{h_i \partial u^i}$. Note that we keep using the contravariant notation (such as A^i, u^i...) despite the fact they are same in orthogonal curvilinear coordinates. The expressions for the gradient, div, curl and Laplacian are obtained from the $\boldsymbol{\nabla}$ operator as done in Cartesian coordinates. Thus:

$$\begin{aligned}
\boldsymbol{grad}\phi &= \boldsymbol{e}_i \frac{\partial}{h_i \partial u^i}\phi \\
\text{div } \boldsymbol{A} &= \boldsymbol{e}_i \frac{\partial}{h_i \partial u^i} \cdot \boldsymbol{A} = \boldsymbol{e}_i \frac{\partial}{h_i \partial u^i} \cdot (h_j A^j \boldsymbol{e}_j) = \frac{1}{h_1 h_2 h_3}\left(\frac{\partial}{\partial u^i}(h_j h_k A^i)\right), \quad i,j,k = 1,2,3 \\
\boldsymbol{curl}\ \boldsymbol{A} &= \boldsymbol{e}_i \frac{\partial}{h_i \partial u^i} \times \boldsymbol{A} = \boldsymbol{e}^i \frac{\partial}{h_i \partial u^i} \times (h_j A^j \boldsymbol{e}_j) = \frac{1}{h_1 h_2 h_3}\begin{vmatrix} h_1 \boldsymbol{e}_1 & h_2 \boldsymbol{e}_2 & h_3 \boldsymbol{e}_3 \\ \frac{\partial}{\partial u^1} & \frac{\partial}{\partial u^2} & \frac{\partial}{\partial u^3} \\ h_1 A^1 & h_2 A^2 & h_3 A^3 \end{vmatrix} \\
\Delta\phi &= \boldsymbol{\nabla} \cdot \boldsymbol{\nabla}\phi = \boldsymbol{e}_i \frac{\partial}{h_i \partial u^i} \cdot \boldsymbol{e}_j \frac{\partial}{h_j \partial u^j}\phi = \frac{1}{h_1 h_2 h_3}\left[\frac{\partial}{\partial u^i}\left(\frac{h_j h_k}{h_i}\frac{\partial \phi}{\partial u^i}\right)\right], \quad i,j,k = 1,2,3
\end{aligned}$$

In order to evaluate the Laplacian of a vector field [14, 15] (called the Beltrami operator) in coordinates other than Cartesian, one resorts to the double curl formula derived above: $\Delta \boldsymbol{A} = \boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \boldsymbol{A}) - \boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \boldsymbol{A})$.

D. Differential operators in non-orthogonal curvilinear coordinates

In non-orthogonal curvilinear coordinates, one distinguishes covariant from contravariant quantities as well as dependence of $\boldsymbol{e}^i, \boldsymbol{e}_i$ on u^j, u_j. The line-element squared versus metric tensor is expressed as:

$$ds^2 = d\boldsymbol{r} \cdot d\boldsymbol{r} = \left(\frac{\partial \boldsymbol{r}}{\partial u_i}\right) du_i \cdot \left(\frac{\partial \boldsymbol{r}}{\partial u_j}\right) du_j \equiv g^{ij} du_i du_j \tag{16}$$

The $\boldsymbol{\nabla}$ operator in curvilinear coordinates is written as: $\boldsymbol{\nabla} = \boldsymbol{e}^i \frac{\partial}{\partial u^i}$ without using any scale factors [13] and consequently possessing un-normalized $\boldsymbol{e}^i, \boldsymbol{e}_i$.

The gradient [16] of a scalar field $\phi(\boldsymbol{r})$ is $\boldsymbol{\nabla}\phi = \boldsymbol{e}^i \frac{\partial \phi}{\partial u^i}$ corresponding to the same expression as in the orthogonal case (with the scale factors $h_i = 1$). This is not true for the divergence, curl and Laplacian where the covariant derivative intervenes because of the appearance of the Jacobian terms (cf Appendix B).

The divergence of a vector field $\boldsymbol{A}$ is written as: $\boldsymbol{\nabla} \cdot \boldsymbol{A} = \boldsymbol{e}^j \frac{\partial}{\partial u^j} \cdot (A^i \boldsymbol{e}_i) = \boldsymbol{e}^j \cdot [(\frac{\partial A^i}{\partial u^j}\boldsymbol{e}_i) + A^i \Gamma^k_{ij} \boldsymbol{e}_k]$. The term $[(\frac{\partial A^i}{\partial u^j}\boldsymbol{e}_i) + A^i \Gamma^k_{ij} \boldsymbol{e}_k]$ is transformed into $[(\frac{\partial A^i}{\partial u^j}) + A^k \Gamma^i_{kj}]\boldsymbol{e}_i$ (cf Appendix B) containing $\boldsymbol{A}$ covariant derivative $D_j A^i = [(\frac{\partial A^i}{\partial u^j}) + A^k \Gamma^i_{kj}]$. Thus the divergence of a vector field $\boldsymbol{A}$ is $\boldsymbol{e}^j \cdot D_j A^i \boldsymbol{e}_i$ is similar to the Cartesian case with the covariant derivative replacing the ordinary one. This can be further expressed compactly using $\Gamma^i_{ij} = \frac{1}{2} g^{lk} \frac{\partial g_{lk}}{\partial u^j}$ (cf Appendix B) as: $\frac{1}{\sqrt{g}} \frac{\partial}{\partial u^k}(\sqrt{g} A^k)$ where $g = det[g_{ij}]$.

Similarly, the curl of a vector field $\boldsymbol{A}$ is defined by: $\boldsymbol{\nabla} \times \boldsymbol{A} = \boldsymbol{e}^i \frac{\partial}{\partial u^i} \times A^j \boldsymbol{e}_j = (\frac{\partial A^k}{\partial u^i} + A^i \Gamma^k_{ij})(\boldsymbol{e}_k \times \boldsymbol{e}_j)$. Again it is similar to the Cartesian case, the covariant derivative replacing the ordinary one.

The scalar Laplacian is obtained from a double application of the covariant derivative following the Cartesian case: $\Delta\phi = \partial_i \partial_i \phi$. Starting from $\Delta\phi = D_i D^i \phi$, we introduce the metric tensor [7] such that:
$\Delta\phi = D_i (g^{ij} D_j \phi) = [\frac{\partial (g^{ij} D_j \phi)}{\partial u^i} + (g^{ij} D_j \phi)\Gamma^k_{ij}] = \frac{1}{\sqrt{g}} \frac{\partial}{\partial u^j}(\sqrt{g} g^{jk} \frac{\partial \phi}{\partial u^k})$.

In order to evaluate the vector Laplacian (Beltrami operator) we follow Hirota *et al.* [15] work who have explicitly shown that the operators $\Delta = \boldsymbol{\nabla} \cdot \boldsymbol{\nabla}$ and $\boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot) - \boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times)$ are same, since the equivalence taken for granted from the Cartesian case is not acceptable. Thus we have: $\Delta \boldsymbol{A} = \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} \boldsymbol{A} = \boldsymbol{e}^i \frac{\partial}{\partial u^i} \cdot \boldsymbol{e}^j \frac{\partial}{\partial u^j} \boldsymbol{A} = g^{ij}\left(\frac{\partial^2}{\partial u^i \partial u^j} - \Gamma^k_{ij} \frac{\partial}{\partial u^k}\right)\boldsymbol{A}$.

