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Weakly nonlocal continuum theories of granular media: restrictions from the Second Law

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Abstract

The classical continuum mechanical model of granular media of rational thermodynamics results in a Coulomb–Mohr type equilibrium stress–strain relation. The proof is based on a two component material model introducing a scalar internal variable. Here we will show how one can get similar stress–strain relations without assuming a balance of substructural interactions, considering only the restrictions of the Second Law of thermodynamics.

Keywords: Continuum theories of granular material; Second Law; Nonequilibrium thermodynamics

1. Introduction

In their classical paper Goodman and Cowin derived a material model of porous and granular media using pure thermodynamic reasoning (Goodman and Cowin, 1972). They considered a material where the density of the solid component is γ, the total density is ρ and the *volume distribution function* v is defined by the following formula

$$\rho = v\gamma.$$

Later the scalar internal variable v was interpreted as *roughness* and its (substantial) time derivative $\dot{v}$ as *abrasion* (Kirchner, 2002; Kirchner and Teufel, 2002). Goodman and Cowin assumed a material with incompressible solid component and with a balance form dynamic equation for the abrasion, a balance of substructural interactions (Goodman and Cowin called it balance of equilibrated force) (Capriz, 1989; Mariano, 2002):

$$\gamma\ddot{v} = \nabla \cdot \mathbf{h} + \sigma_{\dot{v}},$$

where $\mathbf{h}$ is the conductive current and $\sigma_{\dot{v}}$ is the production of $\dot{v}$. After introducing a suitable constitutive space they investigated the requirements coming from the Second Law of thermodynamics with

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Coleman–Noll procedure. Their final result was a definition of *Coulomb granular material* by the following stress function

$$\mathbf{T}^e = (\beta_0 - \beta v^2 + \alpha\nabla v \cdot \nabla v + 2\alpha v \Delta v)\mathbf{I} - 2\alpha \nabla v \circ \nabla v + \lambda \mathrm{Tr}(\boldsymbol{\epsilon})\mathbf{I} + 2\mu\boldsymbol{\epsilon},$$

where β_0, β, α are material parameters, λ, μ are the Lamé coefficients. $\mathbf{I}$ is the second order unit tensor, $\circ$ denotes the tensorial product and Tr is the trace. As one can see an ideal elastic behavior is coupled to the gradient dependent characteristic part, represented by the first two terms.

In this paper we will show, that a similar material model can be derived without assuming a balance of substructural interactions (equilibrated forces), with the very same weakly nonlocal extension of the configurational space as in the model of Goodman and Cowin. In the following Liu's theorem will play an important technical role. Details of the different state spaces, more detailed description of thermodynamic concepts, the applied mathematical methods (especially Liu procedure) can be found in Muschik et al. (2001), regarding the weakly nonlocal extension see Ván (2002, 2003). A thermodynamic background of continuum field theories is in Verhás (1997).

2. Weakly nonlocal fluids—granular media

In our treatment the *basic state space* of granular media is spanned by the density of the solid component, the volume distribution function and the velocity $(\gamma, v, \mathbf{v})$. This basic state space is the simplest large deformation treatment and considers the possibility of changes in the topological structure typical in fluids. With this basic state we are constructing a constitutive model of a *dilatant granular material*, because ρ is not necessarily constant. The *constitutive state space* contains gradients of the basic state variables as in case of classical fluids. Therefore, it is spanned by the variables $(\gamma, \nabla\gamma, v, \nabla v, \mathbf{v}, \nabla\mathbf{v})$. The functions interpreted on the constitutive space are the *constitutive functions*. The *space of independent variables* is spanned by the next time and space derivatives of the constitutive variables $(\dot{\gamma}, \nabla\dot{\gamma}, \nabla^2\gamma, \dot{v}, \nabla\dot{v}, \nabla^2 v, \dot{\mathbf{v}}, \nabla\dot{\mathbf{v}}, \nabla^2\mathbf{v})$, as a consequence of the entropy inequality. Here ∇^2 denotes the second space derivative.

In the following we will assume that the solid part of the material is nearly incompressible, therefore the deformation is due to the changes in the volume distribution function. This condition can be expressed as

$$\dot{\gamma} = 0. \tag{1}$$

Considering (1) the continuity equation can be written as

$$\dot{v} + v\nabla \cdot \mathbf{v} = 0. \tag{2}$$

(1) and (2) are constraints of the independent variables, and are to be considered in the application of the Liu procedure. Moreover, the structure of the constitutive state space implies that the space derivatives of the above equations contain terms solely from the space of independent variables, therefore they are also constraints. The derivative of (1) is

$$\nabla\dot{\gamma} = \mathbf{0}, \tag{3}$$

and the derivative of (2) results in

$$\nabla\dot{v} + \nabla v \nabla \cdot \mathbf{v} + v\nabla\nabla \cdot \mathbf{v} = 0. \tag{4}$$

