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Kinematics of Media with Continuously Changing Topology

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The fundamental postulate of continuum mechanics states that a body is a three-dimensional differentiable manifold and its motions are diffeomorphisms. Simple thought experiments with cyclic motions of dislocations show that they do not preserve topology (set of neighborhoods). The same is valid for chaotic and turbulent motions with coarse-graining. To describe such motions, kinematics of a generalized continuum mechanics is suggested. Observables are defined operationally in the laboratory system which is not anymore equivalent to the Lagrangian picture. The body is a submanifold of a higher-dimensional space and generalized motions are its diffeomorphisms. In a gauge-theoretic interpretation, the motion is a translational connection with the curvature identified as a "dislocation" density-flux.

1. INTRODUCTION

Elasticity and plasticity, fracture and viscoplasticity, laminar and turbulent flows are quite different physical phenomena, but they have a common denominator in their mathematical description: kinematics of a continuum medium. In the scope of continuum mechanics any body is considered as a (material) three-dimensional manifold. Its motion is a time-dependent family of diffeomorphisms completely characterized by basic kinematic fields: velocity, deformation gradient, strain, etc. As a result, the motion preserves topology of the body (close points remain close) and there are two equivalent descriptions: with respect to a reference state (material or Lagrangian) and with respect to a current state (spatial or Eulerian). Diversity of the mentioned phenomena is reflected in constitutive laws and some additional fields such as plastic strain, damage, etc.

Historically, the first mathematical models were developed for elastic deformations and laminar flows. Description of these motions as diffeomorphisms and of the bodies as differentiable manifolds is completely

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adequate physically. On the other hand, extension of these mathematical models to plastic, turbulent, mixing motions is conceptually troubling and may be justified by arguments of mathematical convenience only: if motion is not a diffeomorphism, then what is it?

The purpose of this paper is to show that mixing-type motions which do not preserve (three-dimensional) topology may be described as diffeomorphisms of an extended phase space and thus a body still is a material manifold, but of a higher dimension. In Section 2, the basic notions of classical continuum mechanics (in a space-time form) are briefly outlined. In Section 3, thought experiments with cyclic motions of dislocations in an ideal crystal are considered. The motions visually illustrate a phenomenon of *perestroika*: initially neighboring atoms travel far from each other, though the crystal remains ideal. In this sense, the motions do not preserve the topology (the set of neighborhoods) of the crystal. The same is valid for chaotic (turbulent) motions. Formally, they are described as families of diffeomorphisms, but the slightest coarse-graining does not preserve the topology. Basic problems are formulated: how to describe such motions in the scope of continuum mechanics, what are the defining measurable observables, what is a body, what is the role of coarse-graining?

In Section 4, an outline of kinematics of a generalized continuum mechanics (GCM) is given. The basic observables of GCM admit operational definitions in the laboratory system. Only the current state has a definite physical meaning, and the Eulerian and Lagrangian pictures are not equivalent anymore. The body is a material manifold, but of a higher dimension and motions are its diffeomorphisms.

In Section 5, a gauge-theoretic approach is considered. Motions in GCM are identified with a translational connection. The corresponding curvature has the meaning of a dislocation density-flux. Coarse-graining as a bridge between mixing (turbulent) motions and GCM is discussed in the last section.

2. KINEMATICS IN CLASSICAL CONTINUUM MECHANICS

Continuum mechanics (CM) identifies a body $\mathfrak{B}$ with a three-dimensional differentiable manifold, and motions are families of time-dependent diffeomorphisms χ_t of $\mathfrak{B}$ into the Euclidean space E_3 (see, e.g., Truesdell, 1977). Let us fix a rectilinear coordinate system in E_3 and let X^i and x^i be the coordinates of a material point $\mathbf{X}$ at $t=0$ and its position $\mathbf{x}$ at the time t, i.e.,

$$\chi_t: \quad \mathbf{X} \to \mathbf{x}: \quad x^i = x^i(\mathbf{X}, t) \tag{2.1}$$

The basic kinematic fields are the velocity $\mathbf{V}(\mathbf{X}, t)$ and the deformation gradient $\Phi(\mathbf{X}, t)$

$$V^i = \partial_t x^i(\mathbf{X}, t), \qquad \Phi^i_j = \frac{\partial x^i(\mathbf{X}, t)}{\partial X^j} \tag{2.2, 2.3}$$