IV. TENSOR EXTENSION AND REDUCTION OF PHYSICAL QUANTITIES

A. Tensor extension of physical quantities

Many possibilities exist to extend the attributes [17–19] of any physical quantity initially attached to isotropic media (non-crystalline) to some corresponding anisotropic medium (crystalline).

For example, in electrostatics of isotropic media, the relation: $\boldsymbol{D} = \epsilon \boldsymbol{E}$ with $\boldsymbol{D} \parallel \boldsymbol{E}$ when extended to crystals becomes $D_i = \epsilon_{ij} E_j$ with $\boldsymbol{D} \nparallel \boldsymbol{E}$.

Similarly, in magnetostatics: $\boldsymbol{B} = \mu \boldsymbol{H}$ translates to $B_i = \mu_{ij} H_j$.

Electric conduction in materials is described by Ohm's law $\boldsymbol{J} = \sigma \boldsymbol{E}$ that translates into $J_i = \sigma_{ij} E_j$ in the anisotropic case. The resistivity tensor ρ_{ij} inverse of the conductivity tensor σ_{ij} allows us to rewrite Ohm's law in the following form: $E_i = \rho_{ij} J_j$.

In magnetic (anisotropic) crystals, the susceptibility defined by $M_i = \chi_{ij} H_j$ where $\boldsymbol{M}$ is the magnetization induced by a magnetic field $\boldsymbol{H}$ is extended from the simple case where $M = \chi H$ with $M \parallel H$ and χ a scalar.

In metallic, semiconducting and insulating crystals, anisotropic effective mass that originated from ordinary mass of Newton's law $\boldsymbol{F} = m\boldsymbol{\gamma}$ would be translated into $F_i = m_{ij}\gamma_j$ where $\boldsymbol{\gamma}$ is acceleration.

In piezoelectric crystals [20–22], a stress σ creates a polarization P such that $P = d\sigma$ with d the piezoelectric modulus. In the anisotropic case, a stress σ_{jk} creates a polarization P_i such that $P_i = d_{ijk}\sigma_{jk}$ with d_{ijk} a rank-3 tensor of piezoelectric moduli since it relates a rank-2 (stress) and a rank-1 (polarization) tensors.

When a magnetic field $\boldsymbol{H}$ is applied to a metal or a semiconductor traversed by an electric current density $\boldsymbol{J}$, the Hall effect arises as a voltage, transverse to $\boldsymbol{J}$, described by an electric field $E_i = \rho_{ijk} J_j H_k$ where ρ_{ijk} is a rank-3 tensor relating three vectors $\boldsymbol{E}, \boldsymbol{J}$ and $\boldsymbol{H}$.

It is tempting to generalize Ohm and Hall results by introducing [17] an ordered field expansion:
$E_i = \rho^{(0)}_{ij} J_j + \rho^{(1)}_{ijk} J_j H_k + \rho^{(2)}_{ijkl} J_j H_k H_l ...$ where $\rho^{(0)}_{ij}$ is zero order (no field present) resistivity (Ohm), $\rho^{(1)}_{ijk}$ is first-order (field present) Hall effect, $\rho^{(2)}_{ijkl}$ is second-order (field present) Hall effect... Note that only $\rho^{(0)}_{ij}$ has dimension of resistivity whereas higher order tensors $\rho^{(n)}_{ijk...}, n \geq 1$ do not, because of the presence of magnetic field powers.

Maxwell equations can be rewritten in a tensorial covariant fashion by encapsulating the scalar Φ and vector $\boldsymbol{A}$ potentials into a single 4-potential $A^\alpha = (\Phi, \boldsymbol{A})$ where $\alpha = 0, 1, 2, 3$. Time corresponds to $\alpha = 0$ whereas 3D spatial degrees of freedom are represented by $\alpha = 1, 2, 3$. This leads to write the charge continuity equation $\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{J} = 0$ as $\partial_\alpha J^\alpha = 0$ with $J^\alpha = (c\rho, \boldsymbol{J})$ where c is light velocity.

The antisymmetric rank-2 electromagnetic tensor given by $F^{\alpha,\beta} = \partial^\alpha A^\beta - \partial^\beta A^\alpha$ allows to encapsulate the inhomogeneous Maxwell equations: $\boldsymbol{\nabla} \cdot \boldsymbol{E} = 4\pi\rho, \boldsymbol{\nabla} \times \boldsymbol{B} - \frac{1}{c}\frac{\partial \boldsymbol{E}}{\partial t} = \frac{4\pi}{c}\boldsymbol{J}$ into a covariant form given [23] by: $\partial_\alpha F^{\alpha,\beta} = \frac{4\pi}{c} J^\beta$.

B. Reduction to a scalar by projection along a single or two orthogonal directions

A physical property written by a rank-2 tensor like $\overset{\leftrightarrow}{\epsilon}$, for example, associated with the dielectric constant appearing in $D_i = \epsilon_{ij} E_j$, can be estimated according to a direction given by the unit vector $\boldsymbol{n}$ like ϵ_n in the following way: $\epsilon_n = \epsilon_{ij} \boldsymbol{n}_i \boldsymbol{n}_j$.

We contract the tensor ϵ_{ij} with the components $\boldsymbol{n}_i, \boldsymbol{n}_j$ direction $\boldsymbol{n}$ to make it a representative scalar ϵ_n. To prove this, let D_n be the projection of $\boldsymbol{D}$ following a field $\boldsymbol{E}$ parallel to $\boldsymbol{n}$. This gives $D_n = \boldsymbol{D} \cdot \boldsymbol{E}/|E|$ with $D_n = \epsilon_n |E|$. We then obtain $\epsilon_n |E| = \boldsymbol{D} \cdot \boldsymbol{E}/|E|$.

We get: $\epsilon_n |E| = \overset{\leftrightarrow}{\epsilon}\ \boldsymbol{E} \cdot \boldsymbol{E}/|E|$ and $\epsilon_n = \overset{\leftrightarrow}{\epsilon}\ \boldsymbol{E} \cdot \boldsymbol{E}/(|E||E|) = \overset{\leftrightarrow}{\epsilon}\ (\boldsymbol{E}/|E|) \cdot (\boldsymbol{E}/|E|)$. Now $\boldsymbol{n} = \boldsymbol{E}/|E|$ and therefore: $\epsilon_n = \epsilon_{ij} \boldsymbol{n}_i \boldsymbol{n}_j$.

A physical property expressed as a rank-2 tensor like the dielectric constant ϵ_{ij} or Shear elastic modulus $G(\boldsymbol{n}, \boldsymbol{q})$ can be probed along two different directions (generally orthogonal) carried by two unit vectors $\boldsymbol{n}$ and $\boldsymbol{q}$. Projecting along those two directions, we obtain: $\epsilon_{\boldsymbol{n},\boldsymbol{q}} = \epsilon_{ij} \boldsymbol{n}_i \boldsymbol{q}_j$.

C. Symmetry reduction

Starting from the fact that a component tensor $T_{ij...} \sim x_i x_j x_k ...$ according to Fumi rule [24], we can easily simplify tensors by exploiting crystal symmetry.
Let us consider a rank-2 tensor in 3D and carry on simplification of its components as we we go along triclinic to monoclinic to orthorhombic, tetragonal and finally cubic symmetry.

