

# Mechanical modeling of growth considering domain variation. Part I: constitutive framework

Jean-François Ganghoffer <sup>a,\*</sup>, Bernard Haussy <sup>b</sup>

<sup>a</sup> LEMTA—ENSEM, 2, Avenue de la Forêt de Haye, BP 160, 54054 Vandoeuvre Cedex, France

<sup>b</sup> Ecole Supérieure d'Electronique de l'Ouest, 4, rue Merlet de la Boulaye, BP 30926, 49009 Angers Cedex, France

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## Abstract

The growth of biological tissues is described as the volumetric production of mass within tissue elements, considered as one component potential sites for tissue renewal/resorption at a mesoscopic scale of description. The growth is characterized by a growth transformation gradient, which is accompanied by an additional accommodation transformation, so that the total transformation gradient defines a compatible global displacement field. The continuous change of the domain occupied by each tissue element during growth is considered, hence the mechanical balance laws are written, accounting for the additional terms due to the domain variation. The principle of virtual power is then expressed, considering that the power of internal forces originates from both volumic and surface potentials. The surface potential is thought to express configurational forces tied to the interface motion, extent and orientation. The equilibrium equations of the growing tissue element then follow, associated to surface and line boundary conditions. The writing of the second principle of thermodynamics for a tissue element continuously receiving matter due to transport phenomena allows to identify the driving forces linked to growth, and provides the evolution laws for the growth velocity. The large strains compatibility conditions that characterize the accommodation tensor are further considered as an important aspect of growth. A first insight into the numerical solutions of the compatibility conditions is given, envisaging the situation of radial growth.

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\* Corresponding author. Tel.: +33 383595724; fax: +33 383595551.

E-mail addresses: [jfgangho@ensem.inpl-nancy.fr](mailto:jfgangho@ensem.inpl-nancy.fr) (J.-F. Ganghoffer), [bernard.haussy@eseo.fr](mailto:bernard.haussy@eseo.fr) (B. Haussy).

## Nomenclature

$\underline{X}$	material point position on the initial configuration
$\underline{X}_g$	(resp. $\underline{x}_g$ ) position field on the growing surface $S_{0g}$ (resp. $S_g$ )
$\underline{U}$	displacement field
$\underline{F}$	transformation gradient— $\underline{F}_g$ growth transformation— $\underline{F}_a$ growth accommodation
$\underline{E}$	total lagrangian strain tensor— $\underline{E}_a$ lagrangian accommodation strain
$\underline{D}_g$	(resp. $\underline{D}_a$ ) growth deformation rate (resp. accommodation rate)
$\underline{d}, \underline{d}_g, \underline{d}_a$	Eulerian volumetric, surface and line growth velocity gradient resp.
$\tilde{\underline{d}}, \tilde{\underline{d}}_g, \tilde{\underline{d}}_a$	surface total, growth and accommodation deformation rates resp.
$\underline{\tilde{E}}$	(resp. $\underline{\tilde{E}}_a$ ) surface (resp. accommodation) deformation tensor
$\underline{J}_g$	(resp. $\underline{J}_{sg}$ ) volume Jacobean (resp. surface Jacobean)
$\underline{D}$	rate of deformation tensor— $\delta/\delta t$ domain derivative
$\underline{\Omega}_{0g}$	(resp. $\underline{\Omega}_g$ ) initial (resp. actual) tissue element configuration
$S_{0g}(S_g)$	growth surface in the lagrangian (resp. Eulerian) configuration
$\underline{N}_g$	(resp. $\underline{n}_g$ ) normal to the surface $S_{0g}$ (resp. $S_g$ )
$\underline{L}_g := \nabla_{S_g} \underline{n}_g$	curvature tensor of the surface $S_g$
$\underline{\tau}_{0g}$	(resp. $\underline{\tau}_g$ ) tangent vector to the contour $\partial S_{0g}$ in the tangent plane to $S_{0g}$ (resp. $\partial S_g$ )
$\underline{\nu}_{0g}$	(resp. $\underline{\nu}_g$ ) normal to the contour $\partial S_{0g}$ in the tangent plane to $S_{0g}$ (resp. to the contour $\partial S_g$ )
$\Gamma$	rate of mass change
$\underline{J}_i$	diffusion flux for the $i$ th constituent— $\Phi_{\rho_i}$ conduction flux for the $i$ th constituent
$M_i$	molecular weight of the $i$ th constituent— $\frac{v_{ij}}{M_i}$ stoichiometric coefficients
$\sigma_\rho$	global source of mass— $A_k$ chemical affinity— $R_k$ velocity of the $k$ th chemical reaction
$\mu^v$	(resp. $\mu^s$ ) volumic (resp. surface) chemical potential— $M$ chemical potential field
$\psi^v, \psi^s$	volumetric and surface density resp.
$\underline{A}_s$	surface growth driving force— $C_s$ orientation configurational driving force
$\underline{F}^{IR}, \tilde{\underline{F}}^{IR}, \tilde{\tilde{\underline{F}}}^{IR}$	irreversible volumic, surface and line driving forces for growth resp.

## 1. Introduction

One outstanding problem in developmental biology is the understanding of the factors that may promote the generation of biological form, involving the processes of growth (change of mass), remodeling (change of properties), and morphogenesis (shape changes), a classification suggested by [Taber \(1995\)](#). It is clear that these three aspects of the development of a biological structure have tied connections to each other, and are due to a combination of both genetic and epigenetic factors, such as chemical agents and mechanical stress and strain. There is a vast literature on this subject, tracing back to Galilei Galileo, who suggested that the size and forms of animal bones are determined by their function and their weight. The excellent review by [Taber \(1995\)](#) gives a nice survey of the existing literature, both from theoretical and experimental point of view.

More recent contributions analyze the problem of growth in terms of the evolution of a growth tensor, associated to a natural configuration of the living body, which proves convenient to set up an objective constitutive law ([Epstein and Maugin, 2000](#); [Rodriguez et al., 1994](#); [Ambrosi and Mollica, 2002](#); [Lubarda and Hoger, 2002](#)). [Taber and Humphrey \(2001\)](#), although referring to remodeling (microstructural reconfigura-

tion within the tissue, see Garikipati et al. (2003)), rather describe growth. The further concept of ‘natural configurations’ has been introduced by Rajagopal (1995) and Rajagopal and Srinivasa (1998) in various contexts, see also Humphrey and Rajagopal (2002), as an adequate framework in the modeling of growth.

Adopting a slightly different point of view, creation of mass within a solid body may naturally fit within the framework and objectives of configurational mechanics: mention for instance the ‘accretive forces’ introduced by Gurtin (1995), who complemented the more classical mechanical forces by configurational forces, that describe the internal structure of the material. Configurational mechanics also recently irrigated the field of biomechanics, where the computation of material forces in open systems under growth gives further insight into the morphological changes of the body, see Kuhl and Steinmann (2004), and the references therein.

An alternative route is followed in the present contribution, which analyses the thermomechanics of tissue growth, considering the variation of the domain occupied by the material points when mass is continuously added in both their volume and on their surface. The growth is assumed to occur at the scale of tissue elements, defined as small regions of space (representative volume elements) at a mesoscopic level of description, that receive nutrients and chemical species via diffusion processes, from an externally assumed existing reservoir (Ambrosi and Mollica, 2002). The present approach is similar in spirit to the recent work by Garikipati et al. (2003, 2004), who model the coupling of mass transport and mechanics within the framework of porous media theory. Accordingly, the sources and fluxes of mass are incorporated into the various balance laws, adopting the thermodynamics of irreversible and open systems as a natural framework that allows a physically consistent treatment of the coupling between mechanics and mass transport (Ganghoffer, 2003).

The main issue and originality of the present contribution is to analyze the impact of the domain variation of the tissue element on the balance laws and on the resulting driving forces for growth. Specifically, contributions due to the surface evolution (due to growth) and the boundary line separating the growing surface from the non-growing surface shall be highlighted. Note the recent contribution on the difficult problem of surface growth by Huang (2004), who introduced a new derivative, called the ‘material accretion derivative’, that accounts for surface growth, and a coupling function of growth, leading to a consistent form of the equilibrium equation and to accretive boundary conditions of the growing deformable body.

An outline of the paper is the following: the total potential energy of an evolving structure is written from the setting up of a volumic term and a surface expression, that represents the surface energy of the growing germ. The principle of virtual power is obtained from the stationnarity of the total potential energy (Section 3), in Eulerian form. The writing of the second principle of thermodynamics (Section 4) then enables to identify the driving forces for the growth, some of them being in duality pairing with the surface and line growth velocities. Since the growth is generally not compatible from kinematic point of view, another additional strain is needed in order to preserve the integrity of the displacement field. A numerical solution (Section 5) of the kinematic compatibility condition within a large transformation framework is obtained in the case of a radial growth assumption. Finally (Section 6), a conclusion and some perspectives are given.

The following conventions shall be used in the sequel: vectors are underlined once, and second order tensors twice. The transpose of a vector or a tensor is noted with a superscript “t”, thus for instance  $\underline{A}^t$  is the transpose (line vector or covector) of the column vector  $\underline{A}$ . The convention of implicit summation of a repeated index in any monomial is systematically used. Considering a surface  $S$ , part of the boundary of a volume  $V$ , any field  $A(\underline{x})$  having its domain within the volume  $V$  shall have a counterpart (that can be envisaged as its trace) on the surface  $S$ , using the same variable with a tilde  $\tilde{A}$ , and a line trace on the edge of  $S$  ( $\partial S$ , when the surface is not closed), noted with a double tilde  $\tilde{\tilde{A}}$ . Accordingly, the position vector field  $\underline{x}$  within the volume  $V$  shall have a surface and a line counterpart, noted, respectively  $\tilde{\underline{x}}$  and  $\tilde{\tilde{\underline{x}}}$ . The main advantage of using this last notation is the ability to differentiate fields having their domain distinctly within a volume, a surface or an edge, respectively. This notation shall be used in a systematic manner in the sequel, unless the status of the fields is explicitly stated. The infinitesimal volume, surface and line elements

shall be noted  $dx$ ,  $d\sigma$ , and  $dl$ , respectively; distinctions between volume elements appearing in different configurations shall be done when necessary. The partial derivative of a field  $f(x)$  with respect to the variable  $x$  is noted in abbreviated form, viz  $f_{,x} := \frac{\partial f}{\partial x}$ . Considering a second order tensor  $\underline{\underline{B}}$ , the left divergence of  $\underline{\underline{B}}$  is the vector  $\text{div}_g \underline{\underline{B}}$ , having the components  $(B_{ij,i})_j$ .

## 2. Kinematics of growth

Adopting the point of view of the growing material as a single phase continuum, in which growth is envisaged as an increase of mass of the existing particles (and not an increase of the particle number), Ambrosi and Mollica (2002), the particles (thought as a population of cells in the case of biological tissues) can be labeled in any configuration of the body.

Since the number of particles is the same in any configuration, a motion that connects all configurations can be defined. The initial (Lagrangian) and final (Eulerian) configurations are denoted respectively  $\Omega_{0g}$  and  $\Omega_g$ ; an intermediate configuration  $\Omega_{ig}$  due to growth is further introduced, so that a tangent mapping between the material point  $\underline{X}$  and its counterpart in  $\Omega_{ig}$  (after growth) exists (Rodriguez et al., 1994), thereby defining the growth transformation tensor  $\underline{\underline{F}}_g(\underline{X}, t)$ . The natural state of each particle is then defined as the state reached when cutting the particle and relieving its state of stress while keeping the mass constant; the natural configuration of the body (at a given time) is then the collection of all particles in their natural states (Rajagopal, 1995; Rajagopal and Srinivasa, 1998; Humphrey and Rajagopal, 2002). Since the local (at each material point) change of zero stress state during growth is different from point to point, the growth transformation gradient does not necessarily generate by itself a global compatible displacement field. An additional deformation is needed to restore the continuity of the global displacement field over the whole body: this deformation field shall be called the growth accommodation tensor  $\underline{\underline{F}}_a$  in the sequel. Accordingly, shape changes of a growing tissue (initially supposed to be in a stress-free state) are due to the addition/removal of material (the material added may be different from the existing material) and to an additional deformation needed to accommodate the change of tissue configuration, i.e. shape and volume changes that may otherwise introduce discontinuities within the body.

The classical multiplicative decomposition (Rodriguez et al., 1994) of the transformation gradient

$$\underline{\underline{F}} = \nabla_{\underline{X}} \underline{x}(\underline{X}, t)$$

with  $\underline{X}$  and  $\underline{x}$  the lagrangian end Eulerian positions, respectively, as the product of the growth deformation gradient tensor  $\underline{\underline{F}}_g$  and the growth accommodation tensor  $\underline{\underline{F}}_a$  (reminiscent of large strains plasticity theory) is then introduced:

$$\underline{\underline{F}} = \underline{\underline{F}}_a \cdot \underline{\underline{F}}_g \quad (2.1)$$

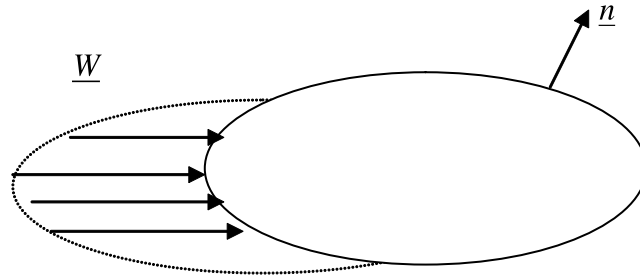
The transformation gradients  $\underline{\underline{F}}_g$ ,  $\underline{\underline{F}}_a$  and  $\underline{\underline{F}}$  define the mappings of the tangent spaces to the configurations  $\Omega_{0g}$ ,  $\Omega_{ig}$  and  $\Omega_g$ , called, respectively  $T_{\Omega_{0g}}$ ,  $T_{\Omega_{ig}}$ , and  $T_{\Omega_g}$ , thus keeping within the framework of simple materials in the sense of Noll (Truesdell and Noll, 1992). Considering the mere kinematic aspect of growth at the present stage, no further specification is needed. The following lagrangian measures of deformation are further introduced:

- the total lagrangian strain tensor is defined as

$$\underline{\underline{E}} := \frac{1}{2} (\underline{\underline{F}}^t \cdot \underline{\underline{F}} - I)$$

- the growth deformation tensor is elaborated as

$$\underline{\underline{E}}_g := \frac{1}{2} (\underline{\underline{F}}_g^t \cdot \underline{\underline{F}}_g - I)$$

Fig. 1. Transport of the material domain  $\Omega_t$  by the velocity field  $\underline{W}$ .