Finally, the balance of momentum is written as

$$\gamma v \dot{\mathbf{v}} + \nabla \cdot \mathbf{P} = 0. \tag{5}$$

Here $\mathbf{P}$ is the pressure tensor. The requirement of nonnegativity of the entropy production is

$$\gamma v \dot{s} + \nabla \cdot \mathbf{j}_s = \sigma_s \geqslant 0, \tag{6}$$

where the specific entropy s, the conductive current of the entropy $\mathbf{j}_s$ and the pressure $\mathbf{P}$ are the constitutive quantities, functions interpreted on the constitutive space. With given constitutive functions the dynamic equations of the granular continua are (1), (2) and (5). According to the Second Law we are to find these constitutive functions that the entropy production be nonnegative. In this way the nonnegativity will be a pure material property, independent of the initial conditions. Liu procedure is applied with the multiplier form (see Liu, 1972; Ván, 2002)

$$\rho\dot{s} + \nabla\cdot\mathbf{j}_s - \Gamma_1\dot{\gamma} - \Gamma_2\nabla\dot{\gamma} - \Gamma_3(\dot{v} + v\nabla\cdot\mathbf{v}) - \Gamma_4(\nabla\dot{v} + \nabla v\nabla\cdot\mathbf{v} + v\nabla\nabla\cdot\mathbf{v}) - \Gamma_5(\gamma v\dot{\mathbf{v}} + \nabla\cdot\mathbf{P}) \geqslant 0.$$

Here we introduced Lagrange–Farkas multipliers Γ_1, Γ_2, Γ_3, Γ_4 and Γ_5 for the constraints (1), (3), (2), (4) and (5) respectively. In deriving the Liu equations one should consider that the substantial time derivative does not commute with the space derivative. The following identity is to be applied

$$(\nabla\dot{a}) = \nabla\dot{a} - \nabla\mathbf{v}\cdot\nabla a.$$

Now the multipliers of the independent variables give the Liu equations, respectively. Introducing a shorthand notation for the partial derivatives of the constitutive quantities as e.g. $\partial_\gamma = \frac{\partial}{\partial\gamma}$ we get

$$\rho\partial_\gamma s = \Gamma_1, \tag{7}$$

$$\rho\partial_{\nabla\gamma} s = \Gamma_2, \tag{8}$$

$$\rho\partial_v s = \Gamma_3, \tag{9}$$

$$\rho\partial_{\nabla v} s = \Gamma_4, \tag{10}$$

$$\rho\partial_{\mathbf{v}} s = \rho\Gamma_5, \tag{11}$$

$$\rho\partial_{\nabla\mathbf{v}} s = \mathbf{0}, \tag{12}$$

$$(\partial_{\nabla v}\mathbf{j}_s - \Gamma_5\partial_{\nabla v}\mathbf{P})^{\mathrm{s}} = \mathbf{0}, \tag{13}$$

$$(\partial_{\nabla\gamma}\mathbf{j}_s - \Gamma_5\cdot\partial_{\nabla\gamma}\mathbf{P})^{\mathrm{s}} = \mathbf{0}, \tag{14}$$

$$(\partial_{\nabla\mathbf{v}}\mathbf{j}_s - \Gamma_4 v\mathbf{I} - \Gamma_5\cdot\partial_{\nabla\mathbf{v}}\mathbf{P})^{\mathrm{s}} = \mathbf{0}. \tag{15}$$

The superscript s denotes the symmetric part of the corresponding function. Eqs. (7)–(11) determine the Lagrange–Farkas multipliers. The solution of (12) results in an entropy that is independent of the gradient of velocity, therefore (15) can be integrated and a particular form of $\mathbf{j}_s$ is determined. Substituting that form of $\mathbf{j}_s$ into (13) and (14) we get two equations that are fulfilled if

$$\partial_{v\nabla v} s = \mathbf{0}, \quad \partial_{v\nabla\gamma} s = \mathbf{0}, \quad \partial_{\nabla v\nabla v} s = \mathbf{0}, \quad \partial_{\nabla v\nabla\gamma} s = \mathbf{0}. \tag{16}$$

The most general generalized entropy function, isotropic and second order in $\mathbf{v}$ and in $\nabla\gamma$ that satisfies the above conditions is the following

$$s(v, \nabla v, \gamma, \nabla\gamma, \mathbf{v}) = s_{\mathrm{e}}(v,\gamma) - m(v,\gamma)\frac{\mathbf{v}^2}{2} - \alpha(v,\gamma)\frac{(\nabla\gamma)^2}{2}. \tag{17}$$

