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Green's formula and singularity at a triple contact line. Example of finite-displacement solution

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ABSTRACT

The various equations at the surfaces and triple contact lines of a deformable body are obtained from a variational condition, by applying Green's formula in the whole space and on the Riemannian surfaces. The surface equations are similar to the Cauchy's equations for the volume, but involve a special definition of the 'divergence' (tensorial product of the covariant derivatives on the surface and the whole space). The normal component of the divergence equation generalizes the Laplace's equation for a fluid–fluid interface. Assuming that Green's formula remains valid at the contact line (despite the singularity), two equations are obtained at this line. The first one expresses that the fluid–fluid surface tension is equilibrated by the two surface stresses (and not by the volume stresses of the body) and suggests a finite displacement at this line (contrary to the infinite-displacement solution of classical elasticity, in which the surface properties are not taken into account). The second equation represents a strong modification of Young's capillary equation. The validity of Green's formula and the existence of a finite-displacement solution are justified with an explicit example of finite-displacement solution in the simple case of a half-space elastic solid bounded by a plane. The solution satisfies the contact line equations and its elastic energy is finite (whereas it is infinite for the classical elastic solution). The strain tensor components generally have different limits when approaching the contact line under different directions. Although Green's formula cannot be directly applied, because the stress tensor components do not belong to the Sobolev space $H^1(V)$, it is shown that this formula remains valid. As a consequence, there is no contribution of the volume stresses at the contact line. The validity of Green's formula plays a central role in the theory.

1. Introduction

Surface properties of deformable bodies have been continually studied since the early work of Gibbs (1878) until recent mechanical or thermodynamic studies, e.g. Gurtin et al. (1998), Simha and Bhattacharya (2000), Rusanov (2005), Steinmann (2008) and Olives (2010a). They have many applications, e.g. in adhesion, coating and nanosciences (since small and thin objects are deformable and have a high surface/volume ratio). A previous paper (Olives, 2010a) was devoted to the physical basis of the theory: application of the equilibrium criterion of Gibbs; introduction of the new concept of 'ideal transformation', i.e., the homogeneous extrapolation of the deformation, in the interface film, up to the dividing surface; determination of the thermodynamic variables of state of a surface; definition of the surface stress tensor; surface and line equations. Moreover, for an elastic solid, it is known that classical elasticity predicts a singularity with an infinite displacement (and an infinite elastic energy) at a solid–fluid–fluid triple contact line, owing to the fluid–fluid surface tension which is a force concentrated on this line (Shanahan and de Gennes, 1986; Shanahan, 1986). Although some authors tried to overcome this problem, by introducing some fluid–fluid interface thickness (Lester, 1961; Rusanov, 1975), some cut-off radius near the contact line (Shanahan and de Gennes, 1986; Shanahan, 1986) or some new elastic force at this line (Madasu and Cairncross, 2004), this situation makes very difficult to write any equilibrium equation at the contact line.

The present paper concerns the mathematical foundation of the theory. A sketch of the proof of the surface and contact line equations is presented (no proof was given in the previous physical paper Olives, 2010a), which shows (i) the importance of the validity of Green's formula at the contact line (despite the singularity) and (ii) owing to the surface properties, the probable existence of a finite-displacement solution (consequence of the line equations, based themselves on the assumption of the validity of Green's formula). These two points are justified with an explicit example of finite-displacement solution, in the simple case of a half-space solid, bounded by a plane, and subjected to a normal force concentrated on a straight line of its surface. This solution also

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shows that the elastic energy is finite and that Green's formula remains valid at the contact line.

