The interface between phases as a layer, Part II. A H-order model for two dimensional nonmaterial continua

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THE INTERFACE BETWEEN PHASES AS A LAYER, PART II
A H-ORDER MODEL FOR TWO DIMENSIONAL NONMATERIAL CONTINUA

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ABSTRACT

We model the interlayer between phases as a 2D continuum accounting for its actual "3D" nature. This is done by defining on a reference surface interfacial quantities in the form of integrals along the thickness of the layer. Therefore it is possible to deduce the general surface balance law from the 3D one. The balance laws are derived for of all the first H moments of mass, linear momentum and angular momentum. This procedure yields surface angular momentum balances Galilean invariant. Finally a Kirchhoff-Love type interface is defined and shortly discussed by means of a first-order model.

1. INTRODUCTION

Capillarity or *Surface Phenomena* occur when significant amounts of physically relevant quantities are *localized* in a region, henceforth called *a layer* $\mathfrak{L}$, whose thickness is *small.*

1.1 Assumptions

We start considering a 3D continuum $\mathfrak{C}$ occupying at instant t the region C(t) and moving with the velocity $\underline{v}$. We assume that the layer $\mathfrak{L}$ is located in $\mathfrak{C}$. We shall model $\mathfrak{L}$ as a *2D nonmaterial continuum* $\mathcal{S}$ whose balance equations for surface densities of mass, linear and angular momenta, are formulated *taking into account the 3D nature* of $\mathfrak{L}$ itself. Here by the term *nonmaterial continuum* we mean that the motion of the layer can be different from that determined by the field $\underline{v}$.

Following [1)] we assume that:

There exists a regular surface $\Sigma \subset \mathfrak{L}$, which models the spatial evolution and geometrical properties of $\mathfrak{L}$ itself in such a way that

$$\mathfrak{L} = \bigcup_{\ell \in I} \Sigma^{\ell} \qquad (1.1)$$

where $I \equiv [-z/2, +z/2]$ (we denote $\pm z/2 \equiv z^{\pm}$), z being the thickness of the layer which in a first approach we assume to be constant, and

$$\Sigma^{\ell} \equiv \left\{ \underline{x} \in \mathfrak{E} \mid \exists! \ \underline{r} \in \Sigma : \underline{x} = \underline{r} + \ell \, \underline{n} \ , \ \underline{n} \equiv \text{unit normal to } \Sigma \text{ at } \underline{r} \right\}$$

Let us notice that the regular surface Σ is chosen with no particular reference to thermomechanical quantities defined in $\mathfrak{E}$ as it is used to be done when introducing Gibbs' dividing surfaces.

The remaining material structure of $\mathfrak{L}$ is preserved by equipping the surface Σ with a structure of 2D continuum. It is done by defining surface densities and flux of physical quantities as suitable integrals of the corresponding volume ones along the thickness of $\mathfrak{L}$. The procedure makes possible an identification of surface quantities which appear in surface balance laws even when dealing with nonmaterial continua. Moreover, this allows for a more careful discussion of the Galilean invariance of the balance laws.

1.2 H-th Order Models For $\mathfrak{L}$.

Following [1)] for every volume density ψ whose flux is $\underline{w}$ and production is $\underline{p}$, we can define the corresponding surface density and production functions as

$$f^{S} \equiv \int_{z^-}^{z^+} j(\ell,\underline{r}) f(\underline{r}+\ell\underline{n}(\underline{r}),t)\,d\ell \equiv \langle j\ f \rangle \ \text{(if } f \text{ stands for } \underline{p} \text{ or } \psi) \qquad (1.2)$$

and the surface flux as

$$\underline{W}^{S'}\{\ \psi\ \} \equiv \langle \psi \otimes (\underline{v}+\ell \operatorname{grad}_{S} c_{n})\ \underline{A}_{S}(\ell) \rangle + \langle \underline{w}\ \underline{A}_{S}(\ell) \rangle, \qquad (1.3)$$

where $j(\ell,\underline{r}) \equiv 1 - 2H(\underline{r})\ell + K(\underline{r})\ell$. Here $H(\underline{r})$ and $K(\underline{r})$ are, respectively, the mean and Gauss curvatures of Σ at $\underline{r}$, the tensors $\underline{b}_0$ and $\mathbb{I}_S$ are the surface curvature and metric tensors of the moving surface Σ, respectively, c_n its geometrical normal speed and $\underline{A}_S(\ell) \equiv (1-2H\ell)\mathbb{I}_S + \ell\underline{b}_0$ is a tensor field which depends of course on $\underline{r}$ and t.

