

# DIRECT EXPRESSION OF INCOMPATIBILITY IN CURVILINEAR SYSTEMS

Nicolas van Goethem

# ▶ To cite this version:

Nicolas van Goethem. DIRECT EXPRESSION OF INCOMPATIBILITY IN CURVILINEAR SYSTEMS. 2016. hal-01236130v2

# HAL Id: hal-01236130 https://hal.science/hal-01236130v2

Preprint submitted on 20 Apr 2016

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

### DIRECT EXPRESSION OF INCOMPATIBILITY IN CURVILINEAR SYSTEMS

NICOLAS VAN GOETHEM

ABSTRACT. With this note, we would like present a method to compute the incompatibility operator in any system of curvilinear coordinates/components. The procedure is independent of the metric in the sense that the expression can be expressed by means of the basis vectors only, which are first defined as normal and tangent to the domain boundary and then extended to the whole domain. It is in some sense an intrinsic method, since the chosen curvilinear system depends solely on the geometry of the domain boundary. As an application, the in extense expression of incompatibility in a spherical system is given.

#### 1. INTRODUCTION

Let us consider a smooth body  $\Omega \subset \mathbb{R}^3$ . The incompatibility is a well-known operator in elasticity, since as applied to the linearized strain tensor  $\epsilon$ , it determines whether the strain derives from a displacement field. Specifically, let the elastic strain be obtained by a constitutive law from the stress tensor  $\sigma$ , i.e.,  $\epsilon = \mathbb{C}\sigma$ , with  $\mathbb{C}$  the compliance fourth-rank tensor, then inc  $\epsilon = 0$  if and only if  $\epsilon = \nabla^S u$  for some displacement field u. If on the contrary it turns out not to vanish, then Kröner's works [6] tell us that dislocations are present, preventing the existence of a well-defined displacement field defined in the whole body. In general a dislocation is a three-dimensional line singularity for the strain field, reducing to a straight line in some simplified cases where a 2D treatment is sufficient, cf., e.g., [13]). Specifically, Kröner's relation reads

$$\operatorname{Curl} \kappa = \operatorname{inc} \epsilon, \tag{1.1}$$

where the contortion tensor  $\kappa$  is related to the tensor-valued dislocation density  $\Lambda$  by  $\kappa = \Lambda - \frac{1}{2} \operatorname{tr} \Lambda \mathbb{I}_2$ . At the mesoscopic scale the dislocation density reads  $\Lambda = \Lambda_{\mathcal{L}} = \tau \otimes b\mathcal{H}^1_{\mathbb{L}\mathcal{L}}$ , where  $\mathcal{H}^1_{\mathbb{L}\mathcal{L}}$  stands for the one-dimensional Hausdorff measure concentrated in the dislocation loop  $\mathcal{L}$ . At the mesoscale, Kröner's relation also holds, as proved in [10, 11]. At the macro (or continuous) scale (which is the scale considered in the present work),  $\Lambda$  is a smooth tensor obtained from its mesoscopic counterpart by some regularization. The fact that at the mesoscale dislocations are closed loops or end at the boundary implies that div  $\Lambda = 0$ . However div  $\kappa \neq 0$  except in particular cases, for instance if one considers pure edge dislocation loops in 3D, i.e., satisfying tr  $\Lambda = 0$ , and therefore the knowledge of the right-hand side of (1.1) is in general not sufficient to uniquely determine the field  $\kappa$ . Note that in this case, The Frank tensor Curl<sup>t</sup>  $\epsilon$  and the dislocation density are univoquely related, since (1.1) reduces to Curl<sup>t</sup>  $\epsilon = \kappa$  in  $\Omega$  with  $\epsilon \times N = 0$  on  $\partial\Omega$ , by virtue of (1.4) and a uniqueness result as proved in [9].

Being a symmetric tensor, the elastic strain satisfies by Beltrami decomposition [7],

$$\epsilon = \nabla^S u + \epsilon^0 \tag{1.2}$$

with u a vector field and where  $\epsilon^0 = \text{inc } F$  represents in a Cartesian system the incompatible part of the strain, for some symmetric and solenoidal second-rank tensor F. Thus, the field F, related to the presence of dislocations satisfies by (1.1) and (1.3) an equation of the following form:

inc inc 
$$F = \operatorname{Curl} \kappa$$
, (1.3)

which is proven in [1] to be well posed (with appropriate boundary conditions on F and  $\operatorname{Curl}^{t} F \times N$ ), provided the dislocation density is given (here we assume that  $\kappa$  is known, for instance by solving a transport-reactiondiffusion equation, as done for point-defects in [12]).

The incompatibility operator on second-rank tensors is classically defined as

$$\operatorname{inc} T := \operatorname{Curl} \operatorname{Curl}^{\mathsf{t}} T, \tag{1.4}$$

<sup>2010</sup> Mathematics Subject Classification. 35J48,35J58,53A05,74A45,74B99.

Key words and phrases. incompatibility, dislocations, elasticity, differential geometry, curvilinear basis, spherical system.

meaning (in a Cartesian system) that the curl is taken over the rows and the columns of a second-rank tensor T, consecutively. In the present work, our concern is to compute the incompatibility in a subset of  $\Omega$ , say an inclusion, whose shape might be arbitrary, or solution of a geometric optimization problem. For this reason, there is a need to express incompatibility in curvilinear systems, chosen to fit the inclusion geometry.

In a general curvilinear system, the same definition (1.4) holds, but care must be taken, since the covariant derivatives do not commute in general because the basis vectors depend on the position, and hence must also be differentiated in (1.4). We will write the general second-rank tensor as T in the Cartesian basis as  $T = T_{ij}^{\text{CART}} e^i \otimes e^j$ , and in the curvilinear basis as  $T = T_{ij}^{\text{CURV}} g^i \otimes g^j$ . Our point of view is that the basis  $\{g^i\}_i = \{N, \tau_R\}$  for R = A, B, where  $\tau_R$  are tangent to the boundary, and N is its unit outwards normal, is first defined on the domain boundary  $\partial\Omega$  and then extended in  $\Omega$ , where its differentials can be computed. This latter operation gives rise to 5 numbers:  $\kappa^R$ , the 2 surface curvatures,  $\gamma^R$ , the 2 divergences of  $\tau^R$ , and  $\xi$ , the deviation with respect to the principal directions. From these five numbers, the Christoffel symbols can be found and hence the covariant derivatives, thus the expression of the curvilinear curl, and eventually of the incompatibility. An important preliminary step is to express the differentials of the basis vectors in terms of  $\kappa^R, \gamma^R, \xi$ , which is given in Theorem 3.2 whose proof can be found in [1]. The curvilinear coordinates are simply the abscissae of the curves with tangent vector  $\tau^R$ , and the radial coordinate r associated to N.

Expressions of the incompatibility in a general curvilinear system are rarely found in extenso in the literature. Let us mention L. E. Malvern's textbook [8], where an expression can be found in Appendix II, expressed in terms of the metric factors  $h_i$  defining the intrinsic metric. Our approach can be considered as an metric-free alternative, since we base our method on the sole geometry of the domain boundary and on the natural orthogonal basis that we may define on it. In Section 5, we apply our method to the spherical system, and provide explicit expressions of all six components of inc T.

Applications of this method can be found in dislocation theory, where the incompatibility in an inclusion is to be found, in order to determine its dislocation content, and design an optimization method where inclusions are inserted as to obtain a maximal increase (or decrease) of certain functionals.

Notations and conventions. Let  $\Omega$  be a bounded domain of  $\mathbb{R}^3$  with smooth boundary  $\partial\Omega$ . By smooth we mean  $C^{\infty}$ , but this assumption could be considerably weakened. Curl, incompatibility and cross product with 2nd order tensors are defined componentwise as follows with the summation convention on repeated indices. Here, E represents 2nd rank tensors, N is a vector, and  $\epsilon$  is the Levi-Civita 3rd rank tensor. One has:

$$(\operatorname{Curl} E)_{ij} := (\nabla \times E)_{ij} = \epsilon_{jkm} \partial_k E_{im}, (\operatorname{inc} E)_{ij} := (\operatorname{Curl} \operatorname{Curl}^{\mathrm{t}} E)_{ij} = \epsilon_{ikm} \epsilon_{jln} \partial_k \partial_l E_{mn}$$

Note that the transpose of Curl *E* will be denoted by Curl<sup>t</sup> *E*. Moreover the tensorial product of two vectors *a* and *b* will be denoted by  $a \otimes b$ , while  $a \odot b = \frac{1}{2}(a \otimes b + b \otimes a)$ .

# 2. Some physical motivations

In this section, we provide two examples of models in which the incompatibility plays a crucial role and must be expressed in a curvilinear system.

2.1. The incompatibility operator in linearized elasticity with dislocations. The strain energy density in small-strain elasticity of an isotropic material reads

$$W_{\rm e}(\epsilon) = \frac{1}{2} \mathbb{A}\epsilon \cdot \epsilon, \qquad (2.1)$$

where  $\epsilon$  is the linearized elastic strain tensor. The stress tensor is classically defined as  $\sigma := \frac{\partial W_e}{\partial \epsilon} = \mathbb{A}\epsilon$ . Furthermore, by the symmetry property of  $\epsilon$ , Beltrami decomposition (1.3) holds. The potential energy is defined as

$$\mathcal{W}(\epsilon) = \int_{\Omega} \left( W_{\rm e}(\epsilon) - f \cdot u - \mathbb{G} \cdot F \right) dx, \tag{2.2}$$

which, in the absence of dislocations, i.e., as F = 0, yields by minimization the standard Equilibrium equation,

$$-\operatorname{div} (\mathbb{A}\epsilon) = -\operatorname{div} (\mathbb{A}\nabla^{S}u) = f, \qquad (2.3)$$

with f the body force and u the displacement field.

