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Geometry of Material Space : Its Consequences in Modern Computational Means

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Applications of the concepts of material manifold, pseudo-momentum and Eshelby stress (canonical « material » momentum and stress) to efficient numerical schemes in the thermomechanics of solids are given. These schemes are that of the finite-element method *whose uncritical application may cause the appearance of spurious configurational forces, that for the* finite-element method *where the balance of canonical momentum provides a powerful tool to study the accuracy of the constructed scheme, natural boundary conditions in gradient theories, and a perturbational approach to localized nonlinear waves, and that of the* finite-volume method *which seems to be particularly well adapted to treat the numerics of wave-like motions in thermomechanical theories of materials. The latter method here is akin to a continuous cellular automaton.*

1 Introduction

In recent years we have devoted much energy to the development of what we called indifferently the *mechanics of continua on the material manifold*, *Eshelby's continuum mechanics*, or, more fancyfully, $\boldsymbol{M}^3$, the *«Material Mechanics of Materials »*. The essential idea of this formulation is that a *canonical* formulation of continuum mechanics (and more generally physics) can only be given on the *material manifold*, i.e., the continuous set of material points that build up the body under consideration (cf. Maugin, 1993, 1995), this in contrast to the classical formulation in physical space, the space of *placements* as the body evolves in time. The main ingredient in this formulation is the expression of the *balance of « pseudo-momentum »* (also called material momentum or canonical momentum) which appears to be generated by virtual displacements or velocities on the material manifold (a change of « particle » or « labelling » rather than an actual change of physical placement of the same particle). This somewhat original viewpoint, that is desorienting and puzzling to many engineers, in fact is the arena of the *intrinsic* formulation of structural rearrangements manifested by the presence of a continuous distribution of defects such as dislocations (cf. Epstein and Maugin, 1990), of anelasticity (cf. Epstein and Maugin, 1995, 1996, 1997; Cleja-Tigoiu and Maugin, 1999), growth (Epstein and Maugin, 1999), phase transitions (Maugin and Trimarco, 1995), damage, etc. It is also the stage on which *driving forces* on micro and macro-defects play, whether in fracture (cf. Maugin and Trimarco, 1992) or more generally at singular sets of points in a material body (cf. Maugin, 1998a). Most of these are reviewed in a synthesis work (Maugin, 1999a) that emphasizes the fact that the balance equation of pseudo-momentum plays the same ontological role as the energy balance, i.e., it is canonical and gathers contribution of *all fields* involved in the considered theory of continua. This relates to the fact that it is the *conservation law* that is associated with the spatial parametrization of the physical modelling and this parametrization applies to all fields involved, whether of mechanical nature or not. Simultaneously, it is the equation that brings up the notion of *material inhomogeneity* to the foreground.

It is usually, and correctly, remarked that at all regular material points, the balance of pseudo-momentum is « equivalent » to the balance of physical momentum. The reason for this is that at all such points, the former can be deduced from the latter by some algebraic and analytic operations allowed by the smoothness of the fields. That is, at such points the balance of pseudo-momentum is an *identity*. However, it is not exactly true that both equations of momentum are operationally equivalent, being then only two different « projections » on different manifolds, of the same equation, because they *cannot* play the same role in problem solving. This is due to the fact that, whether we like it or not, applied forces - which are real physical forces in the Newtonian-Euler-Cauchy sense - are prescribed in physical space (a world to which they belong by definition) so that they intervene in problem solving in the equations (field equations and boundary conditions) expressed in that space. Therefore, initial-value boundary-value problems are, of necessity, solved, analytically or numerically, in physical space. The question then arises of the usefulness of the balance of pseudo-momentum at regular material points, its role in capturing singularities being clear at singular points. This usefulness resides is the redundancy between the two (essentially vectorial) equations as it can be exploited thus. While the balance of physical momentum - and other equations governing other fields than deformation -, are used in the direct problem solving, the balance of pseu-

do-momentum (or its « equilibrium » form where this applies) is to be exploited either in the form of a *criterion* to be satisfied by the already obtained point-wise field solution (e.g., in fracture, phase-transition, anelasticity, etc), or as a way to checking globally the accuracy and quality of the obtained solution. This is very similar to the exploitation of the energy balance in the numerics of hyperbolic systems where the accurarcy of the adopted scheme is measured by a global energy criterion (i.e., does the scheme conserve energy ?). Herein below we focus attention on such an application of the balance of pseudo-momentum in various numerical techniques, noting in passing that the notion of momentum is vectorial, and therefore « directional », and thus richer than that of energy (a scalar) which addresses only magnitude. Three numerical techniques are briefly examined in the light of recent progresses. Before, however, a simple reminder of basic equations is useful.