Using absolute parallelism in E_3 these fields can be shifted from the initial (reference) point $\mathbf{X}$ to the current point $\mathbf{x}$ defining

$$v^i(\mathbf{x}, t) = V^i(\mathbf{X}(\mathbf{x}, t), t), \qquad F^i_j(\mathbf{x}, t) = \Phi^i_j(\mathbf{X}(\mathbf{x}, t), t) \tag{2.4}$$

Similarly, all other fields, such as strain, stress, etc., may be considered as functions of $\mathbf{X}$, t or $\mathbf{x}$, t. It is said that the body is considered in the reference state (Lagrangian picture) or in the current state (Eulerian picture, laboratory system), respectively. It is important that the Lagrangian and Eulerian pictures are equivalent.

Notice that $3+9$ fields (2.3) or (2.4) are defined by 3 fields (2.1) and thus are not independent. The corresponding integrability conditions are given below. Let $X = (t, \mathbf{X})$ and $x = (t, \mathbf{x})$ be points of the Galilean space-time E_G and let us introduce 4-velocity $v = (1, \mathbf{v})$, 4-gradient

$$h = \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{v} & F \end{pmatrix} \tag{2.5}$$

and its inverse

$$h^{-1} = \begin{pmatrix} 1 & \mathbf{0}^T \\ -F^{-1}\mathbf{v} & F^{-1} \end{pmatrix} \tag{2.6}$$

The form of h is dictated by the Galilean invariance.

It can be shown (Kunin and Kunin, 1986) that the integrability condition in the laboratory system has the form

$$\Omega(x) \equiv h(x)\partial \wedge h^{-1}(x) = 0 \tag{2.7}$$

or, in components,

$$\Omega^\mu_{\alpha\beta} = h^\mu_\lambda[\partial_\alpha(h^{-1})^\lambda_\beta - \partial_\beta(h^{-1})^\lambda_\alpha] = 0 \tag{2.8}$$

where $\partial_\alpha = \partial/\partial x^\alpha$ and $\alpha, \beta, \ldots = 0, 1, 2, 3$. In the space representation, this is equivalent to the conditions

$$\nabla \wedge F^{-1} = 0, \qquad (\partial_t + \mathbf{v} \cdot \nabla + \nabla \mathbf{v})F^{-1} = 0 \tag{2.9}$$

At a point $x \in E_G$, the tensor h_x defines an invertible linear transformation of (tangent) vectors, i.e., $h_x \in GL(4)$ [more exactly, h_x belongs to a subgroup of matrices of the form (2.5) invariant with respect to the Galilean transformations]. The tensor field $h(x)$ is an element of a group H of space-time-dependent linear transformations. The elements satisfying the integrability conditions (2.7) will be called holonomic transformations.

The one-to-one correspondence between the motions (modulo rigid body translations) and holonomic transformations permits one to identify them and call them holonomic motions (to be distinguished from more general motions below).

3. MOVING DEFECTS, DISLOCATIONS

An important part of solid state physics and material science is devoted to the description of moving defects: point defects, dislocations, cracks, crazes, etc. At a macrolevel of CM these phenomena are modeled as diffusion, plasticity, damage, fracture, etc. Still, the fundamental postulate states that the body is a material manifold and motion is a family of its diffeomorphisms χ_t (plus motion of defects). As a result, the Lagrangian and Eulerian pictures remain equivalent. To examine the validity of this postulate, let us consider a thought experiment with cyclic dislocation fluxes.

Figure 1 shows the result of passing of a dislocation pileup through an ideal crystal from the left to the right. We denote this operation by the arrow $\rightarrow$. Similarly, $\downarrow$, $\leftarrow$, $\uparrow$ denote the same motions of dislocations in the directions of arrows. We call the composition of the operations $\uparrow\leftarrow\downarrow\rightarrow$ a cycle.

Figure 2a shows a crystal with some of its atoms marked (others are not shown). Positions of the marked atoms after 2 and 4 cycles are shown in Figures 2b and c, respectively. For simplicity, periodic boundary conditions are assumed. In Figure 3, the marked atoms form initially a grid.