Now, in the general case where dislocation lines are present, the minimum problem writes as

$$\min_{\epsilon} \mathcal{W}(\epsilon) = \min_{\substack{\epsilon = \nabla^{s} u + \text{ inc } F}} \mathcal{W}(\epsilon).$$
(2.4)

Letting  $\tilde{u}$  and  $\tilde{F}$  be variations in appropriate function spaces with vanishing boundary conditions, Euler-Lagrange equations read

$$0 = \langle \frac{\delta \mathcal{W}(\epsilon)}{\delta u}, \tilde{u} \rangle = \int_{\Omega} \left( \sigma \cdot \nabla^{S} \tilde{u} - f \cdot \tilde{u} \right) dx,$$
  

$$0 = \langle \frac{\delta \mathcal{W}(\epsilon)}{\delta F}, \tilde{F} \rangle = \int_{\Omega} \left( \sigma \cdot \operatorname{inc} \tilde{F} - \mathbb{G} \cdot \tilde{F} \right) dx,$$
(2.5)

providing after some easy part integrations, the strong forms

$$\begin{cases} -\operatorname{div} \sigma &= f, \\ \operatorname{inc} \sigma &= \mathbb{G}, \end{cases}$$

which appear clearly as a generalization of (2.3). Recalling (1.3), the complete problem consists in solving the coupled problem with unknowns u and F:

$$\begin{cases} -\operatorname{div} (\mathbb{A}\nabla^{S} u) &= f + \operatorname{div} (\mathbb{A}\operatorname{inc} F), \\ \operatorname{inc} (\mathbb{A}\operatorname{inc} F) &= \mathbb{G} - \operatorname{inc} (\mathbb{A}\nabla^{S} u). \end{cases}$$
(2.6)

Material isotropy yields  $\mathbb{A} = \mu \mathbb{I}_4 + \lambda \mathbb{I}_2 \otimes \mathbb{I}_2$  and hence (2.8) rewrites as

$$\begin{cases} -\operatorname{div} \left(\mathbb{A}\nabla^{S} u\right) &= f + \operatorname{div} \left(\lambda \operatorname{tr} \epsilon^{0} \mathbb{I}_{2}\right), \\ \operatorname{inc} \left(\mathbb{A}\operatorname{inc} F\right) &= \mathbb{G} - \operatorname{inc} \left(\lambda \operatorname{div} u \mathbb{I}_{2}\right). \end{cases}$$
(2.7)

Note that the decoupled problem is found as soon as either  $\lambda = 0$ , or incompressibility is assumed, i.e., tr  $\epsilon = \text{tr } \epsilon^0 = \text{div } u = 0$ , and reads

$$\begin{cases} -\operatorname{div} \left( \tilde{\mathbb{A}} \nabla^{S} u \right) &= f \\ \operatorname{inc} \left( \tilde{\mathbb{A}} \operatorname{inc} F \right) &= \mathbb{G} \end{cases} \quad \text{in} \quad \Omega,$$

where the special form of  $\tilde{\mathbb{A}}$  due to incompressibility can be found in [5].

The point here is to observe that according to the geometry of  $\Omega$  it is usefull to have an expression of incompatibility in curvilinear coordinates/components systems according to the geometry of  $\Omega$ .

#### 2.2. Dislocation-induced dissipation. Let us define the system Helmholtz free energy density as

$$\Psi := W_e(\epsilon) + W_{\text{defect}}(\operatorname{Curl} \kappa), \qquad (2.8)$$

whose elastic part is simply the strain energy of previous section, and whose defect part is assumed to depend on the curl of the contortion tensor  $\kappa$ . Therefore, the free energy  $\Psi$  is partially of second-order in the sense that the defect internal variable appears in the form of its derivatives (here its curl). For simplicity, let us assume a quadratic law in the higher-order terms, viz.,  $W_{\text{defect}}(\text{Curl }\kappa) = \frac{1}{2}\mathbb{M}\text{Curl }\kappa$ . Curl  $\kappa$ , with  $\mathbb{M}$  a positive-definite fourth-rank tensor. By Kröner's relation (1.1), the energy of an inclusion  $\omega \subset \Omega$  reads

$$\mathcal{W}_{\text{defect}} := \int_{\omega} \frac{1}{2} \mathbb{M} \operatorname{inc} \epsilon^{0} \cdot \operatorname{inc} \epsilon^{0} dx.$$
(2.9)

Therefore, minimizing this energy will again lead one to evaluate or express the incompatibility in local basis appropriate to the geometry of  $\omega$ .

Note that a full second-order energy density would read for instance  $\Psi := W_e(\epsilon) + \hat{W}_e(\operatorname{Curl}^t \epsilon, \operatorname{div} \epsilon) + \hat{W}_{\operatorname{defect}}(\kappa, \operatorname{Curl} \kappa, \operatorname{div} \kappa) + \overline{W}_{\operatorname{defect}}(\epsilon^0)$ , where  $\operatorname{Curl}^t \epsilon$  is recognized as the Frank tensor, i.e. the gradient of the rotation field.

#### NICOLAS VAN GOETHEM

#### 3. Extension and differentiation of the normal and tangent vectors to a surface

The aim here is to construct a curvilinear basis on the boundary which should be smooth and also orthonormal, starting from the vector  $N_{\partial\Omega}$  normal to the boundary and defining two tangent vectors perpendicular to  $N_{\partial\Omega}$ . This basis is then extended to the whole body. The natural moving frame sought is close in spirit to the Darboux frame of surfaces, though in principle the latter may only be defined at non-umbilical points. As a matter of fact, in order to achieve a certain level of generality, we will not consider principal lines of curvature with their associated principal curvatures, and hence the gradient of the normal vector will be given by a symmetric matrix with possibly non-zero extradiagonal components. Detail on this section, and in particular, the proofs, can be found in [1].

3.1. Signed distance function and extended unit normal. We denote by  $N_{\partial\Omega}$  the outward unit normal to  $\partial\Omega$ , and by b the signed distance to  $\partial\Omega$ , i.e.,

$$b(x) = \begin{cases} \operatorname{dist}(x, \partial \Omega) & \text{if } x \notin \Omega, \\ -\operatorname{dist}(x, \partial \Omega) & \text{if } x \in \Omega. \end{cases}$$

We recall the following results ([3], Chap. 5, Thms 3.1 and 4.3).

**Theorem 3.1.** There exists an open neighborhood W of  $\partial\Omega$  such that

- (1) b is smooth in W;
- (2) every  $x \in W$  admits a unique projection  $p_{\partial\Omega}(x)$  onto  $\partial\Omega$ ;
- (3) this projection satisfies

$$p_{\partial\Omega}(x) = x - \frac{1}{2}\nabla b^2(x), \qquad x \in W;$$
(3.1)

(4) it holds

$$\nabla b(x) = N_{\partial\Omega}(p_{\partial\Omega}(x)), \qquad x \in W.$$

In particular, this latter property shows that  $\nabla b(x) = N_{\partial\Omega}(x)$  for all  $x \in \partial\Omega$  and  $|\nabla b(x)| = 1$  for all  $x \in W$ . Therefore, we define the extended unit normal by

$$N(x) := \nabla b(x) = N_{\partial\Omega}(p_{\partial\Omega}(x)), \qquad x \in W.$$
(3.2)

3.2. Tangent vectors on  $\partial\Omega$ . For all  $x \in \partial\Omega$ , we denote by  $T_{\partial\Omega}(x)$  the tangent plane to  $\partial\Omega$  at x, that is, the orthogonal complement of  $N_{\partial\Omega}(x)$ . As  $\partial\Omega$  is smooth, there exists a covering of  $\partial\Omega$  by open balls  $B_1, \ldots, B_M$  of  $\mathbb{R}^3$  such that, for each index k, two smooth vector fields  $\tau^A_{\partial\Omega}, \tau^B_{\partial\Omega}$  can be constructed on  $\partial\Omega \cap B_k$  where, for all  $x \in \partial\Omega \cap B_k, (\tau^A_{\partial\Omega}(x), \tau^B_{\partial\Omega}(x))$  is an orthonormal basis of  $T_{\partial\Omega}(x)$ . In all the sequel, the index k will be implicitly considered as fixed and the restriction to  $B_k$  will be omitted. In fact, for our needs, global properties and constructions will be easily obtained from local ones through a partition of unity subordinate to the covering.