2 Reminder

For the sake of example, we consider as *field* the deformation of a materially homogeneous, finitely deformable elastic body (no thermal effects). The *field* therefore is the so-called *placement*

$$\mathbf{x} = \chi(\mathbf{X}, t) \tag{1}$$

where $(\mathbf{X}, t)$ provides the *space-time parametrization*. $\mathbf{X}$ represents the material point or « particle » on the material manifold (in fact the three *material* coordinates), and t is the Newtonian time. The same parametrization would hold for other physical fields such as the scalar electric potential and the magnetic vector potential of electromagnetism, or any other field of interest (e.g., a microstructure). The peculiarity of equation (1) is that the field itself, $\mathbf{x}$, is a space parametrization, but in *physical space* E^3. Let $\mathbf{f^0}$ be an applied (physical) body force. Then the local balance equations of mass, linear (physical) momentum, energy, and canonical (material or « pseudo ») momentum are given by :

$$\left.\frac{\partial \rho_0}{\partial t}\right|_{\mathbf{X}} = 0 \tag{2}$$

$$\left.\frac{\partial \mathbf{p}}{\partial t}\right|_{\mathbf{X}} - div_R \mathbf{T} = \mathbf{f}^0 \tag{3}$$

$$\left.\frac{\partial H}{\partial t}\right|_{\mathbf{X}} - \nabla_R.(\mathbf{T}.\mathbf{v}) = \mathbf{f}^0.\mathbf{v} \tag{4}$$

$$\left.\frac{\partial P}{\partial t}\right|_{\mathbf{X}} - div_R \mathbf{b} = \mathbf{F}^0 \tag{5}$$

where we have set

$$\mathbf{v} = \left.\frac{\partial \chi}{\partial t}\right|_{\mathbf{X}} \qquad \mathbf{F} = \left.\frac{\partial \chi}{\partial \mathbf{X}}\right|_{t} = \nabla_R \chi \tag{6}$$

$$H = K + W \qquad K = \frac{1}{2}\rho_0 \mathbf{v}^2 \qquad W = W(\mathbf{F}) \tag{7}$$

$$\mathbf{p} = \rho_0 \mathbf{v} \qquad \mathbf{T} = \partial W / \partial \mathbf{F} \tag{8}$$

$$P = -\mathbf{p}.\mathbf{F} \qquad \mathbf{F}^0 = -\mathbf{f}^0.\mathbf{F} \qquad \mathbf{b} = (W - K)\mathbf{1}_R - \mathbf{T}.\mathbf{F} \tag{9}$$

Here $\mathbf{p}$ is the linear (physical) momentum with components in physical space, $\mathbf{T}$ is the first Piola-Kirchhoff stress, P is the so-called « pseudo-momentum » - it has covariant components on the material manifold - , $\mathbf{b}$ is the *Eshelby (material) stress tensor*, and $\mathbf{F^0}$ is a material force. But this one is simply the pull-back of a physical force onto the material manifold. Had we considered a materially inhomogeneous body (explicitly $\mathbf{X}$- dependent ρ_0 and W), we would have found in the right-hand side of equation (5) an additional term reflecting directly this

inhomogeneity. From the point of view of *invariance*, equation (3) reflects the lack of invariance of the physical system under physical-space translations because of the presence of a physical forces $\mathbf{f}^0$, equation (4) relates to the invariance, of lack of invariance, under time translations, and equation (5) relates to the invariance or lack of invariance under translation on the material manifold (**X** translation). The first one relates to a field, the other two to the space-time parametrization. This would follow from the application of Noether's second theorem, had we considered a Hamiltonian-Lagrangian variational formulation. But, in truth, equation (5) can be deduced identically from equation (3) by mutliplying the latter to the right by **F** and integrating by parts (for well-behaved **F**s), and this constitutes the essence of the *Ericksen-Noether identity*. For instance, in *quasi-statics* (neglect of inertia terms), equations (3)-(5) reduce to