- In the triclinic case (no symmetry):
  We have 3x3=9 components: $\begin{pmatrix} T_{xx} & T_{xy} & T_{xz} \\ T_{yx} & T_{yy} & T_{yz} \\ T_{zx} & T_{zy} & T_{zz} \end{pmatrix}$.
  For any physical tensor (conductivity, permittivity, etc...) the symmetry $T_{ij} = T_{ji}$ is true in general since corresponding energy is akin to a quadratic form (for example, electric energy is $\sigma_{ij} E_i E_j$ with σ_{ij} the conductivity tensor and E_i the electric field). This symmetry leads to only six non-zero components.

- Monoclinic symmetry:
  We have a mirror plane perpendicular to the elementary mesh: $z \to -z$, which causes all components containing

z once to be removed by symmetry. There are four components left: $\begin{pmatrix} T_{xx} & T_{xy} & 0 \\ T_{yx} & T_{yy} & 0 \\ 0 & 0 & T_{zz} \end{pmatrix}$

- Orthorhombic symmetry:
  We have 3 possible mirror planes: $x \to -x, y \to -y, z \to -z$. The non-zero components of the tensor are those containing even combinations of x, y, z. We then have three components: $\begin{pmatrix} T_{xx} & 0 & 0 \\ 0 & T_{yy} & 0 \\ 0 & 0 & T_{zz} \end{pmatrix}$

- Tetragonal symmetry:
  We have the equivalence $x \leftrightarrows y$: $\begin{pmatrix} T_{xx} & 0 & 0 \\ 0 & T_{xx} & 0 \\ 0 & 0 & T_{zz} \end{pmatrix}$

- Cubic symmetry:
  We have the equivalence $x \leftrightarrows y \leftrightarrows z$: $\begin{pmatrix} T_{xx} & 0 & 0 \\ 0 & T_{xx} & 0 \\ 0 & 0 & T_{xx} \end{pmatrix} = T_{xx}\mathbb{1}$ with $\mathbb{1}$ the unit matrix.

NB: All matrix representations of the tensors mentioned above are made in the orthonormal basis $\{xyz\}$.

V. APPLICATION TO ANISOTROPIC ELASTICITY

Pressure possesses a tensor character since it involves a force $\boldsymbol{dF}$ and a surface $\boldsymbol{dS} = \boldsymbol{n}dS$ that are both represented mathematically by vectors. Pression is therefore a rank-2 tensor since it associates two vectors (rank-1 tensors). It is represented by the stress tensor σ_{ij} that originates from force i component i "divided" by surface $\boldsymbol{n}$ component j. Mathematically it is written to bypass division operation as $dF_i = \sigma_{ij} dS_j$.

Stress can be applied to an object in various fashions:

1. Uniaxial stress: $\sigma_{ij} = \sigma n_i n_j$ with σ applied along $\boldsymbol{n}$ orthogonal to a surface element.
2. Hydrostatic stress: $\sigma_{ij} = -\sigma\delta_{ij}$ with σ applied equally along three directions.
3. Simple shear stress: $\sigma_{ij} = \sigma(n_i q_j + n_j q_i)$ where σ is applied along direction $\boldsymbol{n}$ belonging to a surface element orthogonal to $\boldsymbol{q}$.

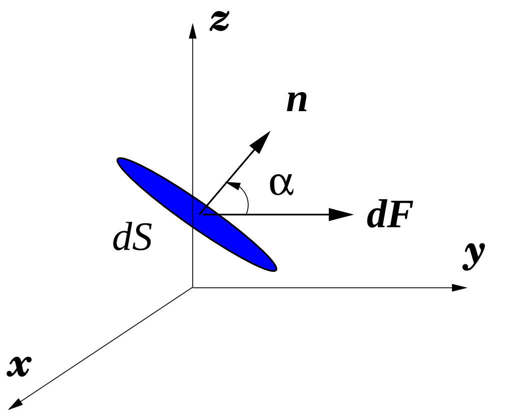

FIG. 4: (Color online) Applied pressure with non collinear force $\boldsymbol{F}$ and normal $\boldsymbol{n}$ to (blue) surface element. When $\alpha = 0$, we get the ordinary scalar pressure $P = \frac{dF}{dS}$. Moving on to arbitrary $\alpha \neq 0$ yields the stress tensor: $\sigma_{ij} \sim \frac{dF_i}{dSn_j}$ rigorously written as $dF_i = \sigma_{ij} dSn_j$

A. Elasticity tensors

A displacement field $\boldsymbol{\delta}(\boldsymbol{r})$ represents local geometrical alterations of a continuum (isotropic or anisotropic), when subjected to internal or external mechanical efforts.

Adopting the same notation as in ECP we consider x^i in a reference frame and call its correspondent $\bar{x}^i$ in the deformed reference (cf fig.5). Deformation alters basis vectors in a way such that they are $\bar{\boldsymbol{e}}_i$ in the deformed object whereas they are given by $\boldsymbol{e}_i$ in the undeformed one (cf fig. 5).

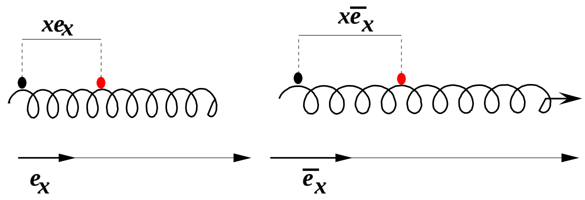

FIG. 5: (Color online) Applying stress to an object results in displacement. This 1D diagram shows an undeformed spring (at left) with a given red marker at $x\boldsymbol{e}_x$ displaced to a new position $x\bar{\boldsymbol{e}}_x$ after applying stretch. The value x does not change since we are defining positions with respect to corresponding basis vectors $\boldsymbol{e}_x$ (initial) and $\bar{\boldsymbol{e}}_x$ (stretched) yielding the 1D displacement field as $\boldsymbol{\delta}(\boldsymbol{x}) = x(\bar{\boldsymbol{e}}_x - \boldsymbol{e}_x)$. One may assume that $\bar{\boldsymbol{e}}_x = E\boldsymbol{e}_x$ where E is the stretching coefficient.

Extending the deformation picture illustrated in fig. 5 from 1D to 3D we define the i-th component of the displacement field as $[\boldsymbol{\delta}(\boldsymbol{r})]^i = x^i(\bar{\boldsymbol{e}}_i - \boldsymbol{e}_i)$ (no summation involved). Thus it suffices to define a deformation matrix $E_{ij}, i,j = 1,2,3$ transforming the basis vectors $\boldsymbol{e}_j$ into $\bar{\boldsymbol{e}}_i$ such that $\bar{\boldsymbol{e}}_i = E_{ij}\boldsymbol{e}_j$, allowing us to define the displacement vector field as: $\boldsymbol{\delta}(\boldsymbol{r}) = x^i(\bar{\boldsymbol{e}}_i - \boldsymbol{e}_i)$ (with summation).