2. Surface and contact line equations

For a general deformable body b in contact with various immiscible fluids f, f′,...(with no mass exchange between the body and the fluids), the mechanical equilibrium condition relative to the body, including its body–fluid surfaces (bf, bf′,...) and its body–fluid–fluid triple contact lines (bff′,...), may be written as

$$\int_{\mathrm{b}} \pi : \delta e\, dv_0 - \int_{\mathrm{b}} \rho \bar{g} \cdot \delta x\, dv - \sum_{\mathrm{bf}} \int_{\mathrm{bf}} p\, n \cdot \delta x\, da - \sum_{\mathrm{bf}} \int_{\mathrm{bf}} \rho_s \bar{g} \cdot \delta x\, da + \sum_{\mathrm{bf}} \int_{\mathrm{bf}} \pi_s : \delta e_s\, da_0 - \sum_{\mathrm{bff'}} \int_{\mathrm{bff'}} \gamma_{\mathrm{ff'}}\, v_{\mathrm{ff'}} \cdot \delta X\, dl + \sum_{\mathrm{bff'}} \int_{\mathrm{bff'}} (\gamma_{0,\mathrm{bf}} - \gamma_{0,\mathrm{bf'}})\, \delta X_0\, dl_0 = 0 \quad (1)$$

(: means double contraction; see Olives, 2010a for the physical basis of the theory), in which δ is an arbitrary variation such that, on the closed surface Σ which bounds the system, the points of the body and the points of the body–fluid–fluid lines remain fixed. In this expression, π is the Piola–Kirchhoff stress tensor (i.e., the Lagrangian form, relative to a reference state of the body) at equilibrium, e the Green–Lagrange strain tensor (also relative to this reference state), dv and dv_0 are respectively the volume measures in the present state and in the reference state, ρ is the mass per unit volume, $\bar{g}$ the (constant) gravity vector field, δx the displacement of a point of the body, p the fluid pressure, n the unit vector normal to the bf surface, oriented from f to b, da and da_0 are respectively the area measures in the present state and in the reference state, ρ_s is the mass per unit area (excess on the dividing surface S_{bf} defined by the condition: no excess of mass of the constituent of the body), π_s the (Lagrangian) surface stress tensor at equilibrium, defined in Olives (2010a), e_s the (Lagrangian) surface strain tensor, defined in Appendix A, $\gamma_{\mathrm{ff'}}$ the fluid–fluid surface tension, $v_{\mathrm{ff'}}$ the unit vector normal to the bff′ line, tangent to the ff′ surface, and oriented from the line to the interior of ff′, δX the (vector) displacement of the bff′ line, perpendicular to the line (in the present state), dl and dl_0 are respectively the length measures in the present state and in the reference state, γ_0 is the surface grand potential (excess on the dividing surface), per unit area in the reference state, and δX_0 the (scalar) displacement of the bff′ line, measured in the reference state, perpendicular to that line in the reference state, and positively considered from bf to bf′ (see also Fig. 2, below).

This variational equilibrium condition leads to various equations at the surfaces and the triple contact lines of the body. Since the preceding paper (Olives, 2010a) was devoted to the physical aspects of the theory, these equations were only written without proof. In this section, a sketch of this proof is presented, which shows the importance of the validity of Green's formula to obtain the contact line equations (despite the line singularity). These equations then suggest the existence of a finite-displacement solution.

In order to only have quantities or variables (such as points, forces, etc.) which refer to the present equilibrium state in these equations, we first need to transform all the Lagrangian terms in (1) (i.e., those related to the 'undeformed' reference state) into Eulerian forms (i.e., related to the deformed present state). It is well known that the Eulerian forms of the above (volume) stress and strain tensors, π and δe, are the Cauchy stress tensor σ and the infinitesimal strain tensor $\delta\varepsilon$ defined below in the next paragraph (see e.g. Mandel, 1966, tome I, annexe II). Note that e measures the strain between the 'undeformed' reference state and the deformed present state, so that its components e_{ij} may have arbitrary values, since large strains may occur in highly deformable bodies (even when subjected to capillary forces or surface stresses). Note also that $\delta\varepsilon$, which measures the infinitesimal strain between the present state and its varied state (i.e., after the variation δ), is not the variation of some strain tensor, but it is related to the variation δe of the Lagrangian tensor e by

$$\delta e = \Phi_0^* \cdot \delta\varepsilon \cdot \Phi_0,$$

where Φ_0 is the deformation gradient between the reference state and the present state and Φ_0^* its adjoint. Classically, the work of deformation of a volume element (first term of (1)) may be written in the Eulerian form

$$\pi : \delta e\, dv_0 = \sigma : \delta\varepsilon\, dv \quad (2)$$

(see Mandel, 1966, ibid.), i.e., with arbitrary Cartesian coordinates in the three-dimensional space E