Here m and α are arbitrary nonnegative functions. We can see, that entropy is a concave function of the variables $\mathbf{v}$ and $\nabla\gamma$. Moreover, the entropy is independent of ∇v. Considering (17), the solution of the last Liu equation (15) gives the entropy current as

$$\mathbf{j}_s = -m\mathbf{v}\cdot\mathbf{P} + \mathbf{j}_1(v,\gamma,\mathbf{v}). \tag{18}$$

Here $\mathbf{j}_1$ is an arbitrary function. Applying (17) and (18) the dissipation inequality simplifies to

$$\nabla \cdot \mathbf{j}_1 - \nabla(m\mathbf{v}) : \mathbf{P} + \rho(\alpha\nabla\gamma \circ \nabla\gamma - v\partial_v s\mathbf{I}) : \nabla\mathbf{v} \geqslant 0.$$

If $\mathbf{j}_1 \equiv \mathbf{0}$ and $m = 1$ (as usual) then the dissipation inequality can be transformed into a solvable form. Introducing the notation $p = -v\rho\partial_v s_e$ entropy inequality further simplifies to

$$-\left(\mathbf{P} - \left(p + \rho\partial_v\alpha\frac{(\nabla\gamma)^2}{2}\right)\mathbf{I} - \rho\alpha\nabla\gamma\nabla\gamma\right) : \nabla\mathbf{v} \geqslant 0.$$

The notation is not arbitrary, because $\partial_v s_e = \partial_\rho s_e \partial_v \rho = -\frac{\tilde{p}(v,\gamma)}{T_0\rho^2}$, where $\tilde{p}$ is the scalar pressure according to the traditional thermostatic definition, corresponding to the Gibbs relation. Or, alternatively investigating a pure mechanical system one can recognize that our s function is still connected to the entropy only in some properties, therefore one can introduce the physical entropy $\tilde{s} = \frac{s}{T_0}$. In this case p is the scalar pressure, T_0 is a constant temperature and all the considerations above are valid. Let us underline here, that there is nothing mysterious in the above identifications that would weaken the above reasoning. Our whole procedure is based on the existence of a constitutive function with the nonnegative balance, a kind of general stability requirement. One can exploit this property and recognize the physical meaning of the corresponding quantities later. On the other hand we should not forget that the introduced $\tilde{s}$ is a kind of generalized, nonequilibrium "physical" entropy with rather strange variables (velocity and gradients) and there is no unique nomination for such quantities (coarse grained kinetic potential?).

The inequality above contains only the pressure tensor $\mathbf{P}$ as constitutive quantity that depends on the velocity gradient, therefore it is solvable. The general solution is

$$\mathbf{P} - \mathbf{P}_e = \mathbf{P}_v = -\mathbf{L}(\nabla\mathbf{v}),$$

where $\mathbf{P}_v$ is the viscous part of the pressure, $\mathbf{L}$ is a nonnegative constitutive function. Here we assumed a symmetric pressure tensor as it is usual for materials without internal moment of momentum. Furthermore, the equilibrium, static part of the pressure is $\mathbf{P}_e$ and it is defined as

$$\mathbf{P}_e = \left(p + \rho\partial_v\alpha\frac{(\nabla\gamma)^2}{2}\right)\mathbf{I} - \rho\alpha\nabla\gamma\nabla\gamma. \tag{19}$$

A material defined by this equilibrium pressure tensor will be called *Coulomb–Mohr material.*

3. Coulomb–Mohr materials

The pressure tensor (19) has several remarkable properties. First of all, the static shear stress is not zero, and $\nabla\gamma$ is an eigenvector of $\mathbf{P}_e$. Furthermore, introducing an arbitrary direction with a unit vector $\mathbf{n}$, one can define a pressure normal to the direction $\mathbf{n}$ as

$$N := \mathbf{n} \cdot \mathbf{P}_e \cdot \mathbf{n} = \hat{p} - \rho\alpha(\nabla\gamma \cdot \mathbf{n})^2,$$

where $\hat{p} = p + \rho\partial_v\alpha(\nabla\gamma)^2/2$. Denoting the shear pressure by $S := P - N$ one can get

$$S^2 + N^2 = (\mathbf{P}_e \cdot \mathbf{n}) \cdot (\mathbf{P}_e \cdot \mathbf{n}) = \hat{p}^2 - 4\rho\alpha\hat{p}(\nabla\gamma \cdot \mathbf{n})^2 + 4(\rho\alpha)^2(\nabla\gamma)^2(\nabla\gamma \cdot \mathbf{n})^2.$$

After a short calculations it follows that

$$S^2 + (N - t)^2 = r^2 \quad \text{where } t = \hat{p} - r \text{ and } r = \rho\alpha(\nabla\gamma)^2.$$

Hence, the possible Mohr circles in the material have a special structure, their envelope from above is a straight line, the material satisfies a failure criteria of Coulomb–Mohr kind, as the Coulomb material of

Goodman and Cowin (Fig. 1). One can check that this is really a failure criteria, the second derivative of the entropy function (17) become semidefinite on the Coulomb–Mohr line and the line separates the region of the state space where the thermodynamic stability is violated from the region where it is fulfilled.

