

## Macro-homogeneous strain fields with arbitrary local inhomogeneity

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FIRST, HILL'S analysis of the macro-homogeneity of the stress and strain fields in an inhomogeneous continuum is reviewed and extended. It is examined which precise requirements must be satisfied by the fluctuating part of the displacement field. The macro-homogeneity conditions are extended to aggregates with spatial correlations. Then, a general construction of macro-homogeneous strain fields is proposed in a general aggregate, which enables accounting for unrestricted local inhomogeneity: arbitrary volume averages of the strain field may be imposed uniformly inside the constituents, provided their distribution has one well-defined volume and linear macro-average. This throws some new light on the classical "compatibility problem", which the models for deformed aggregates have to deal with. Whereas this problem is shown to have no solution when piecewise uniform fields are considered, it thus has always one in the sense of the local volume average. However, the obtained strain fields fluctuate with an unknown amplitude, increasing with inhomogeneity of the imposed strain distribution. It is concluded that the models for deformed aggregates should be interpreted in a statistical sense.

Na wstępie omówiono i rozszerzono uzyskane przez Hilla wyniki dotyczące analizy makrojednorodności pól naprężeń i odkształceń w ośrodku niejednorodnym. Ustalono ściśle warunki jakie spełniać muszą podlegające fluktuacjom składowe pola przemieszczenia. Warunki makrojednorodności rozszerzono na przypadek agregatów o korelacjach przestrzennych. Zaproponowano następnie ogólne zasady konstrukcji makrojednorodnych pól odkształceń w agregatach, pozwalające względnie niejednorodność lokalną. Rozważania te rzucają nowe światło na klasyczny problem „warunków nierozdzielności”, które spełnić muszą modele odkształconego agregatu. Stwierdzono, że problem ten jest nierozwiązalny w przypadku pól odcinkami jednorodnych, ma jednak zawsze rozwiązanie w sensie lokalnych średnich objętościowych. Otrzymane w ten sposób pola podlegają fluktuacjom o nieznanym amplitudzie, wzrastającej wraz z niejednorodnością przyjętego rozkładu odkształceń. Stwierdzono, że modele odkształconych agregatów należy interpretować w sensie statystycznym.

Во введении обсуждены и расширены, полученные Хиллом, результаты, касающиеся анализа макроодностей полей напряжений и деформаций в неоднородной среде. Установлены точные условия каким должны удовлетворять подлежащие флуктуациям составляющие поля перемещений. Условия макроодности расширены на случай агрегатов с пространственными корреляциями. Затем предложены общие принципы конструкции макроодных полей деформаций в агрегатах, позволяющие учитывать локальную неоднородность. Эти рассуждения бросают новый свет на классическую проблему „условий нераздельности”, которым должны удовлетворять модели деформируемого агрегата. Констатируется, что проблема нерешаемая в случае полей отрезками однородных, имеет однако всегда решение в смысле локальных объемных средних. Полученные таким образом поля подлежат флуктуациям с неизвестной амплитудой, возрастающей совместно с неоднородностью принятого распределения деформаций. Констатируется, что модели деформируемых агрегатов следует интерпретировать в статистическом смысле.

## Introduction

IN CONTINUUM physics of inhomogeneous media, it is often necessary to consider the material at different scales. The most important thing is of course to specify the "macroscopic" scale, which is the directly relevant one for discussing the effect of systematic variations in the external solicitations. However, one wants to study the influence of "local" inhomogeneities, the size of which is small compared with the macroscopic size. In order to do that within the framework of continuum physics, one must introduce an even smaller scale: the "microscopic" one, where the material is still assumed to behave as a continuum; in that way, fields can be defined and studied within the microstructural elements constituting the local inhomogeneities. Whereas this procedure is rigorously applied in the homogenization theory for periodic media (SANCHEZ-PALENCIA [27], SUQUET [28]), it is sometimes overlooked in the models for random media, especially those for aggregates such as polycrystals. When discussing models for deformed polycrystals, "microscopic" strains and stresses are often referred to, but it is not always clear whether this designates a mean value of the corresponding field in one constituent crystal or the value of this field at one particular point. One result of the analysis presented here is that the "microscopic" stresses and strains which are predicted by the polycrystal models can not be considered as local values of these fields, and even are difficult to regard as true volume averages of the fields in individual constituents. Rather, these predicted values should be interpreted in a statistical sense, as outlined in the earlier work on the self-consistent model (KRÖNER [20], HILL [13]) or in the generalization [1] of the "relaxed Taylor theory" [16, 19, 26, 29]; this interpretation is more or less implicit in more recent self-consistent approaches of BERVEILLER and ZAOUÏ [5], IWAKUMA and NEMAT-NASSER [18], MOLINARI *et al.* [24], LIPÍŃSKI *et al.* [22].

In this paper we focus on the direct definition of the inhomogeneous distributions, i.e. on the fields and their mean values in the geometrically defined constituents. Specifically, a general construction of strain fields in a random aggregate is presented; this construction allows to obtain macro-homogeneous strain fields having an almost unrestricted local inhomogeneity, in the sense that the distribution of the mean strains in the constituents is only assigned to satisfy an asymptotic condition of statistical homogeneity, without any restriction to the individual values. For the purpose, the Hill macro-homogeneity condition is first discussed and extended. In short, the Hill or Hill-Mandel condition [14, 15, 23] means that the displacement field fluctuates about a linear mean field with a bounded amplitude and a small pseudo-period. It will be shown that these two conditions are not exactly necessary, and indeed cannot be met in a general aggregate where spatial correlations can exist.

The second step is the construction of compatible strain (rate) fields whose mean values in the contiguous constituents of a bounded aggregate are prescribed. The principle of the construction is simple, but leads to an irregular velocity field, only defined on the faces of a cubic lattice (similar displacement fields have been introduced by HAVNER [12] in a particular case). It is really necessary to regularize and to extend this field for obtaining a meaningful construction, but the quite technical procedure is left to appendices. Our analysis is presented in terms of velocities, i.e. a velocity field is built whose unsymmetrical gradient tensor (strain rate *plus spin*, in fact) has prescribed mean values. The macro-homogeneous character of the obtained strain rate and spin field (for statistically homogeneous distributions of its mean values) is most easily seen in a space-filling aggregate, in view of the asymptotic nature of the macrohomogeneity condition. However, the obtainable approximation in a real, bounded aggregate is also given. Finally, the possibility of fulfilling a macro-homogeneity condition separately inside each constituent, or "meso-homogeneity" (the mean value of the gradient fields differing from one constituent to another) is examined. Such a possibility would allow to consider that the discretization operated in the models of deformed polycrystals does correspond to the separation of the polycrystal into homogeneous crystals, thus capturing the very idea of a polycrystal.

In most parts of the paper, the velocity field may be replaced by a vector field of an arbitrary nature and the corresponding gradient. To remain with deformed aggregates, the displacement field and the corresponding finite transformation gradient may be substituted, as in [12] and [15].

## 2. The macro-homogeneity condition for a strain field

### 2.1. The no-correlation condition

In a fundamental study of the extremum principles governing crystal plasticity and their transmission from the crystal level up to the macroscopic one, BISHOP and HILL [6] assumed that, in addition to have well-defined macroscopic volume averages  $\bar{\sigma}$  and  $\bar{\mathbf{D}}$ , the microscopic fields of stress and strain-rate  $\sigma$  and  $\mathbf{D}$  have no macroscopic correlation: this condition ensures the upwards transmission of the principles. Let us note that the virtual work equation does in fact imply this condition for truly macro-homogeneous fields; while the left-hand side of the "no-correlation condition",

$$(2.1) \quad \overline{\sigma : \mathbf{D}} = \bar{\sigma} : \bar{\mathbf{D}}$$

is the macroscopic rate of work per unit volume, as expressed in terms of the microscopic fields, the right one is the same in terms of the macroscopic fields. This justification of Eq. (2.1) is also valid for non-associated stress and strain-rate fields. It is assumed that the fields  $\boldsymbol{\sigma}$  and  $\mathbf{D}$  are homogeneous at the macro-level, i.e. that the volume averages  $\overline{\boldsymbol{\sigma}}^\Omega$  and  $\overline{\mathbf{D}}^\Omega$  are independent of the macro-element  $\Omega$  in which they are taken: in that case, one may consider  $\overline{\boldsymbol{\sigma}}$  and  $\overline{\mathbf{D}}$  in Eq. (2.1) as uniform fields, well-defined at the macroscopic level. In the same way, the microscopic fields  $\boldsymbol{\sigma}$  and  $\mathbf{D}$  have a sense above a certain scale only, i.e. they also are averaged upon certain "micro-elements" but they do depend on the position of the micro-element. The necessity of condition (2.1) has been stated in a neighbouring way by KRÖNER [21], in connection with the assumed existence of a macroscopic behaviour.