- the lagrangian accommodation strain  $\underline{E}_a$  is further defined as

$$\underline{E}_a := \frac{1}{2} (\underline{F}_a^t \cdot \underline{F}_a - I)$$

Noting  $\underline{U} := \underline{x} - \underline{X}$  the displacement field, the total velocity  $\underline{V} = \frac{d\underline{U}}{dt}$  induces a variation of the initial domain occupied by the tissue element under growth. The prescription of the displacement field  $\underline{U}$  is tantamount to the motion of the material domain with a certain velocity field, allowing the calculation of the derivative of functions or functionals having their range on this domain (Allaire and Henrot, 2001). Consider first  $b(\underline{x}, t)$  a scalar valued field defined in the Eulerian coordinates; the time derivation following a point or a domain in its own motion, characterized by a velocity  $\underline{W}$ , is elaborated as

$$\frac{\delta b}{\delta t} := \frac{\partial b}{\partial t} + \underline{W} \cdot \underline{\text{grad}}(b) \quad (2.2)$$

using the symbol  $\delta/\delta t$  to denote this specific derivation. The generalization to a derivation of a functional with respect to a domain  $\Omega_t$  having its own motion defined by the velocity field  $\underline{W}$  (Fig. 1), consists in writing the domain derivative of the integral  $B = \int_{\Omega_t} b(\underline{x}, t) d\underline{x}$  (here,  $b(\underline{x}, t)$  represents a volumic density) as

$$\frac{\delta B}{\delta t} = \int_{\Omega_t} \frac{\partial b}{\partial t} d\underline{x} + \int_{S_t} b \underline{W} \cdot \underline{n} d\sigma \quad (2.3)$$

with  $\underline{n}$  the outward normal to the boundary  $S_t = \partial\Omega_t$ . The generalization to vectorial functions  $\underline{b}(\underline{x}, t)$  is straightforward, since Eqs. (2.2) and (2.3) remain valid.

Note that if  $\underline{W}$  vanishes on a part of the boundary  $\partial\Omega_t$ , only the complementary portion of the boundary (on which  $|\underline{W}| \neq 0$ ) needs effectively to be considered in (2.3). This domain derivation coincides with the material derivative of a volume integral (the volume motion is given by that of the material points) given by Reynold's transport theorem (Truesdell and Noll, 1992).

### 3. Balance laws

In this section, a lagrangian point of view is adopted, so that the energy densities are referred to the initial configuration occupied by the material points of the solid body. Note that any anisotropy (being reflected in the form taken by the strain energy density) can be lost during ongoing deformation, thus is only valid—a priori—in the initial configuration.

The growing solid shall be divided into so-called tissue material elements, considered as the equivalent at a continuum level of the individual cells within a biological context. Although being heterogeneous, the

tissue element is supposed to build a physical entity at a mesoscopic scale of description, exchanging work and matter with the surrounding tissue elements.

**Remark 1.** This mesoscopic viewpoint proves convenient when dealing with a large population of tissue elements. Although it does not allow the consideration of the fine details of the tissue evolution (such as in cellular adhesion process, whereby interfacial processes play a major role (Mefti et al., 2004)), it proves compatible with a treatment using continuum mechanics (with variants at hands, such as the use of mixture theory (Rajagopal, 1995) or (Rajagopal and Srinivasa, 1998)).

A tissue element of matter receiving continuously new matter from outside (due to diffusion processes not being explicitly considered in this contribution) is accordingly considered as the elementary volume of analysis  $\Omega_{0g}$  in the initial configuration (recall that its Eulerian counterpart is noted  $\Omega_g$ ). During growth, matter is then added in the bulk of  $\Omega_{0g}$  and on the portion  $S_{0g}$  (its Eulerian counterpart is noted  $S_g$ ) of the surface  $\partial\Omega_{0g}$  (the change of the surface being induced by that of the bulk); accordingly, the domain occupied by the tissue element changes. When growth does not occur on the whole of  $\partial\Omega_{0g}$ ,  $S_{0g}$  is not a close surface, thus it has a boundary (Fig. 2), noted  $\partial S_{0g}$  (its Eulerian counterpart is noted  $\partial S_g$ ), which is not reduced to the empty space. The normal to the surface  $S_{0g}$  (resp.  $S_g$ ) is noted  $\underline{N}_g$  (resp.  $\underline{n}_g$ ), the tangent vector to the contour  $\partial S_{0g}$  in the tangent plane to  $S_{0g}$  (resp.  $\partial S_g$ )  $\underline{\tau}_{0g}$  (resp.  $\underline{\tau}_g$ ), and the normal to the contour  $\partial S_{0g}$  in the tangent plane to  $S_{0g}$  (resp. to the contour  $\partial S_g$ )  $\underline{\nu}_{0g}$  (resp.  $\underline{\nu}_g$ ).

The impact of the domain variation on the balance laws shall be assessed in the sequel, considering the balance of mass, the momentum conservation equation, and the second principle of thermodynamics. As a matter of simplification, we shall focus on the case of isothermal growth in this contribution.

### 3.1. Balance of mass and transport phenomena

Adopting an Eulerian point of view, the mass variation due to the transport phenomena is written as the following integral

$$\frac{dm}{dt} = \int_{\Omega_g} \Gamma \rho dx_g \quad (3.1)$$

with  $\rho$  the density in the final configuration, and  $\Gamma$  the rate of mass variation due to growth and growth accommodation (a quantity having the dimension of the inverse of time).

Expressing the total mass of the domain  $\Omega_g$  as  $m(\Omega_g) = \int_{\Omega_g} \rho(x) dx$ , we get the following expression of the material derivative:

$$\frac{dm}{dt} = \int_{\Omega_g} \left[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underline{V}) \right] dx_g \quad (3.2)$$

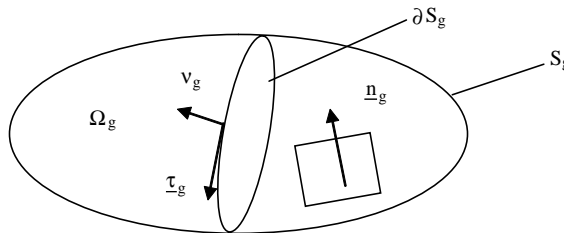


Fig. 2. Tissue element under growth (Eulerian view).

with  $\underline{V}$  the domain variation velocity. Since the equalities (3.1) and (3.2) hold true for any subvolume of  $\Omega_g$ , we obtain the following local condition of mass conservation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underline{V}) = \Gamma \rho \quad (3.3)$$

Assuming that no explicit time dependence occurs, equality (3.3) allows to identify the rate of mass variation, viz  $\Gamma = \frac{1}{\rho} \nabla \cdot (\rho \underline{V})$ . Furthermore, the divergence of the velocity field is equal to the trace of the rate of deformation tensor  $\underline{\underline{D}} := \frac{1}{2}(\nabla \underline{V} + \nabla^t \underline{V})$ , viz

$$\operatorname{div} \underline{V} = \operatorname{Tr}(\underline{\underline{D}}) \quad (3.4)$$

By the application of Green's formula, one immediately obtains

$$\int_{\Omega_g} \operatorname{div} \underline{V} \, dx_g = \int_{\partial \Omega_g} \tilde{V}_N \, d\sigma_g \quad (3.5)$$

thus addition (removal) of matter at the surface occurs when the flux expressed by the surface integral is positive (resp. negative), thus  $\tilde{V}_N := \underline{V} \cdot \underline{N} > 0$  (resp.  $\tilde{V}_N < 0$ ). A few considerations regarding the balance of mass in connection with transport phenomena and chemical reactions are in order. Introducing at this stage the diffusion phenomena leading to creation/resorption of mass, we consider the tissue element as an open system with  $r$  constituents, undergoing chemical reactions. Since the growing tissue element is here viewed as a single-phase continuum, the different constituents are in fact indistinguishable from each other.

Each constituent (labeled with the index  $i$ ) satisfies the mass balance equation

$$\dot{\rho}_i + \rho_i \operatorname{div}(\underline{v}) + \operatorname{div} \underline{J}_i = \Phi_{\rho i} + \sum_{j=1}^r v_{ij} R_j \quad (3.6)$$

in which  $\underline{v}$  is the barycentric velocity,  $\underline{J}_i := \rho_i(\underline{v}_i - \underline{v})$  is a diffusion flux (due to the relative velocity  $(\underline{v}_i - \underline{v})$  of the individual particles,  $\Phi_{\rho i}$  a conduction flux for the  $i$ th constituent, and  $R_j$  the velocity of the chemical reaction for the  $j$ th constituent. The coefficients  $\frac{v_{ij}}{M_i}$  are the stoichiometric coefficients, with  $M_i$  the molecular weight of the  $i$ th constituent. The global mass balance is further obtained by summation of the partial Eq. (3.6):

$$\dot{\rho} + \rho \operatorname{div}(\underline{v}) = \Phi_{\rho} + \sum_{i=1}^r \sum_{j=1}^r v_{ij} R_j \quad (3.7)$$

with  $\Phi_{\rho}$  the total flux of conduction (the summation of the partial Eq. (3.6) cancels the diffusion fluxes). The chemical origin of the rate of mass variation is given by

$$\Gamma = \Phi_{\rho} + \sigma_{\rho} \quad (3.8)$$

with  $\sigma_{\rho} = \sum_{i=1}^r \sum_{j=1}^r v_{ij} R_j$  the source of mass.

In the forthcoming paragraph, the balance of momentum for a growing tissue element shall be expressed.

### 3.2. Balance of momentum

The principle of virtual power expresses the conservation of momentum in weak form, in the sense of distribution theory. However, the fundamental problem here is due to the mixing of the time variation (occurring in the virtual velocities) and the simultaneous domain variation, pointing towards the need for a non-incremental principle at the outset. The writing of the minimum of the total potential energy  $V[\Omega_g]$  of the tissue element at true equilibrium as the nil derivative of  $V[\Omega_g]$  with respect to the (varying) domain leads to a generalized version of the principle of virtual power accounting for the domain variation.



Proceeding in this way enables to start from a quantity (the total potential energy, to be elaborated in the sequel) that involves finite quantities (instead of rates), thus its domain variation can be evaluated without any possible bias due to the occurrence of rates. In the sequel, the velocities shall be considered as virtual variations of the corresponding displacements, and the displacements as virtual variations of the associated positions.

### 3.2.1. Volumic and surface energies for a growing germ

The total mechanical energy of a growing tissue element is set up from a volumetric density  $\psi^V(\underline{X}_g, \underline{E})$  in the initial configuration, depending upon the total lagrangian strain  $\underline{E}$ , and possibly on the position field  $\underline{X}_g$ , and a surface density  $\psi^S(\underline{\tilde{X}}_g, \underline{N}_g, \underline{\tilde{E}})$  in  $\Omega_{0g} \cup S_{0g}$ , depending upon the surface lagrangian strain  $\underline{\tilde{E}}$ , the normal  $\underline{N}_g$  to the surface  $S_{0g}$ , and possibly on the position field  $\underline{\tilde{X}}_g$  on  $S_{0g}$ , in order to account for the heterogeneous nature of growth. We assume that the support (in the mathematical sense) of the density  $\psi^S$  restricts to the sole growing surface  $S_{0g}$ , which in physical terms expresses as the assumption that the surface energy contribution of the (non-growing) surface  $\partial\Omega_{0g}/S_{0g}$  can be neglected.

The selected arguments (as well as the form) of  $\psi^S$  reflect the fact that the surface energy contains:

- A contribution arising from the variations of the dimensions of any infinitesimal element of the growing surface, accounted for by the surface strain tensor  $\underline{\tilde{E}}$ . Since the material added (or removed) from the initial surface  $\partial\Omega_{0g}$  may be different from the initial material, a specific constitutive behaviour needs to be assigned to the surface  $S_{0g}$ . The partial derivative of the surface density with respect to  $\underline{\tilde{E}}$  defines a surface growth driving force  $\underline{\tilde{A}} := \psi^S_{,\underline{\tilde{E}}}$  that triggers the variation of the surface  $S_g$ .
- A contribution arising from the change of configuration of the surface  $S_g$  during its growth: the configuration is characterized by the surface orientation, defined by the normal  $\underline{N}_g$ , in addition to the amount of surface created. Recall the transformation rule of surface elements known as Nanson formula (Truesdell and Noll, 1992)  $\underline{n}_g \, ds = J_g \underline{F}^{-t} \cdot \underline{N}_g \, dS$ , with  $J_g := \det(\underline{F})$ , considering the tangent mapping  $\underline{F}$  between two configurations (the elements attached to the initial configuration, i.e. the oriented surface element  $\underline{N}_g \, dS$ , are noted using capital letters). The partial derivative of the surface energy density with respect to  $\underline{N}_g$  defines an orientational configuration force  $\underline{C}_s := \psi^S_{,\underline{N}}$  conjugated to the change of local surface orientation see Norris (1998), or Freund (1998).

**Remark 2.** Several living tissues primarily grow by accretion or resorption of mass, as pointed in Taber (1995). Tissues or materials such as bones—see e.g. the bio-chemo approach by Silva and Ulm (2002)—shells, horns or branches fall into this category. Regarding surface growth, we herewith advocate a novel contribution, due to a specific consideration of the surface behaviour, in terms of surface energy and equilibrium/boundary conditions. The surface energy clearly plays an important role in growth phenomena, since growth basically occurs by cell adhesion mechanisms (in the case of bones, growth and remodeling are due to the relative activity of two specialized cells, named osteoblasts and osteoclasts (Cowan, 1983)) (Mefti et al., 2004).