$$div_R \mathbf{T} + \mathbf{f}^0 = \mathbf{0} \tag{10}$$

$$\left.\frac{\partial W}{\partial t}\right|_{\mathbf{X}} = \nabla_R.(\mathbf{T}.\mathbf{v}) + \mathbf{f}^0.\mathbf{v} \tag{11}$$

$$div_R \mathbf{b} + \mathbf{F}^0 = \mathbf{0} \tag{12}$$

respectively. At all regular material points **X** we have the following *Ericksen-Noether identity*

$$\left(div_R \mathbf{T} + \mathbf{f}^0\right)\mathbf{F} + \left(div_R \mathbf{b} + \mathbf{F}^0\right) = \mathbf{0} \tag{13}$$

Note that equation (10), valid at all regular points $\mathbf{X}$ *in* Ω_t, and the associated *natural boundary* condition at $\partial\Omega_t$,

$$\mathbf{N}.\mathbf{T} = \mathbf{t}^0 \tag{14}$$

are equivalent to the following *weak formulation* (principle of virtual power)

$$P^*_{(i)} + P^*_{(c)} + P^*_{(v)} = 0 \tag{15}$$

where

$$P^*_{(i)} = -\int_{\Omega_t} \mathrm{T} : (\nabla_{\mathrm{R}} \mathbf{v}^*)^T \, d\Omega \qquad P^*_{(c)} = \int_{\partial\Omega_t} \mathbf{t}^0.\mathbf{v}^* \, dS \qquad P^*_{(v)} = \int_{\Omega_t} \mathbf{f}^0.\mathbf{v}^* d\Omega \tag{16}$$

Equation (15) holds for all sufficiently smooth vectorial test functions (physical velocity fields) $\mathbf{v}^*$. It is the basis of *finite-element computations*. What is the consequence for the variational equation satisfied by **b** ? To see this multiply equation (13) by $\mathbf{F}^{-1}$ to the right, multiply the result scalarly by the test function $\mathbf{v}^*$, and account for equation (15) to obtain the following expression:

$$-\int_{\Omega_t} \mathbf{b} : (\nabla_R \mathbf{V}^*)^T \, d\Omega + \int_{\partial\Omega_t} \mathbf{N}.\mathbf{b}.\mathbf{V}^* \, dS + \int_{\Omega_t} \mathbf{F}^0.\mathbf{V}^* \, d\Omega = 0 \tag{17}$$

for all *virtual material* velocity fields $\mathbf{V}^* = -\mathbf{F}^{-1}.\mathbf{v}^*$. This is formally equivalent to equation (15). But one should note that the second term in equation (17) does not correspond to a prescribed surface stress. Because of this, equation (17) is not applicable as such, i.e., as a weak formulation of the original boundary-value problem. Rather, we note that for any velocity field we have

$$\int_{\partial\Omega_t} \mathbf{N}.\mathbf{b}.\mathbf{V}^* \, dS = \int_{\partial\Omega_t} (\mathbf{N}.\mathbf{V}^*) W \, dS + \int_{\Omega_t} \mathbf{t}^0.\mathbf{v}^* d\Omega \tag{18}$$

so that we obtain the following **original** result (note that **N** is directed outward):

$$G(\Omega_t; \mathbf{V}^*) \equiv -\int_{\partial\Omega_t} W(\mathbf{N}.\mathbf{V}^*) dS = -\int_{\Omega_t} \mathbf{b} : (\nabla_R \mathbf{V}^*)^T \, d\Omega + \int_{\Omega_t} \mathbf{T} : (\nabla_R \mathbf{v}^*)^T \, d\Omega \tag{19}$$

