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Technical note: Coordinate representations of important differential operations in continuum mechanics

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In memory of DSc Djebbar Baroudi and Lic Jari Laukkanen

This note is the last part in the trilogy *Tensors in Continuum Mechanics*. The first part was focused on the representations of m-linear functions on tensor spaces, especially on their duals and transpositions [1]. The second part was dedicated to the memory of Prof. T. Salmi, and it was focused on the curvilinear coordinate systems in continuum mechanics [2] (in Finnish). Because the relationship between stress and their strain conjugates has been discussed in several papers [3, 4, 5], the focus in the present third part is on a more specific area of continuum mechanics: representations of important differential operations (the gradient, divergence, rotor, and Laplace) in curvilinear coordinate systems. Many well-known textbooks on continuum mechanics begin with an introduction to basic mathematical concepts (vector and tensor algebra) [6, 7, 8, 9, 10, 11]. In these presentations, the coordinate systems of space are tacitly assumed to be generally known (Euclidean E^3 , rectangular), in which case they are not defined in more detail. Without exception, the definition of the coordinate system is completely ignored in the articles (assumed rectangular and normalized) [12, 13, 14, 15, 16]. An interesting exception is the recent paper which deals with the fourth order tensors and their dot products [17]. When restricted to Christoffel symbols (mandatory for the representations of differential operations in curvilinear coordinates), only a few recent papers can be found [18, 19]. Ultimately, however, in order to present the results or (numerically) calculate them, the coordinate system must always be defined. This article examines the Cartesian spatial coordinate systems, generalized curvilinear coordinate systems, and representations of important differential operations in these coordinate systems (Euclidean geometry applies). The representations are based on the transformations between the linear rectangular and generalized curvilinear coordinate systems. The key feature of generalization is the unequivocal definition of the base system of rectangular coordinate system. Certain curvilinear rectangular coordinate systems, such as the polar coordinate system, are commonly used in numerical solvers, such as commercial finite element method (FEM) packages. Proposed explicit differential operations make numerical iterative solvers more efficient. Relevant examples concern representations of the differential operations in the important rectangular curvilinear coordinate systems (cylindrical and spherical), and the so-called Christoffel symbols

needed in the representations.

Basis of the coordinate systems

Although the concept of a coordinate system has only been known for a few centuries, coordinate systems as such have been implicitly used for millennia: information about places on the earth's surface and the location of the stars in the sky. The Greek *Claudius Ptolemaios* (~85—165 A.D) proposed longitude and latitude to determine the location on the earth's surface. His work *Almagest* (consisting of books I-XIII [20]) covered also solar systems (book VI) and star catalogues of 1022 stars (books VII-VIII). After the Dark Ages, the first real rectangular coordinate systems were defined by the French *Rene Descartes* (*Discours de la Methode*, in 1637). An interesting detail is that *Isaac Newton* published his *Principian* (in 1687) [21], that is only a few decades later. Moreover, the principal of the canon of music, the *Tocatta and Fugue by J. S. Bach* (1685–1750) [22], was published right after this fruitful period. Later, numerous mathematicians and physicists have developed the theory of coordinate systems. It is natural that the subject has since been discussed also in continuum mechanics, [7, 10, 23, 24, 25].

The spatial coordinate system is formed by choosing a point O as the origin. The coordinate system includes three curves passing through the origin, which are not in the same plane. Figure 1 shows a rectangular coordinate system $X^1X^2X^3$ connected to an origin O , point P , and a so-called position vector

$$\mathbf{r} = x^1\mathbf{e}_1 + x^2\mathbf{e}_2 + x^3\mathbf{e}_3 \quad (1)$$

associated with the point P . The vectors $x^i\mathbf{e}_i$, $i=1,2,3$, are the components of \mathbf{r} and the real numbers x^i denote the coordinates of the point P (usually, the origin O corresponds to $x^i = 0$) [2]. Vectors \mathbf{e}_i are the base vectors of the system $X^1X^2X^3$. If the axis lines are at right angles to each other, we speak of a rectangular or orthogonal coordinate system.