## 2.2. Hill's analysis

Since the macroscopic fields are volume averages of their microscopic counterparts which are inhomogeneous, the macroscopic homogeneity cannot be exact. It should rather be defined as an asymptotic property of the microscopic fields and the no-correlation condition should be deduced from this property. Using the classical transformation of the volume integral of  $\boldsymbol{\sigma} : \mathbf{D}$  into a surface integral, HILL [14] formulated sufficient conditions which the microscopic fields  $\boldsymbol{\sigma}$  and  $\mathbf{D}$  should satisfy in order that they have well-defined macro-averages and fulfil the condition (2.1). Later on, HILL [15] extended his analysis to a pair of unsymmetrical tensors, namely the nominal stress  $\mathbf{N}$  and the transformation gradient. Equivalently, this analysis is here reviewed in rate form. Thus we introduce a (microscopic) velocity field  $\mathbf{V}$  with gradient tensor  $\mathbf{L} = \nabla \mathbf{V}$  and an unsymmetrical tensor field  $\mathbf{T}$  satisfying the equilibrium condition  $\text{div } \mathbf{T} = \mathbf{0}$ ; this could be the material derivative of the transpose  ${}^t\mathbf{N}$ , as in [12] and [18]. The divergence theorem implies:

$$(2.2) \quad \int_{\Omega} \mathbf{T} \cdot {}^t\mathbf{L} \, dv = \int_{\partial\Omega} (\mathbf{T} \cdot \mathbf{n}) \otimes \mathbf{V} \, d\mathcal{S}.$$

The volume averages  $\overline{\mathbf{T}}^\Omega$  and  $\overline{\mathbf{L}}^\Omega$  in the macro-element  $\Omega$  satisfy the relation

$$\overline{(\mathbf{T} - \overline{\mathbf{T}}^\Omega) \cdot {}^t(\mathbf{L} - \overline{\mathbf{L}}^\Omega)}^\Omega = \overline{\mathbf{T} \cdot {}^t\mathbf{L}}^\Omega - \overline{\mathbf{T}}^\Omega \cdot {}^t\overline{\mathbf{L}}^\Omega$$

whence, by applying Eq. (2.2) to  $\mathbf{T} - \overline{\mathbf{T}}^\Omega$  and  $\mathbf{V} - \overline{\mathbf{L}}^\Omega \cdot \mathbf{x}$ :

$$(2.3) \quad \overline{\mathbf{T} \cdot {}^t\mathbf{L}}^\Omega - \overline{\mathbf{T}}^\Omega \cdot {}^t\overline{\mathbf{L}}^\Omega = \frac{1}{v(\Omega)} \int_{\partial\Omega} [(\mathbf{T} - \overline{\mathbf{T}}^\Omega) \cdot \mathbf{n}] \otimes (\mathbf{V} - \overline{\mathbf{L}}^\Omega \cdot \mathbf{x}) \, d\mathcal{S}(\mathbf{x}).$$

Hence, the "tensor" correlation of the tensor products is expressed in terms of the non-uniform part of the surface data: stress vector and velocity field [15]. The trace of the tensor products (2.3) gives the "scalar" correlation:

$$(2.4) \quad \Delta_{\Omega} = \overline{\mathbf{T}:\mathbf{L}^{\Omega}} - \overline{\mathbf{T}}^{\Omega}:\overline{\mathbf{L}}^{\Omega} = \frac{1}{v(\Omega)} \int_{\partial\Omega} [(\mathbf{T} - \overline{\mathbf{T}}^{\Omega}) \cdot \mathbf{n}] \cdot (\mathbf{V} - \overline{\mathbf{L}}^{\Omega} \cdot \mathbf{x}) d\mathcal{S}(\mathbf{x}).$$

The right-hand side of Eq. (2.4) is not changed if one surface field is substituted to its non-uniform part, because this latter has nil average [15]:

$$(2.5) \quad \Delta_{\Omega} = \frac{1}{v(\Omega)} \int_{\partial\Omega} (\mathbf{T} \cdot \mathbf{n}) \cdot (\mathbf{V} - \overline{\mathbf{L}}^{\Omega} \cdot \mathbf{x}) d\mathcal{S}(\mathbf{x}) = \frac{1}{v(\Omega)} \int_{\partial\Omega} [(\mathbf{T} - \overline{\mathbf{T}}^{\Omega}) \cdot \mathbf{n}] \cdot \mathbf{V} d\mathcal{S}.$$

Here, Hill introduces the notions of micro-uniform (surface) data (such that the non-uniform part identically vanishes) and macro-uniform data, (such that the non-uniform part is *bounded* and fluctuates randomly about 0 with a pseudo-period of order  $d$ , the order of magnitude of the linear heterogeneity, e.g. the typical grain size). If one of the surface data, e.g. the velocity field, is micro-uniform, then  $\Delta_{\Omega} = 0$ , by Eq. (2.5). A more realistic situation is also considered, in which one only knows that one of the surface data is macro-uniform. If the *velocity field* is so, the first integral in Eq. (2.5) shows that for a bounded field  $\mathbf{T}$ ,  $\Delta_{\Omega}$  is  $O(R^2)/R^3 = O(1/R)$  where  $R = R(\Omega)$  is the size of the macro-element  $\Omega$ , assumed cubic. Thus  $\Delta_{\Omega}$  becomes negligible if  $R$  is sufficiently large, but it seems difficult to understand the statement of HILL [14] that the small size  $d$  should intervene directly, in an upper bound of Eq. (2.5). Moreover, this way of reasoning cannot be used if the *stress vector* is known to be macro-uniform. In [15] the essential role is played by a "boundary layer argument" according to which the effect of the non-uniformity of the surface data decays with depth and is negligible beyond a layer a few wavelengths thick: thus, except in a volume of order  $R^2d$ , the analysis for micro-uniform data would be applicable to macro-uniform data. Clearly, this argument refers to the mechanical behaviour and for this reason might be more or less valid, depending on the particular material and boundary conditions (Hill emphasizes the case of an elastic material and the extension to highly nonlinear behaviour is not straightforward). Hereafter, no relation between  $\mathbf{T}$  and  $\mathbf{L}$  is assumed; Hill's reasoning for a macro-uniform  $\mathbf{V}$  is extended, and the role of the fluctuation distance  $d$  is clarified.

### 2.3. Amplitude and characteristic distance of the fluctuation

The way in which the deviation  $\Delta_\Omega$  was proved to decay with the increasing size  $R(\Omega)$  for a "macro-uniform" velocity field, remains valid if  $\mathbf{V}$  is more generally assumed to have the form:

$$(2.6) \quad \mathbf{V}(\mathbf{x}) = \mathbf{L}_0 \cdot \mathbf{x} + \mathbf{u}(\mathbf{x}), \quad \mathbf{L}(\mathbf{x}) = \mathbf{L}_0 + \nabla \mathbf{u}(\mathbf{x}),$$

where the nonlinear part  $\mathbf{u}$  may be *unbounded*, but satisfies

$$(2.7) \quad \frac{1}{v(\Omega)} \int_{\partial\Omega} \|\mathbf{u}\| d\mathcal{S} \rightarrow 0, \quad R(\Omega) \rightarrow \infty$$

(in a real, bounded observation domain, the quantity in relations (2.7) should become negligible, when  $\Omega$  is the largest possible, as compared with  $\|\mathbf{L}_0\|$ ). To see this, we first deduce from relations (2.6) and (2.7) that

$$(2.8) \quad \bar{\mathbf{L}}^\Omega = \frac{1}{v(\Omega)} \int_{\Omega} \mathbf{L} dv \rightarrow \mathbf{L}_0, \quad R(\Omega) \rightarrow \infty,$$

since formula (2.2) yields for  $\mathbf{T} \equiv \mathbf{1}$ :

$$(2.9) \quad \int_{\Omega} \mathbf{L} dv = \int_{\partial\Omega} \mathbf{V} \otimes \mathbf{n} d\mathcal{S}.$$

Hence, in view of Eqs. (2.6), the deviation  $\Delta_\Omega$  (Eq. (2.4)) is for large  $R$  equivalent to  $\overline{\mathbf{T}:\nabla \mathbf{u}}^\Omega$ , but Eq. (2.2) implies if  $\mathbf{T}$  is bounded ( $\|\mathbf{T}(\mathbf{x})\| \leq \sigma$  for every  $\mathbf{x}$ ):

$$(2.10) \quad \left| \overline{\mathbf{T}:\nabla \mathbf{u}}^\Omega \right| = \frac{1}{v(\Omega)} \left| \int_{\partial\Omega} (\mathbf{T} \cdot \mathbf{n}) \cdot \mathbf{u} d\mathcal{S} \right| \leq \frac{\sigma}{v(\Omega)} \int_{\partial\Omega} \|\mathbf{u}\| d\mathcal{S}.$$

Conditions (2.6) and (2.7) are thus sufficient to ensure that the velocity gradient  $\mathbf{L}$  is macro-homogeneous in the desired sense. It would be more appropriate to qualify such velocity fields as "macro-linear". We notice here that no bound of a real heterogeneity field  $\mathbf{u}$  in an aggregate, can be deduced from the knowledge of the typical (or maximal) heterogeneity  $\|\delta \mathbf{u}\|$  across one typical (or even maximal) constituent. Indeed, the heterogeneities of the velocity field through successive constituents, may as well pile up one over another as compensate one another: For the macro-homogeneity to hold, it is only necessary that, at some larger scale, the sum of successive

heterogeneities becomes negligible in the average. The number of constituents to be taken into account in order that this average compensation approximately occurs, may depend strongly on the particular structure of the aggregate, and has no a priori bound. In other words, the fluctuating character of the heterogeneity field may well be more complex than that of a bounded wave oscillating about 0 with a pseudo-period of order  $d$ , the mean size of the constituents. Moreover this character — and especially the smallness of the fluctuation distance — does not play an apparent role in the macrolinearity condition (2.6)–(2.7).