For a self-equilibrated (Piola-Kirchhoff) stress field ($\mathbf{f}^0 = \mathbf{0}, \mathbf{t}^0 = \mathbf{0}$), we have

$$\int_{\Omega_t} \mathbf{T} : (\nabla_R \mathbf{v}^*)^T \, d\Omega \equiv 0 \tag{20}$$

so that (19) reduces to the following formula for the *flux of elastic energy outward* the material volume Ω_t for a material velocity field $\mathbf{V}^*$:

$$G(\Omega_t; \mathbf{V}^*) = -\int_{\Omega_t} \mathbf{b} : (\nabla_R \mathbf{V}^*)^T \, d\Omega \tag{21}$$

The quantity G is is usually called an *energy-release rate* (compare to the general definition involving the influx of the Hamiltonian density in Dascalu and Maugin, 1993). The result (21) was hinted at in a conversation with Paul Steinmann (Kaiserslautern, Sept.1998).

Equation (3) through (17) can be generalized to more involved cases including additional degrees of freedom (e.g., a microstructure such as in micropolar elastic bodies, Maugin, 1998b) or electromagnetic deformable bodies (cf. Maugin, 1999b) or *nonsimple* elastic media accounting for the second gradient of strain (so-called *second-gradient* theory ; cf. Maugin and Trimarco, 1992). This second case is particularly relevant to the contents of Section 4 below.

3 Finite-Element Method

In classical elastic engineering computations, when true material inhomogeneities or defects (field singularities) are absent, the *Finite-Element Method* (FEM) is based on a discretization of equation (15) by introducing interpolations of test functions. Imagine that the computation is also made in the absence of applied body forces ($\mathbf{f}^0 = \mathbf{0}$). Then $div_R \mathbf{T} = \mathbf{0}$ is solved by the FEM and this yields a solution that depends on the location of nodes of the FEM net on the material manifold. Knowing such an FEM field solution, the quantities $\mathbf{b}$ and $div_R \mathbf{b}$ can be evaluated, and this may yield

$$div_R \mathbf{b} \neq \mathbf{0} \left(say \mathbf{F}^{err} \right) \tag{22}$$

i.e., there may exist a spatial distribution of spurious material forces $\mathbf{F}^{err}$, where there should be none according to the Ericksen-Noether identity. Equation (22) says something about the faithfulness of the FEM net and the question naturally arises of the tailoring of a finite-element net in such a way that these spurious *configurational forces* be made to vanish. They are *configurational* forces as they do depend on the location of nodes on the material manifold. One may think to release (or make float) the inner material nodes so as to make these spurious material forces vanish, or at least to minimize them. This idea belongs to Braun (1997) and Steinmann (Kaiserslautern; Sept. 1998). In particular, the first author has shown that a distribution of practically vanishing configurational nodal forces could be obtained. Simultaneously, the total energy is reduced in the process and, therefore, becomes closer to the minimum attained by the exact solution. Unfortunately, this optimization procedure may be accompanied by the formation of badly shaped elements which may not improve the finite-element solution. In the process of the above FEM, since all required quantities are already computed in this optimization procedure, equation (21) affords a particularly economical and rapid means of computation of the energy-release rate, if the latter is needed in some criterion of progress.

4 Finite-Difference Method

The *Finite-Difference Method* (FDM) is the numerical realm of nonlinear hyperbolic systems. This discretization method finds its origin in analysis and the approximation of space derivatives of various orders by finite differences. The school of Courant (Lax, Wendroff, etc) in the USA and that of Godunov and Yanenko in Russia are responsible for its successes in treating problems including sharp field discontinuities such as shock waves in fluids. The accuracy of the devised FDM schemes is measured by their property to more or less conserve the global energy of the system. That is, in the present case, the numerical simulation of nonlinear-wave propagation is performed on the FDM discretized version of the *field* equation (3) and, for a conservative system ($\mathbf{f}^0 = \mathbf{0}$), it is

checked whether the global (space integral) version of the energy equation (4) holds for the numerically obtained solution. The result of this check is expressed by announcing that e.g., « energy is conserved up to x% », values of the order of 10^{-3} being quite normal. From that viewpoint, checking that the global version of the here redundant pseudomomentum balance law (5) holds for the numerical solution obtained is also a valid criterion for the accuracy of the scheme of the FDM scheme, except for the *vectorial nature* of that equation which may mean a check along three different axes instead of the conservation of a single scalar entity as is the case for the energy equation. This places energy and pseudomomentum on equal footing or, as we like to say, on the same *ontological level.* In particular, for systems of field equations, both canonical equations and accuracy criteria concern the global physical system and not only one degree of freedom in spite of the 3D vectorial nature of pseudomomentum. Thus, following Christov and Maugin (1999), we may thus speak of FDM schemes that more or less conserve *both* energy and canonical momentum.