Change of basis: consider curvilinear coordinate systems generalized from a Cartesian normalized coordinate system which has the base \mathbf{e}_i , $i=1,2,3$. The position vector (1) is given by

$$\tilde{\mathbf{r}} = y^1\mathbf{e}_1 + y^2\mathbf{e}_2 + y^3\mathbf{e}_3,$$

where y^i , $i = 1, 2, 3$, are the transformed coordinates of (1), that is, the presented transformations leave the space unchanged. In the deformation theory of continuum mechanics, the transformed or deformed coordinates y^i are known as Euler's spatial coordinates and the original coordinates (without deformation) as Lagrange's material coordinates, see further details (change of basis) in Holopainen [2] and textbooks [7, 10].

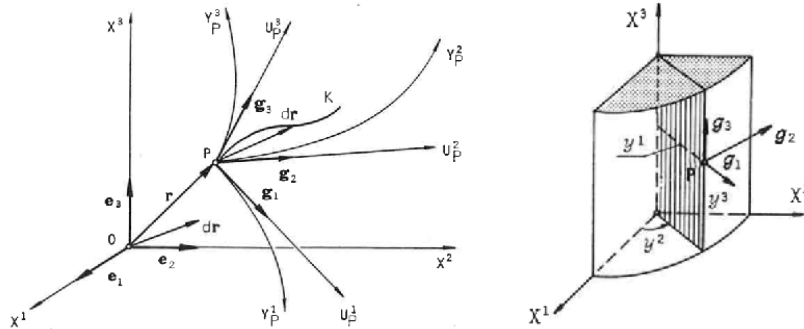


Figure 1. On the left, a rectangular linear coordinate system $X^1X^2X^3$, Cartesian local tangent coordinate system U_P^i , and local coordinate lines Y_P^i of a curvilinear system. The global and local bases are indicated by vectors \mathbf{e}_i and $\mathbf{g}_i = \partial\mathbf{r}/\partial y^i$, $i=1,2,3$. On the right, the observation of the cylindrical rectangular coordinate system.

Coordinate representations of differential operations

Rectangular curvilinear coordinate systems are an important group from the point of view of applications, because the important partial differential equations defined in them, such as *Laplace* and *Helmholtz* equations, are separated. Examples of rectangular curvilinear coordinate systems are planar (e.g., polar coordinate systems), cylindrical, and spherical coordinate systems [2, 7, 9]. Consider a scalar-valued function ϕ of vectors $\phi : \mathbf{r} \rightarrow c$ or alternatively $c = \phi(\mathbf{r})$, where $\mathbf{r} \in \mathbb{E}^3$.

Definition. A scalar-valued linear operator, $\mathbf{A}(\mathbf{r})\circ$, defined by

$$\phi(\mathbf{r} + \Delta\mathbf{r}) - \phi(\mathbf{r}) = \mathbf{A}(\mathbf{r})\Delta\mathbf{r} + \|\Delta\mathbf{r}\|a(\mathbf{r}; \Delta\mathbf{r}), \quad \lim_{\|\Delta\mathbf{r}\| \rightarrow 0} |a(\mathbf{r}; \Delta\mathbf{r})| = 0, \quad (2)$$

is the total differential operator at the point defined by \mathbf{r} .

The total differential is unique; when writing shortly the left hand side of (2) as $\Delta\phi = \phi(\mathbf{r} + \Delta\mathbf{r}) - \phi(\mathbf{r})$ and let $\Delta\mathbf{r} \rightarrow d\mathbf{r}$, when $\mathbf{r} + \Delta\mathbf{r} \rightarrow \mathbf{r} + d\mathbf{r}$ and $\Delta\phi(\mathbf{r}) \rightarrow d\phi(\mathbf{r})$, one can write that

$$d\phi(\mathbf{r}) = \mathbf{A}(\mathbf{r})d\mathbf{r}. \quad (3)$$

When substituting the differential $d\mathbf{r} = dx^i d\mathbf{e}_i$ into (3), one obtains

$$d\phi(\mathbf{r}) = \mathbf{A}(\mathbf{r})d\mathbf{r} = \mathbf{A}(\mathbf{r})dx^i d\mathbf{e}_i = dx^i \mathbf{A}(\mathbf{r})\mathbf{e}_i = dx^i A_i. \quad (4)$$