Stress efforts are represented by rank-2 tensor $\sigma_{ij}(\boldsymbol{r})$ and displacement γ_{ij} a rank-2 tensor is defined by $\gamma_{ij} = \frac{\partial \delta^i}{\partial x^j} = E_{ji}$. It is decomposable, like any tensor, into a symmetric ϵ_{ij} (strain/deformation tensor) and an antisymmetric part ω_{ij} (small rotations tensor):

$$\epsilon_{ij} = \frac{1}{2}(\frac{\partial \delta^i}{\partial x^j} + \frac{\partial \delta^j}{\partial x^i}), \quad \omega_{ij} = \frac{1}{2}(\frac{\partial \delta^i}{\partial x^j} - \frac{\partial \delta^j}{\partial x^i}), \quad \gamma_{ij} = \epsilon_{ij} + \omega_{ij} \tag{17}$$

In linear elasticity the extension of Hooke's law $F = -kx$ yields a linear relation between σ and ϵ, $\sigma_{ij} = C_{ij,kl}\epsilon_{kl}$ obtained from the correspondence: $F \leftrightarrow \sigma, -k \leftrightarrow C_{ij,kl}, x \leftrightarrow \epsilon_{kl}$. For a general solid, the 1D spring elastic constant k transforms into a rank-4 tensor $C_{ij,kl}$ containing elastic constants linking σ and ϵ that are both rank-2 tensors.

Elastic energy writes: $U_E = \frac{1}{2}C_{ij,kl}\epsilon_{ij}\epsilon_{kl}$ extending the 1D spring energy definition $U_E = \frac{1}{2}kx^2$. Thus: $\sigma_{ij} = \frac{\partial U_E}{\partial \epsilon_{ij}}$ and since ϵ is symmetric ($\epsilon_{ij} = \epsilon_{ji}$) we infer σ is as well ($\sigma_{ij} = \sigma_{ji}$). Hooke's law is extended to: $C_{ij,kl} = \frac{\partial^2 U_E}{\partial \epsilon_{ij}\partial \epsilon_{kl}}$.

Instead of using Hooke's law, we might use the relationship $\epsilon_{ij} = S_{ij,kl}\sigma_{kl}$ with $S_{ij,kl}$ the compliance tensor inverse of $C_{ij,kl}$. $S_{ij,kl}$ possesses the same symmetry properties as $C_{ij,kl}$.

B. Elastic moduli

Elastic moduli [25] (Young, shear G, bulk K) and Poisson ratio are given generally along a single direction $\boldsymbol{n}$ or a pair of orthogonal directions $\boldsymbol{n}, \boldsymbol{q}$ with the following operations:

- Strain represented by ϵ_{ij} tensor along single direction $\boldsymbol{n}$:

$$(\Delta l/l)_n = \epsilon_n = \epsilon_{ij}\boldsymbol{n}_i\boldsymbol{n}_j \tag{18}$$

  with l the initial and Δl its stress induced extra lengths.

- Strain represented by ϵ_{ij} tensor along two orthogonal directions $\boldsymbol{n}, \boldsymbol{q}$:

$$(\Delta l/l)_{nq} = \epsilon_{nq} = \epsilon_{ij}\boldsymbol{n}_i\boldsymbol{q}_j \tag{19}$$

  with l the initial and Δl_{nq} its stress induced extra lengths.

1. Young modulus (see for instance example [26]) along a given direction $E(\boldsymbol{n})$
Applying a stress σ_n i.e. a pressure p along direction $\boldsymbol{n}$ induces a strain ϵ_n along same direction yielding Young modulus $E(\boldsymbol{n})$:

$$\frac{1}{E(\boldsymbol{n})} = \frac{\epsilon_n}{\sigma_n} \tag{20}$$

Relating ϵ_n to σ_n is done using $\sigma_{ij} = C_{ij,kl}\epsilon_{kl},\ \epsilon_{ij} = S_{ijkl}\sigma_{kl}$:

$$\sigma_n = \sigma_{ij}n_i n_j,\ \epsilon_n = \epsilon_{ij}n_i n_j \tag{21}$$

Introducing $\sigma_{ij} = pn_i n_j$ with p the pressure into $\sigma_n = \sigma_{ij}n_i n_j$, we get Young modulus as:

$$\frac{1}{E(\boldsymbol{n})} = \frac{\epsilon_n}{\sigma_n} = \frac{pS_{ijkl}n_i n_j n_k n_l}{p} = S_{ijkl}n_i n_j n_k n_l \tag{22}$$

Using Voigt notation (see Appendix) we get the expression of $E(\boldsymbol{n})$ in the triclinic case for any orientation [27] as:

$$\begin{aligned}\frac{1}{E(\boldsymbol{n})} &= s_{11}n_1^4 + s_{22}n_2^4 + s_{33}n_3^4 + (s_{44} + 2s_{23})n_2^2 n_3^2 \\ &+ (s_{55} + 2s_{31})n_3^2 n_1^2 + (s_{66} + 2s_{12})n_1^2 n_2^2 \\ &+ 2n_2 n_3[(s_{14} + s_{56})n_1^2 + s_{24}n_2^2 + s_{34}n_3^2] \\ &+ 2n_3 n_1[s_{15}n_1^2 + (s_{25} + s_{46})n_2^2 + s_{35}n_3^2] \\ &+ 2n_1 n_2[s_{16}n_1^2 + s_{26}n_2^2 + (s_{36} + s_{45})n_3^2]\end{aligned} \tag{23}$$

Note that we have 15 terms instead of 21 due to the mixed coefficient terms such as $(s_{44}+2s_{23})$ and $(s_{55}+2s_{31})$...
In the cubic case [27], using the conversion rules from triclinic to cubic (see Appendix C):
$s_{22} = s_{33} = s_{11}, s_{55} = s_{66} = s_{44}, s_{13} = s_{23} = s_{12}$,
$s_{14} = s_{15} = s_{16} = s_{24} = s_{25} = s_{26} = s_{34} = s_{35} = s_{36} = s_{45} = s_{46} = s_{56} = 0$, we get:

$$\frac{1}{E(\boldsymbol{n})} = s_{11}(n_1^4 + n_2^4 + n_3^4) + 2(s_{12} + \frac{1}{2}s_{44})(n_1^2 n_2^2 + n_2^2 n_3^2 + n_3^2 n_1^2) \tag{24}$$

The example of Silver is displayed in Fig. 6.

2. Poisson ratio
Applying a pressure p along $\boldsymbol{n}$ and measuring deformation along $\boldsymbol{q}$ perpendicularly to $\boldsymbol{n}$ yields Poisson coefficient (see for instance example [26]) from deformation ratio along directions $\boldsymbol{q}$ and $\boldsymbol{n}$:

$$\nu(\boldsymbol{n}, \boldsymbol{q}) = -\frac{(\Delta l/l)_q}{(\Delta l/l)_n} \tag{25}$$

Uniaxial pressure p is related to stress tensor by: $\sigma_{kl} = pn_k n_l$ whereas strains are given by:

$$(\Delta l/l)_n = \epsilon_{ij}n_i n_j,\ (\Delta l/l)_q = \epsilon_{ij}q_i q_j \tag{26}$$

Using compliance tensor relations:

$$\epsilon_{ij} = S_{ijkl}\sigma_{kl},\ \sigma_{kl} = pn_k n_l, \tag{27}$$

we obtain: $\epsilon_{ij} = S_{ijkl}pn_k n_l$.