Both densities  $\psi^V$  and  $\psi^S$  are incorporated into the total mechanical energy, expressed first in the initial configuration  $\Omega_{0g}$ , then pushed forward onto the final configuration  $\Omega_g$ , viz

$$E = \int_{\Omega_{0g}} \psi^V dX + \int_{S_{0g}} \psi^S d\Sigma = \int_{\Omega_g} \psi^V J_g^{-1} dx_g + \int_{S_g} \psi^S J_{sg}^{-1} d\sigma_g \equiv \int_{\Omega_g} \psi^V j_g dx_g + \int_{S_g} \psi^S j_{sg} d\sigma_g \quad (3.9)$$

with  $j_g := J_g^{-1}$  and  $j_{sg} := J_{sg}^{-1}$  the inverses of the volume Jacobian  $J_g$  and the surface Jacobian  $J_{sg} := d\Sigma/d\sigma_g$ , respectively. The surface Jacobian expresses as:  $J_{sg} := J_g/(\underline{n}_g \cdot \underline{F}_g \cdot \underline{N}_g)$ .



In (3.9), the symbols  $dx_g$ ,  $d\sigma_g$  represent the volume and surface differential elements, respectively. Since mass is continuously changing,  $\psi^V$  is defined as a volumic density—instead of a quantity defined per unit mass; following the same idea,  $\psi^S$  is defined as a quantity per unit surface (the quantity of mass attached to a surface has no true physical sense), which potentially reflects more than the mere idea of a surface energy (viewed as a scalar), since the consideration of the normal to the growing surface  $S_g$  introduces an additional orientational dependence. It is clear that the orientation of the surface, together with the amount of surface created, are variables that characterize the configuration of the interface between neighboring tissue elements. The present choice of a lagrangian description is tied to the fact that the deformation due to the accommodation of growth is likely to change the state of anisotropy of the tissue from its state in the initial configuration. Conversely, it may happen that the growth does not change by itself the state of anisotropy, if for instance the same material is smoothly accommodated by the tissue. An explicit dependence on the position of both volumic and surface potentials has been introduced, via the position variables  $\underline{X}_g$  and  $\tilde{\underline{X}}_g$ , respectively, so that the growth is here envisioned as a heterogeneous process occurring in a uniform material body. Recall that a body is called materially uniform when all its points are made of the same material (Epstein and Maugin, 2000); the non-homogeneous character of the growth means that the material points do attain different stages at the same common time (otherwise said, all the material points do not attain the same state at the same instant). However, if the volume of the tissue element is small enough, it can be considered as nearly uniform.

In the case of soft tissue such as the arterial wall, diverse constitutive models for the volumetric energy density  $\psi^V(\underline{X}_g, \underline{E})$  have been proposed in the literature, see Holzapfel and Weizsäcker (1998), Holzapfel et al. (2000) and Holzapfel and Gasser (2001). The novel contribution here is the consideration of the surface energy density term  $\psi^S(\tilde{\underline{X}}_g, \underline{N}_g, \underline{\tilde{E}})$ , the form of which can be built from the two pseudo-invariants of the right-Cauchy Green tensor  $\underline{\tilde{C}} := \underline{\tilde{E}}^T \cdot \underline{\tilde{E}}$  and the two pseudo-invariants of its surface counterpart  $\underline{\tilde{\underline{C}}} := \underline{\tilde{\underline{E}}}_0^T \cdot \underline{\tilde{\underline{E}}}_0$  (itself being constructed from the curvature tensor of the surface  $S_{0g}$ , see the Appendix 1, viz  $\underline{\tilde{\underline{L}}}_{0g} := \nabla_S \underline{N}_g$ ). The surface transformation gradient is here defined in its Lagrangian format as

$$\underline{\tilde{\underline{E}}}_0 = \underline{\tilde{\underline{E}}} \cdot P_0 = \underline{\tilde{\underline{E}}} \cdot (I - \underline{N}_g \otimes \underline{N}_g)$$

with  $P_0 = I - \underline{N}_g \otimes \underline{N}_g$  the Lagrangian projection operator. These four invariants are defined as the following scalar products:

$$I_1 = \underline{N}_g \cdot \underline{\tilde{\underline{C}}} \cdot \underline{N}_g; \quad I_2 = \underline{N}_g \cdot \underline{\tilde{\underline{C}}}^2 \cdot \underline{N}_g; \quad I_3 = \underline{N}_g \cdot \underline{\tilde{\underline{C}}} \cdot \underline{N}_g; \quad I_4 = \underline{N}_g \cdot \underline{\tilde{\underline{C}}}^2 \cdot \underline{N}_g$$

The two first pseudo-invariants are deformation measures in the direction of the normal to the growing surface, while the two last invariants are curvature measures in the same direction. Accordingly, the proposed form of the surface strain energy density will be

$$\psi^S \equiv \psi^S(I_1, I_2, I_3, I_4)$$

Note that more general forms of the volumetric and surface energy densities can be obtained from the representation theorems in Wang (1971).

The total potential energy of the growing tissue element is then the difference between the total energy and the work of the external forces  $W^{\text{ext}}$ :

$$V[\Omega_g] = E - W^{\text{ext}}$$

using a bracket notation to remind that  $V[\Omega_g]$  is considered as a functional of the tissue element configuration. We assume that the equilibrium equations of the growing tissue element are obtained from the annihilation of the Gateaux derivative of  $V[\Omega_g]$ , in the direction of the admissible set of directions  $(\underline{V}, \underline{\tilde{V}}, \underline{\tilde{\underline{V}}})$  representing the directions of volumetric, surface and line growth, respectively.

The work of the external forces is successively expressed in Eulerian and lagrangian format as

$$\begin{aligned} W^{\text{ext}} &:= \int_{\Omega_g} \underline{f}_0 \cdot \underline{u}(\underline{x}) \, d\underline{x}_g + \int_{\partial\Omega_g} \underline{t}_0 \cdot \underline{\tilde{u}}(\underline{\tilde{x}}) \, d\sigma_g + \int_{\partial S_{gt}} p_0 \cdot \underline{\tilde{u}}(\underline{\tilde{x}}) \underline{\tau}_{0g} \, dI_g \\ &= \int_{\Omega_{0g}} \underline{f}_0 \cdot \underline{u}(\underline{X}) J_g \, dX_g + \int_{\partial\Omega_{0g}} \underline{t}_0 \cdot \underline{\tilde{u}}(\underline{\tilde{X}}) J_{sg} \, d\Sigma_g + \int_{\partial S_{0g}} p_0 \cdot \underline{\tilde{u}} \underline{F} \cdot \underline{\tau}_g \, dL_g \end{aligned} \quad (3.10)$$

with  $\underline{f}_0$  the volumetric body forces,  $\underline{t}_0 = \underline{\sigma} \cdot \underline{n}$  the traction vector, product of the Cauchy stress tensor  $\underline{\sigma}$  with the normal  $\underline{n}$  on the boundary  $\partial\Omega$ ,  $p_0$  the (scalar valued function) density of line forces (acting on the close edge  $\partial S_g$ ), and  $(\underline{u}, \underline{\tilde{u}}, \underline{\tilde{u}})$  the triplet of volumetric, surface, and line displacements, respectively. We again refer the reader to the clarifying picture (Fig. 2). Note that the existence of the stress tensor results from the classical Cauchy's tetrahedron argumentation; the traction's acting on the whole boundary of the solid tissue element physically reflect the contact forces exerted by the neighboring tissue elements.

In the forthcoming, the variation of the potential energy of the tissue element is evaluated, accounting for the domain variation due to the growth. Following the previous discussion, the domain variation of any quantity  $(\cdot)$  is noted equivalently  $\frac{d(\cdot)}{d\Omega}$  or  $\frac{\delta}{\delta t}$  in the sequel; a very detailed account of domain derivatives of volume and surface integrals is given in Petryk and Mroz (1986). Accordingly, the domain variation of the total energy expresses in Eulerian form as

$$\begin{aligned} \frac{\delta E}{\delta t} &= \int_{\Omega_g} j_g \delta\psi^V \, d\underline{x}_g + \int_{\Omega_g} \psi^V \delta(j_g) \, d\underline{x}_g - \int_{\Omega_g} \nabla_X(j_g \psi^V) \cdot \delta \underline{U} \, d\underline{x}_g + \int_{S_g} j_g \psi^V \delta \underline{\tilde{U}} \cdot \underline{n}_g \, d\sigma_g \\ &\quad + \int_{S_g} j_{sg} \delta\psi^S \, d\sigma_g + \int_{S_g} \psi^S \delta(j_{sg}) \, d\sigma_g + \int_{S_g} j_{sg} \psi^S \text{div}_S \delta \underline{\tilde{U}} \, d\sigma_g \end{aligned} \quad (3.11)$$

identifying the velocity field  $\underline{V}$  to a virtual variation of the displacement  $\underline{U}$ . The virtual variation can in turn be identified to a virtual velocity; this point of view shall be adopted in the sequel. The three first integrals in (3.11) account for the volumetric part of the growth, while the last four integrals account for the surface growth, occurring on  $S_g$ . Note that the displacement field tied to the domain variation is zero on the surface  $\partial\Omega_g \setminus S_g$ . In order to evaluate the domain variation of the total potential energy, some elements of differential geometry are needed (and made specifically differential geometry of surfaces), which are given in Appendix 1.

### 3.2.2. Equilibrium equations and boundary conditions

In order to set the stage, a decomposition of the kinematics into elements that belong to the tangent plane to the growing surface  $S_g$ , and to its normal shall be performed. The velocity field is being decomposed into a tangential and a normal contribution

$$\underline{V} = \underline{V}_T + V_N \underline{n}_g$$

with  $\underline{V}_T$  the tangential part of  $\underline{V}$ , i.e. its projection onto the tangent plane to  $S_g$ , and  $V_N := \underline{V} \cdot \underline{n}_g$  the—scalar—normal component of  $\underline{V}$ . The surface deformation gradient is further defined as the projection of  $\underline{F}$  onto the tangent plane to  $S_g$ , viz

$$\underline{\tilde{F}} := \underline{F} \cdot (I - \underline{n}_g \otimes \underline{n}_g)$$

Accounting for the dependencies

$$\psi^V = \psi^V(\underline{x}_g, \underline{E}); \psi^S = \psi^S(\underline{\tilde{x}}_g, \underline{n}_g, \underline{\tilde{E}})$$

in the actual configuration, the variations  $\delta\psi^V$  and  $\delta\psi^S$  in (3.11) express as

$$\delta\psi^V = \psi^V_{,E} : \delta \underline{E} + \psi^V_{,x_g} \cdot \delta \underline{x}_g; \quad \delta\psi^S = \psi^S_{,x_g} \cdot \delta \underline{\tilde{x}}_g + \psi^S_{,n_g} \cdot \delta \underline{n}_g + \psi^S_{,E} : \delta \underline{\tilde{E}} \quad (3.12a, b)$$

The displacement field is defined from the comparison of the initial and final position fields as:

$$\underline{U} = \underline{x} - \underline{X}$$

thus by taking the variation:

$$\delta \underline{U} = \delta \underline{x} - \delta \underline{X}$$

By definition of the total transformation gradient  $\underline{\underline{F}}$ , we have

$$\delta \underline{x} = \underline{\underline{F}} \cdot \delta \underline{X}$$

thus giving the variation of the position field vs. the displacement variation

$$\delta \underline{x} = (I - \underline{\underline{F}}^{-1})^{-1} \cdot \delta \underline{U} \quad (3.13)$$

Using the previous equality, the variation of the volumic density is obtained after some elementary calculations as

$$\delta \psi^V = \frac{1}{2} (\psi_{,E}^{Vt} + \psi_{,E}^V) \cdot \underline{\underline{F}}^t : \delta \underline{\underline{F}} + \psi_{,x_g}^V \cdot (I - \underline{\underline{F}}^{-1})^{-1} \cdot \delta \underline{U} \quad (3.14)$$

Combining the surface divergence theorem recalled in the [Appendix 1](#) with the equalities (A1.1) through (A1.7) established in [Appendix 1](#) and the above expression (3.14), gives after a lengthy calculation the (virtual) variation of the total mechanical energy of the germ:

$$\begin{aligned} \delta E = & - \int_{\Omega} \text{div}_g \left[ \frac{1}{2} j(\psi_{,E}^{Vt} + \psi_{,E}^V) \cdot \underline{\underline{F}}^t \right] \cdot (I - \underline{\underline{F}}^{-1})^{-1} \cdot \delta \underline{U} dx_g + \int_{S_{gt}} \underline{n}_g^t \cdot \frac{1}{2} j(\psi_{,E}^{Vt} + \psi_{,E}^V) \cdot \underline{\underline{F}}^t \cdot (I - \underline{\underline{F}}^{-1})^{-1} \\ & \cdot \delta \underline{\underline{U}} d\sigma_g + \int_{\Omega} \psi_{,x_g}^V \cdot (I - \underline{\underline{F}}^{-1})^{-1} \cdot \delta \underline{U} dx_g + \int_{\Omega} \nabla(j\psi^V) \cdot \delta \underline{U} dx_g - \int_{S_{gt}} j\psi^V \delta \underline{\underline{U}} \cdot \underline{n}_g d\sigma_g \\ & + \int_{S_{gt}} (\psi_{,x_g}^S)^t \cdot (I - \underline{\underline{F}}^{-1})^{-1} \cdot \delta \underline{\underline{U}} d\sigma_g - \int_{S_{gt}} \text{div}_s \left[ \frac{1}{2} j_s(\underline{\underline{A}}^{St} + \underline{\underline{A}}^S) \cdot \underline{\underline{F}}^t \right] \cdot (I - \underline{\underline{F}}^{-1})^{-1} \cdot \delta \underline{\underline{U}} d\sigma_g \\ & + \int_{S_{gt}} (\psi_{,n}^S)^t \cdot \underline{\underline{L}} \cdot \underline{\underline{P}} \cdot \delta \underline{\underline{U}} d\sigma_g + \int_{\partial S_{gt}} \frac{1}{2} j_s(\underline{\underline{A}}^{St} + \underline{\underline{A}}^S) \cdot \underline{\underline{F}}^t \cdot (I - \underline{\underline{F}}^{-1})^{-1} \cdot \delta \underline{\underline{U}} \cdot \underline{\tilde{v}} \cdot d\mathbf{l}_g \\ & - \int_{S_{gt}} jJ_s(\underline{\underline{F}} \cdot \underline{\underline{N}}_g)^t \cdot \underline{\underline{L}} \cdot \underline{\underline{P}} \cdot \delta \underline{\underline{U}} d\sigma_g + \int_{S_{gt}} [\nabla_s(\psi^S)]^t \cdot \delta \underline{\underline{U}} d\sigma_g - \int_{\partial S_{gt}} \psi^S \delta \underline{\underline{U}} \cdot \underline{\tilde{v}} \cdot d\mathbf{l}_g \\ & - \int_{S_{gt}} jJ_s[\text{div}_s(\underline{\underline{N}}_g \otimes \underline{\underline{n}}_g)]^t \cdot \delta \underline{\underline{U}} d\sigma_g + \int_{\partial S_{gt}} jJ_s(\underline{\underline{N}}_g \otimes \underline{\underline{n}}_g) \cdot \delta \underline{\underline{U}} \cdot \underline{\tilde{v}} \cdot d\mathbf{l}_g \end{aligned} \quad (3.15)$$

