STRUCTURAL INTERFACES IN SOLID MECHANICS: A VIEW TO APPLICATIONS IN BIOLOGICAL SYSTEMS

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ABSTRACT

The concept of structural interface is introduced focussing on potential applications in the field of bioengineering. In particular, some structural interfaces in biological systems are identified, with emphasis on the periodontal ligament in the tooth-bone system and the articular cartilage in diarthrodial joints. Speculations on possible applications in the modelling of receptor-ligand binding between proteins close the paper.

INTRODUCTION

The connexion between two solid bodies usually consist in a thin, deformable layer of peculiar mechanical characteristics. In particulate composite materials, for instance, a thin interphase often joints the inclusions to the matrix. In biological systems, the periodontal ligament and the articular cartilage represent examples of thin layers connecting bones. In contact mechanics, an interfacial layer separates the two bodies in contact. In all these cases, compared to the connected solids, the interfacial layer:

- has small dimension,
- suffers large strains,
- is characterized by a strongly nonlinear behaviour.

A trivial way to model the above systems is to treat the interface layer as a third body, characterized by nonlinear constitutive laws and subject to large strains. A numerical treatment of this problem is straightforward on one hand -in the sense that it can be pursued in principle with any commercial f.e. code- but highly unsatisfactory on the other. Several difficulties result in fact hidden in this approach. First, a fine, three dimensional mesh is required to model the interface layer, yielding an unnecessary dense mesh in the connected bodies. Second, a large strain formulation of all the system is required, even in the common case in which the solids connected are subject to small strains. Third, f.e. techniques are known to become inaccurate where stress concentrations may arise, and these may occur at the interface. A classical remedy to these inconveniences is represented by the concept of imperfect interface. Following this approach, the thickness of the interface layer is condensed to zero, but instead of the usual transmission conditions across the interface

$$[[\boldsymbol{\sigma}]]\,\mathbf{n} = \mathbf{0}, \qquad \mathbf{u} = \mathbf{0}, \tag{1}$$

(where **n** is the unit vector normal to the interface, $\boldsymbol{\sigma}$ and **u** are the stress tensor and the displacement vector, respectively, and the operator $[[\cdot]]$ denotes a jump in the relevant argument) an interfacial constitutive law is prescribed

$$[[\boldsymbol{\sigma}]]\,\mathbf{n} = \mathbf{0}, \qquad \boldsymbol{\sigma}^{+}\,\mathbf{n} = \mathbf{f}\,([[\mathbf{u}]]), \tag{2}$$

where $\boldsymbol{\sigma}^{+}$ is the stress at one side of the interface and **f** denotes a tensorial function of the displacement jump. When this function is linear and positive definite, the formulation results strongly simplified, but it allows unphysical interpenetration of the material in contact when the interface is subject to compressive tractions. Interfacial nonlinearity may avoid the interpenetration, but may promote instabilities and bifurcations of different nature [1]. Several interfacial constitutive laws have been proposed of the type (2), see for instance [2] and [3], however, a common feature of these models is the fact that the interface has a null thick-ness. Recently, Bigoni and Movchan [4] have introduced the concept of structural interface, possessing finite width and possibly inertia. Mechanical effects differentiating this model from conventional zero-thickness interfaces have been explored for static and dynamic problems and are summarized in the next Section. The focus here is to analyze possibility of employing the model in the analysis of biological systems. In these systems, interfaces are common enough and sometimes characterized by well defined microstructures. For instance, we quote two examples: the famous metacarpal bone from a vulture's wing reported by Thompson [5] (Fig. 1) and the skeleton of the echinoderm keyhole urchin (Mellita quinquiesperforata, Fig. 2), the former similar to a Warren truss and the latter to a strut structure.

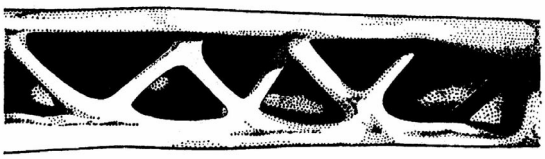


Figure 1. Metacarpal bone from a vulture's wing (after Thompson [5]).

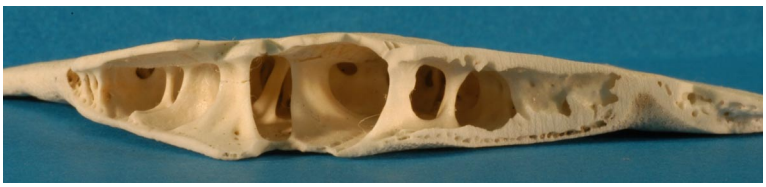


Figure 2. Internal structure from a skeleton of keyhole urchin (Mellita quinquiesperforata, photograph by D. Bigoni).