$$\pi^{ij}\, \delta e_{ij}\, dv_0 = \sigma^{ij}\, \delta\varepsilon_{ij}\, dv,$$

where Latin indices $i, j, k, \ldots$ belong to $\{1, 2, 3\}$ and summation is performed over repeated indices. In a similar way, these concepts are extended to the surfaces in Appendix A, where the Lagrangian surface strain tensor e_s, the Eulerian infinitesimal surface strain tensor $\delta\varepsilon_s$ and the Eulerian surface stress tensor σ_s are defined. The work of deformation of a surface element (fifth term of (1)) may then be written in the Eulerian form (A.12).

Let us first consider the simple case of a bounding surface Σ which only encloses one fluid f and the body b. The equilibrium condition (1) may then be written as

$$\int_{\mathrm{V}} \sigma : \delta\varepsilon\, dv - \int_{\mathrm{V}} \rho \bar{g} \cdot w\, dv - \int_{\mathrm{S}} p\, n \cdot w\, da - \int_{\mathrm{S}} \rho_s \bar{g} \cdot w\, da + \int_{\mathrm{S}} \sigma_s : \delta\varepsilon_s\, da = 0,$$

where $w = \delta x$, V is the bounded open set of E occupied by the part of the body enclosed in Σ, and S the bounded part of S_{bf} enclosed in Σ. Since $\delta\varepsilon = \frac{1}{2}((\mathrm{D}w)^* + \mathrm{D}w)$ and

$$\int_{\mathrm{V}} \mathrm{tr}(\sigma \cdot \delta\varepsilon)\, dv = \int_{\mathrm{V}} \mathrm{tr}\left(\frac{\sigma^* + \sigma}{2} \cdot \mathrm{D}w\right) dv = \int_{\mathrm{V}} \mathrm{tr}(\sigma^* \cdot \mathrm{D}w)\, dv + \int_{\mathrm{V}} \mathrm{tr}\left(\frac{\sigma - \sigma^*}{2} \cdot \mathrm{D}w\right) dv,$$

by application of Green's formula (with $w = 0$ on Σ)

$$\int_{\mathrm{V}} \mathrm{tr}(\sigma^* \cdot \mathrm{D}w)\, dv = -\int_{\mathrm{V}} \mathrm{div}(\sigma^*) \cdot w\, dv - \int_{\mathrm{S}} (\sigma^* \cdot w) \cdot n\, da = -\int_{\mathrm{V}} \mathrm{div}(\sigma^*) \cdot w\, dv - \int_{\mathrm{S}} (\sigma \cdot n) \cdot w\, da \quad (3)$$

(if the components of σ and w belong to $C^1(\bar{\mathrm{V}})$; e.g. Allaire, 2007, Section 3.2.1), this leads to the classical Cauchy's equations for the body

$$\mathrm{div}\, \bar{\sigma} + \rho \bar{g} = 0 \quad (4)$$

$$\sigma^* = \sigma, \quad (5)$$

where $\mathrm{div}\, \bar{\sigma}$ is the vector associated to the linear form $\mathrm{div}(\sigma^*)$, and the remaining condition for the surface

$$-\int_{\mathrm{S}} (\sigma \cdot n) \cdot w\, da - \int_{\mathrm{S}} p\, n \cdot w\, da - \int_{\mathrm{S}} \rho_s \bar{g} \cdot w\, da + \int_{\mathrm{S}} \sigma_s : \delta\varepsilon_s\, da = 0 \quad (6)$$

for any variation such that $w = 0$ on the closed curve $\Gamma = S_{\mathrm{bf}} \cap \Sigma$ which bounds S. Note that, if volume moments $\bar{M}\, dv$ were present, the new term $-\int_{\mathrm{V}} \frac{1}{2} \mathrm{tr}(M^* \cdot \mathrm{D}w)\, dv$[1] would appear in the equilibrium condition, and (5) would become $\sigma - \sigma^* + M = 0$.

[1] M is the endomorphism defined by $(M \cdot x) \cdot y = [\bar{M}, x, y]$, for any vectors x and $y \in \mathrm{E}$; it satisfies $M^* = -M$.