The order of magnitude of the nonlinear part (or heterogeneity):

$$(2.11) \quad \mathbf{u}(\mathbf{x}) = \mathbf{u}_\Omega(\mathbf{x}) = \mathbf{V}(\mathbf{x}) - \bar{\mathbf{L}}^\Omega \cdot \mathbf{x}$$

across an observation domain  $\Omega$ , may be known from experiments such as grid measurements. Then by comparison of  $\sigma \|\bar{\mathbf{L}}^\Omega\|$  with the upper bound in Eq. (2.10), the reliability of the no-correlation condition can be physically assessed. In this, the fluctuation distance again plays no role. However, suppose that  $\mathbf{u}$  is known to fluctuate in such a way that  $\int_{\Gamma_k} \mathbf{u} d\mathcal{S} = \mathbf{0}$  for each  $\Gamma_k$ , where the subdomains  $\Gamma_k$ , with size smaller than  $d$ , build a partition of the boundary  $\partial\Omega$  (in view of the relative homogeneity inside the grains or constituents, the  $\Gamma_k$  should *overlap* the sections of neighbouring grains by the surface of the sample). If moreover the spatial variation rate of the "stress" (or stress rate) field is bounded:

$$(2.12) \quad \|\mathbf{T}(\mathbf{x}) - \mathbf{T}(\mathbf{y})\| \leq K \|\mathbf{x} - \mathbf{y}\|,$$

then a different upper bound is found for  $\Delta_\Omega$ :

$$(2.13) \quad \Delta_\Omega \leq \frac{Kd}{v(\Omega)} \int_{\partial\Omega} \|\mathbf{u}\| d\mathcal{S}.$$

Indeed, we have from Eqs. (2.5) and (2.11) and the fluctuation condition:

$$\Delta_\Omega = \frac{1}{v(\Omega)} \sum_k \int_{\Gamma_k} (\mathbf{T} \cdot \mathbf{n}) \cdot \mathbf{u} d\mathcal{S} = \frac{1}{v(\Omega)} \sum_k \int_{\Gamma_k} [(\mathbf{T} - \bar{\mathbf{T}}^{\Gamma_k}) \cdot \mathbf{n}] \cdot \mathbf{u} d\mathcal{S}$$

(where  $\bar{\mathbf{T}}^{\Gamma_k}$  is the surface average in  $\Gamma_k$ ) and by Eq. (2.12)

$$\int_{\Gamma_k} [(\mathbf{T} - \bar{\mathbf{T}}^{\Gamma_k}) \cdot \mathbf{n}] \cdot \mathbf{u} d\mathcal{S} \leq \mathcal{X} \delta \int_{\Gamma_k} \|\mathbf{u}\| d\mathcal{S}.$$

In the upper bound (2.13), the maximum "stress" (or stress-rate)  $\sigma$  of the upper bound (2.10) has been replaced by the maximum *variation*  $\delta\sigma = Kd$  of the "stress" through a fluctuation domain of the velocity (or displacement) field about the linear mean field. Thus the fluctuation distance of the velocity field does play a role in setting bounds to the deviation (2.5) from the no-correlation condition, *if* the spatial fluctuation of the "stress" is correspondingly bounded.

### 3. A general construction of macro-homogeneous strain fields

#### 3.1. The compatibility problem in deformed aggregates

In a coherent aggregate, the microscopic behaviour is rather uniform inside the constituents, but varies abruptly at their boundaries, while the stress and velocity vectors should remain continuous. A well-known consequence is that both local fields ( $\mathbf{T}$  and  $\mathbf{L}$ ) must be non-uniform and might only be obtained numerically, which would imply a precise knowledge of the behaviour and arrangement of the constituents; even for a small, non-representative number of grains, the calculations are formidable. Nevertheless, such complete simulations of the deformation of a crystalline assembly open a new way for discussing the different polycrystal models [11].

In all operative models for deformed aggregates, each constituent  $\Omega_k$  is given by its local "state" (crystallographic orientation, critical shear stresses, geometrical parameters,...) assumed uniform inside  $\Omega_k$  [2, 3]. In the place of local fields, such models predict *one* tensor  $\mathbf{L}^k$  and  $\mathbf{T}^k$  for one constituent  $\Omega_k$ . The global deformation rate being given by the macroscopic velocity gradient  $\mathbf{L}_0$ , a consistent model should predict a discrete distribution  $(\mathbf{L}^k)_{k=1,\dots,N}$  and  $(\mathbf{T}^k)_{k=1,\dots,N}$  such that the macroscopic average  $\bar{\mathbf{L}}^k$  is the given  $\mathbf{L}_0$ . The "compatibility problem" may then be formulated in the following way: is it always possible (as it should be) to associate a macro-linear velocity field  $\mathbf{V}$  (Eqs. (2.6)–(2.7)) to the distribution  $(\mathbf{L}^k)$ , and in which sense? Do certain models behave more gently in this regard? The predicted  $\mathbf{L}^k$  (or the predicted strain rates  $\mathbf{D}^k$ ) are often interpreted as the local values of the field  $\mathbf{L}$  (or  $\mathbf{D}$ ) in the constituents. Since these latter are assumed homogeneous, the velocity gradient, or only the strain rate  $\mathbf{D}$ , is thus supposed to be a piecewise uniform field. However, we state that *no* compatible strain rate field can be piecewise uniform, unless it is a uniform strain rate and spin field. Indeed, it follows from the compatibility equations that the spin is uniform in a domain  $\Omega$  where the strain rate is so: hence the velocity field is linear in  $\Omega$ ,  $\mathbf{V}(\mathbf{x}) = \mathbf{L}_\Omega \cdot \mathbf{x} + \mathbf{a}_\Omega$ . At the interface  $S$  between two linear domains  $\Omega$  and  $\Omega'$  of  $\mathbf{V}$ , we have  $\mathbf{L}_\Omega \cdot \mathbf{x} + \mathbf{a}_\Omega = \mathbf{L}_{\Omega'} \cdot \mathbf{x} + \mathbf{a}_{\Omega'}$ , or  $(\mathbf{L}_{\Omega'} - \mathbf{L}_\Omega) \cdot (\mathbf{y} - \mathbf{x}) = 0$  if  $\mathbf{x}$  and  $\mathbf{y}$  belong to  $S$ .

Except for the very special case where  $S$  is plane, it will contain four non-coplanar points  $\mathbf{x}, \mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3$ . The above equation then implies that  $L_{\Omega'} - L_{\Omega}$  cancels for three independent vectors, whence  $L_{\Omega} = L_{\Omega'}$ , and our statement is proved. Even in the highly improbable case of all polyhedral constituents, the complex system of the above continuity relations would only have non-uniform solutions in very particular situations, the treatment of which would require the complete knowledge of the spatial arrangement. Thus it is more realistic to consider  $L^k$  and  $T^k$  as the *average* values of the strain and stress rates in a constituent  $\Omega_k$ . Nevertheless, the generic model predicts  $L^k$  and  $T^k$  as mutually associated by an assumed constitutive relation of the constituent. As for a macroscopic relation, this is only justifiable if the field  $L = \nabla V$  has reasonable properties of "macro-homogeneity" but *in every given constituent*. In precise words: in every given  $\Omega_k$ ,  $L$  must fluctuate about  $L^k$  as in Eq. (2.6):  $L(\mathbf{x}) = L^k + \nabla \mathbf{u}^k(\mathbf{x})$ , in such a way that the integral (2.7) (with  $\mathbf{u}^k$  in place of  $\mathbf{u}$ ) is negligible with respect to  $L^k$  when  $\Omega$  is any sufficiently large subdomain of the constituent  $\Omega_k$ . In what follows, we address the question of whether this "meso-homogeneity" condition may be reached for any distribution ( $L^k$ ) of the mean values. Moreover, it is proved that, under two conditions of statistical homogeneity for the distribution ( $L^k$ ) the true macro-homogeneity (Eqs. (2.6)–(2.7) as they stand, for the whole aggregate and the macro-average  $L_0$ ) may be ascertained.