Using that the Jacobian matrix  $DN(x) = D^2b(x)$  of N(x) is symmetric, differentiating the equality  $|N(x)|^2 = 1$  entails

$$\partial_N N(x) = DN(x)N(x) = 0, \qquad x \in W.$$
(3.3)

In other words, N(x) is an eigenvector of DN(x) for the eigenvalue 0. For all  $x \in \partial\Omega$ , the system  $(\tau^A_{\partial\Omega}(x), \tau^B_{\partial\Omega}(x), N_{\partial\Omega}(x))$  is an orthonormal basis of  $\mathbb{R}^3$ . In this basis, DN(x) takes the form

$$DN(x) = \begin{pmatrix} \kappa_{\partial\Omega}^A(x) & \xi_{\partial\Omega}(x) & 0\\ \xi_{\partial\Omega}(x) & \kappa_{\partial\Omega}^B(x) & 0\\ 0 & 0 & 0 \end{pmatrix}, \qquad x \in \partial\Omega,$$
(3.4)

where  $\kappa_{\partial\Omega}^A$ ,  $\kappa_{\partial\Omega}^B$  and  $\xi$  are smooth scalar fields defined on  $\partial\Omega$ .

If  $R \in \{A, B\}$ , we denote by  $R^*$  the complementary index of R, that is,  $R^* = B$  if R = A and  $R^* = A$  if R = B.

#### 3.3. Extended tangent vectors in $\Omega$ and their curvilinear differentials. Let d be defined in W by

$$d = \left(1 + b \kappa_{\partial\Omega}^{A} \circ p_{\partial\Omega}\right) \left(1 + b \kappa_{\partial\Omega}^{B} \circ p_{\partial\Omega}\right) - \left(b \xi_{\partial\Omega} \circ p_{\partial\Omega}\right)^{2}.$$

Possibly adjusting W so that d(x) > 0 for all  $x \in W$ , we define in W, and for R = A, B,

$$\tau^{R} = \tau^{R}_{\partial\Omega} \circ p_{\partial\Omega}, \qquad \kappa^{R} = d^{-1} \left( (1 + b \kappa^{R^{*}}_{\partial\Omega} \circ p_{\partial\Omega}) (\kappa^{R}_{\partial\Omega} \circ p_{\partial\Omega}) - b (\xi_{\partial\Omega} \circ p_{\partial\Omega})^{2} \right), \tag{3.5}$$

$$\xi = d^{-1}\xi_{\partial\Omega} \circ p_{\partial\Omega}, \kappa = \kappa^A + \kappa^B, \qquad \gamma^R = \operatorname{div} \tau^R.$$
(3.6)

Obviously, for each  $x \in W$ , the triple  $(\tau^A(x), \tau^B(x), N(x))$  forms an orthonormal basis of  $\mathbb{R}^3$ . Next, we compute the normal and tangential derivatives of these vectors. We denote the tangential derivative  $\partial_{\tau^R}$  by  $\partial_R$  for simplicity, i.e.,  $\partial_R u := Du\tau^R$ , where Du stands for the differential of u, and  $\partial_R u$  its value in the direction  $\tau^R$ .

**Theorem 3.2** ([1]). It holds in W:

$$\partial_N \tau^R = 0, \partial_R N = \kappa^R \tau^R + \xi \tau^{R^*}, \partial_R \tau^R = -\kappa^R N - \gamma^{R^*} \tau^{R^*}, \partial_{R^*} \tau^R = \gamma^R \tau^{R^*} - \xi N,$$
  
div  $N = \text{tr } DN = \Delta b = \kappa.$  (3.7)

**Corollary 3.3** ([1]). If f is twice differentiable in  $\Omega$  it holds

$$\partial_R \partial_N f = \partial_N \partial_R f + \kappa^R \partial_R f + \xi \partial_{R^*} f. \tag{3.8}$$

# 4. DIFFERENTIAL GEOMETRY ON THE BOUNDARY WITH CURVINORMAL BASIS

At each point  $x \in \partial\Omega$  the curvilinear basis  $(g^i(x))_{i=A,B,N} := (\tau^A(x), \tau^B(x), N_{\partial\Omega}(x))$  is orthonormal and differentiable by Theorem 3.2. Therefore it will be called *curvinormal*. Remark that indices P, Q, R will stand for A or B, and denote one of the two orthogonal tangent vectors on the boundary, whereas index N will always be associated to the normal  $N_{\partial\Omega}$ . In some sense, the chosen curvilinear basis is a generalization to general surfaces of the spherical or cylindrical basis. We recall that  $\partial_i$  means the differential in the direction  $g^i$ . Let u be a scalar. Then,  $\partial_i u = \partial_R u = \tau^R \cdot \nabla u = Du\tau^R$  for R = A, B, or  $\partial_N u = N \cdot \nabla u = DuN$  for i = N, with  $\nabla = e^i \partial_{x_i}$  the Cartesian gradient operator, where  $e^i$  stands for the *i*th Cartesian basis vector. For instance, the gradient in spherical coordinates reads  $\nabla u = \partial_r u e_r + \frac{1}{r} \partial_{\phi} u e_{\Phi} + \frac{1}{r \sin \phi} \partial_{\theta} u e_{\theta}$  and hence  $\partial_A = \frac{1}{r} \partial_{\phi}$ and  $\partial_B = \frac{1}{r \sin \phi} \partial_{\theta}$ . Recall that partial curvilinear derivatives do not commute, as shown in Corollary 3.3.

4.1. Christoffel symbols and Riemannian curvature. A general vector field will be written as  $v = v_i g^i$ with  $v_i$  its covariant components. Moreover, the extrinsic metric is Euclidean, since  $g^{ij} := g^i \cdot g^j = \delta^{ij}$ . Let  $g_i := g_{ij}g^j$  be the dual of the basis vector. The second Christoffel symbol  $\Gamma_{ij}^p$  is defined as the linear operator such that [2]

$$\partial_j g^p = -\Gamma^p_{ij} g^i. \tag{4.1}$$

In other words,  $\Gamma_{ij}^p := -g_i \cdot \partial_j g^p$ . Note also that since  $\Omega$  is embedded in a Euclidean space, one has  $\partial_j g^i = \partial_j g_i$ . Connection. As a consequence, for vector v it holds

$$\partial_j v = \partial_j (v_i g^i) = (\partial_j v_i - \Gamma^p_{ij} v_p) g^i = v_{i\parallel j} g^i, \tag{4.2}$$

where the covariant derivative of the covariant component of v reads

$$v_{i\parallel j} := \partial_j v_i - \Gamma^p_{ij} v_p. \tag{4.3}$$

Thus, for vector  $v = v_i g^i = \hat{v}_j e^j$ , one has  $(\nabla v)_{mn} = \partial_{x_m} u_n$ , and hence

$$\operatorname{rad} v := (\nabla v)_{mn} e^m \otimes e^n = v_{i||j} g^i \otimes g^j = \partial_j v \otimes g^j.$$

$$(4.4)$$

Accordingly, the curl of a vector in the curvinormal basis writes as

g

$$\operatorname{Curl} v := (\operatorname{Curl} v)_k g^k = \epsilon_{kij} v_{i\parallel j} g^k.$$

$$(4.5)$$

Curvilinear coordinates. Let  $q_R \in \omega^R$  be the curvilinear coordinate associated to  $g^R$  in the sense that  $g^R = \frac{\partial_{q_R} x}{G_R}$ , with  $G_R := \|\partial_{q_R} x\|$ , and where x stands for the position vector of a point. Otherwise said,  $q_R$  is the curvilinear abcissa of the curve with tangent vector  $\tau^R$ . In general one has

$$\partial_{q_R} u = \partial_{x_i} u \frac{\partial x_i}{\partial_{q_R}} = g_R G_i^R \partial_{x_i} u = G_R \partial_R u.$$
(4.6)

Hence the gradient of scalar u reads

$$\operatorname{grad} u = \partial_i u g^i = \frac{1}{G_i} \partial_{q_i} u g^i, \tag{4.7}$$

and of vector  $v = v_i g^i$  as

$$\operatorname{grad} v = \partial_j v \otimes g^j = \frac{1}{G_j} \partial_{q_j} v \otimes g^j.$$
 (4.8)

#### NICOLAS VAN GOETHEM

We call the curvilinear expression of the gradient the operator  $\nabla^{\text{CURV}}(\cdot) := h_j \partial_{q_j}(\cdot) g^j$  with  $h_j := \frac{1}{G_j}$ , the *j*th metric factor. Remark that the  $\partial_R$  derivatives do not commute, contrarily to  $\partial_{q_R}$ , because of the factors  $G_R$ . As an example, consider the spherical base system, where  $G_N = G_r = 1, G_A = G_{\phi} = \frac{1}{r}, G_B = G_{\theta} = \frac{1}{r \sin \phi}$ , and  $q_A = \phi$  (polar angle),  $q_B = \theta$  (azimuthal angle); it holds,

$$(\partial_A \partial_r - \partial_r \partial_A) = \frac{1}{r^2} \partial_\phi, \ (\partial_B \partial_r - \partial_r \partial_B) = \frac{1}{r^2 \sin \phi} \partial_\theta, \ (\partial_B \partial_A - \partial_A \partial_B) = \frac{1}{r^2 \sin \phi \tan \phi} \partial_\theta.$$
(4.9)

Christoffel symbols in the curvinormal basis. By Theorem 3.2, it is easily deduced by identification with (4.1) that the only nonvanishing components of  $\Gamma_{ij}^p$  read (with no sum on repeated indices)

$$\Gamma_{RR^*}^N = -\xi, \ \Gamma_{RR}^N = -\kappa^R, \ \Gamma_{NR}^{R^*} = \xi, \ \Gamma_{R^*R}^R = \gamma^{R^*}, \ \Gamma_{NR}^R = \kappa^R, \ \Gamma_{R^*R^*}^R = -\gamma^R.$$
(4.10)