The above definitions give at the same time the only possible relationships between the surface quantities and their bulk counterparts (better to say - their primitives), in order the interfacial balance law localized on the surface Σ were compatible and derivable from the 3D law. The latter is postulated for ψ in the integral form as well as in the following local one:

$$\frac{\partial}{\partial t}\,\psi + \mathrm{div}\,(\psi\otimes\underline{v} + \underline{w}) = \underline{p}\ . \tag{1.4}$$

On the other hand using the model developed in [1,2] one could not completely take into account [*1*] the influence of the thickness of the layer on the thermomechanical behaviour of phase interfaces. Quoted model we shall call a *0-th order model*.

In order to resolve the aforementioned difficulty an H-th order model is proposed, introducing the k-th moments ($k \le H$) of a typical quantity f by

$${}^{k}f \equiv \ell^{k}(\underline{x},t)\ f \qquad \text{when } \underline{x} \in \mathfrak{L}. \tag{1.5}$$

here ℓ^k means the k-th power of ℓ. One should mention at this point the approach used by Dumais [3], who already introduced the concept of the higher order moments in modelling interface phenomena. The following local balance equation for ψ can be easily derived from (1.4) and properties of the function $\ell(\underline{x},t)$ (see Lemma 2.9 in [1]) :

$$\frac{\partial}{\partial t}{}^{k}\psi + \mathrm{div}\,({}^{k}\psi\otimes\underline{v} + {}^{k}\underline{w}) = {}^{k}\underline{p} + k\left({}^{k-1}\psi\otimes(\underline{v}\cdot\underline{n}-c_n) + {}^{k-1}\underline{w}\cdot\underline{n}\right) \tag{1.6}$$

Regarding (1.6) as a particular case of (1.4) and recalling the results in Sec. 2 of [1], we get the following surface balance equation:

$$\begin{aligned}\frac{\delta n}{\delta t}\,{}^{k}\psi^{s} - 2Hc_n\,{}^{k}\psi^{s} + \mathrm{div}_s\left(\langle{}^{k}\psi\otimes(\underline{v}+\ell\,\mathrm{grad}_s c_n)\,\underline{A}_s(\ell)\rangle + \langle{}^{k}\underline{w}\,\underline{A}_s(\ell)\rangle\right) &= \\ = [\![j({}^{k}\psi(\underline{v}-\underline{c}) - {}^{k}\underline{w}\,]\!]\cdot\underline{n} + {}^{k}p^{s} + \langle jk\left({}^{k-1}\psi\otimes(\underline{v}\cdot\underline{n}-c_n) + {}^{k-1}\underline{w}\cdot\underline{n}\right)\rangle,\end{aligned} \tag{1.7}$$

where $\frac{\delta n}{\delta t}$, grad_s and div_s denote respectively the surface Thomas derivative, gradient and divergence operators. This equation is valid for any $k \ge 1$. If $k = 0$ the primitive interfacial balance law found in [1,2] is the counterpart of (1.4). In this particular case the last term of its L.H.S. is given by (1.3) and its last term of the R.H.S. vanishes.

[*1*] The authors gratefully acknowledge having this drawn to their attention by Professor S. RIONERO.

It can however arise a question concerning the mathematical completeness of this kind of approach. To answer this question one should first notice that the k-th moment of a typical function f in (1.5) (regarded as a function of ℓ only) defines the projection of f on the polynomial ℓ^k belonging to the basis formed by all polynomialsof the function space $L^2([\mathfrak{z}^-,\mathfrak{z}^+],\ d\mu = j d\ell)$. The measure μ is positive and absolutely continuous with respect to the Lebesgue measure as long as j is positive and H and K are finite; this corresponds to the hypothesis H3.1 in [1] on the thickness of the layer $\mathfrak{L}$. Therefore the H-order theory deals with truncated expansions along the thickness of the layer of physical quantities to be balanced.