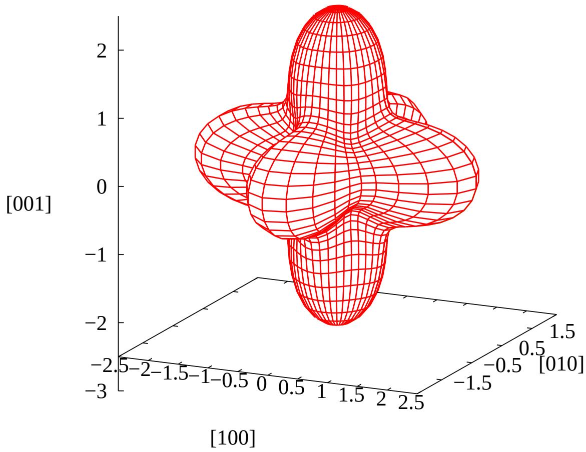

FIG. 6: Inverse Young modulus $\frac{1}{E(\boldsymbol{n})}$ of Silver versus direction $\boldsymbol{n}$. Silver compliances [28] are $s_{11} = 2.29, s_{12} = -0.983, s_{44} = 2.17$ in 1/[100GPa]. Calculated [29] values along all directions are in 1/[100GPa] units.

Using the above relations, the Poisson ratio is given by:

$$\begin{aligned} \nu(\boldsymbol{n},\boldsymbol{q}) &= -\frac{\epsilon_{ij}q_iq_j}{\epsilon_{ij}n_in_j} \\ &= -\frac{S_{ijkl}\ q_iq_jn_kn_l}{S_{ijkl}\ n_in_jn_kn_l} \end{aligned} \tag{28}$$

In the triclinic case we get for the numerator (21 terms):

$$\begin{aligned} S_{ijkl}\ q_iq_jn_kn_l &= s_{11}n_1^2q_1^2 + s_{22}n_2^2q_2^2 + s_{33}n_3^2q_3^2 \\ &+ s_{44}n_2n_3q_2q_3 + s_{55}n_1n_3q_1q_3 + s_{66}n_1n_2q_1q_2 \\ &+ s_{12}n_1^2q_2^2 + s_{13}n_1^2q_3^2 + s_{14}n_1^2q_2q_3 + s_{15}n_1^2q_1q_3 \\ &+ s_{16}n_1^2q_1q_2 + s_{23}n_2^2q_3^2 + s_{24}n_2^2q_2q_3 \\ &+ s_{25}n_2^2q_1q_3 + s_{26}n_2^2q_1q_2 \\ &+ s_{34}n_3^2q_2q_3 + s_{35}n_3^2q_1q_3 + s_{36}n_3^2q_1q_2 \\ &+ s_{45}n_2n_3q_1q_3 + s_{46}n_2n_3q_1q_2 + s_{56}n_1n_3q_1q_2 \end{aligned} \tag{29}$$

whereas the denominator is $E(\boldsymbol{n})$ (see eq. 23).
In the cubic case [30], the Poisson ratio is (using the conversion rules in Appendix C):

$$\nu(\boldsymbol{n},\boldsymbol{q}) = -\frac{s_{12} + (s_{11} - s_{12} - \frac{1}{2}s_{44})(n_1^2q_1^2 + n_2^2q_2^2 + n_3^2q_3^2)}{s_{11} - 2((s_{11} - s_{12} - \frac{1}{2}s_{44})(n_1^2n_2^2 + n_2^2n_3^2 + n_1^2n_3^2)} \tag{30}$$

The $\nu(\boldsymbol{n},\boldsymbol{q})$ example of Silver with $\boldsymbol{n}$ in a plane orthogonal to $\boldsymbol{q} = [001]$ is displayed in Fig. 7.

3. Shear modulus
It is defined by $G = \frac{\text{Shear stress}}{\text{Angular shear strain}}$ (see for instance example [31]) with two efforts are applied along $\boldsymbol{n}$ and $\boldsymbol{q}$ with $\boldsymbol{n}\perp\boldsymbol{q}$ as required by shear stress. Like Poisson ratio it is a symmetric function of $\boldsymbol{n}$ and $\boldsymbol{q}$ given by $G(\boldsymbol{n},\boldsymbol{q})$ defined as inverse ratio of angular shear deformation over shear stress:

$$\frac{1}{G(\boldsymbol{n},\boldsymbol{q})} = \left[\frac{2\epsilon_{ij}}{\sigma_{ij}}\right]_{nq} \tag{31}$$

This is a generalization of formula 18 to the $\langle nq\rangle$ symmetric case to express stress and strain in a symmetric fashion. $\langle nq\rangle$ symmetrized angular shear strain is given by:

$$[2\epsilon_{ij}]_{nq} = 2\epsilon_{ij}n_iq_j = 2S_{ijkl}\sigma_{kl}n_iq_j \tag{32}$$

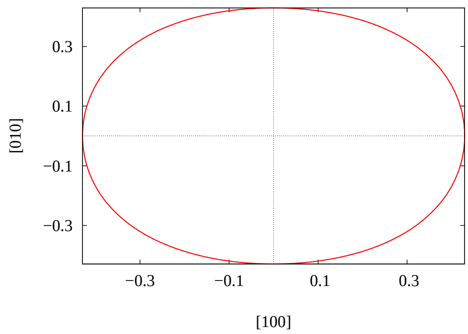

FIG. 7: Calculated [29] Poisson ratio $\nu(\boldsymbol{n},\boldsymbol{q})$ of Silver versus $\boldsymbol{n}$ angle in [100], [010] plane orthogonal to $\boldsymbol{q} = [001]$. Silver compliances [28] are $s_{11} = 2.29, s_{12} = -0.983, s_{44} = 2.17$ in 1/[100GPa].

We get the symmetrized stress as:

$$[\sigma_{ij}]_{nq} = \sigma_{ij} n_i q_j = \sigma(n_i q_j + n_j q_i) n_i q_j = \sigma \tag{33}$$

Shear modulus is given by:

$$\begin{aligned} \frac{1}{G(\boldsymbol{n},\boldsymbol{q})} &= \frac{2\epsilon_{ij}\; n_i q_j}{\sigma_{ij} n_i q_j} \\ &= \frac{2S_{ijkl}\sigma_{kl}\; n_i q_j}{\sigma} \\ &= 2S_{ijkl}\;(n_k q_l + n_l q_k)\; n_i q_j \end{aligned} \tag{34}$$

Using Tensor symmetry $S_{ijkl} = S_{ijlk}$, we finally obtain:

$$\frac{1}{4G(\boldsymbol{n},\boldsymbol{q})} = S_{ijkl}\; n_i q_j n_k q_l \tag{35}$$

Using Voigt notation (cf. Appendix B) we get the expression of $\frac{1}{4G(\boldsymbol{n},\boldsymbol{q})}$ in the triclinic case for any orientation [27] as:

$$\begin{aligned} \frac{1}{G(\boldsymbol{n},\boldsymbol{q})} &= 4[2s_{12} - (s_{11} + s_{22} - s_{66})]n_1 q_1 n_2 q_2 \\ &+ 4[2s_{23} - (s_{22} + s_{33} - s_{44})]n_2 q_2 n_3 q_3 \\ &+ 4[2s_{31} - (s_{33} + s_{11} - s_{55})]n_3 q_3 n_1 q_1 \\ &+ 4(n_1 q_2 + n_2 q_1)[(s_{16} - s_{36})n_1 q_1 + (s_{26} - s_{36})n_2 q_2] \\ &+ 4(n_2 q_3 + n_3 q_2)[(s_{24} - s_{14})n_2 q_2 + (s_{34} - s_{14})n_3 q_3] \\ &+ 4(n_3 q_1 + n_1 q_3)[(s_{35} - s_{25})n_3 q_3 + (s_{15} - s_{25})n_1 q_1] \\ &+ s_{44}(n_2 q_3 - n_3 q_2)^2 + s_{55}(n_3 q_1 - n_1 q_3)^2 \\ &+ s_{66}(n_1 q_2 - n_2 q_1)^2 + 2s_{45}(n_2 q_3 + n_3 q_2)(n_3 q_1 + n_1 q_3) \\ &+ 2s_{56}(n_3 q_1 + n_1 q_3)(n_1 q_2 + n_2 q_1) \\ &+ 2s_{64}(n_1 q_2 + n_2 q_1)(n_2 q_3 + n_3 q_2) \end{aligned} \tag{36}$$