With the introduction of localized nonlinear waves of the solitary-wave type (kinks, humps, bound states, soliton complexes) in nonlinear *dispersive* systems of field equations, the exploitation of the pseudomomentum balance law is even more fruitfull. This is easily understood by examining two specific questions. First, in a general way, for such systems, the field equations (equation 3 and the equations governing additional fields if any) present both nonlinearities and high-order space or mixed derivatives. This is the case when treating an elastic crystal in which both nonconvexity of the strain energy and a weak nonlocality (gradient effects) are taken into account (e.g., in shape-memory alloys). An example of such systems is the following 1D generalized Boussinesq equation (cf. Maugin and Christov, 1999) where subscripts t and X stands for partial derivatives, s is a strain (e.g., one shear component), $F(s)$ is a polynomial in s starting with second degree, and β is a positive or negative parameter:

$$s_{tt} - c_T^2 s_{XX} - \left[F(s) - \beta s_{XX} + s_{XXXX}\right]_{XX} = 0 \tag{23}$$

A *stiff* mathematical system such as this one, although one dimensional in space, requires devising a high-performance FDM scheme (see, e.g., Christov and Maugin, 1993, 1995). This makes that FDM is also an art. We do not write here the pseudomomentum balance equation (5) that corresponds to the field equation (23) because the formal expression (5) suffices for our general purpose. Imagine that we have obtained analytically (with some luck) or numerically, strongly localized solitary-wave-like solutions of equation (23) thats we call « shapes » S. These corresponds usually to spatially uniform solutions at infinity. First the writing of the global form-by integration over the real line R in the absence of force $\mathbf{f}^0$- of equation (5) provides theoretically an equation of the following type

$$\frac{d\mathbf{P}}{dt} = \mathbf{0} \qquad \mathbf{P} := \int_R P dX \tag{24}$$

This is a Newtonian-like equation of inertial motion for the « shape » S. There is no term in the right-hand side of equation $(24)_1$ because all field derivatives go to zero at infinity for these solutions S which, therefore, are steadily progressing. As a matter of fact imposing the vanishing in the right-hand side of equation $(24)_1$ reveals the *natural limit* conditions on higher-order field derivatives, that classical types of boundary conditions do not consider. But in the numerical simulation of the steady propagation of « *shapes* » S, we have to work either on a periodic landscape arrangement or on a finite space interval. The satisfaction of these conditions is a necessity for the realization of the inertial motion globally governed by equation (24). Otherwise, the nonzero values at the interval boundaries will in fact create a perturbing *driving force* that will accelerate or slow down the supposedly steadilly moving shape, with a motion equation

$$\frac{d\mathbf{P}}{dt} = \mathbf{F}^{driving} \neq \mathbf{0} \tag{25}$$

replacing then equation $(24)_1$. Making $\mathbf{F}^{driving}$ zero or minimal is a justified endeavour. But it is clear that the same scheme - equations $(24)_1$ and (25) - can also be exploited to treat the influence of nonzero applied forces (or any term that can be viewed as a perturbation on the inertial motion of undeformed « shapes » present in the right-hand side of equation (2) to start with. Then the initial « shape » solutions are found - with some freedom left to some of their parameters - on the basis of the homogeneous form of equation (2). Equation (25) where the right hand-side is then given by the space-integrated materially-convected form of this perturbing force, provides

the time-evolution equation of these gross parameters (e.g., speed) in solutions (transient nonlinear localized wave forms) that cannot be obtained through any other known method.