From the other hand, the total differential of the scalar-valued vector function is

$$d\phi(\mathbf{r}) = \frac{\partial\phi}{\partial x^i} dx^i. \quad (5)$$

Comparing equations (4) and (5), both of which are valid with arbitrary differentials dx^1 , dx^2 , dx^3 , we arrive at the result

$$A_i = \frac{\partial\phi}{\partial x^i}, \quad i = 1, 2, 3, \quad (6)$$

which result, as such, is valid in both rectangular and curvilinear coordinate systems. Define the vector-valued scalar function $\mathbf{grad} : R \rightarrow \mathbb{E}^3$ such that

$$\mathbf{grad}\phi(\mathbf{r}) \bullet \circ = \mathbf{A}(\mathbf{r}) \circ. \quad (7)$$

The vector $\mathbf{grad}\phi$ is termed the gradient of function ϕ at \mathbf{r} . By substituting the expression $d\mathbf{r} = dx^i \mathbf{e}_i$ in the relation (3) and taking into account the definition (7), one obtains $d\phi(\mathbf{r}) = \mathbf{A}(\mathbf{r})d\mathbf{r} = \mathbf{grad}\phi(\mathbf{r}) \bullet d\mathbf{r} = (\mathbf{grad}\phi(\mathbf{r}))_i \mathbf{e}^i \bullet dx^j \mathbf{e}_j$ and then

$$d\phi(\mathbf{r}) = (\mathbf{grad}\phi(\mathbf{r}))_i dx^j \delta_j^i = (\mathbf{grad}\phi(\mathbf{r}))_i dx^i. \quad (8)$$

When the result (8) is compared with the formula (5) and taking into account that the differentials dx^i , $i = 1, 2, 3$, are arbitrary, it follows that $(\mathbf{grad}\phi(\mathbf{r}))_i = \partial\phi/\partial x^i$ or

$$\nabla\phi := \mathbf{grad}\phi = \frac{\partial\phi}{\partial x^i} \mathbf{e}^i, \quad (9)$$

where ∇ is the so-called nabla operator. Let's further define the scalar-valued divergence operator $\text{div} : \mathbb{E}^3 \rightarrow R$ such that

$$\text{div} \mathbf{f} := \mathbf{e}^i \bullet \mathbf{A}\mathbf{e}_i = \frac{\partial\phi}{\partial x^i} \mathbf{e}^i. \quad (10)$$

Taking into account the operation $A_j^i = v_j^i = \mathbf{e}^i \bullet \mathbf{A}\mathbf{e}_j$ for a vector \mathbf{v} , one can define the relation $\text{div} \mathbf{v} := v_i^i$ which in rectangular coordinate systems takes the form

$$\text{div} \mathbf{v} := \frac{\partial v^i}{\partial x^i}, \quad i = 1, 2, 3, \quad (11)$$

whereas in curvilinear coordinate systems the form is

$$\operatorname{div} \mathbf{v} := \frac{\partial v^i}{\partial y^i} + \binom{i}{ij} v^j, \quad i, j = 1, 2, 3, \quad (12)$$

where the second term includes the Christoffel's symbol. Actually, it can be shown that

$$\frac{\partial}{\partial y^i} \ln \sqrt{g} = \binom{\alpha}{i\alpha}, \quad \alpha = 1, 2, 3, \quad g = \det(\mathbf{g}) > 0, \quad (13)$$

when the result (12) takes the form

$$\operatorname{div} \mathbf{v} := \frac{\partial v^i}{\partial y^i} + \frac{\partial v^j}{\sqrt{g}} \frac{\partial \sqrt{g}}{\partial y^j} \quad \text{or} \quad \operatorname{div} \mathbf{v} := \frac{1}{\sqrt{g}} \frac{\partial}{\partial y^i} (v^i \sqrt{g}). \quad (14)$$