A comment about these thought experiments should be made. If we assume that the marked atoms are initially true neighbors, then the corresponding dislocation density would be unrealistically high. To achieve the same qualitative results in the case of more realistic dislocation densities, the number of cycles should be greater (by a factor of 10^2–10^3). The

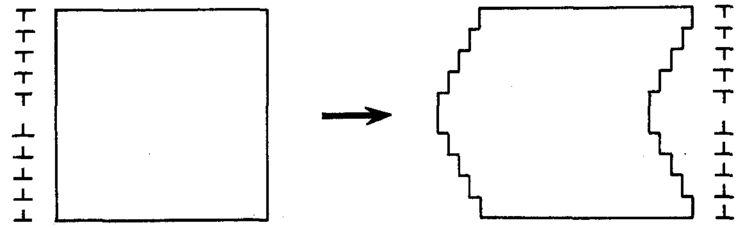

Fig. 1. The result of passing of the dislocation pileup.

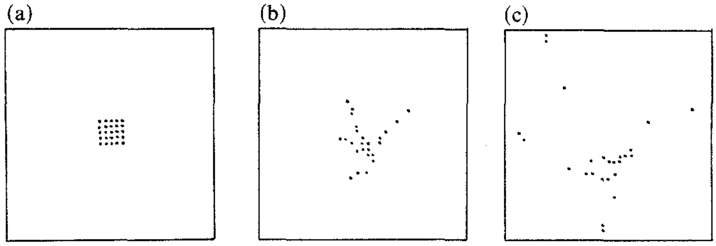

Fig. 2. (a) A crystal with some of its atoms marked (others are not shown). (b) After 2 cycles. (c) After 4 cycles.

conclusion is that cyclic motions of dislocations result in a phenomenon of mixing (*perestroika*) and that these effects may be important.

As an example, one can point to metallurgical rolling (Metals Handbook, 1985). At the crystallographic scale, the process qualitatively may be similar to that shown above. At the scale of the grains, the process results in curly grain structures, slip lines, deformation twins, kink bands. At the next microscopic scale, the characteristic features include material fibering, flow lines, shear bands, and Lüders lines. Finally, at the macroscopic CM scale, the process is described as a continuous plastic deformation and all information on *perestroika* is lost.

An important lesson is that *perestroika* is intimately related to coarse-graining. Notice that, for the thought experiments indicated above, the crystal structure (or discreteness of slip lines) played the role of coarse-graining. After establishing a quantitative measure for *perestroika*, the transition to a continuum description is possible and quite natural. On the contrary, assuming the dislocation flux to be continuous from the very beginning misses the effect of *perestroika* completely. Thus, the order of transitions to limits is essential.

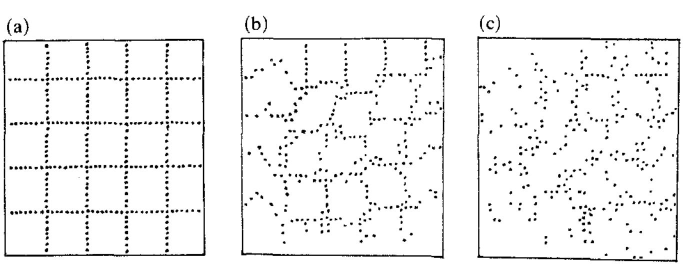

Fig. 3. The same as Figure 2, with marked atoms forming initially the grid.

A similar situation arises if we want to describe mixing properties of a Hamiltonian system (Guckenheimer and Holmes, 1983). Let $\Delta\Gamma$ be the volume of a phase space droplet which does not depend on time (Liouville theorem). If the motion is mixing, the droplet spreads out over the phase space as $t \to \infty$. Let us assume that the phase space is ε-coarse-grained and let $\Delta_\varepsilon\Gamma(t)$ be the corresponding coarse-grained volume of the droplet. It is clear that $\Delta_\varepsilon\Gamma(t)$ asymptotically increases with time. The Kolmogrov entropy K defined as

$$K = \lim_{\varepsilon \to 0} \lim_{t \to 0} \ln \Delta_\varepsilon \Gamma(t) \tag{3.1}$$

is a measure of mixing. The measure does not depend on a choice of coarse-graining, but the order of limits is essential.

Note that the Kolmogrov entropy K is closely related to the Liapunov exponent λ and the correlation time τ. Namely, $K \sim \lambda \sim \tau^{-1}$. The computations provided for the above cycles of ideal dislocation flows are in agreement with these estimates.

Now we are in a position to formulate the basic problem: how do we incorporate *perestroika*-type phenomena which do not preserve topology (the set of neighborhoods) into the formalism of continuum mechanics? In particular: what is a body, what is a motion, what are the basic measurable quantities? As a partial answer to these questions, we outline a mathematical structure for the kinematics of a generalized continuum mechanics.