Examples of applications of the ideas presented in this Section are given in Christov *et al* (1996), Maugin and Christov (1999) and Maugin (1999b). Note that like in the previous section, and in accord with the general philosophy of this presention, the field equations, *per se*, serve one purpose, while the energy and/or pseudomomentum equations serve another one. Note by way of conclusion that equations (24) and (25) do not presuppose that the *point mechanics* (relationships between mass, momentum, velocity and energy) satisfied by the « shapes » in question is Newtonian. These relationships are part of the problem.

5 Finite-Volume Method - Continuous Cellular Automata: Thermodynamically based Numerical Scheme

The *Finite-Volume Method* (FVM) considers a fixed grid and cells, rather than discrete points, as discrete elements. It directly reflects the notion of conservation laws which apply to these cells. The theory presented in Section 2 clearly emphasizes the notion of conservation laws. Therefore, the FVM seems, at the price of some adjustments, to be appropriate to the treatment of dynamical problems such as generally posed in Section 2. It is all the more true that cells thus considered may also be viewed as the elementary blocks of a thermodynamics of so-called *discrete systems* in the manner of Schottky (cf. Muschik, 1990). In this thermodynamics the state in one discrete system (e.g., one of the above cells) is defined in terms of its environment which may or may not be in thermodynamical equilibrium. *Contact thermodynamical quantities* (e.g., contact temperature, contact stresses) are introduced to characterize the state of the discrete system (in fact defined at the boundary surface of a cell in the FVM). This idea of making a cell's state depend on that of its neighbors is tantamount to introducing a *strategy* for the propagation of the thermodynamic state. This is akin to introducing the notion of *cellular automaton,* although discretization here is based on continuous balance laws, so that we may refer to this method as that of *continuous cellular automata.* The referred to above strategy is essential in some dynamical thermomechanical problems such as that of the propagation of a *phase-transition front.* It is along this line of thought that our most recent works develop.

In a more traditional, engineering-like approach to that problem, which nonetheless makes use of the notions of canonical momentum and Eshelby stress (cf. Maugin and Trimarco, 1995; Maugin, 1998a, 1999a), a thermodynamically admissible *criterion of progress* for such fronts is decided on the basis of the following assumptions: (i) the phase front is a singular surface of zero thickness; (ii) this front does not present any dislocations, (iii) the criterion is essentially of the plastic or viscoplastic type (i.e., presenting both a threshold and a characteristic time scale). The computational strategy then is the following: at each instant of time, for which we know the location of the transition front, the problem is solved spatially on account of the basic field equations and boundary and matching conditions, for instance by the FEM. Knowing then the fields on both sides of the transition front at all ot its points, the *driving force* is evaluated point wise (it is related to the jump equation associated with the balance of canonical momentum) and the future progress of the front is decided on account of the criterion. This obviously shows again that equations such as (3) and (5) intervene at different steps of the formulation, the second being accounted for on account of the jump-like solution of the first.

In the new scheme developed starting with Berezovski's work of 1997, all thermomechanical balance laws are expressed for each cell, and the bulk quantities within each cell are related to the contact ones through the thermodynamics of discrete systems. A high-performance wave-propagation algorithm is exploited - using Lax-Wendroff and Godunov's ideas - that yields extremely good results in the simulation of the rapid progression of sharp wave fronts in 2D elasticity or thermoelasticity (cf. Berezovski and Maugin, 1999a,b). It is interesting to give a very few elements of that type of approach, for instance in linear isotropic, but materially inhomogeneous, thermoelasticity where the basic field equations are equations (3) and (4), the latter yielding in fact the equation of heat propagation [equation (5) is to be exploited later on]. More precisely, the balance of linear (physical) momentum, the time-rate of change of the Hooke-Duhamel constitutive equation, and the heat-propagation equation read as follows at any regular material point in the absence of body force and heat source:

$$\frac{\partial(\overline{\rho}_0(\mathbf{x})v_i)}{\partial t} - \frac{\partial \sigma_{ij}}{\partial x_j} = 0 \tag{26}$$