Note that we used above the orthogonality of $\boldsymbol{n},\boldsymbol{q}$ translating indicially into $n_i q_i = 0$. We have 15 terms again like in the Young modulus case because of the mixed terms such as $[2s_{12} - (s_{11} + s_{22} - s_{66})]$ or $[2s_{23} - (s_{22} + s_{33} - s_{44})]$ when considered as a single elastic coefficient ... In the cubic case, we get (using conversion rules of Appendix C):

$$\frac{1}{G(\boldsymbol{n},\boldsymbol{q})} = s_{44} + 4(s_{11} - s_{12} - \frac{1}{2}s_{44})(n_1^2 q_1^2 + n_2^2 q_2^2 + n_3^2 q_3^2) \tag{37}$$

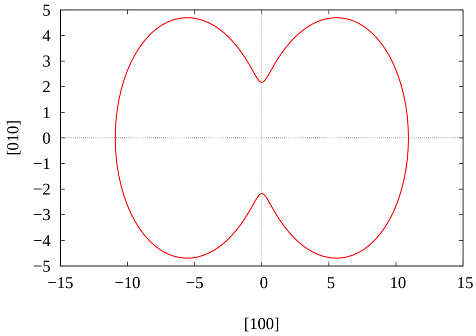

FIG. 8: Calculated [29] inverse shear modulus $\frac{1}{G(\boldsymbol{n},\boldsymbol{q})}$ of Silver versus $\boldsymbol{n}$ angle in $[100],[010]$ plane orthogonal to $\boldsymbol{q}=[001]$. Silver compliances [28] are $s_{11}=2.29, s_{12}=-0.983, s_{44}=2.17$ in 1/[100GPa]. Values along all directions are in 1/[100GPa] units.

The $\frac{1}{G(\boldsymbol{n},\boldsymbol{q})}$ example of Silver versus $\boldsymbol{n}$ in a plane orthogonal to $\boldsymbol{q}=[100]$ is displayed in Fig. 8.

4. Bulk modulus
The definition $K_{T,S}=-\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_{T,S}$ for isothermal or adiabatic bulk modulus implies a change of volume for an applied hydrostatic pressure.
Writing: $K\approx-\frac{1}{V}\left(\frac{\Delta V}{\Delta P}\right)$ and using $\epsilon_{ii}=\frac{\Delta V}{V}$, we get $K\approx-\frac{\epsilon_{ii}}{\Delta P}$. Using $\epsilon_{ij}=S_{ijkl}\sigma_{kl}$ with $\sigma_{kl}=-\Delta P\delta_{kl}$, we finally get: $K=S_{iijj}$.
Thus the most general expression for the bulk modulus exploiting symmetry and Voigt notation (see Appendix B) contains 9 terms since $i,j=1,2,3$:

$$\begin{aligned} K=S_{iijj} &= s_{11}+s_{12}+s_{13}+s_{21}+s_{22} \\ &+ s_{23}+s_{31}+s_{32}+s_{33} \\ &= s_{11}+s_{22}+s_{33}+2(s_{12}+s_{23}+s_{13}) \end{aligned} \tag{38}$$

VI. CONCLUSION AND PERSPECTIVES

Tensor calculus is powerful and very useful for Physics students since it provides them not only with elegant procedures to simplify complicated algebraic, vectorial expressions but also to describe anisotropic materials by extending simple scalar physical properties to more general appropriate mathematical expressions.

Appendix A: Tensor etymology and its evolution

The word tensor originally pertains to muscular taxonomy (extensor is a type of muscle implicated in stretch effort as opposed to flexor implicated in angular effort) then moved to differential geometry and more recently to computer science and neural networks. Recently Google built TPU (Tensor Processing Units) for dealing with deep learning problems of Artificial Intelligence deals with cognitive problems such as chess and go games, face recognition, speaker recognition... TPU-based processors are fast because of the massive parallelism of their architecture specially tailored for tackling stacked layers in deep neural network problems. They are faster that traditional CPU (Von Neumann architecture or with some modifications for speedup) and GPU (Graphic Processing Units) dedicated to graphic (Video) operations possessing a Harvard architecture like DSP (Digital signal processor) chips targeted for real-time applications.

Google TPU are made of parallel (systolic) arrays that contain each 65,536 (256 x 256) circuits called "Tensor Processing Elements (TPE)" that perform matrix multiplication with 8-bit based multiply-and-accumulate (MAC) operations in a single clock cycle. The TPU runs at 700 MHz, thus it can compute 65,536x7x10 ^{8} = 46x10 ^{12} MAC per second [32].

From data compute element point of view, a CPU processes (1×1) data units (such as product of two scalars), a GPU a $(1 \times N)$ data unit (such as the scalar product of two N dimensional vectors) whereas TPU processes $(N \times N)$ data units (such as the product of two $N \times N$ matrices). A CPU may perform tens of instructions per cycle (IPS), a GPU $\sim 10^4$ IPS whereas a TPU may crunch several $\sim 10^5$ IPS.

Appendix B: Covariant derivative

In general, the derivative of a tensor (with rank $\neq 0$) is not a tensor, since the derivative of the Jacobian terms intervene violating the tensor character as prescribed by ECP. As an example let us take the derivative [33, 34] of a a contravariant vector field (eq. 10) and examine its transformation according to ECP:

$$\frac{\partial A^i}{\partial u^k} = \frac{\partial^2 u^i}{\partial u^k \partial \bar{u}^j}\bar{A}^j + \frac{\partial u^i}{\partial \bar{u}^j}\frac{\partial \bar{A}^j}{\partial u^k} \tag{B1}$$

The first term in the RHS breaks ECP since we were expecting a single term with Jacobian factors. Thus we have to introduce a special derivative (called covariant derivative) that absorbs the derivative terms of the Jacobian factors. This mathematical problem disappears in the Cartesian case since the basis vectors do not depend on local coordinates.

Let us define the derivative of the covariant basis vector $\frac{\partial \boldsymbol{e}_i}{\partial u^j} = \Gamma^k_{ij}\boldsymbol{e}_k$ such that the vector differential $d\boldsymbol{A} = d(A^i\boldsymbol{e}_i) = (\frac{\partial A^i}{\partial u^j}du^j)\boldsymbol{e}_i + A^i\frac{\partial \boldsymbol{e}_i}{\partial u^j}du^j = [(\frac{\partial A^i}{\partial u^j}\boldsymbol{e}_i) + A^i\Gamma^k_{ij}\boldsymbol{e}_k]du^j$. Note that the coefficients Γ^k_{ij} that are called Christoffel symbols are not tensors.

The covariant derivative $[(\frac{\partial A^i}{\partial u^j}\boldsymbol{e}_i) + A^i\Gamma^k_{ij}\boldsymbol{e}_k]$ can be rewritten by exchanging the dummy indices i, k in the second term to yield: $[(\frac{\partial A^i}{\partial u^j}) + A^k\Gamma^i_{kj}]\boldsymbol{e}_i$. This allows us to rewrite $d\boldsymbol{A} = d(A^i\boldsymbol{e}_i) = (D_jA^i)\boldsymbol{e}_i du^j$ where the covariant derivative $D_jA^i = [(\frac{\partial A^i}{\partial u^j}) + A^k\Gamma^i_{kj}]$ is a rank-2 tensor containing the Jacobian factor derivative.