Let's further define the so-called vector-valued rotor operator $\mathbf{rot} : E^3 \rightarrow E^3$ such that

$$\mathbf{rot} \mathbf{f} := \mathbf{e}^i \times \mathbf{A} \mathbf{e}_i. \quad (15)$$

From the equation $A_i^j = g^j \bullet \mathbf{A} \mathbf{g}_i$ follows in curvilinear coordinate system $Y^1 Y^2 Y^3$ that $\mathbf{A} \mathbf{g}_i = A_i^j \mathbf{g}_j$, $i = 1, 2, 3$. Then, from eq. (15) follows for a vector $\mathbf{v} = \mathbf{f}(\mathbf{r})$ that

$$\mathbf{rot} \mathbf{v} := \mathbf{g}^i \times A_i^j \mathbf{g}_j = A_i^j \mathbf{g}^i \times g_{kj} \mathbf{g}^k = A_i^j g_{kj} \mathbf{g}^i \times \mathbf{g}^k = A_{ki} \mathcal{E}^{ikm} \mathbf{g}_m = A_{kj} \mathcal{E}^{jki} \mathbf{g}_i = v_{k,j} \mathcal{E}^{jki} \mathbf{g}_i. \quad (16)$$

Finally, the scalar-valued Laplace operator $\operatorname{Lap} : R \rightarrow R$ important for applications is

$$\operatorname{Lap} \phi = \operatorname{div} \mathbf{grad} \phi = \nabla^2 \phi = \Delta \phi. \quad (17)$$

Using equations (20) and (14), one obtains

$$\operatorname{Lap} \phi = \operatorname{div} \mathbf{grad} \phi = \frac{1}{\sqrt{g}} \frac{\partial}{\partial y^i} \left(\frac{\partial \phi}{\partial y^j} g^{ji} \sqrt{g} \right). \quad (18)$$

Especially, in an orthonormal Cartesian coordinate system $X^1 X^2 X^3$, $g^{ij} = \delta^{ij}$ and $g = 1$ hold, when

$$\operatorname{Lap} \phi = \frac{\partial^2 \phi}{\partial (x^i)^2}, \quad i = 1, 2, 3. \quad (19)$$

Example 1. Calculate the gradient of the function ϕ , the divergence and rotor of the vector \mathbf{v} at \mathbf{r} , and the Laplace operator of the function ϕ at \mathbf{r} in the cylindrical and spherical coordinates $Y^1 Y^2 Y^3$, when the base vectors are $\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3$ and $\mathbf{g}^1, \mathbf{g}^2, \mathbf{g}^3$.

Solution. The gradient is defined using the total derivative:

$$\mathbf{grad} \phi := \frac{\partial \phi}{\partial y^i} \mathbf{g}^i = \frac{\partial \phi}{\partial y^i} g^{ij} \mathbf{g}_j \quad (20)$$

in which latter result the index reduction rule was applied [2]. Using the metric matrices in the cylindrical coordinates [2]

$$g_{ij} := \mathbf{g}_i \cdot \mathbf{g}_j = \begin{bmatrix} 1 & 0 & 0 \\ 0 & (y^1)^2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad g^{ij} := \mathbf{g}^i \cdot \mathbf{g}^j = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1/(y^1)^2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

one obtains

$$\mathbf{grad} \phi = \frac{\partial \phi}{\partial y^1} \mathbf{g}_1 + \frac{1}{(y^1)^2} \frac{\partial \phi}{\partial y^2} \mathbf{g}_2 + \frac{\partial \phi}{\partial y^3} \mathbf{g}_3.$$

The determinant of the metric matrix is $g = (y^1)^2$, when from eq. (14) follows that

$$\operatorname{div} \mathbf{v} = \frac{1}{y^1} \frac{\partial}{\partial y^i} (v^i y^1) = \frac{v^1}{y^1} + \frac{\partial v^i}{\partial y^i}, i = 1, 2, 3.$$