$$\frac{\partial \sigma_{ij}}{\partial t} = \lambda(\mathbf{x})\frac{\partial v_k}{\partial x_k}\delta_{ij} + \mu(\mathbf{x})\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) + m(\mathbf{x})\frac{\partial T}{\partial t}\delta_{ij} \tag{27}$$

$$\frac{\partial (C(\mathbf{x})T)}{\partial t} = \frac{\partial}{\partial x_i}\left(k(\mathbf{x})\frac{\partial T}{\partial x_i}\right) + m(\mathbf{x})\frac{\partial v_k}{\partial x_k} \tag{28}$$

where ρ_0 is the density of matter, σ is Cauchy's stress, λ and μ are Lamé coefficients, $m = -\alpha(3\lambda+2\mu)$ is the thermoelastic coupling coefficient if α is the dilatation coefficient, C is the heat capacity, and k is the heat-conduction coefficient; T denotes the small deviation of temperature. The material inhomogeneity is explicitly indicated by the **x**-dependence of some of these coefficients. By integration over a cell or finite-volume element V, we obtain the following system of FVM balance equations:

$$\frac{\partial}{\partial t}\int_V \rho_0 v_i dV = \int_{\partial V} \Sigma_{ij} n_j dA \tag{29}$$

$$\frac{\partial}{\partial t}\int_V \varepsilon_{ij} dV = \int_{\partial V} H_{ijk} n_k dA \tag{30}$$

$$\frac{\partial}{\partial t}\int_V \sigma_{ij} dV = \int_{\partial V} \left(2\mu H_{ijk} n_k + \lambda \delta_{ij} V_k n_k\right) dA + \varphi_{ij} \tag{31}$$

$$\frac{\partial}{\partial t}\int_V CT dV = \int_{\partial V} \left(k(\mathbf{n}.\nabla)T + mV_k n_k\right) dA + \varphi^{inh} \tag{32}$$

where

$$H_{ijk} \equiv (1/2)\left(\delta_{ik}V_j + \delta_{jk}V_i\right) \tag{33}$$

and source terms due to material inhomogeneities (labelled « *inh* ») and thermoelastic couplings (labelled « *te* ») are given by

$$\varphi_{ij} = \varphi_{ij}^{te} + \varphi_{ij}^{inh} \tag{34}$$

$$\varphi_{ij}^{te} = \int_V m\delta_{ij}\frac{\partial T}{\partial t} dV \tag{35}$$

$$\varphi_{ij}^{inh} = -\int_V \left(v_k \frac{\partial \lambda}{\partial x_k}\delta_{ij} + v_i \frac{\partial \mu}{\partial x_j} + v_j \frac{\partial \mu}{\partial x_i}\right) dV \tag{36}$$

$$\varphi^{inh} = -\int_V v_k \frac{\partial m}{\partial x_k} dV \tag{37}$$

Herein above V_i and Σ_{ij} are the « contact » velocity and Cauchy stress defined at the FV element boundary of unit outward normal n_i. Θ denotes the « contact temperature ». Contact and bulk quantities are related by thermodynamic constraints such as the following one for the stress [labels (1) and (2) refer to two neighboring cells].

$$\sigma_{ij}^{(1)} + \Sigma_{ij}^{(1)} - T^{(1)}\left(\frac{\partial \sigma_{ij}^{(1)}}{\partial T}\right)_\varepsilon - \Theta^{(1)}\left(\frac{\partial \Sigma_{ij}^{(1)}}{\partial T}\right)_\varepsilon = \sigma_{ij}^{(2)} + \Sigma_{ij}^{(2)} - T^{(2)}\left(\frac{\partial \sigma_{ij}^{(2)}}{\partial T}\right)_\varepsilon - \Theta^{(2)}\left(\frac{\partial \Sigma_{ij}^{(2)}}{\partial T}\right)_\varepsilon \tag{38}$$