Moreover, it is observed that  $\Gamma_{ij}^p$  is not symmetric, i.e.,  $\Gamma_{ij}^p \neq \Gamma_{ij}^p$ . Therefore, the torsion is nonvanishing, and reads

$$T_{ij}^p := \Gamma_{ij}^p - \Gamma_{ji}^p$$

In the curvinormal basis, it is easily computed that the only nonvanishing components of  $T_{ij}^p$  are

$$T_{ij}^{R} = \kappa^{R} \delta_{iN} \delta_{jR} + \xi \delta_{iN} \delta_{jR^{*}} + (\gamma^{R^{*}} - \gamma^{R}) \delta_{iR^{*}} \delta_{jR}.$$

Note that the Riemann curvature tensor is defined as [4]

$$\operatorname{Riem}_{ijk}^{q} := \partial_{k} \Gamma_{ij}^{q} - \partial_{j} \Gamma_{ik}^{q} + \Gamma_{ij}^{p} \Gamma_{pk}^{q} - \Gamma_{ik}^{p} \Gamma_{pj}^{q}.$$

$$\tag{4.11}$$

Spherical system. As an example, in a spherical coordinates/components system, it holds<sup>1</sup>  $i, j \in \{\phi, \theta\}, \kappa^R = \frac{1}{r}, \gamma^{\phi} = \frac{1}{\tan \phi}, \gamma^{\theta} = 0$ , and hence

$$\Gamma_{ij}^{r} = \begin{pmatrix} 0 & 0 & 0\\ 0 & -\frac{1}{r} & 0\\ 0 & 0 & -\frac{1}{r} \end{pmatrix}, \ \Gamma_{ij}^{\phi} = \begin{pmatrix} 0 & \frac{1}{r} & 0\\ 0 & 0 & 0\\ 0 & 0 & -\frac{1}{r\tan\phi} \end{pmatrix}, \ \Gamma_{ij}^{\theta} = \begin{pmatrix} 0 & 0 & \frac{1}{r}\\ 0 & 0 & \frac{1}{r\tan\phi}\\ 0 & 0 & 0 \end{pmatrix}.$$
(4.12)

Hence, the torsion reads

$$T_{ij}^{r} = 0, \ T_{ij}^{\phi} = \begin{pmatrix} 0 & \frac{1}{r} & 0\\ -\frac{1}{r} & 0 & 0\\ 0 & 0 & 0 \end{pmatrix}, \ T_{ij}^{\theta} = \begin{pmatrix} 0 & 0 & \frac{1}{r}\\ 0 & 0 & \frac{1}{r\tan\phi}\\ -\frac{1}{r} & -\frac{1}{r\tan\phi} & 0 \end{pmatrix}.$$
 (4.13)

Accordingly the covariant derivative reads

$$\left( v_{i\parallel j} \right)_{ij} = \begin{pmatrix} \partial_r v_r & \frac{1}{r} \partial_\phi v_r - \frac{v_\phi}{r} & \frac{1}{r\sin\phi} \partial_\theta v_r - \frac{v_\theta}{r} \\ \partial_r v_\phi & \frac{1}{r} \partial_\phi v_\phi + \frac{v_r}{r} & \frac{1}{r\sin\phi} \partial_\theta v_\phi - \frac{v_\theta}{r\tan\phi} \\ \partial_r v_\theta & \frac{1}{r} \partial_\phi v_\theta & \frac{1}{r\sin\phi} \partial_\theta v_\theta + \frac{v_r}{r} + \frac{v_\phi}{r\tan\phi} \end{pmatrix}_{ij} .$$

$$(4.14)$$

Hence the curl of a vector,  $(\operatorname{Curl} v)_i := \epsilon_{ikj} v_{k||j}$ , writes by (4.5) and (4.14) as

$$(\operatorname{Curl} v)_{i} = \begin{pmatrix} \frac{1}{r \tan \phi} v_{\theta} + \frac{1}{r} \partial_{\phi} v_{\theta} - \frac{1}{r \sin \phi} \partial_{\theta} v_{\phi} \\ \frac{1}{r \sin \phi} \partial_{\theta} v_{r} - \frac{1}{r} v_{\theta} - \partial_{r} v_{\theta} \\ \frac{1}{r} v_{\phi} + \partial_{r} v_{\phi} - \frac{1}{r} \partial_{\phi} v_{r} \end{pmatrix}_{i}.$$

$$(4.15)$$

4.2. Commutation operator in the curvinormal basis. The covariant components of a second-rank tensor T reads [4]

$$T_{ij\parallel k} = \partial_k T_{ij} - \Gamma^l_{ik} T_{lj} - \Gamma^l_{jk} T_{il}.$$

$$(4.16)$$

Let  $T_{ij} = v_{i||j}$ . Then by (4.16) one has  $v_{i||jk} := (u_{i||j})_{||k}$  and hence

$$\begin{aligned} v_{i\|jk}g^{i} &= \partial_{k}v_{i\|j}g^{i} - (\Gamma_{ik}^{l}v_{l\|j} + \Gamma_{jk}^{l}v_{i\|l})g^{i} = \partial_{k}\left(v_{i\|j}g^{i}\right) + v_{i\|j}\Gamma_{lk}^{i}g^{l} - (\Gamma_{ik}^{l}v_{l\|j} + \Gamma_{jk}^{l}v_{i\|l})g^{i} \\ &= \partial_{k}\left(v_{i\|j}g^{i}\right) - \Gamma_{jk}^{l}v_{i\|l}g^{i}, \end{aligned}$$

where (4.3) and a change of dumb indices have been used. Therefore,

$$\partial_k(\partial_j v) = \left(v_{i||jk} + \Gamma^l_{jk} v_{i||l}\right) g^i.$$
(4.17)

In particular,

$$v_{i\parallel jk} - v_{i\parallel kj} = (\partial_k \partial_j - \partial_l \partial_k) v \cdot g^i - T^l_{jk} v_{i\parallel l},$$
(4.18)

<sup>&</sup>lt;sup>1</sup>Here,  $\phi$  denotes the polar, and  $\theta$  the azimuthal coordinate, respectively.

that following [4] can be rewritten by means of the Riemann curvature as

$$v_{i\|jk} - v_{i\|kj} = \operatorname{Riem}_{iqkj} v_q - T_{jk}^l v_{i\|l}.$$
(4.19)

Remark that in spherical coordinates and by (4.13) and (4.9), (4.18) yields (with a slight abuse of notations, since one writes  $q_R$  instead of R as covariant differentiation indice)

$$v_{i\|r\phi} - v_{i\|\phi r} = v_{i\|r\theta} - v_{i\|\theta r} = v_{i\|\theta\phi} - v_{i\|\phi\theta} = 0,$$
(4.20)

that is, the second covariant derivatives commute in spherical coordinates/components. In particular, one has  $\epsilon_{ljk}v_{i||jk} = \epsilon_{ljk}(v_{i||j})_{||k} = 0$  in spherical coordinates/components. Note that the identity Curl  $\nabla u = 0$  holds simply by Schwarz lemma if u is a scalar, whereas its vector counterpart Curl  $\nabla v$  reads

$$\operatorname{Curl} \nabla v = \operatorname{Curl} \left( (\nabla v)_{ij}^{\operatorname{CART}} e^i \otimes e^j \right) = \operatorname{Curl} \left( (\nabla v)_{ij}^{\operatorname{CURV}} g^i \otimes g^j \right),$$

that is, in the Cartesian system,

$$\operatorname{Curl}\left((\nabla v)_{ij}^{\operatorname{CART}} e^{i} \otimes e^{j}\right) = -\epsilon_{ljk}(v_{i,j})_{,k} e^{i} \otimes e^{l} = 0.$$

by Schwarz lemma. However, in a general curvilinear system, one has

$$\operatorname{Curl}\left((\nabla v)_{ij}^{\operatorname{CURV}}g^{i}\otimes g^{j}\right) = \nabla^{\operatorname{CURV}}(\nabla v)_{ij}^{\operatorname{CURV}}\times g^{i}\otimes g^{j} + (\nabla v)_{ij}^{\operatorname{CURV}}\operatorname{Curl}^{\operatorname{CURV}}(g^{i}\otimes g^{j}) = 0,$$

and hence

$$\nabla^{\text{CURV}}(\nabla v)_{ij}^{\text{CURV}} \times (g^i \otimes g^j) = (v_{i||j})_{||k} g^i \otimes \epsilon_{lkj} g^l = -(\nabla v)_{ij}^{\text{CURV}} \text{Curl}^{\text{CURV}}(g^i \otimes g^j).$$
(4.21)

Remark that in the spherical system, the first term on the RHS of (4.21) vanishes by (4.20).

Summarizing, Eq. (4.21) shows that the non-commutation operator in the RHS of (4.19) is related in the curvilinear system to the curl of the basis diads. This fact will appear crucial in the calculations of the following sections.