The evaluation of the Christoffel symbol consists of taking the scalar product with $\boldsymbol{e}^l$ of $\frac{\partial \boldsymbol{e}_i}{\partial u^j} = \Gamma^k_{ij}\boldsymbol{e}_k$. Thus $\boldsymbol{e}^l \cdot \frac{\partial \boldsymbol{e}_i}{\partial u^j} = \Gamma^k_{ij}\boldsymbol{e}^l \cdot \boldsymbol{e}_k = \Gamma^k_{ij}\delta^l_k = \Gamma^l_{ij}$ using the orthogonality of $\boldsymbol{e}^l$ and $\boldsymbol{e}_k$.

The relation $\Gamma^l_{ij} = \boldsymbol{e}^l \cdot \frac{\partial \boldsymbol{e}_i}{\partial u^j}$ implies symmetry of the Christoffel symbol $\Gamma^l_{ij} = \Gamma^l_{ji}$ since $\Gamma^l_{ij} = \boldsymbol{e}^l \cdot \frac{\partial^2 \boldsymbol{r}}{\partial u^i \partial u^j}$ after using the definition $\boldsymbol{e}_i = \frac{\partial \boldsymbol{r}}{\partial u^i}$ and allows to relate Γ^l_{ij} to the metric tensor by taking its spatial derivative: $\frac{\partial g_{ij}}{\partial u^k} = \frac{\partial(\boldsymbol{e}_i \cdot \boldsymbol{e}_j)}{\partial u^k} = \boldsymbol{e}_i \cdot \frac{\partial \boldsymbol{e}_j}{\partial u^k} + \boldsymbol{e}_j \cdot \frac{\partial \boldsymbol{e}_i}{\partial u^k}$. Combining the spatial derivatives we finally get: $\Gamma^l_{ij} = \frac{g^{lk}}{2}\left(\frac{\partial g_{jk}}{\partial u^i} + \frac{\partial g_{ki}}{\partial u^j} - \frac{\partial g_{ij}}{\partial u^k}\right)$.

Contracting Γ^l_{ij} yields: $\Gamma^i_{ij} = \frac{1}{2}g^{lk}\frac{\partial g_{lk}}{\partial u^j}$ since the last two terms cancel by symmetry and index transformation. Using the derivative of determinant $g = det[g_{ij}]$ formula [35] given by $\frac{\partial g}{\partial u^j} = gg^{ik}\frac{\partial g_{ik}}{\partial u^j}$, the contracted Christoffel symbol is rewritten as: $\Gamma^i_{ij} = \frac{1}{\sqrt{g}}\frac{\partial \sqrt{g}}{\partial u^j}$.

Appendix C: Voigt notation

- Symmetry of elastic constants
  Elastic energy $U_E = \frac{1}{2}C_{ij,kl}\epsilon_{ij}\epsilon_{kl}$ is invariant under $i \leftrightarrow j$ and $k \leftrightarrow l$ interchange. Moreover it is invariant under $\{ij\} \leftrightarrow \{kl\}$ interchange. Thus we infer $C_{ij,kl} = C_{ji,kl} = C_{ij,lk} = C_{kl,ij}$. Thus we may replace a couple of indices ij with a single index I and replace rank-4 tensor $C_{ij,kl} =$ with its matrix representation C_{IJ} with $I, J = 1...6$.

  The index replacement is done according to the recipe:
  $11 \to 1$, $22 \to 2$, $33 \to 3$, $23 \to 4$, $13 \to 5$, $12 \to 6$. This can be written in a more compact way as:
  $ii \to i, ij \to 9 - (i + j)$ when $i \neq j$

  The 6×6 matrix (36 components) represents completely $C_{ij,kl}$ with its $3^4 = 81$ components taking account of symmetry. This matrix is in fact symmetric $C_{ij,kl} = C_{kl,ij}$ originating from the property of elastic energy $\frac{1}{2}C_{ij,kl}\epsilon_{ij}\epsilon_{kl}$ providing another justification for practicality of Voigt notation. We end up with 21 components (since [36-6]/2 +6, i.e. 15+6=21) for the triclinic crystal.

- Application to the cubic crystal case
  The number of components in the cubic case can be done along the same lines we treated rank-2 tensors previously.

Contrary to simple intuition (like in the rank-2 case) leading to a single elastic constant in a cubic solid, three elastic constants C_{11}, C_{12} and C_{44} (using Voigt notation explained in Appendix B) are needed in this case yielding: $C_{11} = C_{xx,xx} = C_{yy,yy} = C_{zz,zz}, C_{12} = C_{xx,yy} = C_{xx,zz} = C_{yy,zz}, C_{44} = C_{xy,xy} = C_{xz,xz} = C_{yz,yz}, C_{xy,xz} = C_{xy,yz} = C_{xz,yz} = 0$. This means one has to distinguish between geometrical symmetry and mechanical symmetry.

Consequently we have a hierarchy of symmetries:

1. Cubic symmetry (3 constants: C_{11}, C_{12} and C_{44}).
2. Isotropic elasticity with rotational symmetry about some reference direction (2 constants: Lamé $\{\lambda, \mu\}$ coefficients or Young and Poisson $\{E, \nu\}$).
3. Full isotropy in all directions like in a Newtonian fluid (1 constant).

Taking x, y, z along cubic axes, we write $C_{xy} = C_{44}$ and $C_{zz} = \frac{1}{2}(C_{11} - C_{12})$. Consequently, the elastic constant tensor writes:

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix} \tag{C1}$$

Stresses in the cubic case are: $\sigma_{xx} = C_{11}\epsilon_{xx} + C_{12}\epsilon_{yy} + C_{12}\epsilon_{zz}, \sigma_{yy} = C_{12}\epsilon_{xx} + C_{11}\epsilon_{yy} + C_{12}\epsilon_{zz}\sigma_{zz} = C_{12}\epsilon_{xx} + C_{12}\epsilon_{yy} + C_{11}\epsilon_{zz}\sigma_{xy} = 2C_{44}\epsilon_{xy}, \sigma_{xz} = 2C_{44}\epsilon_{xz}, \sigma_{yz} = 2C_{44}\epsilon_{yz}$

Particular case: In the isotropic elastic case we have only two elastic constants with $C_{xy} = C_{zz}$, leading to a couple of Lamé coefficients $\lambda = C_{12}$ and $\mu = C_{xy} = C_{zz}$ yielding: $\sigma_{ij} = \lambda\epsilon_{kk}\delta_{ij} + 2\mu\epsilon_{ij}$. This means a stress σ_{11} induces a longitudinal strain ϵ_{11} and transverse identical values $\epsilon_{22} = \epsilon_{33}$ resulting in: $\sigma_{12} = 2\mu\epsilon_{12}$ and $G = \mu$.

- Compliance tensor
  Given the symmetry with respect to pairs of indices $S_{ij,kl} = S_{ji,kl}, S_{ij,kl} = S_{ij,lk}$..., we can proceed to a matrix representation $s_{I,J}$ of $S_{ij,kl}$ with $I, J = 1...6$ with the same rules as in the elastic tensor case. Hence the full matrix $s_{I,J}$ with its 6×6 (36 components) represents S_{ijkl} tensor with its 81 components. Since $s_{I,J}$ is symmetric the number of components is only 21.