Proceeding in a similar manner, the variation of the work of external forces acting on the tissue element (using the Eulerian form of (3.10)) is obtained as

$$\begin{aligned} \delta W^{\text{ext}} = & \int_{\Omega_g} \underline{f}_0 \cdot \delta \underline{U} dx_g - \int_{\Omega_g} \nabla_X(\underline{f}_0 \cdot \underline{u}) \cdot \delta \underline{U} dx_g + \int_{S_{gt}} \underline{f}_0 \cdot \underline{\tilde{u}} \delta \underline{\underline{U}} \cdot \underline{n}_g d\sigma_g + \int_{\partial \Omega} \underline{t}_0 \cdot \delta \underline{\underline{U}} d\sigma_g \\ & - \int_{S_{gt}} \nabla_s(\underline{t}_0 \cdot \underline{\tilde{u}})^t \cdot \delta \underline{\underline{U}} d\sigma_g + \int_{\partial S_{gt}} \underline{t}_0 \cdot \underline{\tilde{u}} \delta \underline{\underline{U}} \cdot \underline{\tilde{v}}_g d\mathbf{l}_g + \int_{\partial S_{gt}} p_0 \delta \underline{\underline{U}} \cdot \underline{\tau}_g d\mathbf{l}_g \\ & - \int_{\partial S_{gt}} p_0 \underline{\underline{U}} \cdot \underline{\tau} \underline{\underline{L}} \cdot \underline{\underline{P}} \cdot \delta \underline{\underline{U}} \underline{\underline{n}}_g d\mathbf{l}_g - \int_{\partial S_{gt}} \text{div}_s[(p_0 \underline{\underline{U}} \cdot \underline{\tau}) \cdot \underline{\tau}_g \otimes \underline{\tau}_g] \cdot \delta \underline{\underline{U}} d\mathbf{l}_g \end{aligned} \quad (3.16)$$

In (3.16), one has to distinguish the actual displacement  $\underline{u}$  (lower case letters) from its virtual variation (written with capital letters). The stationnarity condition of the total potential energy  $V[\Omega_g]$  at equilibrium is further exploited: the arbitrariness of the variations  $(\delta \underline{U}, \delta \underline{\tilde{U}}, \delta \underline{\tilde{\tilde{U}}})$ —traducing the independence of the variations of the displacement vector  $\underline{U}$  on the volume, surface and line, respectively—wherein the tangential and normal variations are mutually independent, then gives the set of mechanical equilibrium equations (we again refer to Fig. 2 for the definition of the geometrical entities attached to the germ):

(i) *Volume equilibrium*: The following vectorial equation is obtained

$$-\text{div}_g \left[ \frac{1}{2} j (\psi_{,E}^{\text{vt}} + \psi_{,E}^{\text{v}}) \cdot \underline{\underline{F}}^{\text{t}} \right] (I - \underline{\underline{F}}^{-1})^{-1} + (I - \underline{\underline{F}}^{-1})^{-1} \cdot \psi_{,x_g}^{\text{v}} + \nabla_X (j \psi^{\text{v}}) = \underline{f}_0 - \nabla_X (\underline{f}_0 \cdot \underline{u}) \quad (3.17)$$

The following surface and line equations are the natural boundary conditions associated to the previous equilibrium equation:

(ii) *Surface boundary condition*: the equilibrium is described by the vectorial equation

$$\begin{aligned} \frac{1}{2} j \left\{ (\psi_{,E}^{\text{vt}} + \psi_{,E}^{\text{v}}) \cdot \underline{\underline{F}}^{\text{t}} \cdot (I - \underline{\underline{F}}^{-1})^{-1} \right\} - j \psi^{\text{v}} \cdot \underline{n}_g + (I - \underline{\underline{F}}^{-1})^{-1} \cdot \psi_{,x_g}^{\text{S}} - \text{div}_S \left[ \frac{1}{2} j_s (\underline{\underline{A}}^{\text{St}} + \underline{\underline{A}}^{\text{S}}) \cdot \underline{\underline{F}}^{\text{t}} \right] \cdot (I - \underline{\underline{F}}^{-1})^{-1} \\ + \underline{\underline{L}} \cdot \underline{\underline{P}} \cdot \psi_{,n}^{\text{S}} - j J_s \cdot \underline{\underline{L}} \cdot \underline{\underline{P}} \cdot (\underline{\underline{F}} \cdot \underline{N}_g) + \nabla_S (\psi^{\text{S}}) - j J_s [\text{div}_S (\underline{N}_g \otimes \underline{n}_g)] = (f_0 \cdot \underline{u})(I - P) \cdot \underline{n}_g + t_0 - \nabla_S (t_0 \cdot \underline{u}) \end{aligned} \quad (3.18)$$

When deriving the surface boundary condition, only the part of the boundary where growth occurs ( $S_{g_t}$ ) has been considered.

(iii) *Line boundary condition*: the projection on the direction  $\underline{v}$  gives the following scalar equation

$$\begin{aligned} \frac{1}{2} j_s \underline{v}_g^{\text{t}} \cdot (\psi_{,E}^{\text{St}} + \psi_{,E}^{\text{S}}) \cdot \underline{\underline{F}}^{\text{t}} \cdot (I - \underline{\underline{F}}^{-1})^{-1} \cdot \underline{v}_g - \psi^{\text{S}} + j J_s \underline{v}^{\text{t}} (\underline{N}_g \otimes \underline{n}_g) \cdot \underline{v}_g \\ = t_0 \cdot \underline{\tilde{u}} - p_0 \underline{\tilde{U}} \cdot \underline{\underline{\tau}}_g \cdot \underline{\underline{L}} \cdot \underline{\underline{P}} \cdot \underline{v}_g - \underline{v}_g^{\text{t}} \cdot \text{div}_S [(p_0 \underline{\tilde{U}} \cdot \underline{\underline{\tau}}_g) \cdot \underline{\underline{\tau}}_g \otimes \underline{\underline{\tau}}_g] \end{aligned} \quad (3.19)$$

Conversely, the projection on the orthogonal direction  $\underline{\tau}$  gives the scalar boundary equation

$$j_g J_s \underline{v}_g^{\text{t}} (\underline{N}_g \otimes \underline{n}_g) \cdot \underline{\underline{\tau}}_g = p_0 - p_0 \underline{\tilde{U}} \cdot \underline{\underline{\tau}}_g \cdot \underline{\underline{L}} \cdot \underline{\underline{P}} \cdot \underline{\underline{\tau}}_g - \underline{\underline{\tau}}^{\text{t}} \cdot \text{div}_S [(p_0 \underline{\tilde{U}} \cdot \underline{\underline{\tau}}_g) \cdot \underline{\underline{\tau}}_g \otimes \underline{\underline{\tau}}_g] \quad (3.20)$$

Note that the methodology of domain variation adopted in the present contribution gives a point of view equivalent to the one developed in Huang (2004), since the additional surface term due to domain variation includes both a contribution due to the variation of the actual domain due to domain deformation (due to growth and growth accommodation) and a second contribution due to mass exchange—through the boundary  $S_g$ —with the surrounding tissue elements. Rewrite indeed the domain derivative of any quantity  $B = \int_{\Omega_t} b(\underline{x}, t) \text{d}x$  (here,  $b(\underline{x}, t)$  represents a volumic density) as

$$\frac{\delta B}{\delta t} = \int_{\Omega} \frac{\partial b}{\partial t} \text{d}x + \int_{\partial \Omega \setminus S_g} b \underline{U} \cdot \underline{n} \text{d}\sigma + \int_{S_g} b \underline{U}_g \underline{n}_g \text{d}\sigma$$

The two first terms can be identified to contributions of points that are in one-to-one correspondence with their homologues on the initial configuration, while the last term on the r.h.s. represents the contribution of the accretive material particles (on the portion of surface  $S_g$  where growth occurs). This brings an explanation of the origin of the material accretion derivative introduced by Huang (2004). According to this, the previous surface and line boundary conditions can be seen as accretive boundary conditions.

The virtual power of the internal forces is then identified to the Gateaux derivative of the total mechanical energy of the tissue element  $E$  in the direction given by the set of variations, replacing the variations by the triplet of virtual volumic, surface, and line velocities  $(\underline{V}, \underline{\tilde{V}}, \underline{\tilde{V}})$ :

$$\begin{aligned}
 p_i = & \int_{\Omega_g} \text{div}_g \left[ \frac{1}{2} j(\psi_{,E}^{\text{vt}} + \psi_{,E}^{\text{v}}) \cdot \underline{\underline{F}}^{\text{t}} \right] \cdot (I - \underline{\underline{F}}^{-1})^{-1} \cdot \underline{V} \, \text{d}x_g - \int_{S_g} \underline{n}_g^{\text{t}} \cdot \frac{1}{2} j(\psi_{,E}^{\text{vt}} + \psi_{,E}^{\text{v}}) \cdot \underline{\underline{F}}^{\text{t}} \cdot (I - \underline{\underline{F}}^{-1})^{-1} \cdot \underline{\tilde{V}} \, \text{d}\sigma_g \\
 & - \int_{\Omega_g} \psi_{,x_g}^{\text{v}} \cdot (I - \underline{\underline{F}}^{-1})^{-1} \cdot \underline{V} \, \text{d}x_g - \int_{\Omega_g} \nabla(j\psi^{\text{v}}) \cdot \underline{V} \, \text{d}x_g + \int_{S_g} j\psi^{\text{v}} \underline{\tilde{V}} \cdot \underline{n}_g \, \text{d}\sigma_g \\
 & - \int_{S_g} (\psi_{,x_g}^{\text{s}})^{\text{t}} \cdot (I - \underline{\underline{F}}^{-1})^{-1} \cdot \underline{\tilde{V}} \, \text{d}\sigma_g + \int_{S_g} \text{div}_s \left[ \frac{1}{2} j_s(\underline{\underline{A}}^{\text{st}} + \underline{\underline{A}}^{\text{s}}) \cdot \underline{\underline{F}}^{\text{t}} \right] \cdot (I - \underline{\underline{F}}^{-1})^{-1} \cdot \underline{\tilde{V}} \, \text{d}\sigma_g \\
 & - \int_{S_g} (\psi_{,n}^{\text{s}})^{\text{t}} \cdot \underline{\underline{L}} \cdot \underline{\underline{P}} \cdot \underline{\tilde{V}} \, \text{d}\sigma_g - \int_{\partial S_g} \frac{1}{2} j_s(\underline{\underline{A}}^{\text{st}} + \underline{\underline{A}}^{\text{s}}) \cdot \underline{\underline{F}}^{\text{t}} \cdot (I - \underline{\underline{F}}^{-1})^{-1} \cdot \underline{\tilde{V}} \cdot \underline{\tilde{v}}_g \cdot \text{d}l_g \\
 & + \int_{S_g} jJ_s(\underline{\underline{F}} \cdot \underline{\underline{N}}_g)^{\text{t}} \cdot \underline{\underline{L}} \cdot \underline{\underline{P}} \cdot \underline{\tilde{V}} \, \text{d}\sigma_g - \int_{S_g} [\nabla_s(\psi^{\text{s}})]^{\text{t}} \cdot \underline{\tilde{V}}_g \, \text{d}\sigma_g + \int_{S_g} jJ_s[\text{div}_s(\underline{\underline{N}}_g \otimes \underline{n}_g)]^{\text{t}} \cdot \underline{\tilde{V}} \, \text{d}\sigma_g \\
 & - \int_{\partial S_g} jJ_s(\underline{\underline{N}}_g \otimes \underline{n}_g) \cdot \underline{\tilde{V}} \cdot \underline{\tilde{v}}_g \cdot \text{d}l_g
 \end{aligned} \quad (3.21)$$

The virtual power of the external forces is obtained from (3.16) as

$$\begin{aligned}
 p_e = & \int_{\Omega_g} \underline{f}_0 \cdot \underline{V} \, \text{d}x_g - \int_{\Omega_g} \nabla_X(\underline{f}_0 \cdot \underline{u}) \cdot \underline{V} \, \text{d}x_g + \int_{S_g} \underline{f}_0 \cdot \underline{\tilde{V}} \cdot \underline{n}_g \, \text{d}\sigma_g + \int_{\partial\Omega_g} \underline{t}_0 \cdot \underline{\tilde{v}} \, \text{d}\sigma_g \\
 & - \int_{S_g} \nabla_s(\underline{t}_0 \cdot \underline{\tilde{u}})^{\text{t}} \cdot \underline{\tilde{V}} \, \text{d}\sigma_g + \int_{\partial S_g} \underline{t}_0 \cdot \underline{\tilde{u}} \underline{\tilde{V}} \cdot \underline{\tilde{v}}_g \, \text{d}l_g + \int_{\partial S_g} p_0 \underline{\tilde{V}} \cdot \underline{\tau}_g \, \text{d}l_g \\
 & - \int_{\partial S_g} p_0 \underline{\tilde{U}} \cdot \underline{\tau}_g \underline{\underline{L}} \cdot \underline{\underline{P}} \cdot \underline{\tilde{V}} \underline{n}_g \, \text{d}l_g - \int_{\partial S_g} \text{div}_s[(p_0 \underline{\tilde{U}} \cdot \underline{\tau}_g) \cdot \underline{\tau}_g \otimes \underline{\tau}_g] \cdot \underline{\tilde{V}} \, \text{d}l_g
 \end{aligned} \quad (3.22)$$

The principle of virtual power expresses in the final configuration in a quasi-static situation (the power of inertial forces is neglected) as

$$p_i + p_e = 0 \quad (3.23)$$

In the sequel, the power of the internal forces is fully expressed in terms of Eulerian kinematic quantities (volumetric terms in (3.21) indeed involve lagrangian strain and stress measures). The additive decomposition of the total deformation rate is then postulated

$$\underline{\underline{D}} := \text{sym}(\underline{\underline{L}}) \quad (3.24)$$

with

$$\underline{\underline{L}} := \dot{\underline{\underline{F}}} \cdot \underline{\underline{F}}^{-1} \quad (3.25)$$

the velocity gradient, sum of a growth deformation rate  $\underline{\underline{D}}_g$ , and an accommodation rate  $\underline{\underline{D}}_a$ :

$$\underline{\underline{D}} = \underline{\underline{D}}_g + \underline{\underline{D}}_a \quad (3.26)$$

The assumption behind this decomposition is that the addition of matter occurring within the growing body is smooth enough so that the resulting accommodation strain can be neglected with respect to the growth deformation (identified to a smooth growth); it is indeed believed that nature knows the best way to generate a self-accommodating growth.