4. GENERALIZED KINEMATICS

As a key step, let us first define measurable quantities (basic observables). All other observables will be uniquely determined through the basic ones. An operational requirement: all measurable quantities must be defined in the laboratory system.

We restrict ourselves to the following minimal set of basic observables: the mass density $\rho(\mathbf{x}, t)$, the velocity $\mathbf{v}(\mathbf{x}, t)$, and the rate of deformation $\dot{F}(\mathbf{x}, t)$. It is essential that $\mathbf{v}$ and $\dot{F}$ are considered as independently measurable quantities, for example, by an appropriate averaging of the mass and momentum fluxes, respectively. Here we do not go into the details of the operational definitions.

The velocity field $\mathbf{v}(\mathbf{x}, t)$ defines a holonomic motion χ_t and the corresponding deformation gradient $F_0(\mathbf{x}, t)$ as a solution of the integrability equations (2.9) with the initial data $F_0(\mathbf{x}, 0) = I$ (unit tensor). Similarly, $\dot{F}(\mathbf{x}, t)$ defines the deformation tensor field $F(\mathbf{x}, t)$ modulo initial data $F(\mathbf{x}, 0)$. Then the equation $F = F_0 F_*$ defines a decomposition of F into the holonomic F_0 and nonholonomic (plastic) $F_* = F_0^{-1} F$ components. It is worth mentioning that $\mathbf{v}$ is a coarse-graining-based velocity. Therefore the family of diffeomorphisms χ_t determined by $\mathbf{v}$ does not describe paths of material particles.

The space-time deformation tensor field

$$h(x) = \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{v} & F \end{pmatrix} \tag{4.1}$$

is identified with a (generally) nonholonomic motion or transformation. A measure of nonholonomicity is given by the tensor field (compare to (2.7))

$$\Omega(x) = h\partial \wedge h^{-1} \tag{4.2}$$

The time and space components of $\Omega(x)$ can be identified with dislocation density and flux, respectively (Kunin and Kunin, 1986). In particular, $F(\mathbf{x}, 0) = F_*(\mathbf{x}, 0)$ is determined by the initial dislocation density. Depending on the scale to which the model applies, Ω describes either dislocations in a crystal or macroscopic sources of plastic deformations (quasidislocations).

There are two possible interpretations of (4.2): first, this is the definition of Ω; second, the dislocation density and flux are independently measurable quantities, and (4.2) is a meaningful equation whose validity has to be checked experimentally.

In the scope of this kinematic model, the state of the body is completely defined by two space-time fields: $\rho(x)$ and $h(x)$ (the extended models may also include internal degrees of freedom as indicated below). Geometrically, the body B is the (4+4)-dimensional tangent bundle TE_G equipped with an extension of the measure ρ. Motions are special diffeomorphisms of TE_G defined by $h \in H$: h_x transforms the tangent space T_xE_G at each point $x \in E_G$.

Generally, nonholonomic $h(x)$ describe underlying microscopic motions in average only. For holonomic h, $\Omega = 0$ and we return to the usual kinematics of CM.

5. A GAUGE-THEORETIC APPROACH

First, it is necessary to clarify in what sense "gauge theory" will be understood here. As a rule, physicists identify gauge theory (GT) with the Yang–Mills gauge theory (YM-GT). The characteristic feature of the YM-GT is the action of a group on internal degrees of freedom rather than on the space-time. In a more general understanding of GT, the group action is extended to the space-time as well, and gauge fields are related to a connection on a principal fiber bundle (Trautman, 1980). The fundamental group of continuum mechanics is the group of affine motions acting on E_G and thus the gauge fields should be related to affine connections rather than to the usual linear connections. Our approach follows Kunin and Kunin (1986). Different models are developed by Kadić and Edelen (1983) and Edelen and Lagoudas (1988).

An affine connection on E_G is a pair (∇, h), where ∇ is a linear connection (covariant derivative) and $h = h(x)$ is a tensor field of type $(1, 1)$ which may be identified with the translational connection (Kobayashi and Nomizu, 1963). The connection (∂, I) corresponds to the usual absolute parallelism in E_G. The deviation from the absolute parallelism is characterized by an affine curvature $\mathfrak{R} = (R, S, \Omega)$. Here $R(x)$ is the curvature of ∇, S is the torsion of ∇ (translational component of (∇, I)), and $\Omega(x)$ is the translational curvature, i.e., the curvature of the pure translational connection (∂, h) [see (5.1) below]. The tensors S and Ω of the type $(1, 2)$ have similar (but not identical) properties and there is a tendency in the literature to confuse them.