3.2. Vector fields with arbitrary local means of their gradient

A bounded aggregate  $\Omega$  is partitioned in its constituents  $\Omega_1, \dots, \Omega_N$  and a family  $(L^k)_{k=1, \dots, N}$  of second-order tensors is given. Except at the boundaries of the constituents, we may associate to every point  $\mathbf{x}$  of the aggregate, the tensor  $\hat{L}(\mathbf{x})$  which is the  $L^k$  corresponding to the unique constituent  $\Omega_k$  containing  $\mathbf{x}$ . Take an orthonormal basis  $(\mathbf{e}_j)_{j=1,3}$  and for  $\mathbf{x} \in \Omega$ , define the intersection  $I_j(\mathbf{x})$  of the segment  $[pr_j(\mathbf{x}), \mathbf{x}]$  ( $pr_j$  is the projection on the plane  $x_j = 0$ ) with  $\Omega$ . Then, three vector fields  $U_j (j=1,3)$  may be defined as the linear integration of the piecewise constant function  $\hat{L}$  in the direction  $\mathbf{e}_j$ :

$$(3.1) \quad U_j(\mathbf{x}) = \int_{I_j(\mathbf{x})} \hat{L}(\mathbf{y}) d\mathbf{y}.$$

Now let  $\mathcal{C}_l$  be a cubic lattice with mesh parameter  $l$ , having its sides parallel to the  $\mathbf{e}_j$ . We define a vector field  $V'_l$  only on the faces of  $\mathcal{C}_l$ :  $V'_l(\mathbf{x}) = U_j(\mathbf{x})$  if  $\mathbf{x}$  belongs to a face perpendicular to  $\mathbf{e}_j$ , and we observe that  $V'_l$  has the following property:

$$(3.2) \quad \int_{\partial C} \mathbf{V}'_i \otimes \mathbf{n} d\mathcal{S} = v(C) \mathbf{L}^k \quad \text{if } C \subset \Omega_k,$$

where  $C$  is one of the cubes of the lattice  $\mathcal{C}_l$  and  $v(C) = l^3$ . This follows from the definition, since  $\mathbf{n}(\mathbf{x}) = \mathbf{e}_j$ ,  $\mathbf{n}(\mathbf{x} - l\mathbf{e}_j) = -\mathbf{e}_j$  and

$$(3.3) \quad \mathbf{V}'_i(\mathbf{x}) - \mathbf{V}'_i(\mathbf{x} - l\mathbf{e}_j) = \mathbf{U}_j(\mathbf{x}) - \mathbf{U}_j(\mathbf{x} - l\mathbf{e}_j) = \mathbf{L}^k \cdot l\mathbf{e}_j,$$

when  $\mathbf{x}$  is on the face of  $C$  with external normal  $\mathbf{e}_j$  (the assumption  $C \subset \Omega_k$  implying that  $\hat{\mathbf{L}} \equiv \mathbf{L}^k$  in  $C$ ).

In general there is no relation between the values  $\mathbf{U}_j$  for different  $j$ , so that the surface field  $\mathbf{V}'_i$  is discontinuous at every ridge of the lattice  $\mathcal{C}_l$ . However  $\mathbf{V}'_i$  may be regularized and then extended into a body field  $\mathbf{V}_{i,\eta}$ , arbitrarily near to  $\mathbf{V}'_i$  in the sense that

$$(3.4) \quad \sum_{C \subset \Omega} \int_{\partial C} \|\mathbf{V}_{i,\eta} - \mathbf{V}'_i\| d\mathcal{S} \leq \eta$$

(Appendix 1). From Eqs. (2.9) and (3.2) it follows that the velocity gradient field  $\mathbf{L}_{i,\eta}$  satisfies if  $C \subset \Omega_k$ :

$$\|v(C) \mathbf{L}^k - \int_C \mathbf{L}_{i,\eta} dv\| = \left\| \int_{\partial C} (\mathbf{V}'_i - \mathbf{V}_{i,\eta}) \otimes \mathbf{n} d\mathcal{S} \right\| \leq \int_{\partial C} \|\mathbf{V}_{i,\eta} - \mathbf{V}'_i\| d\mathcal{S}$$

whence, by inequality (3.4), denoting by  $\Omega_k^{(l)}$  the union of the cubes of the  $\mathcal{C}_l$  lattice which are entirely included in  $\Omega_k$ :

$$(3.5) \quad \sum_k \|v(\Omega_k^{(l)}) \mathbf{L}^k - \int_{\Omega_k^{(l)}} \mathbf{L}_{i,\eta} dv\| \leq \sum_k \sum_{C \subset \Omega_k} \|v(C) \mathbf{L}^k - \int_C \mathbf{L}_{i,\eta} dv\| \leq \eta.$$

(The cubes intersecting the boundaries of the constituents are omitted in inequality (3.5), but their average contribution decays with  $l$ : this is proved by returning to surface integrals as in Eq. (3.2), due to the continuity of  $\mathbf{U}_j \otimes \mathbf{e}_j$  which on the  $j$  faces is equal to  $\pm \mathbf{V}'_i \otimes \mathbf{n}$ ). For sufficiently small  $l$ , the volume averages of  $\mathbf{L}_{i,\eta}$  in the constituents  $\Omega_k$  are thus arbitrarily near to the given tensors  $\mathbf{L}^k$ .

If desired,  $\mathbf{V}_{i,\eta}$  could be replaced by another field, arbitrarily near in the sense of inequality (3.4), but giving exactly the imposed average values of its gradient (Lemma 1 of Appendix 1). Also, if the  $\mathbf{L}^k$  are zero-trace tensors, a vector field with zero divergence may be chosen (Lemma 3 of Appendix 1).

It must be finally mentioned that the way of "transmitting" a vector field from three adjacent faces  $\partial C_-$  of a cube  $C$  to the opposite faces  $\partial C_+$ , by

Eq. (3.3), so as to obtain a given surface integral (3.2), has previously (but independently) been found by HAVNER [12], in the particular case where the  $L^k$  tensors are all the same in the space-filling lattice  $\mathcal{C}_l$ . The aim was to give a general form of macro-homogeneous displacement field (periodic, however). Unfortunately, for a given surface field on  $\partial C_-$ , this directly obtained field is generally discontinuous on every ridge of  $\partial C_+$  and can not be extended in a body field satisfying the divergence theorem and Eq. (2.9). This fact was not pointed out in [12].

### 3.3. Fulfilment of the macro-homogeneity condition

In Sect. 2, the asymptotic nature of the macro-homogeneity condition has been emphasized (see Eqs. (2.7)–(2.8)). Thus we consider a space-filling aggregate, partitioned in an infinite sequence of bounded constituents  $\Omega_1, \dots, \Omega_k, \dots$ . In order to obtain a macro-homogeneous gradient field  $L = \nabla V$  having prescribed volume averages  $L^k$  in the constituents  $\Omega_k$ , we must suppose that the infinite sequence  $(L^k)$  is statistically homogeneous, in the sense that

$$(3.6) \quad \overline{L^k}^\Omega = \frac{1}{v(\Omega)} \int_\Omega \hat{L} dv \rightarrow L_0, \quad R(\Omega) \rightarrow \infty.$$

Here the macroscopic average  $L_0$  is asymptotically reached, *independently of the position* of the macro-element  $\Omega$ . The research of  $L$  is equivalent to that of the associated vector field  $V$ , which must be "macro-linear" in the sense of Eqs. (2.6)–(2.7), in order that  $L$  be macro-homogeneous. In general we only have to find the nonlinear part  $u$  in Eq. (2.6), such that the local averages of  $\nabla u$  are  $L^k - L_0$ . Thus we may assume  $L_0 = 0$ .

The whole construction of Sect. 3.2 remains valid for the space-filling aggregate  $\Omega = \mathbf{R}^3$  (the only questionable point is inequality (3.4) which limits the difference between the irregular surface field  $V'_i$  and the regularized body field  $V_{i,\eta}$ . However, the way in which the regularization process is propagated from one cube to another, allows to obtain Eq. (3.4) for these infinitely many cubes (Appendix 1); this is only a question of convergent series). Now we prove that the obtained field  $V_{i,\eta}$  satisfies condition (2.7) if the *linear* averages of the  $L^k$  tensors are asymptotically equivalent to their volume average  $L_0 = 0$ , when segments  $[\mathbf{x} - R\mathbf{e}_i, \mathbf{x}]$  (parallel to the coordinate axes) are considered:

$$(3.7) \quad \left\| \mathbf{0} - \frac{1}{R} \int_{[\mathbf{x} - R\mathbf{e}_i, \mathbf{x}]} \hat{L}(\mathbf{y}) d\mathbf{y} \right\| \leq \varepsilon(R) \rightarrow 0, \quad R \rightarrow \infty.$$

Indeed, combining (3.7) with the definition (3.1) of  $V'_i$ , we see that to every small number  $\alpha$  we may associate a size  $R_\alpha$  such that

$$(3.8) \quad \|V'_i(\mathbf{x})\| \leq \alpha \|\mathbf{x}\| \quad \text{if } (|x_j| \geq R_\alpha \text{ for all } j = 1, 2, 3).$$

On the other hand, we assume that the  $L^k$  tensors are bounded,  $\|L^k\| \leq A$ , for all  $k$ , which implies:

$$(3.9) \quad \|V'_i(\mathbf{x})\| \leq A \|\mathbf{x}\| \quad \text{for every } \mathbf{x}.$$

Defining the "cross"  $X_\alpha$  ( $|x_j| \leq R_\alpha$  for one  $j$  at least), which is in fact the union of three perpendicular walls, and separating the surface integral of  $\|V'_i\|$  accordingly, we obtain from (3.8) and (3.9):

$$(3.10) \quad \int_{X_\alpha \cap \partial\Omega} + \int_{\partial\Omega \setminus X_\alpha} \|V'_i\| d\mathcal{S} \leq R(\Omega) \cdot (A\mathcal{S}(X_\alpha \cap \partial\Omega) + \alpha\mathcal{S}(\partial\Omega)).$$

Evidently, we may suppose that the cube  $\Omega$  and the "cross" have no common boundary; in that case:

$$\mathcal{S}(X_\alpha \cap \partial\Omega) \leq 6R_\alpha R(\Omega), \quad \mathcal{S}(\partial\Omega) = 6R(\Omega)^2.$$

Thus, Eq. (3.10) implies that

$$\int_{\partial\Omega} \|V'_i\| d\mathcal{S} \leq 6\alpha R(\Omega)^3 \cdot \left(1 + \frac{AR_\alpha}{\alpha R(\Omega)}\right) \sim 6\alpha R(\Omega)^3, \quad R(\Omega) \rightarrow \infty$$

and with (3.4), this proves that  $V_{i,\eta}$  satisfies the macrolinearity condition (2.7), since  $\alpha$  is arbitrary.