4.3. Expression of the incompatibility in the curvinormal basis. Now, the incompatibility operator on a second-rank tensor T is defined as<sup>2</sup>

$$\operatorname{inc} T := \operatorname{Curl} \operatorname{Curl}^{\mathsf{t}} T, \tag{4.22}$$

which in a Cartesian system is equivalent to writing componentwise

inc 
$$T = \epsilon_{ikm} \epsilon_{iln} \partial_k \partial_l T_{mn} e^i \otimes e^j$$
.

In a general curvilinear system, Eq. (4.22) shows that it suffices to express the curl of a tensor and apply twice the curl operator. In fact, (4.22) rewrites as

inc 
$$T = \text{Curl} \left( \text{Curl}^{\text{t}} \left( T_{ij}^{\text{CART}} e^i \otimes e^j \right) \right) = \text{Curl} \left( \text{Curl}^{\text{t}} \left( T_{ij}^{\text{CURV}} g^i \otimes g^j \right) \right),$$

with

$$\operatorname{Curl} \left( T_{ij}^{\operatorname{CURV}} g^i \otimes g^j \right) = \nabla^{\operatorname{CURV}} T_{ij}^{\operatorname{CURV}} \times g^i \otimes g^j + T_{ij}^{\operatorname{CURV}} \operatorname{Curl}^{\operatorname{CURV}} (g^i \otimes g^j).$$
(4.23)

Remark that, as compared with the Cartesian system case, the second term in the RHS is nonvanishing and requires to compute the curl of the basis diads. Summarizing, one has

$$\operatorname{Curl}^{t} \left( T_{ij}^{\operatorname{CURV}} g^{i} \otimes g^{j} \right) = S_{ij}^{\operatorname{CURV}} g^{i} \otimes g^{j}, \tag{4.24}$$

for some components  $S_{ij}^{\text{CURV}}$  obtained by rearranging (4.23). Hence, the incompatibility in the curvilinear system writes as

$$\text{inc } T = \nabla^{\text{CURV}} S_{ij}^{\text{CURV}} \times \left(g^i \otimes g^j\right) + S_{ij}^{\text{CURV}} \text{Curl}^{\text{CURV}}(g^i \otimes g^j)$$
$$= \nabla^{\text{CURV}} S_{ij}^{\text{CURV}} \times \left(g^i \otimes g^j\right) + S_{ij}^{\text{CURV}} \left(\left(\nabla^{\text{CURV}} g^i\right) \times g^j + g^i \otimes \text{Curl}^{\text{CURV}} g^j\right) = \eta_{ij} g^i \otimes g^j.$$
(4.25)

Obviously,  $\eta_{ij}$  is symmetric as soon as T is, by the symmetry property of its Cartesian counterpart  $\epsilon_{ikm}\epsilon_{jln}\partial_k\partial_l T_{mn}$ . Moreover, its explicit expression only requires to determine the gradient of scalar  $S_{ij}^{\text{CURV}}$  in the curvilinear system, which is expressed by means of the tangent vectors as

$$\nabla^{\mathrm{CURV}} S^{\mathrm{CURV}}_{ij} = D S^{\mathrm{CURV}}_{ij}(x) [g^l] g^l = \left(g^l \cdot \nabla S^{\mathrm{CURV}}_{ij}\right) g^l$$

 $<sup>^{2}</sup>$ For some authors, e.g. L. E. Malvern [8] the incompatibility is defined with a minus sign.

(see also Eq. (4.7)), together with the curvilinear differentials of the basis tensors to be found in Section 3.3 (by means of Eq. (4.1), (4.3) and (4.5)), and expressed by means of  $\kappa^R$ ,  $\gamma^R$  and  $\xi$ , which are intrinsic numbers of the boundary as related to the choice of the basis. Note that use has been made of identity

$$\operatorname{Curl} a \otimes b = \nabla a \times b + a \otimes \operatorname{Curl} b. \tag{4.26}$$

### 5. Incompatibility in the spherical system

We recall that we adopt the convention that  $\phi$  be the polar and  $\theta$  be the azimuthal angles. Moreover  $x = rg^r$ , with r the radius. The spherical system consists of the triad  $\{g^r, g^{\phi}, g^{\theta}\}$ , with according to our conventions,  $N = g^r, \tau^A = g^{\phi}$  and  $\tau^B = g^{\theta}$ , the latter two being tangent to the sphere of radius r and normal vector  $g^r$ . We consider a symmetric tensor T whose general form reads

$$T = T_{rr}g^r \otimes g^r + T_{\phi\phi}g^\phi \otimes g^\phi + T_{\theta\theta}g^\theta \otimes g^\theta + 2T_{r\phi}g^r \odot g^\phi + 2T_{r\theta}g^r \odot g^\theta + 2T_{\phi\theta}g^\phi \odot g^\theta.$$
(5.1)

5.1. Curl of the diads. By virtue of (4.14) and (4.15), and recalling (4.26), let us first compute the curl of the base diads.

$$\begin{aligned} \operatorname{Curl} & (g^r \otimes g^r) &= -\frac{1}{r} (g^{\phi} \otimes g^{\theta} - g^{\theta} \otimes g^{\phi}), \\ \operatorname{Curl} & (g^r \otimes g^{\phi}) &= \frac{1}{r} (g^r \otimes g^{\theta} - g^{\theta} \otimes g^r), \\ \operatorname{Curl} & (g^r \otimes g^{\theta}) &= -\frac{1}{r} (g^r \otimes g^{\phi} - g^{\phi} \otimes g^r) + \frac{1}{r \tan \phi} g^r \otimes g^r, \\ \operatorname{Curl} & (g^{\phi} \otimes g^r) &= \frac{1}{r} g^r \otimes g^{\theta} + \frac{1}{r \tan \phi} g^{\theta} \otimes g^{\phi}, \\ \operatorname{Curl} & (g^{\phi} \otimes g^{\phi}) &= -\frac{1}{r \tan \phi} g^{\theta} \otimes g^r + \frac{1}{r} g^{\phi} \otimes g^{\theta}, \\ \operatorname{Curl} & (g^{\phi} \otimes g^{\theta}) &= -\frac{1}{r} (g^r \otimes g^r + g^{\phi} \otimes g^{\phi}) + \frac{1}{r \tan \phi} g^{\phi} \otimes g^r, \\ \operatorname{Curl} & (g^{\theta} \otimes g^r) &= -\frac{1}{r} g^r \otimes g^{\phi} - \frac{1}{r \tan \phi} g^{\phi} \otimes g^{\phi}, \\ \operatorname{Curl} & (g^{\theta} \otimes g^r) &= -\frac{1}{r} (g^r \otimes g^r + g^{\theta} \otimes g^{\theta}) + \frac{1}{r \tan \phi} g^{\phi} \otimes g^{\phi}, \\ \operatorname{Curl} & (g^{\theta} \otimes g^{\phi}) &= \frac{1}{r} (g^r \otimes g^r + g^{\theta} \otimes g^{\theta}) + \frac{1}{r \tan \phi} g^{\phi} \otimes g^r, \\ \operatorname{Curl} & (g^{\theta} \otimes g^{\theta}) &= \frac{1}{r} (g^r \otimes g^r - g^{\theta} \otimes g^r) + \frac{1}{r \tan \phi} g^{\phi} \otimes g^r, \\ \operatorname{Curl} & (g^{\theta} \otimes g^{\theta}) &= \frac{1}{r} (g^r \otimes g^r - g^{\theta} \otimes g^r) + \frac{1}{r \tan \phi} g^{\phi} \otimes g^r. \end{aligned}$$
(5.2)

5.2. inc  $T_{rr}g^r \otimes g^r$ . Let us first compute the curl of  $T = T_{rr}g^r \otimes g^r$ , by using the formulation

$$\operatorname{Curl} \left( T_{ij}g^i \otimes g^j \right) = \nabla T_{ij} \times \left( g^i \otimes g^j \right) + T_{ij} \operatorname{Curl} \left( g^i \otimes g^j \right).$$

One has

$$\operatorname{Curl} T = \nabla T_{rr} \times (g^r \otimes g^r) + T_{rr} \operatorname{Curl} (g^r \otimes g^r) = -\frac{1}{r} \partial_{\phi} T_{rr} g^r \otimes g^{\theta} + \frac{1}{r \sin \phi} \partial_{\theta} T_{rr} g^r \otimes g^{\phi} - \frac{T_{rr}}{r} (g^{\phi} \otimes g^{\theta} - g^{\theta} \otimes g^{\phi}).$$
(5.3)

Hence

5.3. Complete expression of the incompatibility. Collecting (A.1) and all the computations of the Appendix, one arrives at the general formula.