The reader is referred to Berezosvki (1997) and Berezovski and Maugin (1999a,b) for the application to the numerics of smooth elastic and thermoelastic 2D wave propagation. What about the application to the propagation of phase-transition fronts where, of necessity, a criterion of progress (change of thermoelastic phase as the front progresses) is involved. This must necessarily exploit the balance of pseudomomentum in a form adapted to the continuous-cellular automaton formalism. As a matter of fact, in the present case, this additional balance law reads, at each regular material point:

$$\frac{\partial p_i^w}{\partial t} - \frac{\partial b_{ji}^w}{\partial x_j} = f_i^{inh} + f_i^{th} \tag{39}$$

where we have set (W is the free energy per unit volume)

$$p_i^w = -\rho_0 v_j u_{j,i} \qquad b_{ji}^w = -\left(L^{th}\delta_{ji} + \sigma_{jk}u_{k,i}\right) \tag{40}$$

$$L^{th} = \frac{1}{2}\rho_0(\mathbf{x})\mathbf{v}^2 - W\left(\varepsilon_{ij}, T; \mathbf{x}\right) \qquad f_i^{inh} = \left(\frac{\partial L^{th}}{\partial x_i}\right)_{\exp l} \qquad f_i^{th} = S\frac{\partial T}{\partial x_i} \qquad S = -\frac{\partial W}{\partial T} \tag{41}$$

The two source terms in equation (39) are due, respectively, to true material inhomogeneities and pseudo-inhomogeneities caused by thermal effets. (cf. Maugin, 1993, 1995); p_i^w, the purely quadratic part of pseudo-momentum, is called *wave* or *crystal momentum*, and b_{ji}^w is the corresponding part of the Eshelby stress tensor, with u_i the infinitesimal displacement. The integral of equation (39) over a VE cell yields

$$\frac{\partial}{\partial t}\int_V p_i^w dV - \int_{\partial V} n_j B_{ji}^w dA = \Phi_i^w \tag{42}$$

where

$$\Phi_i^w = \int_V \left(f_i^{inh} + f_i^{th}\right)dV \tag{43}$$

and B_{ji}^w is the « contact » Eshelby stress tensor. Together with the Eshelby tensor of the neighboring cell, the Eshelby stress b_{ji}^w satisfies the following time-evolution equation and thermodynamical constraint:

$$\frac{\partial b_{ji}^w}{\partial t} = -\left(\frac{\partial L^{th}}{\partial t}\delta_{ji} + \frac{\partial \sigma_{jk}}{\partial t}\frac{\partial u_k}{\partial x_i} + \sigma_{jk}\frac{\partial v_k}{\partial x_i}\right) \tag{44}$$

and

$$-\frac{\partial}{\partial t}\left(\frac{\partial u_j}{\partial x_p}\right)\left(B_{pj}^w - b_{pj}^{w*}\right) \geq 0 \tag{45}$$

where the minus sign in equation (45) originates from the fact that the Eshelby stress expands power in the « inverse motion » velocity field (Maugin, 1993). A short algebra allows one to show that the volume-element integral of equation (44) yields the following expression:

$$\frac{\partial}{\partial t}\int_V \left(b_{ji}^{w} + \frac{1}{2}\rho_0 \mathbf{v}^2 \delta_{ji} \right) dV = -\int_{\partial V} \left(\Sigma_{jk} V_k n_i \right) dA$$
$$+ \int_V \left(\left(\sigma_{pq} \frac{\partial v_p}{\partial x_q} - C\frac{\partial T}{\partial t} \right) \delta_{ji} - \frac{\partial \sigma_{jk}}{\partial t} \frac{\partial u_k}{\partial x_i} + \frac{\partial \sigma_{jk}}{\partial x_i} v_k \right) dV \tag{46}$$

The integrand in the left-hand volume integral is no other than the « *quasi-static* » Eshelby stress which indeed governs the phase transition. The criterion of progress must, therefore, exploit equations (42) and (46). Related works are in progress.

6 Conclusion

Referring to all above considered cases we must, by way of conclusion, emphasize the different roles played by the field equations, *per se*, and the canonical equation of momentum. The latter proves to be extremely useful, and in fact the only tool available, to devise criteria of progress. This applies in all numerical methods examined, whether of the finite-element, finite-difference, or finite-volume type. These applications succeed in granting a clearly engineering-like flavor to concepts, those of pseudomomentum and Eshelby stress, whose origin is to be found in abstract field theory and the geometry of the material manifold or material space.

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