### 3.4. Discussion

#### 1. Solution of the compatibility problem in the average sense

In Sect. 3.3, the distribution  $(L^k)_{k \geq 1}$  of the mean strain rates and spin rates has demanded the following properties of statistical homogeneity, in order that the construction of Sect. 3.2 lead to a *macro-homogeneous* field  $L = \nabla V$  (such that, moreover,  $\bar{L}^{\Omega_k} = L^k$  for every  $k$ ): the distribution  $(L^k)$  must have an asymptotically well-defined macroscopic average  $L_0$  (Eq. (3.6)) and the *linear* average values of the distribution must be asymptotically equivalent to its *volume* average value  $L_0$  (Eq. (3.7)). These properties are worth discussing within the frame of an asymptotic theory of the distribution of the "states" of the constituents in a random aggregate [2], which is presented

in another paper [3]. In "operative polycrystal models" (Sect. 3.1), the discretization is directly done in terms of the states. When applied to simulate a material with statistically homogeneous distribution of the states of its constituents, any such model will thus provide a distribution ( $L^k$ ) having the desired properties (this statement is precised and proved in [3]). Hence, the compatibility problem (Sect. 3.1) may always be solved in the sense of the prescribed volume averages, by using the construction of Sect. 3.2. In this regard, any of such operative models is satisfactory and no one may be said to be "superior".

## 2. Fulfilment of the meso-homogeneity condition

For sufficiently small  $l$  and  $\eta$ , the volume average of the velocity gradient in any constituent  $\Omega_k$ ,  $\bar{L}_{l,\eta}^{\Omega_k}$ , is arbitrarily near to the prescribed value  $L^k$ , in view of (3.5); actually the second inequality in (3.5) proves more: every average  $\bar{L}_{l,\eta}^C$  in a small cube  $C$  (with size  $l$ ) is nearly the  $L^k$  corresponding to the constituent  $\Omega_k$  containing  $C$ . Thus, as for an exact constituent  $\Omega_k$ , the volume average  $\bar{L}_{l,\eta}^\omega$  is arbitrarily near to  $L^k$  if  $l, \eta$  are small enough and the domain  $\omega$  is included in  $\Omega_k$  — and for an assigned minimum size of  $\omega$ , this holds uniformly with regard to the position of  $\omega$  in the space-filling aggregate. However, the field  $L_{l,\eta}$  is not uniformly bounded with respect to  $l$ , even in integral norm. On the contrary, it is generally true that for a fixed  $\eta$  and for any given domain  $\omega$ :

$$(3.11) \quad \int_{\omega} \|L_{l,\eta}\| dv \rightarrow \infty \quad \text{as} \quad l \rightarrow 0,$$

since  $V_{l,\eta}$  must regularize the discontinuity  $\Delta V$  of  $V_i'$  from one face  $i$  to another  $j \neq i$  of the small cubes  $C$ , the value of  $\Delta V$  being roughly independent of  $l$  — thus leading to an amplitude of order  $\Delta V/l$  for the gradient  $L_{l,\eta}$  and an integral (3.11) of order  $v(\omega)\Delta V/l$ .

In other words: by reducing the size  $l$  of the cubes, the construction allows to obtain the prescribed averages  $L^k$  of  $L$  in smaller and smaller domains located anywhere inside the constituents  $\Omega_k$ , but this also increases the fluctuation amplitude of the obtained strain (rate) field  $L = L_{l,\eta}$ . For a given distribution ( $L^k$ ) of the prescribed mean values, it is hence generally impossible to state in what measure the no-correlation condition inside the constituents may be reached; the same may be said on the fulfilment of the meso-homogeneity condition (Sect. 3.1), since this implies the local no-correlation. This is not a shortcoming of our natural construction, but a necessary consequence of prescribing a non-uniform distribution ( $L^k$ ) of the local means: the degree of the attainable approximate meso-homogeneity depends on the inhomogeneity of both the distribution

and the aggregate itself. Overlooking this point may lead to wrong statements.

As a consequence, it is difficult to regard the mutually associated stresses and strains, predicted by any given "operative model", as the true volume averages of the corresponding fields in the geometrically defined constituents (since the strain field should then be meso-homogeneous). A more realistic objective that the aggregate models should generally pursue, is to predict the stresses and strains, averaged as functions of the local state. This is of course consistent with the discretization in states but, in our opinion, needs to be analysed precisely (such an analyse is proposed in [3]).

On the other hand, exactly as for the macro-homogeneity condition, the meso-homogeneity of *experimental* strain fields may be physically assessed (by measuring the strain inhomogeneity at the scale of the constituents). As far as metallic polycrystals are concerned, this kind of strain inhomogeneity is well evaluated by measuring the variations in the crystal orientation inside a grain, because the strain rate and the lattice spin are bound together. Thus we expect the meso-homogeneity condition to be more precisely verified at low or moderate strains, where the metallurgists clearly identify grains or (later) subgrains and cells (see e.g. [10, 25]), than at high strains (such as those attained during cold-rolling), where large and contiguous zones under continuously heterogeneous strain seem to form at some places (see e.g. [9]). It is worth noting that the strain inhomogeneity is generally agreed to increase with strain, and that our construction clearly links the deviation from the meso-homogeneity, i.e. the *intra-constituent* inhomogeneity, with the differences between the  $L^k$  for different "grains"  $\Omega_k$ , i.e. the *inter-constituent* inhomogeneity. Finally, in so far as the meso-homogeneity of the actual fields is considered to be experimentally consistent, a simple formulation of the model [1] may be given [4]: the meso-homogeneity assumption was implicit in the original formulation. This model is generalized in [3].

### 3. Meaning of the extended macro-homogeneity condition

It may be seen from Eqs. (3.1) and (3.7) that if the heterogeneity field  $u(x) = V(x) - L_0 \cdot x$  has to be *bounded*, then the convergence of the linear averages of the  $L^k$  tensors towards  $L_0$  must be at least of  $O(1/R)$ , where  $R$  is the considered length. Accordingly, the linear distributions of the states of the constituents should converge towards the asymptotic volume distribution like  $1/R$  [2]. This is clearly a restrictive condition. Thus again (see Sect. 2.3), a bounded heterogeneity field may not be expected for general aggregates. In practice, of course, only bounded aggregates are encountered; then a "bounded" heterogeneity means "having an amplitude independent of the size of the measuring base": *this* condition is not to expect general, *real* aggregates, and is not necessary to obtain

macro-homogeneous strain fields. In the same way, we have seen that the condition of a fluctuating heterogeneity field with a characteristic distance having the same order of size as the constituents, is neither necessary nor in general expectable. We conclude that HILL'S and MANDEL'S definition of the macro-homogeneity [14, 15, 23] applies to aggregates which are strongly disordered, whereas an operative macro-homogeneity condition (2.6)–(2.7) may also be defined for aggregates having arbitrarily large "clusters" or spatial correlations.

#### 4. Conclusions

A theoretical analysis of the structure of the strain and spin field in a deformed aggregate has been presented and some parallels have been drawn with both the experimental reality and the operative models, especially in the case of metallic polycrystals. The main results are the following:

1. Hill's macro-homogeneity condition has been reviewed, clarifying the role played by the amplitude and the characteristic distance of the fluctuating part of the displacement. This allows to extend Hill's definitions to more general situations with spatial correlations.

2. The "compatibility problem" in the models for deformed aggregates, has been formulated in a general way. It has no solution if piecewise uniform strain and stress fields are assumed. In an average sense, this problem has always a solution and does not allow us to decide between different models.

3. In order that these models could predict the average strains (and stresses) in the geometrically defined constituents, it is necessary that the strain field be "meso-homogeneous", i.e. fulfil a macro-homogeneity condition separately inside each constituent. The more severe compatibility problem of obtaining a meso-homogeneous strain field cannot be solved for a general distribution of the average strains. It is thus advisable to interpret the predicted strain distributions in a statistical sense, and it is suggested that this needs a rigorous formulation of the local "state" and the corresponding functions.