$$(\operatorname{inc} T)_{rr} = -\frac{2T_{rr}}{r^2} + \left(\frac{\partial_{\theta}^2 T_{\phi\phi} + T_{\phi\phi}}{r^2 \sin \phi} - \frac{\partial_{\phi} T_{\phi\phi}}{r^2 \tan \phi} + \frac{\partial_r T_{\phi\phi}}{r} + \frac{2T_{\phi\phi}}{r^2}\right) + \left(\frac{\partial_{\phi}^2 T_{\theta\theta}}{r^2} + \frac{2\partial_{\phi} T_{\theta\theta}}{r^2 \tan \phi} + \frac{\partial_r T_{\theta\theta}}{r}\right) - \frac{2\partial_{\phi} \left(T_{r\phi} \sin \phi\right)}{r^2 \sin \phi} - \frac{2\partial_{\theta} T_{r\theta}}{r^2 \sin \phi} - \frac{2}{\sin \phi} \left(\frac{\partial_{\theta} \partial_{\phi} T_{\phi\theta}}{r^2} + \frac{\partial_{\theta} T_{\phi\theta}}{r^2 \tan \phi}\right),$$

$$(\operatorname{inc} T)_{\phi\phi} = -\left(\frac{\partial_r T_{rr}}{r} - \frac{\partial_{\phi} T_{rr}}{r^2 \tan \phi} - \frac{\partial_{\theta}^2 T_{rr}}{r^2 \sin^2 \phi}\right) + \left(\partial_r^2 T_{\theta\theta} + \frac{2\partial_r T_{\theta\theta}}{r}\right)$$

$$(5.5)$$

$$- \frac{4T_{r\phi}}{r^2 \tan \phi} - 2\left(\frac{\partial_{\theta} T_{r\phi}}{r^2 \sin \phi} + \frac{\partial_{\theta} \partial_r T_{r\theta}}{r \sin \phi}\right),\tag{5.6}$$

$$(\text{ inc } T)_{\theta\theta} = \left(\frac{\partial_{\phi}^2 T_{rr}}{r^2} - \frac{\partial_r T_{rr}}{r}\right) + \left(\partial_r^2 T_{\phi\phi} + \frac{2\partial_r T_{\phi\phi}}{r}\right) - 2\left(\frac{\partial_r \partial_{\phi} T_{r\phi}}{r} + \frac{\partial_{\phi} T_{r\phi}}{r^2}\right), \tag{5.7}$$

$$(\operatorname{inc} T)_{r\phi} = \frac{\partial_{\phi} I_{rr}}{r^{2}} + \frac{\partial_{r} I_{\phi\phi}}{r \tan \phi} - \left(\frac{\partial_{r} \partial_{\phi} I_{\theta\theta}}{r} + \frac{2\partial_{r} I_{\theta\theta}}{r \tan \phi}\right) - \left(\frac{\partial_{\theta} I_{r\phi}}{r^{2} \sin^{2} \phi} + \frac{2I_{r\phi}}{r^{2}}\right) + \frac{\partial_{\phi} (\partial_{\theta} T_{r\theta} \sin \phi)}{r^{2} \sin^{2} \phi} + \frac{\partial_{\phi} \partial_{r} T_{\phi\theta}}{r \sin \phi},$$
(5.8)

$$(\operatorname{inc} T)_{r\theta} = \frac{\partial_{\theta} T_{rr}}{r^{2} \sin \phi} - \frac{\partial_{r} \partial_{\theta} T_{\phi\phi}}{r \sin \phi} + \frac{1}{\sin \phi} \left( \frac{\partial_{\phi} \partial_{\theta} T_{r\phi}}{r^{2}} - \frac{\partial_{\theta} T_{r\phi}}{r^{2} \tan \phi} \right) - \left( \frac{\partial_{\phi} \left( \partial_{\phi} T_{r\theta} \sin \phi \right)}{r^{2} \sin^{2} \phi} + \frac{T_{r\theta}}{r^{2}} - \frac{T_{r\theta}}{r^{2} \tan^{2} \phi} \right) + \left( \frac{2\partial_{r} T_{\phi\theta}}{r \tan \phi} + \frac{\partial_{r} \partial_{\phi} T_{\phi\theta}}{r} \right),$$
(5.9)  
$$(\operatorname{inc} T)_{\phi\theta} = \frac{1}{r^{2} \sin \phi} \left( \frac{\partial_{\theta} T_{rr}}{\tan \phi} - \partial_{\theta} \partial_{\phi} T_{rr} \right) + \left( \frac{\partial_{r} \partial_{\theta} T_{r\phi}}{r \sin \phi} + \frac{\partial_{\theta} T_{r\phi}}{r^{2} \sin \phi} \right)$$

$$+ \left(\frac{\partial_r \partial_\phi T_{r\theta}}{r} - \frac{\partial_r T_{r\theta}}{r \tan \phi} - \frac{T_{r\theta}}{r^2 \tan \phi} + \frac{\partial_\phi T_{r\theta}}{r^2}\right) - \left(\partial_r^2 T_{\theta\phi} + \frac{2\partial_r T_{\phi\theta}}{r}\right).$$

#### 6. Concluding Remarks

In this note a method to compute the incompatibility operator in a system of curvilinear components/coordinates is proposed. Moreover an in-extenso expression of the incompatibility is given in the spherical system. It has been shown that the incompatibility of the elastic strain is directly linked to the dislocation density of a solid. Therefore our method will allow us, in a first step, to compute the energy related to dislocations in spherical inclusions. In a second step, to optimize the location of these inclusions in the body with a view to minimizing or maximizing certain cost functionals. This will be the purpose of future work. To conclude, a simple application of our full expression will be given.

Application: determining the dislocation-induced force in linearized elasticity. Recall the general form of second-order free energy  $\Psi := W_e(\epsilon) + \hat{W}_e(\operatorname{Curl}^t \epsilon, \operatorname{div} \epsilon) + \hat{W}_{\operatorname{defect}}(\kappa, \operatorname{Curl} \kappa, \operatorname{div} \kappa) + \overline{W}_{\operatorname{defect}}(\epsilon^0)$ . Let  $\varphi_e(u) = \int_{\Omega} W_e(\nabla u) dx$  and  $\varphi_{\operatorname{defect}}(F) = \int_{\Omega} \overline{W}_{\operatorname{defect}}(\operatorname{inc} F) dx$ . The Fréchet derivative of  $\varphi_e$  at u in the direction v reads  $D\varphi_e(u)[v] = \int_{\Omega} \mathbb{A} \nabla u \nabla v dx = -\int \operatorname{div} (\mathbb{A} \nabla u) \cdot v dx$ , that is, the differential  $\varphi'_e(u) := D\varphi_e(u) = f$ , by Riesz theorem. Also,  $D\varphi_{\operatorname{defect}}(F)[V] = \int_{\Omega} \operatorname{inc} \overline{W}'_{\operatorname{defect}}(\operatorname{inc} F) \cdot V dx$  and we set  $\mathbb{G} := \varphi'_{\operatorname{defect}}(F) = \operatorname{inc} \overline{W}'_{\operatorname{defect}}(\operatorname{inc} F)$  which is symmetric and divergence free. Assume also that  $\mathbb{G}$  is independent of  $\epsilon^0$ . Now we would like to solve (2.8) with  $\Omega$  the unit sphere, in the simplified case where  $\mathbb{A} = \alpha \mathbb{I}_4$ , and taking  $\mathbb{G} = g^\theta \otimes g^\theta$ , that is, we seek F such that inc  $(\alpha \operatorname{inc} F) = g^\theta \otimes g^\theta$ .

such that inc  $(\alpha \operatorname{inc} F) = g^{\theta} \otimes g^{\theta}$ . The solution of inc  $T = g^{\theta} \otimes g^{\theta}$  is found by (5.7) as  $T(r)g^r \otimes g^r$  with  $T(r) = -\frac{1}{2}r^2 + c$ . Moreover, by (5.5)  $F = F(r)g^r \otimes g^r$  is a solution with  $F(r) = \frac{1}{4\alpha}r^4 - \frac{c}{2\alpha}r^2$ . Uniqueness is obtained by imposing the natural homogeneous Dirichlet conditions  $F = \operatorname{Curl}^{\mathsf{t}} F \times N = 0$  on  $\partial\Omega$ , i.e., at r = 1, that is, for c = 1/2. Thus  $\epsilon^0 = -\frac{1}{2\alpha}(r^2 - 1)g^r \otimes g^r$ . Now the displacement u is obtained by solving  $-\operatorname{div}(\mathbb{A}\nabla u) = f + \operatorname{div}(\mathbb{A}\epsilon^0)$ , where  $\operatorname{div}(\mathbb{A}\epsilon^0) = -(2r - \frac{1}{r})g^r$  is a radial force due to the presence of dislocations.