**Remark 3.** As pointed in [Taber \(1995\)](#), surface growth often develops without generating residual stresses. Note that volumetric growth is not excluded in cases where the tissue essentially grows by surface accretion of mass. This shows that growth can occur without developing high residual stresses. The consideration of two different time scales in [Skalak \(1981\)](#) and [Skalak et al. \(1982\)](#), despite appearing as a kinematical artifact, might be the correct description (the characteristic relaxation times for growth might be shorter than the time needed for the return to the elastic equilibrium of the body) of how nature in fact proceeds to easily accommodate the growth without generating residual stresses. The problem of growth incompatibility shall nevertheless be tackled in the forthcoming Section 5.

The accommodation strain itself is supposed to be purely elastic, described by lagrangian strain tensors, respectively, the (elastic) volumetric accommodation deformation tensor  $\underline{\underline{E}}_a$ , and the (elastic) surface accommodation deformation tensor  $\underline{\underline{E}}_s$  (defined in Section 2). The total lagrangian strain is then

$$\underline{\underline{E}} = \underline{\underline{E}}_g^t \cdot \underline{\underline{E}}_a \cdot \underline{\underline{E}}_g + \underline{\underline{E}}_g \quad (3.27)$$

Introducing the symmetrical part of the growth velocity gradient:

$$\underline{\underline{D}}_g := \frac{1}{2} (\underline{\underline{d}}_g + \underline{\underline{d}}_g^t) \quad (3.28)$$

with  $\underline{\underline{d}}_g$  the Eulerian growth velocity gradient, a straightforward analogy with plasticity ([Khan and Huang, 1995](#)) gives the relationship

$$\underline{\underline{D}}_g := \underline{\underline{F}}_g^{-t} \cdot \frac{\delta \underline{\underline{E}}_g}{\delta t} \cdot \underline{\underline{F}}_g^{-1} \quad (3.29)$$

Equality (3.29) defines the growth part of the deformation rate in (3.26). These preliminaries at hand, the power of internal forces is next expressed in terms of the Eulerian strain measures introduced the above, from the virtual variation of the total energy of the tissue element (equality (A2.5) in the [Appendix 2](#)):

$$\begin{aligned} p_i = & - \int_{\Omega_g} \underline{\underline{\sigma}} : \underline{\underline{D}} dx_g - \int_{\Omega_g} j(\psi_{,x}^V)^t \cdot \underline{\underline{V}} dx_g - \int_{S_g} \underline{\underline{\tilde{\sigma}}} : \underline{\underline{\tilde{d}}} d\sigma_g + \int_{S_g} \left\{ j_s(\psi_{,n}^S)^t \cdot \underline{\underline{L}} \cdot \underline{\underline{P}} - j_s(\psi_{,x}^S)^t - (\nabla_s \psi^S)^t \right. \\ & \left. + jJ_s(\underline{\underline{F}} \cdot \underline{\underline{N}}_g)^t \cdot \underline{\underline{L}} \cdot \underline{\underline{P}} - \nabla_s \cdot [jJ_s \psi^S(\underline{\underline{n}}_g \otimes \underline{\underline{N}}_g)^t] + \nabla_s(j_s \psi^S) \right\} \cdot \underline{\underline{\tilde{V}}} d\sigma_g \\ & - \int_{\partial S_g} (1 + j_s) \psi^S \underline{\underline{\tilde{V}}} \cdot \underline{\underline{\tilde{v}}}_g dl_g - \int_{\partial S_g} jJ_s(\underline{\underline{n}}_g \otimes \underline{\underline{N}}_g)^t \cdot \underline{\underline{\tilde{V}}} \cdot \underline{\underline{\tilde{v}}}_g dl_g \end{aligned} \quad (3.30)$$

distinguishing between volumetric, surface and line terms successively in the r.h.s. In (3.30), the following conjugated strain and stress measures have been introduced:

$$\underline{\underline{\sigma}} := j \underline{\underline{F}} \cdot \underline{\underline{S}} \cdot \underline{\underline{F}}^t$$

recalling the relationships (see Section 3.2)  $\underline{\underline{D}} = \underline{\underline{F}}^{-t} \cdot \underline{\underline{\dot{E}}} \cdot \underline{\underline{F}}^{-1}$ ;  $\underline{\underline{\tilde{d}}} := \underline{\underline{F}}^{-t} \cdot \underline{\underline{\dot{E}}} \cdot \underline{\underline{F}}^t$ .

The writing of the second principle of thermodynamics will next allow to identify the irreversible forces tied to growth.

#### 4. Second principle and driving forces for growth

The local form of the second principle of the thermodynamics for an open continuous system (control volume fixed in space) has been obtained in the [Appendix 3](#), see also [Munster \(1966\)](#):

$$\underline{\underline{\sigma}} : \underline{\underline{D}} - \underline{\underline{\sigma}} : \underline{\underline{D}}^R - \underline{\underline{J}}_k \cdot \nabla \mu_k + A_k R_k + \underline{\underline{J}}_k \cdot \underline{\underline{F}}_k \geq 0 \quad (4.1)$$

with  $\underline{D}^R$  the reversible part of  $\underline{D}$ ,  $A_k$  the chemical affinity (conjugated to the velocity  $R_k$  of the  $k$ th chemical reaction), and  $\underline{F}_k$  the force vector dual to the heat diffusion flux  $\underline{J}_k$ . Inequality (4.1) expresses the positivity of the internal entropy production, accounting for diffusion of mass (the last term on the l.h.s.), chemical reactions (the fourth term), the non-uniformity of the intensive parameters (here the chemical potential), and the mechanical dissipation (the two first terms).

An expression of the reversible flux  $J_k^e$  versus the normal growth velocity is given by

$$J_k^e = \frac{\rho_k}{M_k} V_N$$

with  $\frac{\rho_k}{M_k}$  the number of moles of the  $k$ -species per unit volume. Considering a growing germ, volumic and surface chemical potentials  $\mu^V$  (respectively  $\mu^S$ ) can be defined from the partial derivatives of  $\psi^V$  and  $\psi^S$  versus the volumic and surface densities, respectively,  $\rho^V$  and  $\rho^S$ :

$$\mu^V := \frac{\partial \psi^V}{\partial \rho^V}; \quad \mu^S := \frac{\partial \psi^S}{\partial \rho^S}$$

A global form of Clausius–Duhem inequality is next obtained, transforming the mechanical dissipation into the difference of (minus) the power of internal forces and the reversible mechanical power

$$\phi^{\text{int}} = -p_i + p_i^R \quad (4.2)$$

The reversible part of the power of internal forces is next identified: it is assumed that the terms involving the growth velocity field, arising from the change of domain tied to growth, are irreversible contributions to the total mechanical power of internal forces. Furthermore, the virtual velocity (in terms of its volumic, surface and line contributions, condensed into the triplet  $(\underline{V}, \underline{\tilde{V}}, \underline{\tilde{\tilde{V}}})$ ) is decomposed into the sum of a growth velocity vector (the triplet  $(\underline{V}_g, \underline{\tilde{V}}_g, \underline{\tilde{\tilde{V}}}_g)$ , using the self-explanatory index ‘g’), and a virtual accommodation velocity vector (the triplet  $(\underline{V}_a, \underline{\tilde{V}}_a, \underline{\tilde{\tilde{V}}}_a)$ , using the self-explanatory index ‘a’)

$$(\underline{V}, \underline{\tilde{V}}, \underline{\tilde{\tilde{V}}}) = (\underline{V}_g, \underline{\tilde{V}}_g, \underline{\tilde{\tilde{V}}}_g) + (\underline{V}_a, \underline{\tilde{V}}_a, \underline{\tilde{\tilde{V}}}_a)$$

It is clear that the growth and accommodation vectors defined by this decomposition do not (in general) define compatible (globally integrable) displacement fields.

Thus, considering the decomposition of the total velocity (3.5), the surface and line contributions in the previous decomposition that express as linear forms of the growth velocities  $\underline{\tilde{V}}_g$  and  $\underline{\tilde{\tilde{V}}}_g$ , respectively, are irreversible contributions to  $p_i$ . Accordingly, considering the decomposition of the total deformation rate, viz  $\underline{D} = \underline{D}_g + \underline{D}_a$ , with  $\underline{D}_a$  considered as being reversible, and the equivalent decomposition of the surface deformation rate  $\underline{\tilde{d}}$

$$\underline{\tilde{d}} = \underline{\tilde{d}}_g + \underline{\tilde{d}}_a$$

with  $\underline{\tilde{d}}_g := \underline{F}_g^{-t} \cdot \underline{\dot{E}}_g \cdot \underline{F}_g^t$  the irreversible surface growth rate deformation tensor, and  $\underline{\tilde{d}}_a$  an additional contribution due to accommodation of growth, one identifies the reversible internal power

$$\begin{aligned} p_i^R := & - \int_{\Omega_g} \underline{\sigma} : \underline{D}_a \, dx_g - \int_{S_g} \underline{\tilde{\sigma}} \\ & : \underline{\tilde{d}}_a \, d\sigma_g - \int_{\Omega_g} j(\psi^V) \cdot \underline{V}_a \, dx_g + \int_{S_g} \underline{\tilde{F}}^{\text{IR}} \cdot \underline{\tilde{V}}_a \, d\sigma_g - \int_{\partial S_g} \underline{\tilde{\tilde{F}}}^{\text{IR}} \cdot \underline{\tilde{\tilde{V}}}_a \cdot \underline{\tilde{v}}_g \, dl_g \end{aligned} \quad (4.3)$$

thus giving the mechanical dissipation

$$\phi^{\text{int}} = \int_{\Omega_g} \underline{F}^{\text{IR}} \cdot \underline{V}_g \, dx_g + \int_{S_g} \underline{\tilde{F}}^{\text{IR}} \cdot \underline{\tilde{V}}_g \, d\sigma_g + \int_{\partial S_g} \underline{\tilde{\tilde{F}}}^{\text{IR}} \cdot \underline{\tilde{\tilde{V}}}_g \cdot \underline{\tilde{v}}_g \, dl_g \quad (4.4)$$



with  $\underline{F}^{\text{IR}} = j(\psi_{,x}^{\text{V}})^{\text{t}} - \text{div} \underline{\underline{\sigma}}$  the irreversible volumic driving force for growth,

$$\begin{aligned} \underline{\underline{\tilde{F}}}^{\text{IR}} := & j_s \underline{\underline{L}} \cdot \underline{\underline{P}} \cdot (\psi_{,n}^{\text{S}}) - j_s (\psi_{,x}^{\text{S}}) - (\nabla_s \psi^{\text{S}}) + j J_s \underline{\underline{L}} \cdot \underline{\underline{P}} \cdot (\underline{\underline{F}} \cdot \underline{\underline{N}}_g) - \nabla_s \cdot [j J_s \psi^{\text{S}} (\underline{\underline{n}}_g \otimes \underline{\underline{N}}_g)^{\text{t}}] \\ & + \nabla_s (j_s \psi^{\text{S}}) + \underline{\underline{\sigma}} \cdot \underline{\underline{n}}_g - \text{div}_s \underline{\underline{\tilde{\sigma}}} \end{aligned}$$

the irreversible surface growth driving force, and

$$\underline{\underline{\tilde{F}}}^{\text{IR}} := (1 + j_s) \psi^{\text{S}} I + j J_s (\underline{\underline{n}}_g \otimes \underline{\underline{N}}_g)^{\text{t}} + \underline{\underline{\tilde{\sigma}}}$$

the irreversible line driving force for growth. Observe that the volumetric and surface growth driving forces are of vectorial nature, while the line growth-driving force has been expressed in a tensorial form (via the identity tensor). Decoupling the mechanical dissipation from the chemical dissipation term  $\phi^{\text{ch}} = -\underline{\underline{J}}_k \cdot \nabla \mu_k + A_k R_k + \underline{\underline{J}}_k \cdot \underline{\underline{E}}_k$ , further gives the inequality

$$\phi^{\text{int}} \geq 0 \quad (4.5)$$

Taking for granted the fact that the continuum tissue behaves as a generalized standard material (Maugin, 1992), inequality (4.5) is satisfied provided a pseudo-potential of dissipation  $\phi^* = \phi^*(\underline{\underline{F}}^{\text{IR}}, \underline{\underline{\tilde{F}}}^{\text{IR}}, \underline{\underline{\tilde{\tilde{F}}}}^{\text{IR}})$  exists, such that the time rates in (4.4) derive from it according to the normality relations

$$\underline{\underline{V}}_g = \phi_{,\underline{\underline{F}}^{\text{IR}}}^*; \underline{\underline{\tilde{V}}}_g = \phi_{,\underline{\underline{\tilde{F}}}^{\text{IR}}}^*; \underline{\underline{\tilde{\tilde{V}}}}_g = \phi_{,\underline{\underline{\tilde{\tilde{F}}}}^{\text{IR}}}^* \quad (4.6)$$

The set of relations (4.6) define the evolution laws for the set of internal variables  $(\underline{\underline{V}}_g, \underline{\underline{\tilde{V}}}_g, \underline{\underline{\tilde{\tilde{V}}}}_g)$ ; they have to be completed by the constitutive law of the tissue, that relates the lagrangian stress  $\underline{\underline{S}}$  to the (elastic) part of the accommodation lagrangian strain  $\underline{\underline{E}}_a$  (in both its volumetric and surface realization); this can be achieved by the setting up of the volumic and surface potentials  $\psi^{\text{V}}$  and  $\psi^{\text{S}}$ , recalling the relationships  $\underline{\underline{S}} := \psi_{,E}^{\text{V}}; \underline{\underline{S}} := \psi_{,E}^{\text{S}}$ .