#### Appendix 1. Regularization of the field $V_i'$ into the field $V_{i,n}$ (or $V$ )

Precisely, we demand that  $V$  is in the simplest Sobolev space  $\mathbf{H}^1(\Omega) = H^1(\Omega)^3$ , i.e. each component  $V_i$  of  $V$  and each partial weak derivative  $\partial V_i / \partial x_j$  is a different function  $\varphi$  whose square  $\varphi^2$  has a finite integral in  $\Omega$  (the set of such  $\varphi$  is classically denoted  $L^2(\Omega)$ ). The space  $\mathbf{H}^1(\Omega)$  is a convenient tool, e.g. the fields considered and practically handled in the numerical approximation of partial differential equations often have exactly this regularity (DAUTRAY and LIONS [7]). Here, an even more essential point is the

validity of the divergence theorem for the fields of  $\mathbf{H}^1(\Omega)$ , involving that of the virtual work equation and the equation (2.2) above [28]. This validity follows from density arguments. However, the fields of  $\mathbf{H}^1(\Omega)$  and their derivatives may be discontinuous and their restrictions or "traces" to the boundary  $\partial\Omega$  are thus defined indirectly (by a continuity extension of the ordinary restriction operator  $\mathbf{V} \rightarrow \mathbf{V}|_{\partial\Omega}$ , as this is defined for the dense subspace of  $\mathbf{H}^1(\Omega)$  containing all the infinitely differentiable fields). Anyway, we still denote such "traces"  $\mathbf{V}|_{\partial\Omega}$ .

The regularization is first done in one cube and then propagated from one cube to another.

#### A1.1. Case of a single cube with an additional vector field on its half-boundary

Let  $\Omega$  be a simple cube. Let us choose a vertex 0, denote  $\partial\Omega_-$  the union of the three faces bordering 0 and  $\partial\Omega_+$  the three opposite faces. For any  $\varepsilon > 0$ , for every given regular vector field  $\mathbf{U}$  on  $\partial\Omega_-$  ( $\mathbf{U} \in \mathbf{H}^1(\partial\Omega_-)$ ) and every 2nd order tensor  $\mathbf{L}^0$ , we are going to build a regular field  $\mathbf{V}$  ( $\mathbf{V} \in \mathbf{H}^1(\Omega)$  and  $\mathbf{V}|_{\partial\Omega_+} \in \mathbf{H}^1(\partial\Omega_+)$ ), such that  $\operatorname{div}\mathbf{V} = 0$  if  $\operatorname{tr}\mathbf{L}^0 = 0$ ,

$$(A.1) \quad \frac{1}{v(\Omega)} \int_{\partial\Omega} \mathbf{V} \otimes \mathbf{n} d\mathcal{S} = \mathbf{L}^0, \quad \mathbf{V}|_{\partial\Omega_-} = \mathbf{U},$$

and

$$(A.2) \quad \int_{\partial\Omega_+} \|\mathbf{V}(\mathbf{x}) - \mathbf{U}(\mathbf{x} - \Delta\mathbf{x}) - \mathbf{L}^0 \cdot \Delta\mathbf{x}\| d\mathcal{S}(\mathbf{x}) \leq \varepsilon.$$

Here  $\Delta\mathbf{x} = l\mathbf{n}(\mathbf{x})$  is the difference vector between the opposite sides of  $\Omega$ ,  $l$  being the size of  $\Omega$ .

Suppose that  $\Omega$  is one cube of the lattice  $\mathcal{C}_l$  of Sect. 3.2 and is included in a constituent having  $\mathbf{L}^0$  as the prescribed mean value. Then, if  $\mathbf{U}$  is the restriction to  $\partial\Omega_-$  of the field  $\mathbf{V}_l$ , the field

$$(A.3) \quad \mathbf{V}^2(\mathbf{x}) = \mathbf{U}(\mathbf{x} - \Delta\mathbf{x}) + \mathbf{L}^0 \cdot \Delta\mathbf{x},$$

for  $\mathbf{x}$  almost everywhere (a.e.) in  $\partial\Omega_+$ , is the restriction to  $\partial\Omega_+$  of the same field  $\mathbf{V}'_l$ . Note that  $\mathbf{V}^2$  satisfies Eq. (A.1). This explains what we are doing.

The boundary  $\partial S = \partial(\partial\Omega_+)$  of  $S = \partial\Omega_+$  is equal to  $\partial(\partial\Omega_-)$ , i.e. to the union of the six two-by-two adjacent ridges of  $\Omega$ , which do contain neither the point 0 nor the opposite vertex. Let us first (incorrectly) deal with traces

in the same way as if they were ordinary restrictions: then,  $V_{|\partial\Omega}$  would be uniquely defined by  $V_{|\partial\Omega^-} = U$  which is known and  $V_{|\partial\Omega^+} = V_{|S}$ , provided that these two coincide at the common (sub-) boundary  $\partial S$ . Thus, we would have to find a field  $V^1 \in H^1(S)$ , satisfying (A.2) in the place of  $V$ , such that:

$$(A.4) \quad \int_{\partial\Omega^+} V^1 \otimes n d\mathcal{S} = \int_{\partial\Omega^+} V^2 \otimes n d\mathcal{S} = - \int_{\partial\Omega^-} U \otimes n d\mathcal{S} + v(\Omega)L^0$$

so as to obtain (4.1), and that  $V^1_{|\partial S} = U_{|\partial S}$ . Actually, this procedure is correct: it is proved in Appendix 2 that a unique field  $V \in H^1(\partial\Omega)$  is found in that way, having  $V_{|\partial\Omega^-} = U$  and  $V_{|\partial\Omega^+} = V^1$  as ordinary restrictions. Once a possible  $V^1$  will be found, we then just will have to extend  $V$  from  $\partial\Omega$  to the inner part of the cube  $\Omega$ .

(i) *Construction of a field  $V^1$  on  $S = \partial\Omega^+$*

If  $E$  is an arbitrary second-order tensor (the space of such tensors will be denoted by  $\mathcal{L}$  and  $\mathcal{L}_0$  will denote the subspace of zero-trace 2nd order tensors), we are able to find in the same way as for  $V^2$  an integrable field  $X(X \in L^1(S))$  such that

$$(A.5) \quad f(X) \equiv \int_S X \otimes n d\mathcal{S} = E.$$

In other words  $f$  defines a linear mapping of  $L^1(S)$  onto  $\mathcal{L}$ . Since this mapping is obviously continuous with respect to the usual norm

$$(A.6) \quad \|X\|_1 = \int_S \|X(x)\| d\mathcal{S}(x)$$

of  $L^1(S)$ , we shall be allowed to use Lemma 1 below. This lemma essentially states that, if we always can find an irregular solution (or even only an approximate one) to a given finite set of linear, scalar functional equations like (A.5), then we also can find, near an irregular solution, an exact and regular one. Then, Lemma 2 will allow us to modify the trace,  $X_{|\partial S}$ , almost without changing  $f(X)$ . By combining these results, we will find a satisfying field  $V^1$ . Lemmas 1 and 2 are proved in Appendix 3.

LEMMA 1

Let  $E$  and  $F$  be two normed linear spaces,  $F$  having finite dimension,  $f$  be a continuous linear mapping of  $E$  onto  $F$  and  $E_0$  be a dense subspace of  $E$ . Then, the restriction  $f_0 = f_{E_0}$  is an open mapping of  $E_0$  onto  $F$ . Moreover, for every open set  $U$  in  $E$ ,  $f(U)$  and  $f_0(U \cap E_0)$  are the same open set in  $F$ .

## LEMMA 2

Let  $\omega$  be a bounded open set in  $\mathbf{R}^n$ , whose boundary  $\partial\omega$  is regular (piecewise  $\mathcal{C}^1$ ) and let  $U$  be a field in  $\mathbf{H}^{1/2}(\partial\omega)$  <sup>(1)</sup>. Then for every  $\varepsilon > 0$  there exists a field  $U^1 = U_\varepsilon^1 \in \mathbf{H}^1(\omega)$  such that

$$(A.7) \quad \int_{\omega} \|U^1(\mathbf{x})\| dv_n(\mathbf{x}) \leq \varepsilon \quad \text{and} \quad U^1|_{\partial\omega} = U.$$

Let us come to the research of a regular field  $V^1$ , arbitrarily near  $V^2$  in the sense that  $\int_S \|V^1 - V^2\| d\mathcal{S} \leq \varepsilon$ , satisfying (A.4) with the given trace  $V^1|_{\partial S} = U|_{\partial S}$ . The subspace  $\mathbf{H}_0^1(S)$  containing those fields  $X \in \mathbf{H}^1(S)$  whose trace  $X|_{\partial S}$  are zero, is dense in  $\mathbf{L}^1(S)$  with respect to the integral norm  $\|X\|_1$ . We thus apply Lemma 1: since the ranges of the open balls  $f(\mathbf{H}_0^1(S) \cap B(V^2, \varepsilon/2))$  and  $f(B(V^2, \varepsilon/2))$  are one and the same open set in  $\mathcal{L}$ , there is a  $\delta > 0$  such that

$$(A.8) \quad B(f(V^2), \delta) \subset f(\mathbf{H}_0^1 \cap B(V^2, \varepsilon/2)).$$

Applying successively Lemma 2 (with  $n = 2$ ) to the three faces of  $S$ , we find a field  $U^1 \in \mathbf{H}^1(S)$  such that  $U^1|_{\partial S} = U|_{\partial S}$  with  $\|U^1\|_1 \leq \text{Min}(\delta, \varepsilon/2)$ .