To calculate the rotor of \mathbf{v} , we refer to (16), when $\operatorname{rot} \mathbf{v} := v_{k,j} \mathcal{E}^{jki} \mathbf{g}_i$, $i = 1, 2, 3$ or

$$\operatorname{rot} \mathbf{v} = (v_{2,3} \mathcal{E}^{321} + v_{3,2} \mathcal{E}^{231}) \mathbf{g}_1 + (v_{1,3} \mathcal{E}^{312} + v_{3,1} \mathcal{E}^{132}) \mathbf{g}_2 + (v_{1,2} \mathcal{E}^{213} + v_{2,1} \mathcal{E}^{123}) \mathbf{g}_3$$

or

$$\operatorname{rot} \mathbf{v} = \frac{1}{\sqrt{g}} ((-v_{2,3} + v_{3,2}) \mathbf{g}_1 + (v_{1,3} - v_{3,1}) \mathbf{g}_2 + (-v_{1,2} + v_{2,1}) \mathbf{g}_3).$$

The only non-zero components of Christoffel symbols at cylindrical coordinates are

$$\begin{pmatrix} 1 \\ 22 \end{pmatrix} = -y^1, \quad \begin{pmatrix} 2 \\ 12 \end{pmatrix} = \begin{pmatrix} 2 \\ 21 \end{pmatrix} = \frac{1}{y^1},$$

when the components of the total derivative of the vector \mathbf{v} are

$$\begin{aligned} v_{1,2} &= \frac{\partial v_1}{\partial y^2} - \begin{pmatrix} k \\ 21 \end{pmatrix} v_k = \frac{\partial v_1}{\partial y^2} - \begin{pmatrix} 2 \\ 21 \end{pmatrix} v_2 = \frac{\partial v_1}{\partial y^2} - \frac{1}{y^1} v_2, \\ v_{2,1} &= \frac{\partial v_2}{\partial y^1} - \begin{pmatrix} k \\ 12 \end{pmatrix} v_k = \frac{\partial v_2}{\partial y^1} - \begin{pmatrix} 2 \\ 12 \end{pmatrix} v_2 = \frac{\partial v_2}{\partial y^1} - \frac{1}{y^1} v_2, \\ v_{1,3} &= \frac{\partial v_1}{\partial y^3} - \begin{pmatrix} k \\ 31 \end{pmatrix} v_k = \frac{\partial v_1}{\partial y^3}, \quad v_{3,1} = \frac{\partial v_3}{\partial y^1} - \begin{pmatrix} k \\ 31 \end{pmatrix} v_k = \frac{\partial v_3}{\partial y^1}, \\ v_{2,3} &= \frac{\partial v_2}{\partial y^3} - \begin{pmatrix} k \\ 32 \end{pmatrix} v_k = \frac{\partial v_2}{\partial y^3}, \quad v_{3,2} = \frac{\partial v_3}{\partial y^2} - \begin{pmatrix} k \\ 23 \end{pmatrix} v_k = \frac{\partial v_3}{\partial y^2}. \end{aligned}$$

Using the components above, the rotor of the vector \mathbf{v} is

$$\operatorname{rot} \mathbf{v} = \frac{1}{y^1} [(-\frac{\partial v_2}{\partial y^3} + \frac{\partial v_3}{\partial y^2}) \mathbf{g}_1 + (\frac{\partial v_1}{\partial y^3} - \frac{\partial v_3}{\partial y^1}) \mathbf{g}_2 + (-\frac{\partial v_1}{\partial y^2} + \frac{\partial v_2}{\partial y^1}) \mathbf{g}_3].$$