## 5. Accommodation of the growth and kinematic compatibility

While preserving the uniform character of the material body, the growth does in general not generate an integrable global displacement field, thus it needs an additional deformation (of elastic or inelastic nature). Physically, the growth ‘strain’ (rather transformation)  $\underline{\underline{E}}_g$  is the strain that would be observed at a point of the tissue if it could be insulated from the surrounding tissue during its growth under zero stress; such isolated elements of matter do not fit together into the whole body when fully grown, thus a residual stress field will be generated in order to maintain the kinematic integrity of the continuous body. The compatibility problem and the genesis of residual stresses was tackled for instance in Skalak et al. (1996), the authors rather focusing on the integrability conditions of the displacement field from an assumed growth strain, in both small and large transformations, however not trying to find explicitly the form of the accommodation tensor for incompatible growth situations.

The kinematic compatibility in general is the cornerstone of Beltrami resolution method in elasticity, whereby the stress tensor is chosen as the primary unknown. We here focus on the expression and satisfaction of the compatibility condition within a large transformation context. A criterion for the kinematic compatibility condition within a large transformations framework is first enunciated, based on considerations that pertain to the differential geometry of kinematics. The curvilinear coordinates lines defined by the equations  $X_I = Cte$ ,  $I = 1, 2, 3$ , in the Lagrange configuration  $\Omega_{0g}$ , become new coordinate-lines  $x_i = Cte$ ,  $i = 1, 2, 3$ , in the Euler configuration  $\Omega_g$ . The tangent vectors to these lines are the basis vectors  $(\underline{\underline{e}}_i)_i$ , that sustain a non-Euclidean space, having the metric tensor components  $g_{ij} = \underline{\underline{e}}_i \cdot \underline{\underline{e}}_j$ . Similarly, the components of the metric tensor in the Lagrange configuration are the scalar products of the lagrangian base vectors,  $G_{IJ} = \underline{\underline{E}}_I \cdot \underline{\underline{E}}_J$ .

For materially simple materials in the sense of Noll, the motion is described by the linear tangent application  $\underline{E}$ , mapping the tangent spaces at homologous points in  $\Omega_{0g}$  and  $\Omega_g$ . Since the tangent space to a differentiable manifold is Euclidean (in the present case the manifold associated to the curvilinear coordinates  $x_i(X_J, t)$ ), the metric of the tangent space  $T_M$  at point  $M \in \Omega_g$ , is given by the expression  $ds^2 = ds_0^2 + 2E_{IJ}(\underline{X}) dX_I dX_J$ . This further leads to the vanishing of the fourth order Riemann–Christoffel curvature tensor, which constitutes the kinematic compatibility condition in a large transformation context, viz

$$R_{imj}^l = \frac{\partial \Gamma_{ij}^l}{\partial u^m} + \Gamma_{ij}^k \Gamma_{mk}^l - \frac{\partial \Gamma_{mj}^l}{\partial u^i} - \Gamma_{mj}^k \Gamma_{ik}^l = 0 \quad (5.1)$$

with  $\{u_i\}_i$  the set of curvilinear coordinates attached to the manifold  $\Omega_g$ .

The compatibility of growth can be stated as the following problem: for a given assumed state of the growth, defined at any instant  $t$  by the tensorial growth field  $\underline{E}_g(\underline{X}, t)$ , find the tensorial field  $\underline{E}_a(\underline{x}_g, t)$  such that the growth state at the same instant  $t$  is compatible, i.e. condition (5.1) is satisfied. The general situation is that of a heterogeneous growth, whereby the material points do not attain the same state of growth at the same time. The growth may in general be influenced by mechanical factors, such as the local state of stress (residual or actual), and the fluxes of the different chemical species. We here assume that the growth develops as a mechanism not being influenced by the current stress state, and consider the instantaneous situation of a growth having developed into a portion of a cylindrical domain (Fig. 3); we deal here with a frozen time  $t_0$  that shall not appear explicitly in the subsequent coordinate transformations. The material point in the initial configuration is assigned the coordinates  $\underline{X} = (R, R\theta, Z)$ , each being homogenous to a length; the coordinates of the material points in the intermediate configuration at the frozen time  $t_0$  are given by  $\underline{x}_g = (\rho, \rho\varphi, \xi)$ .

The growth model then expresses as the following relationship between both coordinate systems:

$$\begin{cases} \rho = f(R) \\ \varphi = K_\theta(R)\theta \\ \xi = Z \end{cases}$$

whereby the setting up of the functions  $f(R)$  and  $K_\theta(R)$  prescribes the growth law along the cylinder radius and in the angular direction, respectively; the angular function  $K_\theta(R)$  has been assumed to depend upon the sole radial variable (and not upon the angle  $\theta$ ), which means that the growth is homogeneous in the ortho-radial direction. The growth displacement vector is then evaluated as the difference between both position fields, as

$$\underline{U}_g = \underline{x}_g - \underline{X} \equiv \begin{pmatrix} \rho - R \\ \rho\varphi - R\theta \\ 0 \end{pmatrix}$$

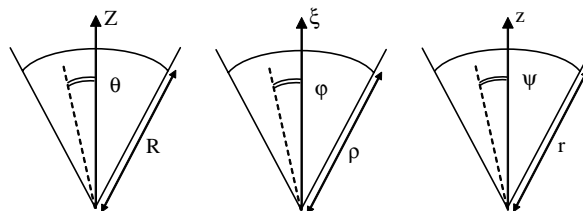


Fig. 3. Cylindrical growth of a continuum biological tissue.

according to previous positions mapping. The growth tensor is then defined as

$$\underline{\underline{F}}_g := I + \nabla_X \underline{U}_g$$

resulting in the following expression

$$\underline{\underline{F}}_g = \begin{pmatrix} \frac{df(R)}{dR} & 0 & 0 \\ 0 & \frac{d}{dR}(\rho K_\theta(R)) & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (5.2)$$

The accommodation of growth is then modeled by the relationship between the coordinates systems in the intermediate and final configurations, viz

$$\begin{cases} r = r(\rho) \\ \psi = \eta_\theta(\rho)\varphi \\ z = \varepsilon\xi \end{cases}$$

with  $\varepsilon$  a constant coefficient, corresponding to a plane strain deformation state. Accordingly, the accommodation tensor expresses (in a two-dimensional representation: according to the invariance with respect to translations in the directions of the axis of the cylinder, one focuses on a planar section of the cylinder) as

$$\underline{\underline{F}}_a = \begin{pmatrix} \frac{dr(\rho)}{d\rho} & 0 \\ 0 & \frac{d}{d\rho}(r(\rho)\eta_\theta(\rho)) \end{pmatrix} \quad (5.3)$$

The product of the growth and accommodation tensors is then

$$\underline{\underline{F}}_{eg} = \begin{pmatrix} \frac{dr(\rho)}{dR} & 0 \\ 0 & \frac{d}{dR}(\rho K_\theta(R)) \frac{d}{d\rho}(r(\rho)\eta_\theta(\rho)) \end{pmatrix}$$

**Remark 4.** We follow in this example the presentation of the kinematics of growth given in Rodriguez et al. (1994). A mapping between the material point  $\underline{X}$  in the initial configuration and its counterpart in  $\Omega_g$  (after growth)  $\underline{x}_g$  is set up, as

$$\underline{X} \in \Omega_0, \quad t \in R^+ \mapsto \underline{x}_g := \underline{X} + \underline{U}_g(\underline{X}, t)$$

with  $\underline{U}_g(\underline{X}, t)$  the growth vector field and  $t$  a time-like parameter. The vector field  $\underline{U}_g(\underline{X}, t)$  is in general non-compatible at the macroscopic scale of the whole body, since a discontinuity or a superposition of material may occur due to the growth: thus, the previous relation establishes  $\underline{x}_g$  as an *anholomic vector field*. However, since one can define the differential of the displacement between two non-holonomic coordinate systems, the variation of the position in  $\Omega_g$  is given by

$$\delta \underline{x}_g = \underline{\underline{F}}_g \cdot \delta \underline{X}$$

introducing thereby the growth transformation gradient  $\underline{\underline{F}}_g$ . Although the coinage displacement cannot be attributed to the previous multivalued function  $\underline{U}_g(\underline{X}, t)$ , it serves as a convenient (and intermediate) object to ascribe the growth kinematics.

Adopting this two-dimensional representation in the remaining of this paragraph, the transport of the tangent vectors to the initial configuration  $(\underline{e}_R, \underline{e}_\theta)$  then defines the tangent vectors on the actual configuration:

$$\underline{f}_1 = \frac{dr}{dR} \underline{e}_R; \quad \underline{f}_2 = \frac{d}{dR}(\rho K_\theta(R)) \frac{d}{d\rho}(r(\rho)\eta_\theta(\rho)) \underline{e}_\theta$$

The Christoffel symbols, projections of the derivatives of these tangent vectors (with respect to the actual coordinates) onto the actual basis vectors  $(\underline{f}_1, \underline{f}_2)$ , are next obtained as

$$\begin{aligned} \Gamma_{11}^1 &= \frac{\partial \underline{f}_1}{\partial r} \cdot \underline{f}_1 = \frac{d^2 r}{dR^2}; \quad \Gamma_{12}^1 = \frac{\partial \underline{f}_1}{\partial \psi} \cdot \underline{f}_1 = 0; \quad \Gamma_{11}^2 = \frac{\partial \underline{f}_1}{\partial r} \cdot \underline{f}_2 = 0; \quad \Gamma_{21}^1 = \frac{\partial \underline{f}_2}{\partial r} \cdot \underline{f}_1 = 0; \\ \Gamma_{12}^2 &= \frac{\partial \underline{f}_1}{\partial \psi} \cdot \underline{f}_2 = \frac{dr}{dR} \frac{d}{dR}(\rho K_\theta) \frac{d^2}{dR^2}(\rho K_\theta) \frac{d}{d\rho}(r\eta_\theta); \quad \Gamma_{22}^1 = \frac{\partial \underline{f}_2}{\partial \psi} \cdot \underline{f}_1 = -\frac{1}{\eta_\theta K_\theta} \frac{d}{dR}(\rho K_\theta) \frac{d}{d\rho}(r\eta_\theta) \frac{dr}{dR}; \\ \Gamma_{21}^2 &= \frac{\partial \underline{f}_2}{\partial r} \cdot \underline{f}_2 = \frac{dR}{dr} \frac{d}{dR}(\rho K_\theta) \frac{d^2}{dR^2}(\rho K_\theta) \left( \frac{d}{d\rho}(r\eta_\theta) \right)^2; \quad \Gamma_{22}^2 = \frac{\partial \underline{f}_2}{\partial \psi} \cdot \underline{f}_2 = 0 \end{aligned}$$

Introducing these expressions into the differential equations (particularization of (5.1)) that express the vanishing of the fourth order curvature tensor, viz

$$\frac{\partial \Gamma_{21}^2}{\partial r} = \Gamma_{11}^1 \Gamma_{21}^2 - \Gamma_{21}^2 \Gamma_{11}^2; \quad \frac{\partial \Gamma_{22}^1}{\partial r} = \Gamma_{12}^2 \Gamma_{22}^1 - \Gamma_{22}^1 \Gamma_{11}^1$$

leads to the two differential equations

$$\begin{aligned} \frac{\partial}{\partial r} \left[ \frac{dR}{dr} \frac{d(\rho K_\theta)}{dR} \frac{d^2(\rho K_\theta)}{dR^2} \left( \frac{d}{d\rho}(r\eta_\theta) \right)^2 \right] &= \frac{dR}{dr} \frac{d(\rho K_\theta)}{dR} \frac{d^2(\rho K_\theta)}{dR^2} \left[ \frac{d^2 r}{dR^2} - \frac{dr}{dR} \frac{d}{dR}(\rho K_\theta) \frac{d}{d\rho}(r\eta_\theta) \right] \\ \frac{\partial}{\partial r} \left[ -\frac{1}{\eta_\theta K_\theta} \frac{d}{dR}(\rho K_\theta) \frac{d}{d\rho}(r\eta_\theta) \frac{dr}{dR} \right] &= -\left( \frac{1}{\eta_\theta K_\theta} \frac{d}{dR}(\rho K_\theta) \frac{d}{d\rho}(r\eta_\theta) \frac{dr}{dR} \right) \left[ \frac{dr}{dR} \frac{d}{dR}(\rho K_\theta) \frac{d}{d\rho}(r\eta_\theta) - \frac{d^2 r}{dR^2} \right] \end{aligned} \quad (5.4a, b)$$

We shall evidence analytical and numerical solutions of these two conditions, making simplifying assumptions of a mathematical and physical nature: it is immediate to observe that Eq. (5.4a) is automatically satisfied when

$$\frac{d^2}{dR^2}(\rho K_\theta) = 0$$

thus leading to the expression

$$\rho(R) = \frac{AR + B}{K_0}$$

considering that the angular growth is homogeneous for each radius, i.e.  $K_\theta(R) = K_0$ .