  Thus the symmetric compliance matrix in the triclinic case can be written as:

$$\begin{pmatrix} s_{11} & s_{12} & s_{13} & s_{14} & s_{15} & s_{16} \\ & s_{22} & s_{23} & s_{24} & s_{25} & s_{26} \\ & & s_{33} & s_{34} & s_{35} & s_{36} \\ & & & s_{44} & s_{45} & s_{46} \\ & & & & s_{55} & s_{56} \\ & & & & & s_{66} \end{pmatrix} \tag{C2}$$

  In the cubic case we have:

$$\begin{pmatrix} s_{11} & s_{12} & s_{12} & 0 & 0 & 0 \\ & s_{11} & s_{12} & 0 & 0 & 0 \\ & & s_{11} & 0 & 0 & 0 \\ & & & s_{44} & 0 & 0 \\ & & & & s_{44} & 0 \\ & & & & & s_{44} \end{pmatrix} \tag{C3}$$

This allows us to find a quick set of rules to convert from triclinic to cubic:
$s_{22} = s_{33} = s_{11}, s_{55} = s_{66} = s_{44}, s_{13} = s_{23} = s_{12}$,
$s_{14} = s_{15} = s_{16} = s_{24} = s_{25} = s_{26} = s_{34} = s_{35} = s_{36} = s_{45} = s_{46} = s_{56} = 0$.

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[1] M. Spiegel, *Vector analysis and an Introduction to Tensor Analysis*, Schaum's outline series in mathematics, McGraw-Hill (1968).

[2] D. Kay, *Tensor calculus*, Schaum's outline series in Mathematics, McGraw-Hill (1988).

[3] When Einstein worked at the Federal Office for Intellectual Property (1903-1909) in Bern (patent office), he was interested in train scheduling and synchronization to manage their circulation and avoid congestion or collisions between them, all over Switzerland. This is how he got involved into moving clocks and frames as well as time evolution differences between railway station and moving train times. The "relativity" word was inspired from Galileo work who first forged the "Principle of Relativity" for Galilean moving frames in 1632.

[4] C. W. Misner, K. S. Thorne and J. A. Wheeler, *Gravitation*, W. H. Freeman San Francisco (1971).

[5] J. D. Norton, Rep. Prog. Phys. **56**, 791 (1993).

[6] C. Kittel *Introduction to Solid State Physics*, 8th edition, Wiley, New York (2006).

[7] G. F. Arfken and H. J. Weber, *Mathematical methods for physicists,* Sixth Edition, Elsevier Academic Press (London, 2005).

[8] C. Dullemond and K. Peeters, *Introduction to Tensor Calculus*, University of Heidelberg booklet (1991).

[9] In general the spatial derivative of a tensor is not a tensor. The covariant derivative is introduced as means to preserve tensor character through the spatial derivation operation.

[10] There are several possibilities for the rank-2 Kroenecker tensor: a- Doubly covariant: $\delta_{ij} = \boldsymbol{e}_i \cdot \boldsymbol{e}_j$, b-Doubly contravariant: $\delta^{ij} = \boldsymbol{e}^i \cdot \boldsymbol{e}^j$ and c- Mixed covariant-contravariant: $\delta_i^j = \boldsymbol{e}_i \cdot \boldsymbol{e}^j$ assuming the right properties of orthonormality of the bases $\boldsymbol{e}_i$ and $\boldsymbol{e}^j$.

[11] Levi-Civita tensors are, strictly speaking, pseudo-tensors since they change sign depending on the frame right-handedness like axial vectors. An example of an axial vector is the angular momentum vector $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$ whose covariant component $L_i = \frac{1}{2}\epsilon_{ijk} L_{jk}$ where rank-2 tensor L_{jk} is given by $L_{jk} = x_j p_k - x_k p_j$. A spatial inversion $\boldsymbol{r} \to -\boldsymbol{r}$ results in $\boldsymbol{v} \to -\boldsymbol{v}$ but $\boldsymbol{L} \to \boldsymbol{L}$ in contrast with polar vectors. Note that covariant Levi-Civita tensor possesses a contravariant version defined by: $\epsilon^{lmn} = (\boldsymbol{e}^l, \boldsymbol{e}^m, \boldsymbol{e}^n)$. Covariant and contravariant versions are related through the metric tensor as: $\epsilon_{ijk} = g_{il} g_{jm} g_{kn} \epsilon^{lmn}$.

[12] In general this is not true but when we are dealing with smooth non singular functions, the symmetry of the tensor $\partial_i \partial_j$ is true.

[13] Scale factors (also called Lamé coefficients) are introduced to make the basis vectors $\boldsymbol{e}_i$ normalized. In orthogonal curvilinear coordinates we obtain from expansion eq. 5 a scale factor $h_i = |\frac{\partial \boldsymbol{r}}{\partial u^i}|$ yielding $\frac{\partial \boldsymbol{r}}{\partial u^i} = h_i \boldsymbol{e}_i$ such that: $d\boldsymbol{r} = h_i \boldsymbol{e}_i du^i$ (summation over i being assumed despite its presence three times) with $\boldsymbol{e}_i$ normalized. The scale factors can be defined with the metric tensor $h_i = \sqrt{\boldsymbol{e}_i \cdot \boldsymbol{e}_i} = \sqrt{g_{ii}}$ (no summation over i). For instance, in cylindrical coordinates, $\{\rho, \phi, z\}$, the scale factors are respectively $h_\rho = 1, h_\phi = \rho, h_z = 1$ whereas in spherical coordinates $\{r, \theta, \phi\}$ we have: $h_r = 1, h_\theta = r, h_\phi = r \sin\theta$.

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[16] The gradient is expressed as: $\boldsymbol{grad}\phi = \frac{1}{h_i}\frac{\partial \phi}{\partial u^i}\boldsymbol{e}^i$ with all $\boldsymbol{e}^i$ normalized. Note that summation over i is done in $\frac{1}{h_i}\frac{\partial \phi}{\partial u^i}\boldsymbol{e}^i$ despite appearance of i three times. It is possible to have the contravariant gradient from the covariant one by contracting with the metric tensor as: $g^{ij}\frac{1}{h_i}\frac{\partial \phi}{\partial u^i}$.

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[26] In this simple example, Young modulus E is obtained from: $\sigma_{11} = 1, \sigma_{ij} = 0\ \forall i, j \neq 1, 1$. The longitudinal strain is given by: $\epsilon_{11} = S_{1111}\sigma_{11}$ leading to: $\sigma_{11} = E\epsilon_{11}$ yielding: $E = 1/S_{1111}$. Transverse deformation is obtained as: $\epsilon_{22} = S_{2211}\sigma_{11}$, in the same fashion: $\epsilon_{33} = S_{3311}\sigma_{11}$. Poisson coefficient ν is the ratio of transverse to longitudinal strains: $\nu = -\frac{\epsilon_{22}}{\epsilon_{11}} = -\frac{S_{2211}\sigma_{11}}{S_{1111}\sigma_{11}} = -ES_{2211}$.

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[31] Shear modulus is obtained by applying a single stress σ_{12} inducing an angular deformation $2\epsilon_{12}$, such that $G = \frac{\sigma_{12}}{2\epsilon_{12}}$.

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