2. MECHANICAL INTERFACIAL BALANCE LAWS

Let ρ be the mass density function for the continuum $\mathfrak{C}$. To make the presentation more compact and to make evident the Galilean invariance of surface balance laws we introduce the following denotation (compare 1.3)

$$\underline{W}^{s'}\{{}^k\rho\} \equiv {}^k\underline{M}^s := \langle {}^k\underline{m}(\ell)\rangle = \langle j\ell^k\rho\underline{v}\mathbb{1}_s\rangle + {}^k\underline{W}_\rho,$$

$${}^k\underline{S}_1\{\psi\} := \left\langle \left(\frac{{}^k\psi}{{}^k\rho} - \frac{{}^k\psi^s}{{}^k\rho^s} \right) \otimes {}^k\underline{m}(\ell)\right\rangle, \quad {}^k\underline{S}_2\{\psi\} := \langle {}^k\underline{w}\ \underline{A}_s(\ell)\rangle, \tag{2.1}$$

where ${}^k\underline{W}_\rho := \langle \ell^k\rho(\underline{A}_s(\ell) - j\mathbb{1}_s)\underline{v} + \ell^{k+1}\rho\ \mathrm{grad}_s c_n\ \underline{A}_s(\ell)\rangle$ can be proved to be Galilean invariant paralleling the proof of Lemma 4.2 in [1] . Moreover it is evident that the ${}^k\underline{S}_m$, m = 1,2, are Galilean invariant, of course, if $\underline{w}$ fulfills the same requirement.

2.1. Balance of Moments of Mass and Linear Momentum

With our denotation the balance equation for the moments of mass will take the following form, where $H \ge k \ge 1$,

$$\frac{\delta n}{\delta t}\,{}^k\rho^s - 2Hc_n\,{}^k\rho^s + \mathrm{div}_s\,{}^k\underline{M}^s = [\![j({}^k\rho(\underline{v}\cdot\underline{n}-c_n)]\!] + k\langle {}^{k-1}\rho\ (\underline{v}\cdot\underline{n}-c_n)\rangle. \tag{2.2}$$

To balance the first H moments of linear momentum with $\underline{w}$ equal to the minus Cauchy stress $\underline{T}$ the following set of equations must be satisfied

$$\frac{\delta n}{\delta t}\left({}^{k}\rho^{s}\,{}^{k}\underline{v}^{s}\right) - 2Hc_n\,{}^{k}\rho^{s}\,{}^{k}\underline{v}^{s} + \mathrm{div}_s({}^{k}\underline{V}\otimes{}^{k}\underline{M}^{s} + {}^{k}\underline{\underline{S}}_1\{\rho\underline{v}\} + {}^{k}\underline{\underline{S}}_2\{\rho\underline{v}\}) = {}^{k}(\rho\underline{b})^{s}$$

$$+ [\![({}^{k}\rho\underline{v}\otimes(\underline{v}\cdot\underline{n}-c_n)-{}^{k}\underline{T}\,\underline{n})j]\!] + \langle j\,k(\,{}^{k-1}\rho\underline{v}\otimes(\underline{v}\cdot\underline{n}-c_n) - {}^{k-1}\underline{T}\cdot\underline{n})\rangle \qquad (2.3)$$

where ${}^{k}\rho^{s}\,{}^{k}\underline{v}^{s} := {}^{k}(\rho\underline{v})^{s}$, ${}^{k}\underline{\underline{S}}_1\{\rho\underline{v}\} = \langle(\underline{v}-{}^{k}\underline{v}^{s})\otimes{}^{k}\underline{m}(\ell)\rangle$, ${}^{k}\underline{\underline{S}}_2\{\rho\underline{v}\} = -\langle{}^{k}\underline{T}\,\underline{A}_s(\ell)\rangle$.

Let us notice that for every $k \le H-2$ the term ${}^{k}\underline{W}_\rho$ is known in terms of moments of mass and linear momentum whose evolution is governed by the balance equations (2.2 -2.3) introduced in H-order models. Therefore in such models constitutive equations for ${}^{H-n}\underline{W}_\rho$ are required, together with constitutive equations for ${}^{k}\underline{\underline{S}}_m\{\rho\underline{v}\}$ where $k=1,\ldots,H$ and $n=0,1$.