One then searches for the combination of the functions  $r = r(\rho)$ ;  $\psi = \eta_\theta(\rho)\varphi$  that render the growth compatible, i.e. that satisfy (5.4b). The further choice of a constant angular accommodation, viz

$$\eta_\theta(\rho) = Cte = \eta_0$$

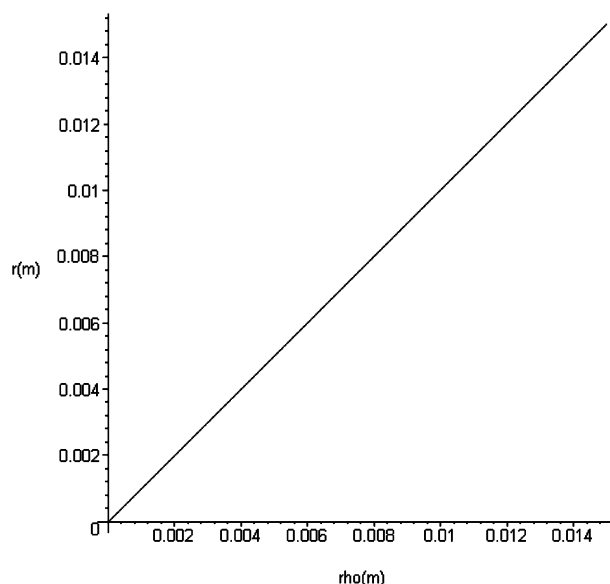


Fig. 4. Distribution of the actual radius  $r$  vs. the initial radius  $\rho$ .  $K_0 = 1.1$ .  $\eta_0 = 1/K_0 \cdot A = 1$ . Initial conditions:  $r(0) = 0$ ;  $r'(0) = 1$ .

then renders the following differential equation, obtained after easy manipulations:

$$-2r''(\rho) + \eta_0 \frac{A^2}{K_0} r'(\rho)^4 - \frac{A^2}{K_0^2} r'(\rho)^2 r''(\rho) = 0 \quad (5.5)$$

noting therein  $r'(\rho) := \frac{dr}{d\rho}$ ;  $r''(\rho) := \frac{d^2r}{d\rho^2}$ .

The second order differential equation (5.5) is solved with the specific boundary conditions  $r(0) = 0$  and  $r'(0) = 1$ , considering as in Rodriguez et al. (1994) the relationship  $\eta_0 = 1/K_0$ .

- In the specific case  $A = 0$ , the previous Eq. (5.5) takes the simple form  $r''(\rho) = 0$ , thus the actual radius  $r$  linearly varies versus  $\rho$ .
- In the general case ( $A$  non-nil), it is then seen (Fig. 4, considering the initial conditions  $r(0) = 0$ ;  $r'(0) = 1$ ) that the actual radius also nearly linearly varies versus  $\rho$ .

In order to conclude this section, note that the growth has been here envisaged—via the kinematic description—as a diffuse mechanism, in fact a volumetric growth. An alternative would be a surface growth process, occurring by the accretion of successive layers of newly added material. The description of surface growth needs however a specific treatment, that lies outside the scope of the present contribution. In general, one is faced with the more involved problem of a time dependent growth, whereby the rate of the growth tensor is related to the actual stress by a specific constitutive law: at each instant, one has to actualize the spatial distribution of the growth tensor, and then to solve the equilibrium equations in terms of the dependence  $\underline{T}(F_a)$ .

**Remark 5.** The analysis of growth incompatibilities points towards a geometrical viewpoint that considers growth as the propagation of defects in the material manifold of the growing body. This viewpoint exploits the fruitful synergy between the continuum theory and the differential geometry, whereby the issue of the existence of a global holonomic configuration (associated to the existence of a global compatible position vector field) is resolved in terms of two central quantities of differential geometry, namely the Cartan

torsion and the Riemann curvature tensor, see the pioneering works of Kondo (1952), Nye (1953) and Kröner (1960), and the more recent contribution of Steinmann (1996).

## 6. Conclusion and perspectives

A mechanical model for tissue growth has been elaborated at the mesoscopic scale of so-called tissue elements, considered as elementary representative volume elements, exchanging work and matter with the surrounding. The change of configuration due to growth is accounted for by a variation of the domain occupied by a tissue element under growth. The kinematics of the growth has been modeled by a growth transformation tensor, which is accompanied by an accommodation tensor that restores the integrity of the global displacement field. The energy of a growing tissue element exchanging and receiving mass both on its surface and in the bulk from transport phenomena and chemical reactions has been expressed, starting from a volume and a surface density, accounting for possible growth heterogeneities. The surface potential has been assumed to depend upon the normal to the growing surface, the total lagrangian strain, and the surface growth transformation tensor; it expresses the surface effects, which can represent an important contribution to the total energy of the growth, especially at small sizes (of the order of the micron and less).

The balance of momentum has been accordingly expressed in weak form, as a result of the vanishing of the gateaux derivative of the total potential energy of the growing germ, accounting for the domain variation (volume, surface and line variations) due to growth. The strong form of the principle of virtual power expressed in static case results in the equilibrium equations, and the associated surface and line (the growing surface of the tissue element is assumed to be non-closed, thus it has a line boundary) boundary conditions.

Considering the growth as being fully irreversible, the writing of the second principle of thermodynamics has further evidenced the volumetric, surface and line thermodynamic forces that trigger the growth.

As an important aspect of growth per se, the writing of the large strains kinematic compatibility condition as the vanishing of the fourth-order Riemann curvature tensors has provided an analytical solution for the accommodation tensor in the case of a radial growth, in the form of two possible families of solutions. It is clear in a general situation of heterogeneous growth that the set of mechanical balance equations have to be combined with both the constitutive equation of the solid growing material and with the transport equations. The numerical simulation of tissue growth is postponed to the second part of this contribution.

In biological systems, the search for a goal function of a living organism is one of the key points in the understanding and modeling of these systems (Wilhelm and Brüggemann, 2000). It is thought that the growth and evolution follow some organization principles regarding both the spatial and the temporal dimensions: we herewith envision the flow of metabolic processes as occurring within a structured well-chosen space–time manifold. The search for new variational principles that shall serve as goal functions is from our point of view an important challenge susceptible to bring a new vision of morphogenesis and evolution for biological tissues under growth.

## Appendix 1. Elements of differential geometry of surfaces

The operator  $\text{div}_S$  in the equality (3.11) denotes the surface divergence (Petryk and Mroz, 1986), defined from the projection of the gradient by the tensorial operator

$$\underline{\underline{P}} := I - \underline{n}_g \otimes \underline{n}_g$$

with  $P \in L(n_g^\perp, R^3)$  called the surface projection operator, such that one formally has  $\nabla_s := P \cdot \nabla$ , which defines the surface gradient in operator form. The surface divergence is then formally defined as the following equality between operators:

$$\text{div}_s(\cdot) := \text{Tr}(\nabla_s(\cdot))$$

Applied to the velocity field  $\underline{V}$ , this definition yields

$$\text{div}_s \underline{V} = \text{Tr}(\nabla_s \underline{V})$$

A superficial second order tensor field  $\underline{\underline{A}}$  on the surface  $S_g$  is a linear transformation from the tangent space of  $S_g$  to  $R^3$ . An extension of the domain of  $\underline{\underline{A}}$  to the whole space is made, requiring that  $\underline{\underline{A}}$  annihilates vectors normal to the tangent plane, i.e.  $\underline{\underline{A}} \cdot \underline{n}_g = 0$ . Tensor  $\underline{\underline{A}}$  then admits a unique decomposition into tangential and normal components  $\underline{\underline{A}}_{\text{tan}}$  and  $\underline{a}$ , viz

$$\underline{\underline{A}} = \underline{\underline{A}}_{\text{tan}} + \underline{n}_g \otimes \underline{a}$$

The surface divergence of a superficial tensor field is then defined by

$$\underline{b} \cdot \text{div}_s \underline{\underline{A}} = \text{div}_s(\underline{\underline{A}}^t \cdot \underline{b})$$

for any constant vector  $\underline{b}$ .

The velocity field is decomposed as the sum of its projections

$$\underline{V} = \underline{V}_T + V_N \cdot \underline{n}_g,$$

with  $\underline{V}_T$  the tangential part of  $\underline{V}$ , i.e. its projection onto the tangent plane to  $S_g$ , and  $V_N := \underline{V} \cdot \underline{n}_g$  the normal component of  $\underline{V}$ , i.e. the projection of  $\underline{V}$  onto the normal to the tangent plane.

According to this, one can explicit the scalar product

$$\nabla \underline{n}_g \cdot \underline{V} = \nabla \underline{n}_g \cdot \underline{V}_T = \nabla_s \underline{n}_g \cdot \underline{V}_T + (\underline{n}_g \otimes \underline{n}_g) \cdot \nabla \underline{n}_g \cdot \underline{V}_T = \nabla_s \underline{n}_g \cdot \underline{V}_T$$

The material derivative of the normal to the evolving surface  $S_g$  is then obtained as

$$\dot{\underline{n}}_g = \frac{\partial \underline{n}_g}{\partial t} + \nabla \underline{n}_g \cdot \underline{V} = \frac{\partial \underline{n}_g}{\partial t} + \underline{\underline{L}}_g \cdot \underline{V}_T \quad (\text{A1.1})$$

The tensor  $\underline{\underline{L}}_g := \nabla_s \underline{n}_g$  is the surface gradient of the normal  $\underline{n}_g$ , representing the curvature tensor of the surface  $S_g$ .

According to these definitions, the so-called surface transformation gradient

$$\underline{\underline{\tilde{F}}} = \underline{\underline{F}} \cdot P = \underline{\underline{F}} \cdot (I - \underline{n}_g \otimes \underline{n}_g)$$

has the material derivative

$$\dot{\underline{\underline{\tilde{F}}}} = \dot{\underline{\underline{F}}} - \dot{\underline{\underline{F}}} \cdot (\underline{n}_g \otimes \underline{n}_g) - (\underline{\underline{F}} \cdot \underline{\underline{L}}_g \cdot \underline{V}_T) \otimes \underline{n}_g - (\underline{\underline{F}} \cdot \underline{n}_g) \otimes (\underline{\underline{L}}_g \cdot \underline{V}_T) \quad (\text{A1.2})$$

or equivalently in component form:

$$\dot{\tilde{F}}_{ij} = \dot{F}_{ij} - \dot{F}_{ik} n_{gk} n_{gj} - F_{ik} n_{gj} L_{kp} V_p^T - F_{ik} n_{gk} L_{gjp} V_p^T$$

A more detailed account regarding surface deformation gradients is given in [Petryk and Mroz \(1986\)](#) and [Gurtin \(1995\)](#). The surface deformation gradient  $\underline{\underline{\tilde{F}}} := \underline{\underline{P}} \cdot \underline{\underline{F}}$  has the property to carry line elements attached to the initial configuration into material line elements of the surface  $S_g$ ; otherwise said, the pull-back of the line elements attached to  $S_g$  defines material line elements in the initial configuration  $\Omega_{0g}$ , forming a patch of tangent planes, the collection of which defines the pull-back of  $S_g$  into  $\Omega_{0g}$ .



The variation of the tangent vector  $\underline{\tau}_g = \underline{F} \cdot \underline{\tau}_{0g}$  (material vector) is evaluated from the orthogonality property  $\underline{\tau}_g \cdot \underline{n}_g = 0$ , thus giving

$$\delta \underline{\tau}_g = -(\underline{\tau}_g \cdot \delta \underline{n}_g) \underline{n}_g = -(\underline{\tau}_g \cdot \underline{L} \cdot \underline{P} \cdot \underline{v}) \underline{n}_g \quad (\text{A1.3})$$

The following divergence theorems are further involved:

$$\int_{\Omega_g} \underline{A} : \delta \underline{F} \, dx_g = - \int_{\Omega_g} \text{div}_g(\underline{A}) \cdot \delta \underline{U} \, dx_g + \int_{S_g} \underline{n}_g^t \cdot \underline{A} \cdot \delta \underline{U} \, d\sigma_g$$

Note that in this transformation, there is no complementary term on the surface  $\partial\Omega_g \setminus S_g$ , since the support of  $\delta \underline{U}$  is restricted to  $S_g$ . One further writes a similar formula for the transformation of the surface integral:

$$\int_{S_g} \underline{\tilde{B}} : \delta \underline{\tilde{F}} \, d\sigma_g = - \int_{S_g} \text{div}_s(\underline{\tilde{B}}) \cdot \delta \underline{\tilde{U}} \, d\sigma_g + \int_{\partial S_g} \underline{n}_g^t \cdot \underline{\tilde{B}} \cdot \delta \underline{\tilde{U}} \cdot \underline{v}_g \, dl_g \quad (\text{A1.4})$$

The two previous equalities are valid for any second order tensors  $\underline{A}$  (having its range in  $\Omega_g$ ) and  $\underline{\tilde{B}}$  (surface tensor having its range on  $S_g$ ).