Since  $\|f(U^1)\| \leq \|U^1\|_1$  by (A.5), we have thus  $f(V^2 - U^1) \in B(f(V^2), \delta)$  whence, from (A.8), we find a field  $V^0 \in \mathbf{H}_0^1(S)$  such that

$$(A.9) \quad f(V^0) = f(V^2 - U^1) \quad \text{and} \quad \|V^0 - V^2\| \leq \varepsilon/2.$$

The field  $V^1 = V^0 + U^1$  satisfies  $f(V^1) = f(V^2)$  and thus also (A.4); moreover,  $V^1|_{\partial S} = U^1|_{\partial S} = U|_{\partial S}$  and  $\|V^1 - V^2\|_1 \leq \|V^0 - V^2\|_1 + \|U^1\|_1 \leq \varepsilon$ , as announced.

(ii) Extension of  $V$  from  $\partial\Omega$  to  $\Omega$ 

The above construction of  $V^1$  provides us with the trace  $V|_{\partial\Omega} = (U|_{\partial\Omega-}, V^1|_{\partial\Omega+})$  (see Appendix 2) of the field  $V$  that we are looking for. From the trace theorem of zero order (see e.g. [7]), it follows that there exists at least one field  $V^3 \in \mathbf{H}^1(\Omega)$  having exactly this trace (actually there are a lot of such fields). Now, we only have to deal with the additional zero divergence condition of the incompressible case. The construction of  $V|_{\partial\Omega}$  ensures that

$$(A.10) \quad \int_{\partial\Omega} V \otimes n d\mathcal{S} = v(\Omega) L^0.$$

<sup>(1)</sup> This Sobolev space is not defined here, since we only use the trace theorem (see below) ensuring that the trace application  $U \rightarrow U|_{\partial\omega}$  maps  $\mathbf{H}^1(\omega)$  onto  $\mathbf{H}^{1/2}(\partial\omega)$ .

The incompressibility condition  $\text{tr} \mathbf{L}^0 = 0$  then takes the form

$$(A.11) \quad 0 = \int_{\partial\Omega} \mathbf{V} \cdot \mathbf{n} d\mathcal{S} = \int_{\Omega} \text{div} \mathbf{V}^3 dv.$$

The range of the div operator, restricted to  $\mathbf{H}_0^1(\Omega)$ , is exactly the set  $L^2(\Omega)/\mathbf{R}$  of the classes of the functions  $p \in L^2(\Omega)$  satisfying  $\int_{\Omega} p dv = 0$ . This follows from [7], (3d vol., p. 828): the inclusion  $\text{div}(\mathbf{H}_0^1(\Omega)) \subset CL^2(\Omega)/\mathbf{R}$  comes from the divergence theorem; the inverse inclusion follows from the fact that the adjoint operator of  $u = \text{div}|_{\mathbf{H}_0^1}$  is  $u^* = \text{grad}|_{L^2(\Omega)/\mathbf{R}}$  by the same theorem, and from an inequality  $\|p\|_{L^2(\Omega)/\mathbf{R}} \leq C(\Omega) \|\text{grad} p\|_{L^2(\Omega)}$  whence  $\text{Ker}(u^*) = \{0\}$ , i.e.  $u(\mathbf{H}_0^1)^\perp = \{0\}$ .

This, combined with (A.11), shows that there is a field  $\mathbf{V}^4 \in \mathbf{H}_0^1(\Omega)$  (that is,  $\mathbf{V}^4|_{\partial\Omega} = 0$ ) such that  $\text{div} \mathbf{V}^4 = -\text{div} \mathbf{V}^3 \in L^2(\Omega)/\mathbf{R}$ . The field  $\mathbf{V} = \mathbf{V}^3 + \mathbf{V}^4$  of  $\mathbf{H}^1(\Omega)$  has the right trace  $\mathbf{V}|_{\partial\Omega}$  and satisfies  $\text{div} \mathbf{V} = 0$  in  $\Omega$ . With the definition (A.3) of the irregular field  $\mathbf{V}^2$ , the proximity condition  $\|\mathbf{V}^1 - \mathbf{V}^2\|_1 \leq \varepsilon$  gives (A.2). *QED.*

**A1.2. Propagation of the regularization process in the lattice**

In the lattice  $\mathcal{C}_l$ , the position of a given cube is directly specified by an integer threesome  $(M,N,P)$  and any volume domain  $\Omega$  is covered by a family of cubes of  $\mathcal{C}_l$ :

$$(A.12) \quad \Omega \subset \left( \bigcup_{(M,N,P) \in I_l} C^{MNP} \right) = \Omega_{(l)}, \quad C^{MNP} \in \mathcal{C}_l.$$

This set of threesomes  $I_l$  is finite if  $\Omega$  is *bounded*. In that case, we may order the  $C^{MNP}$  in the lexicographic way, obtaining the differently indexed cubes  $C_m$ . Here  $m$  takes all values from 1 to an integer  $n = \text{Card}(I_l)$ . For a given  $m > 1$ ,  $C_m$  has at most three common faces with the preceding cubes: indeed, if  $m = m(M,N,P)$ ,  $C_m$  has one and only common face with each of the only three cubes  $C^{M-1,N,P}$ ,  $C^{M,N-1,P}$ ,  $C^{M,N,P-1}$  which may, or not, belong to  $\Omega_{(l)}$ . Also, if  $\Omega$  is *unbounded*, a different order  $(C_m)_{m \geq 1}$  may be defined with the same property. First, in the 2-D case, this order is obtained by describing a square spiral from the origine square to infinity, as indicated.

17	16	15	14	13
18	5	4	3	12
19	6	1	2	11
20	7	8	9	10
21	22	23	24	25

Thus the squares at the boundary of the "large" square (with side  $nl$ ) are successively counted at step  $n$  ( $n = 3, 5, 7, \dots$ ). In the same way, for the 3-D case, the boundary cubes of the large cube  $B_n$  (with side  $nl$ ) are counted at step  $n$ , beginning with the lower face which is described as in the 2-D case; then the square rings at the boundary of  $B_n$  are successively described in the direct sense, upwards from one ring to another; step  $n$  is ended by describing the upper face of  $B_n$  in the same way as the lower one. Only those cubes pertaining to  $\Omega_{(l)}$  are counted.

Now, attributing to each of the so-indexed cubes  $C_m \in \Omega^{(l)}$  the tensor  $L^{k(m)}$  of the subdomain  $\Omega_k$  including  $C_m$  (an arbitrary choice is done at the boundaries  $\partial\Omega_k$ ), we proceed in a recurrent manner. For every cube  $C_m$  there are at least three adjacent faces which are common with no preceding cube  $C_p$  ( $1 \leq p < m$ ). We denote  $\partial C_m^+$  this set of three "free" faces, and  $\partial C_m^-$  the three other faces. On those faces of  $\partial C_m^-$  which are *not* common with a preceding cube (often, there is no such face), a field  $U'_m$  is initialized as  $U'_m = V'_i$ . Thus for the first cube, at the origin:  $U'_1 = \mathbf{0}$  which is in  $H^1(\partial C_1^-)$  and we apply Sect. A1.1 with  $U_1 = U'_1 = \mathbf{0}$  and  $L^{k(1)}$ , obtaining the restriction  $V|_{C_1}$  which satisfies (A.1) and (A.2). Then at step  $m$ , the trace of the field  $V|_{C_1 \cup \dots \cup C_{m-1}}$  is taken as data  $U''_m$  on  $F''_m = \partial C_m^- \cap (\partial C_{1 \cup \dots \cup C_{m-1}})$ , and  $U'_m = V'_i$  on  $F'_m = \partial C_m^- \setminus (\partial C_{1 \cup \dots \cup C_{m-1}})$ . A regularization process is applied as in ((A1.1), (i)) so as to obtain a field  $U_m \in H^1(\partial C_m^-)$  whose restriction  $U_{m|F'}$  is arbitrarily near to  $U'_m$ , while the restriction  $U_{m|F''}$  is *exactly* the previously obtained field  $U''_m = V_{i|F''}$ . The process of Sect. A1.1 is then applied with  $U_m$  and  $L^{k(m)}$ . In order to obtain (3.4) one only has to take the tolerances  $\varepsilon_m$  in (A.2) in the form of a convergent series, e.g.  $\varepsilon_m = \eta/2^m$ .

## Appendix 2. Definition of a field in $H^1(\omega)$ by its restrictions to contiguous subdomains, having common traces

In Appendix 1, it is supposed that a field  $U$  can be defined in  $H^1(\omega)$  by its two restrictions  $U^1$  and  $U^2$  to disjointed open subdomains  $\omega_1$  and  $\omega_2$  having a common boundary  $\Gamma = \partial\omega_1 \cap \partial\omega_2$ , provided that the traces  $U^1|_{\Gamma}$  and  $U^2|_{\Gamma}$  are the same field of  $H^{1/2}(\Gamma)$ . In Appendix 1,  $\omega$  is the boundary  $\partial\Omega$  of the considered cube in  $\mathbf{R}^3$ ,  $\omega_1$  and  $\omega_2$  are two opposite groups of three adjacent faces of  $\Omega$ :  $\omega_1 = \partial\Omega^-$ ,  $\omega_2 = \partial\Omega^+$ . Thus  $\omega$ , in this case, is not an open set of  $\mathbf{R}^3$  but a surface or "two-dimensional manifold" and  $\omega_1$  and  $\omega_2$  are "manifolds with boundary". The Sobolev spaces can be defined on abstract manifolds and the trace theorems can be obtained for manifolds with boundary (HÖRMANDER [17]). However, the involved manifolds are so simple in our case (consisting of a small number of trivial mappings) that the use of this formalism would appear overbearing and unnecessary. The only important feature of the considered situation is the low regularity of these manifolds — namely, they are piecewise  $\mathcal{C}^1$  (continuously differentiable).