#### NICOLAS VAN GOETHEM

# Appendix A. Other terms of the incompatibility

A.1. inc  $T_{\phi\phi}g^{\phi} \otimes g^{\phi}$ . Let us compute the curl of  $T = T_{\phi\phi}g^{\phi} \otimes g^{\phi}$ . One has

$$\operatorname{Curl} T = \nabla T_{\phi\phi} \times (g^{\phi} \otimes g^{\phi}) + T_{\phi\phi} \operatorname{Curl} (g^{\phi} \otimes g^{\phi}) \\ = \partial_r T_{\phi\phi} g^{\phi} \otimes g^{\theta} - \frac{1}{r \sin \phi} \partial_{\theta} T_{\phi\phi} g^{\phi} \otimes g^r + \frac{T_{\phi\phi}}{r} (g^{\phi} \otimes g^{\theta} - \frac{1}{\tan \phi} g^{\theta} \otimes g^r).$$

Hence

$$\begin{aligned} \text{Curl Curl}^{t} T &= \nabla(\partial_{r}T_{\phi\phi}) \times (g^{\theta} \otimes g^{\phi}) - \nabla(\frac{\partial_{\theta}T_{\phi\phi}}{r\sin\phi}) \times (g^{r} \otimes g^{\phi}) + \nabla\left(\frac{T_{\phi\phi}}{r}\right) \times (g^{\theta} \otimes g^{\phi}) \\ &- \nabla\left(\frac{T_{\phi\phi}}{r\tan\phi}\right) \times (g^{r} \otimes g^{\theta}) \\ &+ \partial_{r}T_{\phi\phi} \text{Curl } (g^{\theta} \otimes g^{\phi}) - \frac{\partial_{\theta}T_{\phi\phi}}{r\sin\phi} \text{Curl } (g^{r} \otimes g^{\phi}) \\ &+ \frac{T_{\phi\phi}}{r} \text{Curl } (g^{\theta} \otimes g^{\phi} - \frac{1}{\tan\phi}g^{r} \otimes g^{\theta}) \\ &\text{inc } T &= \left(\frac{\partial_{\theta}^{2}T_{\phi\phi} + T_{\phi\phi}}{r^{2}\sin\phi} - \frac{\partial_{\phi}T_{\phi\phi}}{r^{2}\tan\phi} + \frac{\partial_{r}T_{\phi\phi}}{r} + \frac{2T_{\phi\phi}}{r^{2}}\right) g^{r} \otimes g^{r} + (\partial_{r}^{2}T_{\phi\phi} + \frac{2\partial_{r}T_{\phi\phi}}{r})g^{\theta} \otimes g^{\theta} \\ &+ \frac{2\partial_{r}T_{\phi\phi}}{r\tan\phi}g^{r} \odot g^{\phi} - \frac{2\partial_{r}\partial_{\theta}T_{\phi\phi}}{r\sin\phi}g^{r} \odot g^{\theta}. \end{aligned}$$
(A.1)

A.2. inc  $T_{\theta\theta}g^{\theta} \otimes g^{\theta}$ . Let us compute the curl of  $T = T_{\theta\theta}g^{\theta} \otimes g^{\theta}$ . One has

$$\operatorname{Curl} T = \nabla T_{\theta\theta} \times (g^{\theta} \otimes g^{\theta}) + T_{\theta\theta} \operatorname{Curl} (g^{\theta} \otimes g^{\theta}) \\ = -\partial_r T_{\theta\theta} g^{\theta} \otimes g^{\phi} + \frac{\partial_{\theta} T_{\theta\theta}}{r} g^{\theta} \otimes g^r + \frac{T_{\theta\theta}}{r} (\frac{1}{\tan \phi} g^{\theta} \otimes g^r - g^{\theta} \otimes g^{\phi}).$$

Hence

$$\begin{aligned} \text{Curl Curl}^{\text{t}} T &= -\nabla(\partial_{r}T_{\theta\theta}) \times (g^{\phi} \otimes g^{\theta}) + \nabla(\frac{\partial_{\phi}T_{\theta\theta}}{r}) \times (g^{r} \otimes g^{\theta}) + \nabla(\frac{T_{\theta\theta}}{r}) \times (\frac{1}{\tan\phi}g^{r} \otimes g^{\theta} - g^{\phi} \otimes g^{\theta}) \\ &- \partial_{r}T_{\theta\theta} \operatorname{Curl} (g^{\phi} \otimes g^{\theta}) + \frac{\partial_{\phi}T_{\theta\theta}}{r} \operatorname{Curl} (g^{r} \otimes g^{\theta}) + \frac{T_{\theta\theta}}{r} \operatorname{Curl} (\frac{1}{\tan\phi}g^{r} \otimes g^{\theta} - g^{\phi} \otimes g^{\theta}) \\ &\text{inc } T &= \left(\frac{\partial_{\phi}^{2}T_{\theta\theta}}{r^{2}} + \frac{2\partial_{\phi}T_{\theta\theta}}{r^{2}\tan\phi} + \frac{\partial_{r}T_{\theta\theta}}{r}\right)g^{r} \otimes g^{r} + (\partial_{r}^{2}T_{\theta\theta} + \frac{2\partial_{r}T_{\theta\theta}}{r})g^{\phi} \otimes g^{\phi} \\ &- 2\left(\frac{\partial_{r}\partial_{\phi}T_{\theta\theta}}{r} + \frac{2\partial_{r}T_{\theta\theta}}{r\tan\phi}\right)g^{r} \odot g^{\phi}.\end{aligned}$$

A.3. inc  $2T_{r\phi}g^r \odot g^{\phi}$ . Let us compute the curl of  $T = 2T_{r\phi}g^r \odot g^{\phi}$ . One has

$$\begin{aligned} \operatorname{Curl} T &= 2\nabla T_{r\phi} \times (g^r \odot g^{\phi}) + 2T_{r\phi} \operatorname{Curl} (g^r \odot g^{\phi}) \\ &= \partial_r T_{r\phi} g^r \otimes g^{\theta} + \frac{\partial_{\phi} T_{r\phi}}{r} g^{\phi} \otimes g^{\theta} - \frac{\partial_{\theta} T_{r\phi}}{r \sin \phi} g^r \otimes g^r + \frac{\partial_{\theta} T_{r\phi}}{r \sin \phi} g^{\phi} \otimes g^{\phi}) \\ &+ \frac{T_{r\phi}}{r} (2g^r \otimes g^{\theta} - g^{\theta} \otimes g^r + \frac{1}{\tan \phi} g^{\theta} \otimes g^{\phi}). \end{aligned}$$

Hence

$$\begin{aligned} \text{Curl Curl}^{\text{t}} T &= \nabla(\partial_r T_{r\phi}) \times (g^{\theta} \otimes g^r) - \nabla(\frac{\partial_{\phi} T_{r\phi}}{r}) \times (g^{\theta} \otimes g^{\phi}) - \nabla(\frac{\partial_{\theta} T_{r\phi}}{r \sin \phi}) \times (g^r \otimes g^r) \\ &+ \nabla(\frac{\partial_{\theta} T_{r\phi}}{r \sin \phi}) \times (g^{\phi} \otimes g^{\phi}) + 2\nabla(\frac{T_{r\phi}}{r}) \times (g^{\theta} \otimes g^r) - \nabla(\frac{T_{r\phi}}{r}) \times (g^r \otimes g^{\theta}) \\ &+ \nabla(\frac{T_{r\phi}}{r \tan \phi}) \times (g^{\phi} \otimes g^{\theta}) \\ &+ \partial_r T_{r\phi} \text{Curl } (g^{\theta} \otimes g^r) - \frac{\partial_{\phi} T_{r\phi}}{r} \text{Curl } (g^{\theta} \otimes g^{\phi}) - \frac{\partial_{\theta} T_{r\phi}}{r \sin \phi} \text{Curl } (g^r \otimes g^r) \\ &+ \frac{\partial_{\theta} T_{r\phi}}{r \sin \phi} \text{Curl } (g^{\phi} \otimes g^{\phi}) + \frac{T_{r\phi}}{r} \text{Curl } (2g^{\theta} \otimes g^r - g^r \otimes g^{\theta} + \frac{1}{\tan \phi} g^{\phi} \otimes g^{\theta}) \\ &\text{inc } T &= -2\left(\frac{\partial_{\phi} T_{r\phi}}{r^2} + \frac{T_{r\phi}}{r^2 \tan \phi}\right) g^r \otimes g^r - \frac{4T_{r\phi}}{r^2 \tan \phi} g^{\phi} \otimes g^{\phi} \\ &- 2\left(\frac{\partial_{r} \partial_{\phi} T_{r\phi}}{r} + \frac{\partial_{\phi} T_{r\phi}}{r^2}\right) g^{\theta} \otimes g^{\theta} - 2\left(\frac{\partial_{\theta}^2 T_{r\phi}}{r^2 \sin^2 \phi} + \frac{2T_{r\phi}}{r^2}\right) g^r \odot g^{\phi} \\ &+ 2\left(\frac{\partial_{\phi} \partial_{\theta} T_{r\phi}}{r^2 \sin \phi} - \frac{\partial_{\theta} T_{r\phi}}{r^2 \sin \phi \tan \phi}\right) g^r \odot g^{\theta} + 2\left(\frac{\partial_r \partial_{\theta} T_{r\phi}}{r \sin \phi} + \frac{\partial_{\theta} T_{r\phi}}{r^2 \sin \phi}\right) g^{\phi} \odot g^{\theta}. \end{aligned}$$

A.4. inc  $2T_{r\theta}g^r \odot g^{\theta}$ . Let us compute the curl of  $T = 2T_{r\theta}g^r \odot g^{\theta}$ . One has Curl  $T = 2\nabla T_{r\theta} \times (g^r \odot g^{\theta}) + 2T_{r\theta} \operatorname{Curl} (g^r \odot g^{\theta})$ 

$$\begin{aligned} \operatorname{Curl} T &= 2\nabla T_{r\theta} \times (g^r \odot g^{\theta}) + 2T_{r\theta} \operatorname{Curl} (g^r \odot g^{\theta}) \\ &= -\partial_r T_{r\theta} g^r \otimes g^{\phi} + \frac{\partial_{\phi} T_{r\theta}}{r} (g^r \otimes g^r - g^{\theta} \otimes g^{\theta}) + \frac{\partial_{\theta} T_{r\theta}}{r \sin \phi} g^{\theta} \otimes g^{\phi} \\ &+ \frac{T_{r\theta}}{r} \left( g^{\phi} \otimes g^r - 2g^r \otimes g^{\phi} + \frac{1}{\tan \phi} (g^r \otimes g^r - g^{\phi} \otimes g^{\phi}) \right). \end{aligned}$$