The variation of the normal vector is, according to (3.14), neglecting the explicit time dependence of  $\underline{n}_g$ :

$$\delta \underline{n}_g = \underline{L}_g \cdot \delta \underline{U}_T = \underline{L}_g \cdot \underline{P} \cdot \delta \underline{U} \quad (\text{A1.5})$$

Furthermore, the counterpart of (3.15) in terms of variations is

$$\delta \tilde{F}_{ij} = \delta F_{ij} - \delta F_{ik} n_{gk} n_{gj} - F_{ik} n_{gj} L_{kp} \delta U_p^T - F_{ik} n_{gk} L_{jp} \delta U_p^T \quad (\text{A1.6})$$

The variations of the volume and surface Jacobian express as

$$\delta(j_g) = -\frac{1}{j_g^2} \cdot J_g \text{div}(\delta \underline{U}) = -j_g \text{div}(\delta \underline{U}); \quad \delta(j_{sg}) = -j_{sg} \delta(J_{sg}), \quad \text{with } J_{sg}(\underline{n}_g \cdot \underline{F}_g \cdot \underline{N}_g) = J_g,$$

thus giving after an elementary calculation

$$\delta(J_{sg}) = J_{sg} \nabla_X(\delta \underline{U}) - j_{sg} J_{sg}^2 (\underline{F}_g \cdot \underline{N}_g)^t \cdot \underline{L}_g \cdot \underline{P} \cdot \delta \underline{U} - j_{sg} J_{sg}^2 \underline{n}_g \cdot \nabla_X(\delta \underline{U}) \cdot \underline{N}_g \quad (\text{A1.7})$$

We shall further make use the surface divergence theorem, with two variants:

- (i) considering a surface vector field  $\underline{p}$  (i.e. a vector field attached to the tangent plane of the surface  $S_g$ ) and a surface tensor  $\underline{c}$ , one has

$$\int_{\partial S_g} \underline{c} \cdot \underline{p} \cdot \underline{v}_g \, dl_g = \int_{S_g} (\underline{c} : \nabla_s \underline{p} + \underline{p} \cdot \text{div}_s \underline{c}) \, d\sigma_g$$

- (ii) for a scalar field  $q$  and a superficial vector field  $\underline{d}$ , one writes

$$\int_{\partial S_g} q \underline{d} \cdot \underline{v}_g \, dl_g = \int_{S_g} (\underline{d} \cdot \nabla_s q + q \text{div}_s \underline{d}) \, d\sigma_g$$

## Appendix 2. Variation of the total energy (Eulerian form)

Starting from the expression of the total mechanical energy of the growing tissue element

$$E := \int_{\Omega_g} j \psi^V(\underline{x}_g, \underline{E}) \, dx_g + \int_{S_{gt}} j_s \psi^S(\underline{\tilde{x}}_g, \underline{n}_g, \underline{\tilde{E}}) \, d\sigma_g$$

its domain derivative is easily evaluated as the following lengthy expression:

$$\begin{aligned} \frac{\delta E}{\delta t} = & \int_{\Omega_g} j\psi_{,x}^V \underline{V} dx + \int_{\Omega_g} j\psi_{,E}^V \\ & : \dot{\underline{E}} dx_g + \left\{ - \int_{\Omega_g} j\psi^V \operatorname{div} \underline{V} dx_g - \int_{\Omega_g} \nabla_X (j\psi^V)^t \cdot \underline{V} dx_g + \int_{S_{gt}} j\psi^V \underline{V} \cdot \underline{n}_g d\sigma_g \right\} \\ & + \int_{S_{gt}} j_s [\psi_{,x}^S \cdot \underline{\tilde{V}} - (\psi_{,n}^S)^t \cdot \underline{\underline{L}} \cdot \underline{\underline{P}} \cdot \underline{\tilde{V}} + \underline{\underline{S}} : \underline{\underline{\dot{E}}}] d\sigma_g + \int_{S_{gt}} \psi^S \dot{j}_s d\sigma_g + \int_{S_{gt}} j_s \psi^S \operatorname{div}_S \underline{V} d\sigma_g \end{aligned} \quad (\text{A2.1})$$

The sum of the three terms under the accolade vanish, in view of the equality

$$- \int_{\Omega_g} j\psi^V \operatorname{div} \underline{V} dx_g = \int_{\Omega_g} \nabla_X (j\psi^V)^t \cdot \underline{V} dx_g - \int_{S_{gt}} j\psi^V \underline{V} \cdot \underline{n}_g d\sigma_g$$

One further transforms the homologous surface contribution

$$\int_{S_g} j_s \psi^S \operatorname{div}_S \underline{V} d\sigma_g = - \int_{S_g} \underline{\tilde{V}} \cdot \nabla_S (j_s \psi^S) d\sigma_g + \int_{\partial S_g} j_s \psi^S \underline{\tilde{V}} \cdot \underline{v}_g dl_g \quad (\text{A2.2})$$

Adopting a point of view similar to plasticity (Khan and Huang, 1995), the following identity is easily obtained

$$\int_{\Omega_g} j \underline{\underline{S}} : \dot{\underline{E}} dx_g = \int_{\Omega_g} \underline{\underline{\sigma}} : \underline{\underline{D}} dx_g \quad (\text{A2.3})$$

with  $\underline{\underline{\sigma}} = j \underline{\underline{F}} : \underline{\underline{S}} \cdot \underline{\underline{F}}^t$  and furthermore, the term  $\int_{S_{gt}} \psi^S \dot{j}_s d\sigma_g$  is transformed into

$$\begin{aligned} \int_{S_g} \psi^S \dot{j}_s d\sigma_g = & \int_{S_g} [\underline{\tilde{V}} \cdot \nabla_S \psi^S - j J_s (\underline{\underline{F}} \cdot \underline{\underline{N}}_g)^t \cdot \underline{\underline{L}} \cdot \underline{\underline{P}} \cdot \underline{\tilde{V}} + \nabla_S \cdot (j J_s \psi^S (\underline{\underline{n}}_g \otimes \underline{\underline{N}}_g)^t) \cdot \underline{\tilde{V}}] d\sigma_g \\ & + \int_{\partial S_g} \psi^S \underline{V} \cdot \underline{v}_g dl_g + \int_{\partial S_g} j J_s (\underline{\underline{n}}_g \otimes \underline{\underline{N}}_g)^t \cdot \underline{\tilde{V}} \cdot \underline{v}_g dl_g \end{aligned} \quad (\text{A2.4})$$

Gathering the expressions the above gives the derivative

$$\begin{aligned} \frac{\delta E}{\delta t} = & \int_{\Omega_g} \underline{\underline{\sigma}} : \underline{\underline{D}} dx_g + \int_{\Omega_g} j (\psi_{,X}^V)^t \cdot \underline{V} dx_g + \int_{S_g} \underline{\underline{\sigma}} : \underline{\underline{\dot{d}}} dx_g - \int_{S_g} \left\{ j_s (\psi_{,n}^S)^t \cdot \underline{\underline{L}} \cdot \underline{\underline{P}} - j_s (\psi_{,x}^S)^t - (\nabla_S \psi^S)^t \right. \\ & \left. + j J_s (\underline{\underline{F}} \cdot \underline{\underline{N}}_g)^t \cdot \underline{\underline{L}} \cdot \underline{\underline{P}} - \nabla_S \cdot [j J_s \psi^S (\underline{\underline{n}}_g \otimes \underline{\underline{N}}_g)^t] + \nabla_S (j_s \psi^S) \right\} \cdot \underline{\tilde{V}} d\sigma_g \\ & + \int_{\partial S_g} (1 + j_s) \psi^S \underline{\tilde{V}} \cdot \underline{v}_g dl_g + \int_{\partial S_g} j J_s (\underline{\underline{n}}_g \otimes \underline{\underline{N}}_g)^t \cdot \underline{\tilde{V}} \cdot \underline{v}_g dl_g \end{aligned} \quad (\text{A2.5})$$

expressed in Eulerian format.

### Appendix 3. Thermodynamics of open systems

For material systems that exchange work and mass with their surrounding, the material derivative of the volumic internal energy  $u$  expresses as Munster (1966)

$$\dot{u} = \nabla \cdot (\underline{J}_q) - p_i + \underline{J}_k \cdot \underline{E}_k \quad (\text{A3.1})$$

with  $\underline{J}_q$  the heat diffusion flux (that shall obey a constitutive relationship vs. the temperature  $T$ ),  $p_i = -\underline{\sigma} : \underline{D}(\underline{v})$  the volumetric density of the power of internal forces (expressed here choosing an Eulerian description, with  $\underline{\sigma}$  the Cauchy stress),  $\underline{J}_k$  the diffusion flux of the  $k$ -specie, and  $\underline{F}_k$  an external force acting on the  $k$ -specie.

The entropy balance expresses in terms of the material derivative of the volumic density of entropy  $s$  as

$$T\dot{s} = \dot{u} - \underline{\sigma} : \underline{D}^R - \mu_k \rho_k \dot{c}_k \quad (\text{A3.2})$$

considering  $k = 1, \dots, N$  chemical species (otherwise called constituents) having each the chemical potential  $\mu_k$  and the concentration  $c_k = \frac{\rho_k}{\rho}$  being the ratio of mass densities of the  $k$ th constituent to the total density. The symmetric part of the velocity gradient  $\underline{D}$  is being additively decomposed into a reversible contribution  $\underline{D}^R$  and an irreversible contribution  $\underline{D}^{IR}$ .

The barycentric balance of mass is (for the  $k$ th constituent)

$$\rho \dot{c}_k = -\nabla \cdot (\underline{J}_k) + v_{km} R_m \quad (\text{A3.3})$$

with  $R_j$  the velocity of the chemical reaction for the  $j$ th constituent (a scalar quantity). The (vectorial) flux of mass  $\underline{J}_k$  expresses vs. the local velocity  $\underline{v}_k$ , the barycentric velocity  $\underline{v}$  and the mass density  $\rho_k$  as

$$\underline{J}_k = \rho_k (\underline{v}_k - \underline{v})$$

thus the exchange term on the right-hand side of (A2.3) further expresses in the balance law

$$\frac{\partial \rho_k}{\partial t} = -\nabla \cdot (\rho_k \underline{v}) - \nabla \cdot (\underline{J}_k) = -\nabla \cdot (\underline{\Phi}_{m_k})$$

The flux  $\underline{\Phi}_{m_k}$  decomposes into a convection flux and a diffusion flux  $\underline{J}_k$ . Introducing (A3.3) and (A3.1) into (A3.2) leads to

$$\rho T \dot{s} = \nabla \cdot (\underline{J}_q) - p_i + \underline{J}_k \cdot \underline{F}_k - \underline{\sigma} : \underline{D}^R + \mu_k \nabla \cdot (\underline{J}_k) - \mu_i v_{ij} R_j \quad (\text{A3.4})$$

We further transform in (A3.4) all terms having divergence multiplicative factors, using the general equality

$$\mu_k \nabla \cdot (\underline{J}_k) = \nabla \cdot (\mu_k \underline{J}_k) - \underline{J}_k \cdot \nabla \mu_k$$

thus giving

$$\rho T \dot{s} = \nabla \cdot (\underline{J}_q) - p_i - \underline{\sigma} : \underline{D}^R + \nabla \cdot (\mu_k \underline{J}_k) - \underline{J}_k \cdot \nabla \mu_k + A_k R_k + \underline{J}_k \cdot \underline{F}_k$$

with  $A_k := v_{ik} \mu_i$  the chemical affinities, introduced by De Donder (Munster, 1966). The comparison with the conservation law of the entropy,

$$\dot{s} = \nabla \cdot (\underline{J}_s) + \sigma_s$$

introducing the entropy flux  $\underline{J}_s$  (exchange of entropy with the environment) and the source of entropy  $\sigma_s$  (irreversible contribution), gives by identification (all terms having a divergential form are exchange contributions):

$$\rho T \sigma_s = -p_i - \underline{\sigma} : \underline{D}^R - \underline{J}_k \cdot \nabla \mu_k + A_k R_k + \underline{J}_k \cdot \underline{F}_k \quad (\text{A3.5}_1)$$

$$\underline{J}_s = \underline{J}_q + \mu_k \underline{J}_k \quad (\text{A3.5}_2)$$

The positivity of the entropy source  $\sigma_s = \dot{s}_i$  implies

$$\underline{\sigma} : \underline{D} - \underline{\sigma} : \underline{D}^R - \underline{J}_k \cdot \nabla \mu_k + A_k R_k + \underline{J}_k \cdot \underline{F}_k = \underline{\sigma} : \underline{D}^{IR} - \underline{J}_k \cdot \nabla \mu_k + A_k R_k + \underline{J}_k \cdot \underline{F}_k \geq 0 \quad (\text{A3.6})$$

The entropy source results accordingly from the non-uniformity of the intensive parameters, the conduction of heat (with here the specific case of a uniform temperature) and diffusion of mass, the dissipation of mechanical energy (expressed by the first term in the right hand side of (A3.6)) and the occurrence of chemical reactions.

An alternative expression of the dissipation is obtained by considering the general form of the balance of energy and entropy ( $u$  and  $s$ , respectively, denote the densities of internal energy and entropy, per unit mass):

$$\rho \dot{u} = -\nabla \cdot \underline{J}_q - p_i + \underline{J}_k \cdot \underline{E}_k; \rho \dot{s} = -\nabla \cdot \underline{J}_s + \sigma_s$$

with  $\underline{J}_s := \frac{1}{T}(\underline{J}_q - \mu_i \underline{J}_i)$  the total entropy flux. We then immediately obtain

$$\rho \dot{\psi} = \rho s \dot{T} - \nabla \cdot \underline{J}_q + T \nabla \cdot \underline{J}_s + \underline{J}_k \cdot \underline{E}_k - p_i - \sigma_s$$

with  $\psi := u - Ts$  the free energy. For an isothermal process, the positivity of the entropy production  $\sigma_s$  in previous inequality then expresses as

$$\rho \dot{\psi} \leq -p_i + \underline{J}_k \cdot \underline{E}_k - \nabla \cdot (\mu_i \underline{J}_i) \quad (\text{A3.7})$$

The principle of virtual power,  $\frac{dK}{dt} = P_e + P_i$ , leads to the global form of previous inequality:

$$\frac{dK}{dt} + \int_{\Omega} \rho \dot{\psi} dx \leq P_e + \underline{J}_k \cdot \underline{E}_k + \Phi_m \quad (\text{A3.8})$$

with  $K$  the kinetic energy, and  $\Phi_m := -\int_{\partial\Omega} \mu_i \underline{J}_i \cdot \underline{n} d\sigma$  the flux of mass through the boundary of  $\Omega$ . Previous inequality traduces the fact that the flux of mechanical work and mass increases the kinetic and internal free energy of the system, the difference being dissipated.

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