2.2 Balance of Moments of Angular Momentum

We restrict now ourself only to nonpolar continua. The master angular momentum balance law is well known in the 3D theory; its interfacial counterpart requires to define two quantities for each k-th moment. Namely

$$ {}^{k}\Psi^{s} := \langle j(\underline{r} + \ell\,\underline{n}) \times \ell^{k}\rho\underline{v}\rangle\ ,\quad {}^{k}\Psi_2^{s} := \langle j\ell\,\underline{n} \times \ell^{k}\rho\underline{v}\rangle \qquad (2.4)$$

and the corresponding flux and production terms are

$$ {}^{k}\underline{w}(\ell) = -\,(\underline{r} + \ell\,\underline{n}) \times \ell^{k}\underline{T}, \qquad {}^{k}\underline{w}_2(\ell) = -\,\ell\,\underline{n} \times \ell^{k}\underline{T}$$

$$ {}^{k}\underline{p}^{s} = \langle j(\underline{r} + \ell\,\underline{n}) \times \ell^{k}\rho\underline{b}\rangle, \qquad {}^{k}\underline{p}_2^{s} = \langle j\ell\,\underline{n} \times \ell^{k}\rho\underline{b}\rangle - \langle j\ell^{k}\underline{F}\rangle \qquad (2.5)$$

where (cf.[1]) $j\underline{F} := (j\underline{1}+\ell(\underline{b}_0 - K\ell\mathbb{I}_s)\times\underline{T}\rangle - j\underline{n}\times\underline{T}\cdot\underline{n} - \underline{m}(\ell)\times(\underline{v}\cdot\underline{n})\underline{n} + j\rho\underline{v}\times c_n\underline{n}$.
Making use of the balance law (1.7) substituting ${}^{k}\psi^{s}$ with those defined in (2.4) together with the corresponding terms from (2.5) we arrive at a pair of equations (for any $H \ge k \ge 1$) which generalize (4.17) and (4.22) in [1] . Subtracting the second from the first and using the cross product of $\underline{r}$ with the law (2.3) we end up with

$$\langle\, j(\underline{1} \times \ell^{k}\underline{T})\,\rangle = \underline{0} \qquad (2.6)$$

which is automatically satisfied if $\underline{T}$ is symmetric. On the other hand the H + 1 equations (2.6) with $k = 0,1,\ldots H$ represent the H-th order condition of non-polarity of the layer.

3. SHELL-LIKE INTERFACE OF KIRCHHOFF-LOVE TYPE

Let us consider the particular case of interfaces in which the layer $\mathfrak{L}$ is defined by the kinematics of the continuum $\mathfrak{C}$. We assume that a surface Σ can be found such that the velocity field has the particular form, namely

$$\underline{v}(\ell;\underline{r},t) = \underline{v}_0(\underline{r},t) - \ell(\text{grad}_s w_n + \underline{b}_0\underline{v}_\tau), \quad \text{where } \underline{v}_\tau\cdot\underline{n} = 0 \tag{3.1}$$

This velocity field describes the motion in which particles appearing in the layer on a line tangent to a normal $\underline{n}$ move with equal normal speeds. However if w_n is equal to c_n and $\underline{v}_\tau$ equal to $\underline{v}_0 \mathbb{I}_s$ and the both are independent of ℓ then the aforementioned particles remain on a common line. In this case it turns out that the following relations

$$\underline{v}_0(\underline{r},t)\mathbb{I}_s = j^{-1}(d_z)\underline{A}_s(d_z)(\underline{V}^s + d_z \text{ grad } c_n), \quad (\underline{V}^s - \underline{v}_0)\cdot\underline{n} = 0, \tag{3.2}$$

hold, where $d_{\mathfrak{z}}$ defined by ${}^1\rho^s = d_{\mathfrak{z}}\, \rho^s$ belongs to $[\mathfrak{z}^-, \mathfrak{z}^+]$.

Formula (3.2) shows that the first order model is required for describing the Kirchhoff-Love type interface. More precisely if we consider all together

1) the interfacial linear momentum and mass balance laws

2) the boundary values for ρ^- and ρ^+ (they play the role of constitutive quantities) consistent with the sign of $\underline{v}_0\cdot\underline{n}$,

we obtain a well posed problem for bulk mechanical balance laws. Kirchhoff-Love type interface is a first instance in which the higher order models show their applicability in modelling surface phenomena.

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