Hence

$$\begin{aligned} \text{Curl Curl}^{\mathsf{t}} T &= -\nabla(\partial_r T_{r\theta}) \times (g^{\phi} \otimes g^r) + \nabla(\frac{\partial_{\phi} T_{r\theta}}{r}) \times (g^r \otimes g^r - g^{\theta} \otimes g^{\theta}) + \nabla(\frac{\partial_{\theta} T_{r\theta}}{r \sin \phi}) \times (g^{\phi} \otimes g^{\theta}) \\ &+ \nabla(\frac{T_{r\theta}}{r}) \times \left(g^r \otimes g^{\phi} - 2g^{\phi} \otimes g^r + \frac{1}{\tan \phi}(g^r \otimes g^r - g^{\phi} \otimes g^{\phi})\right) \\ &- \partial_r T_{r\theta} \text{Curl } (g^{\phi} \otimes g^r) + \frac{\partial_{\phi} T_{r\theta}}{r} \text{Curl } (g^r \otimes g^r - g^{\theta} \otimes g^{\theta}) + \frac{\partial_{\theta} T_{r\theta}}{r \sin \phi} \text{Curl } (g^{\phi} \otimes g^{\theta}) \\ &+ \frac{T_{r\theta}}{r} \text{Curl } \left(g^r \otimes g^{\phi} - 2g^{\phi} \otimes g^r + \frac{1}{\tan \phi}(g^r \otimes g^r - g^{\phi} \otimes g^{\phi})\right) \\ &\text{inc } T &= -\frac{2\partial_{\theta} T_{r\theta}}{r^2 \sin \phi} g^r \otimes g^r - 2\left(\frac{\partial_{\theta} T_{r\phi}}{r^2 \sin \phi} + \frac{\partial_{\theta} \partial_r T_{r\theta}}{r \sin \phi}\right) g^{\phi} \otimes g^{\phi} \\ &+ \frac{2}{\sin \phi} \left(\frac{\partial_{\phi} \partial_{\theta} T_{r\theta}}{r^2} + \frac{\partial_{\theta} T_{r\theta}}{r^2 \tan \phi}\right) g^r \odot g^{\phi} \\ &- 2\left(\frac{\partial_r^2 T_{r\theta}}{r^2} + \frac{T_{r\theta}}{r^2} - \frac{T_{r\theta}}{r^2 \tan^2 \phi} + \frac{\partial_{\phi} T_{r\phi}}{r^2 \tan \phi}\right) g^{\phi} \odot g^{\theta} \\ &+ 2\left(\frac{\partial_r \partial_{\phi} T_{r\theta}}{r} - \frac{\partial_r T_{r\theta}}{r \tan \phi} - \frac{T_{r\theta}}{r^2 \tan \phi} + \frac{\partial_{\phi} T_{r\theta}}{r^2}\right) g^{\phi} \odot g^{\theta}. \end{aligned}$$

A.5. inc  $2T_{\phi\theta}g^{\phi} \odot g^{\theta}$ . Let us compute the curl of  $T = 2T_{\phi\theta}g^{\phi} \odot g^{\theta}$ . One has

$$\operatorname{Curl} T = 2\nabla T_{\phi\theta} \times (g^{\phi} \odot g^{\theta}) + 2T_{\phi\theta} \operatorname{Curl} (g^{\phi} \odot g^{\theta}) = \partial_r T_{\phi\theta} (g^{\theta} \otimes g^{\theta} - g^{\phi} \otimes g^{\phi}) + \frac{\partial_{\phi} T_{\phi\theta}}{r} g^{\phi} \otimes g^r - \frac{\partial_{\theta} T_{\theta\phi}}{r \sin \phi} g^{\theta} \otimes g^r + \frac{T_{\phi\theta}}{r} \left( g^{\theta} \otimes g^{\theta} - g^{\phi} \otimes g^{\phi} + \frac{2}{\tan \phi} g^{\phi} \otimes g^r \right).$$
(A.2)

Hence

$$\begin{aligned} \text{Curl Curl} \ T &= \nabla(\partial_r T_{\phi\theta}) \times (g^{\theta} \otimes g^{\theta} - g^{\phi} \otimes g^{\phi}) + \nabla(\frac{\partial_{\phi} T_{\phi\theta}}{r}) \times (g^r \otimes g^{\phi}) - \nabla(\frac{\partial_{\theta} T_{\phi\theta}}{r \sin \phi}) \times (g^r \otimes g^{\phi}) \\ &+ \nabla(\frac{T_{\phi\theta}}{r}) \times \left(g^{\theta} \otimes g^{\theta} - g^{\phi} \otimes g^{\phi} + \frac{2}{\tan \phi}g^r \otimes g^{\phi}\right) \\ &+ \partial_r T_{\phi\theta} \text{Curl } (g^{\theta} \otimes g^{\theta} - g^{\phi} \otimes g^{\phi}) + \frac{\partial_{\phi} T_{\phi\theta}}{r} \text{Curl } (g^r \otimes g^{\phi}) - \frac{\partial_{\theta} T_{\phi\theta}}{r \sin \phi} \text{Curl } (g^r \otimes g^{\theta}) \\ &+ \frac{T_{\phi\theta}}{r} \text{Curl } \left(g^{\theta} \otimes g^{\theta} - g^{\phi} \otimes g^{\phi} + \frac{2}{\tan \phi}g^r \otimes g^{\phi}\right) \\ &\text{inc } T &= -\frac{2}{\sin \phi} \left(\frac{\partial_{\theta} \partial_{\phi} T_{\phi\theta}}{r^2} + \frac{\partial_{\theta} T_{\phi\theta}}{r^2 \tan \phi}\right) g^r \otimes g^r + 2\frac{\partial_{\phi} \partial_r T_{\phi\theta}}{r \sin \phi}g^r \odot g^{\phi} \\ &+ 2\left(\frac{2\partial_r T_{\phi\theta}}{r \tan \phi} + \frac{\partial_r \partial_{\phi} T_{\phi\theta}}{r}\right) g^r \odot g^{\theta} - 2\left(\partial_r^2 T_{\theta\phi} + \frac{2\partial_r T_{\phi\theta}}{r}\right) g^{\phi} \odot g^{\theta}. \end{aligned}$$

#### References

- S. Amstutz and N. Van Goethem. Analysis of the incompatibility operator and application in intrinsic elasticity with dislocations. SIAM J. Math. Anal., 2016.
- [2] P. G. Ciarlet. An introduction to differential geometry with applications to elasticity. J. Elasticity, 78-79(1-3):3–201, 2005.
- [3] M. C. Delfour and J.-P. Zolésio. Shapes and geometries, volume 4 of Advances in Design and Control. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2001. Analysis, differential calculus, and optimization.
- B. A. Dubrovin, A. T. Fomenko, and S. P. Novikov. Modern geometry methods and applications, Part 1 (2nd edn). Cambridge studies in advanced mathematics. Springer-Verlag, New-York, 1992.
- [5] A. Hoger and B. E. Johnson. Linear elasticity for constrained materials: Incompressibility. J. Elasticity, 38(1):69-93, 1995.
- [6] E. Kröner. Continuum theory of defects. In R. Balian, editor, Physiques des défauts, Les Houches session XXXV (Course 3). North-Holland, Amsterdam, 1980.
- [7] G. Maggiani, R. Scala, and N. Van Goethem. A compatible-incompatible decomposition of symmetric tensors in L<sup>p</sup> with application to elasticity. *Math. Meth. Appl. Sci*, 38(18):5217–5230, 2015.
- [8] L.E. Malvern. Introduction to the mechanics of a continuous medium. Prentice-Hall series in engineering of the physical sciences. Prentice-Hall, 1969.
- [9] R. Scala and N. Van Goethem. Dislocations at the continuum scale: functional setting and variational properties. (preprint: www.cvgmt.it), 2014.
- [10] N. Van Goethem. Fields of bounded deformation for mesoscopic dislocations. Math. Mech. Solids, 19(5):579–600, 2014.
- [11] N. Van Goethem. Incompatibility-governed singularities in linear elasticity with dislocations. *Math. Mech. Solids*, page (to appear), 2016.
- [12] N. Van Goethem, A. de Potter, N. Van den Bogaert, and F. Dupret. Dynamic prediction of point defects in Czochralski silicon growth. An attempt to reconcile experimental defect diffusion coefficients with the V/G criterion. J. Phys. Chem. Solids, 69:320–324, 2008.
- [13] N. Van Goethem and F. Dupret. A distributional approach to 2D Volterra dislocations at the continuum scale. Europ. Jnl. Appl. Math., 23(3):417–439, 2012.

UNIVERSIDADE DE LISBOA, FACULDADE DE CIÊNCIAS, DEPARTAMENTO DE MATEMÁTICA, CMAF+CIO, ALAMEDA DA UNIVERSI-DADE, C6, 1749-016 LISBOA, PORTUGAL

E-mail address: vangoeth@fc.ul.pt

12