Using the index raising formula [2], one can write

$$v_i = g_{ij} v^j, \quad i = 1, 2, 3 \Rightarrow v_1 = g_{1j} v^j = g_{11} v^1; \quad v_2 = g_{2j} v^j = g_{22} v^2 = (y^1)^2 v^2; \quad v_3 = g_{3j} v^j = g_{33} v^3 = v^3$$

and the rotor of the vector \mathbf{v} is

$$\operatorname{rot} \mathbf{v} = (\frac{1}{y^1} \frac{\partial v^3}{\partial y^2} - y^1 \frac{\partial v^2}{\partial y^3}) \mathbf{g}_1 + \frac{1}{y^1} (\frac{\partial v^1}{\partial y^3} - \frac{\partial v^3}{\partial y^1}) \mathbf{g}_2 + (2v^2 + y^1 \frac{\partial v_2}{\partial y^1} - y^1 \frac{\partial v_2}{\partial y^1} - \frac{1}{y^1} \frac{\partial v_1}{\partial y^2}) \mathbf{g}_3. \quad (21)$$

Following the steps above, the corresponding results in the spherical coordinate system are obtained, i.e.,

$$\operatorname{grad} \phi = \frac{\partial \phi}{\partial y^1} \mathbf{g}_1 + \frac{1}{(y^1)^2} \frac{\partial \phi}{\partial y^2} \mathbf{g}_2 + \frac{1}{(y^1)^2 \sin^2 y^2} \frac{\partial \phi}{\partial y^3} \mathbf{g}_3, \quad (22)$$

$$\operatorname{div} \mathbf{v} = \frac{\partial v^i}{\partial y^i} + 2 \frac{v^1}{y^1} + v^2 \cot y^2, \quad i = 1, 2, 3, \quad (23)$$

$$\begin{aligned} \operatorname{rot} \mathbf{v} &= (\sin y^2 \frac{\partial v^3}{\partial y^2} - \frac{1}{\sin y^2} \frac{\partial v^2}{\partial y^3} + 2 \cos y^2 v^3) \mathbf{g}_1 + (\frac{1}{(y^1)^2 \sin y^2} \frac{\partial v^1}{\partial y^3} - \sin y^2 \frac{\partial v^3}{\partial y^1} - 2 \frac{\sin y^2}{y^1} v^3) \mathbf{g}_2 + \\ &(\frac{1}{\sin y^2} \frac{\partial v^2}{\partial y^1} - \frac{1}{(y^1)^2 \sin y^2} \frac{\partial v^1}{\partial y^2} + \frac{2v^2}{y^1 \sin y^2}) \mathbf{g}_3. \end{aligned} \quad (24)$$

Because in the cylindrical coordinate system $g = (y^1)^2$ and $g^{ij} = 0$, when $i \neq j$, and $g^{11} = g^{33} = 1$ and $g^{22} = 1/(y^1)^2$, from equation (18) follows that

$$\operatorname{Lap} \phi = \frac{1}{y^1} \frac{\partial}{\partial y^i} (\frac{\partial \phi}{\partial y^j} g^{ji} y^1) = \frac{1}{y^1} [\frac{\partial}{\partial y^1} (\frac{\partial \phi}{\partial y^1} y^1) + \frac{\partial}{\partial y^2} (\frac{\partial \phi}{\partial y^2} \frac{1}{y^1}) + \frac{\partial}{\partial y^3} (\frac{\partial \phi}{\partial y^3} y^1)]$$

or

$$\operatorname{Lap} \phi = \frac{1}{y^1} \frac{\partial \phi}{\partial y^1} + \frac{\partial^2 \phi}{\partial (y^1)^2} + \frac{1}{(y^1)^2} \frac{\partial^2 \phi}{\partial (y^2)^2} + \frac{\partial^2 \phi}{\partial (y^3)^2}. \quad (25)$$

Finally, the Laplace-operator in the spherical coordinate system takes the form

$$\operatorname{Lap} \phi = \frac{2}{y^1} \frac{\partial \phi}{\partial y^1} + \frac{\cot y^2}{(y^1)^2} \frac{\partial \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial (y^1)^2} + \frac{1}{(y^1)^2} \frac{\partial^2 \phi}{\partial (y^2)^2} + \frac{1}{(y^1)^2 \sin^2 y^2} \frac{\partial^2 \phi}{\partial (y^3)^2}. \quad (26)$$

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