The zero order trace theorem is valid for such manifolds (see e.g. [7]). Therefore, we consider it sufficient to prove the following result.

LEMMA 3

Let  $\omega_1$  and  $\omega_2$  be two disjoint open sets of  $\mathbf{R}^n$ , each with a piecewise  $\mathcal{C}^1$  boundary  $\partial\omega_i$ ,  $U^i$  be a function in  $H^1(\omega_i)$ ,  $\gamma_i$  the (well-defined) trace mappings of  $H^1(\omega_i)$  onto  $H^{1/2}(\partial\omega_i)$ , denote  $\Gamma = \partial\omega_1 \cap \partial\omega_2$  and  $\mathcal{S}$  the surface measure on  $\partial\omega_1 \cup \partial\omega_2$ . In order that the function  $U$  defined a.e. on the interior  $\omega$  of  $\omega_1^a \cup \omega_2^a$  by<sup>(2)</sup>

$$(A.12) \quad U(x) = U^i(x) \quad \text{a.e. } x \in \omega_i$$

be in  $H^1(\omega)$ , it is sufficient that

$$(A.13) \quad \gamma_1(U^1) = \gamma_2(U^2), \quad \mathcal{S} \text{ — a.e. in } \Gamma.$$

Note that, if the boundary intersection  $\Gamma$  is  $\mathcal{S}$ -negligible — in particular if  $\Gamma$  is void — no condition is imposed to the traces  $\gamma_i(U^i)$ . Also note that the results will be obviously extended to vector fields  $U^i \in \mathbf{H}^1(\omega_i) = (H^1(\omega_i))^m$ , as this is needed in Sect. 3.

PROOF. Clearly,  $U$  is in  $L^2(\omega)$ . We must show that the weak derivatives  $D_j U$  ( $j = 1, \dots, n$ ) also are functions  $V_j \in L^2(\omega)$ . Denoting  $\mathcal{D}(\omega)$  the space of infinitely differentiable functions with a compact support included in  $\omega$ , we have by definition

$$(A.14) \quad \forall \varphi \in \mathcal{D}(\omega) \quad \langle D_j U, \varphi \rangle = - \langle U, D_j \varphi \rangle = - \sum_{i=1}^2 \int_{\omega_i} U^i D_j \varphi \, dv.$$

Since  $U^i \in H^1(\omega_i)$ , the weak derivatives  $D_j U^i$  are functions  $V_j^i \in L^2(\omega_i)$ . We extend these functions to  $\omega$  by zero in  $\omega \setminus \omega_i$ , with the same notation. We may write for  $i = 1, 2$  and  $j = 1, \dots, n$ :

$$(A.15) \quad \int_{\omega_i} (U^i D_j \varphi + \varphi D_j U^i) \, dv - \int_{\partial\omega_i} \varphi \gamma_i(U^i) n_j^i \, d\mathcal{S} = 0,$$

where  $n_j^i$  ( $j = 1, \dots, n$ ) are the components of the  $\mathcal{S}$  — a.e. defined outer normal  $\mathbf{n}^i$  to  $\partial\omega_i$  ( $i = 1, 2$ ). Indeed, for a fixed  $\varphi \in \mathcal{D}(\omega)$ , this equality writes  $\Phi^i(U^i) = 0$  with a continuous linear form  $\Phi^i$  on  $H^1(\omega^i)$  (the continuity of the first integral follows from the definition of the  $H^1$  space and the Cauchy–Schwartz inequality in  $L^2(\omega_i)$ ; the continuity of the second integral results from the continuity of the trace mapping  $\gamma_i$  and the Cauchy–Schwarz inequality in  $L^2(\partial\omega_i)$ ). Since, by the divergence theorem,  $\Phi^i(U^i) = 0$  when

<sup>(2)</sup> If  $\Omega$  is a subset of  $\mathbf{R}^n$ ,  $\Omega^a$  denotes the closure of  $\Omega$ .

$U^i$  is a function in  $\mathcal{D}(\mathbf{R}^n)$  and since  $\mathcal{D}(\mathbf{R}^n)$  is dense in  $H^1(\omega_i)$ , we have (A.15) for every  $U^i \in H^1(\omega_i)$ . (This implies that  $\gamma_i(\varphi U^i) = \varphi \gamma_i(U^i)$ ). Therefore

$$(A.16) \quad \langle D_j U, \varphi \rangle = \sum_{i=1}^2 \int_{\omega_i} \varphi D_j U^i dv - \sum_{i=1}^2 \int_{\partial\omega_i} \varphi \gamma_i(U^i) n_j^i d\mathcal{S},$$

but the sum of the integrals on  $\partial\omega_i$  vanish, because  $\varphi = 0$  on  $(\partial\omega_1 \cup \partial\omega_2) \setminus \Gamma$  (since this set belongs to  $\partial\omega$ ),  $\mathbf{n}^1 + \mathbf{n}^2 = 0$  and  $\gamma_1(U^1) = \gamma_2(U^2)$   $\mathcal{S}$  — a.e. on  $\Gamma$ . Defining  $V_j = V_j^1 + V_j^2$  in  $L^2(\omega)$ , we have thus

$$(A.17) \quad \langle D_j U, \varphi \rangle = \int_{\omega} V_j \varphi dv = \langle V_j, \varphi \rangle$$

which proves Lemma 3.

### Appendix 3

#### 1. Proof of Lemma 1

Since  $f_0$  is continuous,  $f_0(E_0)$  is dense in  $f(E) = F$  and since  $F$  is finite-dimensional, the linear subspace  $f_0(E_0)$  is closed, hence  $f_0(E_0) = F$ . Let  $p$  be the canonical mapping of  $E_0$  onto  $E'_0 = E_0/\text{Ker } f_0$  and  $f_0 = f'_0 \circ p$  the corresponding factorization. Again, the finite dimension of  $F$  implies that  $f'_0$  is a bicontinuous one-to-one linear mapping of  $E'_0$  onto  $F$ : in particular,  $f'_0$  is an open mapping. That  $p$  also is an open mapping, follows easily from the definitions of the quotient space  $E'_0$  and its topology (e.g. DIEUDONNE [8]). Thus, the composite  $f_0$  is an open mapping. Let  $U$  be an open set in  $E$  and  $X$  an arbitrary point in  $U$ . There is an  $\eta > 0$  such that the open ball  $B(X, 2\eta)$  of radius  $2\eta$  is in  $U$ , hence, for every  $Y \in B(X, \eta)$  the ball  $B(Y, \eta)$  is in  $U$ . Since  $f_0$  is open and linear, it is easy to see that  $f_0$  is "uniformly open", i.e. there is a  $\delta > 0$  such that  $B(f(X_0), \delta) \subset f(B(X_0, \eta) \cap E_0)$  holds for every  $X_0 \in E_0$ . Since  $f$  is continuous, there is an  $\varepsilon > 0$  such that  $f(B(X, \varepsilon)) \subset B(f(X), \delta)$  and it is possible to choose  $\varepsilon \leq \eta$ . The subspace  $E_0$  being dense in  $E$ , there is an  $X_0 \in B(X, \varepsilon) \cap E_0$ , whence  $f(X_0) \in B(f(X), \delta)$  or equivalently  $f(X) \in B(f(X_0), \delta)$  which is in  $f(B(X_0, \eta) \cap E_0)$ . But since  $\varepsilon \leq \eta$ ,  $X_0$  belongs to  $B(X, \eta)$  and thus  $B(X_0, \eta) \subset U$ . Hence  $f(X) \in f(U \cap E_0)$ , which completes the proof. The proof is also valid for metric linear topological spaces.

#### 2. Proof of Lemma 2

Denote

$$A^\delta = \{x; d(x, A) = [\text{Inf}(\|x - y\|; y \in A)] \leq \delta\}.$$

The assumed regularity of  $\partial\omega$  implies that  $v(\partial\omega)^\delta$  vanishes with  $\delta$ . For every  $\delta > 0$  there exists an infinitely differentiable function  $\varphi_\delta$  such that

$0 \leq \varphi_\delta \leq 1$ ,  $\varphi_\delta(x) = 1$  if  $d(x, \partial\omega) \leq \delta/2$  and  $\varphi_\delta(x) = 0$  if  $d(x, \partial\omega) \geq \delta$ . From the "trace theorem of zero order" (e.g. [7]), we know that there exists a field  $\mathbf{W} \in \mathbf{H}^1(\omega)$  such that  $\mathbf{W}|_{\partial\omega} = \mathbf{U}$ . For any  $\delta > 0$ , we have also  $(\varphi_\delta \mathbf{W})|_{\partial\omega} = \mathbf{U}$  and moreover

$$(A.18) \quad \int_{\omega} \|\varphi_\delta \mathbf{W}\| \, dv \leq \int_{(\delta\omega)} \|\mathbf{W}\| \, dv \rightarrow 0 \quad \text{as } \delta \rightarrow 0$$

whence Lemma 2 follows.

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