Material stability in mechanics is far more complex matter than in equilibrium thermodynamics of gases and fluids where it is connected to the appearance of new phases (Goddard, 2002, 2003). On the other hand in a thermodynamic approach the loss of thermodynamic stability means the violation of dynamic stability (e.g. the corresponding partial differential equations loose their hyperbolicity). Stability losses of this kind where treated in connection of rigid, microcracked materials in Ván (2001). There the microstructure was characterized by a vectorial dynamic variable **D** (representing the average crack length, a damage) and two general free energies of the microcracked materials were introduced. There with special material parameters one can arrive to a Coulomb–Mohr failure criteria and pressure tensors similar to (19), but with a local variable called damage vector **D**, instead of the gradient variable $\nabla\gamma$. The role of $\nabla\gamma$ is similar to **D** in every sense. Recalling the quadratic form of the entropy function the loss of thermodynamic stability is not a direct consequence of an increasing $|\nabla\gamma|$. The loss of stability is more involved and always connected to changes in the stress/deformation state and appears only in perpendicular to $\nabla\gamma$, in a 'shear' direction. The complexity of the different kind stability losses is investigated e.g. in Béda (1999, 2000).

Our basic state space and configuration space was that of a fluid. In the one component case, when the configuration state space is $(\rho, \nabla\rho, \mathbf{v}, \nabla\mathbf{v})$ an ideal Euler fluid and the viscous Navier–Stokes fluids appear after similar derivations. Remarkable, that a higher order weakly nonlocal one component fluid, where the constitutive state space contains also the second order derivative of the density, results in the Madelung fluid (known from the hydrodynamic version of quantum mechanics) in the ideal, nondissipative case (Ván and Fülöp, 2003).

According to the comparison of Kirchner and Hutter the model of Goodman and Cowin is the most robust one among several local continuum granular material models of porous and granular media (with scalar internal variables). Interestingly, the other compared models can be considered as relocalized (according to the terminology of Ván (2003)), because they can introduce nonlocality through a generalized entropy current. A different continuum granular model of Aranson and Tsimring introduces also a scalar internal variable with a Ginzburg–Landau dynamics (assumed in an ad hoc way) (Aranson and Tsimring, 2001; Sapozhnikov et al., 2002; Volfson et al., 2003). Their starting point is the granular kinetic theory and thorough calculations and simulations try to understand the connections in that direction. Therefore their model is not compatible with a realistic static case. In understanding the granular phenomena and especially to create an applicable continuum model is a great challenge of physics where definitely a large extension of our understanding of continuum concepts and therefore the extension of continuum theories is

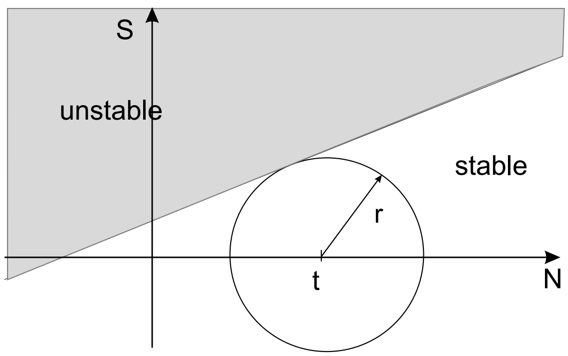

Fig. 1. The envelope of the Coulomb–Mohr circles as a boundary of the stability.

necessary (Capriz, 2003). The simple model shown in this work is a step in that direction demonstrating the capabilities and simplicity of thorough constitutive reasoning.

Finally, it is important to observe the differences in the conditions of the derivation and also in the final results of the model of Goodman–Cowin and the present one. Here the fluid like state space and the large differences in the compressibility were essential conditions in the derivation. There was no need to introduce a balance of substructural interactions (but of course the state space can be extended to include $\ddot{\gamma}$ and one can investigate the consequences). We have got a Coulomb–Mohr failure criteria in the static limit in both cases. However, the structure of the equilibrium pressure tensors and therefore the implied physical reasons were completely different. To investigate the physical relevance of the two models further work is necessary. In this direction the known solutions are very important and generalization of the Goodman–Cowin model like the flow calculations of Wang and Hutter (1999) and Massoudi (2001). Another possibility to test the differences could be to look into static failure data of Coulomb–Mohr materials. Related experimental data regarding porous rocks have been published recently by Vásárhelyi (2002, 2003a,b).

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