From a group-theoretic point of view, it is quite natural to identify the translational component h of the connection (∇, h) with the motion $h(x)$ introduced above. Let u, v be two arbitrary vector fields. Then the translational curvature Ω is given by (Kunin and Kunin, 1986)

$$\Omega(u, v) = h[(\nabla_u h^{-1})v - (\nabla_v h^{-1})u] \tag{5.1}$$

where ∇_u is the covariant derivative in the direction u. For the special case $\nabla = \partial$, $u = \partial_\alpha$, $v = \partial_\beta$, (5.1) specializes to (4.2). It follows that the translational curvature Ω can be identified with the dislocation density-flux (for nontrivial ∇).

The curvature R and torsion S are related to the internal degrees of freedom: disclinations and spin dislocations which have not been considered above. These as well as other internal variables (microcrack density, temperature, etc.) require additional state variables and the corresponding extension of the kinematics.

In the modern approach, CM is represented in a coordinate-free form that leads to a deeper mathematical and physical insight. Notice that "coordinate-free" means invariance with respect to holonomic coordinate transformations. The gauge approach extends essentially the invariance group. The requirement of invariance (covariance) with respect to a group G of gauge transformations is an intrinsic part of GT. In the case of continuum mechanics, G can be isomorphic to H and interpreted as a group of moving nonholonomic frames. As a result, the equations of continuum mechanics can be represented in a gauge-covariant form which is especially useful for nonholonomic motions.

However nice these applications of GT are, the most important contribution of GT can be expected in the construction of complex models for different interacting fields. First, it is important to classify variables into gauge fields and matter fields. For example, with respect to the translation group, motions h and dislocations Ω are gauge fields, whereas temperature, damage, and electromagnetic fields in the medium are matter fields. With respect to other groups, the latter themselves can be Yang–Mills-type gauge fields.

Second, the construction of a complex model can be split into successive "gaugings." For example, let us consider an elastic body as an initial model. Successive gaugings with respect to translations, rotations, etc., lead to the introduction of new kinematic variables corresponding to dislocations, spin dislocations, disclinations, etc.

These examples indicate that the GT approach can be a useful heuristic tool in the development of new complex models.

6. DISCUSSION

It is shown above that the *perestroika*-type motions which do not preserve topology of the 3D body can be described in terms of smooth invertible mappings of an extended space. A bridge between real motions and their mathematical models is an appropriate coarse-graining. In connection with this, two basic questions may be discussed. Is there any trace of coarse-graining in generalized kinematics? Are coarse-graining and generalized kinematics applicable to different types of mixing (turbulent) motions?

Coarse-graining of space-time is characterized by two (small) scales: time τ and length l. Mathematical models taking into account the existence of these elementary scales deal with a quasicontinuum (quantized space-time) rather than with the usual space-time (Kunin, 1980, 1982). In this case an admissible class of (analytic) functions automatically takes care of elementary scales. Another situation arises if the scales τ and l are not fixed, but rather are variable parameters of state (resolution of a microscope). An appropriate kinematic description may be obtained using coherent states or wavelet transforms (Klauder and Skagerstam, 1985).

Now let us consider chaotic (mixing) motion of a Hamiltonian system or the Lorentz-type system. Formally, the motion is a family of diffeomorphisms x_t: $\mathbf{X} \to x(\mathbf{X}, t)$ of initial positions into their images, but for $t \gg \tau = \lambda^{-1}$ (λ is the Liapunov exponent) the motion completely "forgets" the initial data. As a result, the smallest coarse-graining destroys diffeomorphisms and the motion is nonholonomic rather than holonomic.

In the case of turbulent motion of a viscous fluid, in addition to a time scale $\tau \sim \lambda^{-1}$ there exists a characteristic length l (Kolmogorov scale). Typically scales of interest are much bigger than τ and l, which justifies the introduction of coarse-graining and the description of motion as nonholonomic. In particular, in the scope of the generalized kinematics, the rate of rotation can be different from curl **v**. This difference is in principle measurable.

We conclude that the existence of scale parameters in mixing-type motions leads in a natural way to GCM. Conversely, the physical interpretation of GCM is related to an appropriate coarse-graining.

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