THE NOTION OF STRUCTURAL INTERFACE

In order to introduce the concept of structural interface, we refer to the model sketched in Fig. 3, inspired from the internal structure of the keyhole urchin, Fig. 2, and restricted to two-dimensions for simplicity. Two solids denoted by indices + and − are connected through a

finite thickness interface in Fig. 3. The microstructure of the interface is made in a way that only radial forces are transmitted, a situation introduced here for simplicity, but which is used in nanotechnology to represent van der Waals interactions. If the two connected surfaces are described by the position vectors $\mathbf{r}^+$ and $\mathbf{r}^-$ in the form

$$\mathbf{r}^{\pm}(\theta) = f_{\pm}(\theta)\,\mathbf{e}_r, \qquad \theta \in [\theta_1, \theta_2], \tag{3}$$

where f_+ and f_- are generic, but (for simplicity) smooth functions of angle θ and $\mathbf{e}_r$ is the radial unit vector. The elementary surface length dl, the tangent and orthogonal unit vectors $\mathbf{s}$ and $\mathbf{n}$ at a generic θ are

$$dl = |\mathbf{v}|\, d\theta, \qquad \mathbf{s} = \frac{\mathbf{v}}{|\mathbf{v}|}, \qquad \mathbf{n} = \frac{-f\,\mathbf{e}_r + f'\mathbf{e}_\theta}{|\mathbf{v}|}, \tag{4}$$

where

$$\mathbf{v} = f'\,\mathbf{e}_r + f\,\mathbf{e}_\theta\,. \tag{5}$$

Equilibrium conditions of the interfacial structure require that

$$\mathbf{t}_+ = \frac{|\mathbf{v}_-|}{|\mathbf{v}_+|}\,\mathbf{t}_-, \tag{6}$$

where $\mathbf{t}_\pm$ denotes the tractions at the two connected surfaces. The condition that the interface transmits only radial forces and that these are linear functions of the radial difference between displacements at the two connected surfaces gives

$$\mathbf{t}_+ = -k\,(u_r^+ - u_r^-)\,\mathbf{e}_r, \tag{7}$$

where $u_r = \mathbf{u} \cdot \mathbf{e}_r$ is the radial component of displacement and k denotes a positive proportionality constant. Equations (6) and (7) define the behaviour of the structural interface sketched in Fig. 3. It may be worth mentioning that in a specific mechanical problem, the interface enters the formulation only through eqns. (6) and (7), so that further consideration of the interface itself are not needed.

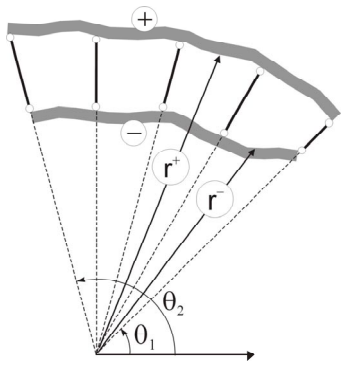


Figure 3. A model of structural interface

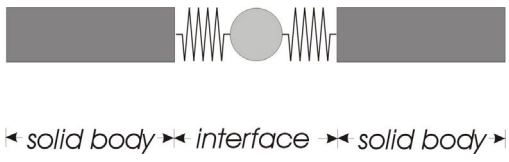


Figure 4. A simple model of structural interface with inertia

It has been shown in [4] with specific examples that for quasi-static problems the thickness of the interface introduces an additional characteristic length, providing a parameter which can serve different design needs, for instance, it may be employed to obtain neutral coated inclusions. In biological systems, however, the interfacial thickness can also be employed to model flux of fluids and the consideration of the morphology of the interfacial microstructure may allow the introduction of rules for morphology evolution and remodelling.
The interfacial structure shown in Fig. 3 does not possess an inertia. Bigoni and Movchan [4] have explored the possibility that interfacial inertia can play a role in dynamics.
A simple spring-mass-spring model of an inertial interface structure is presented in Fig. 4, joining two continuous bars. A periodic version of the semi-discrete model sketched in Fig. 4 has been analyzed in [4]. The analysis has revealed peculiar characteristics, particularly, it has been found that the interfacial inertia strongly affects the dynamic characteristics of the system, which may be designed to possess peculiar filtering properties for elastic waves.

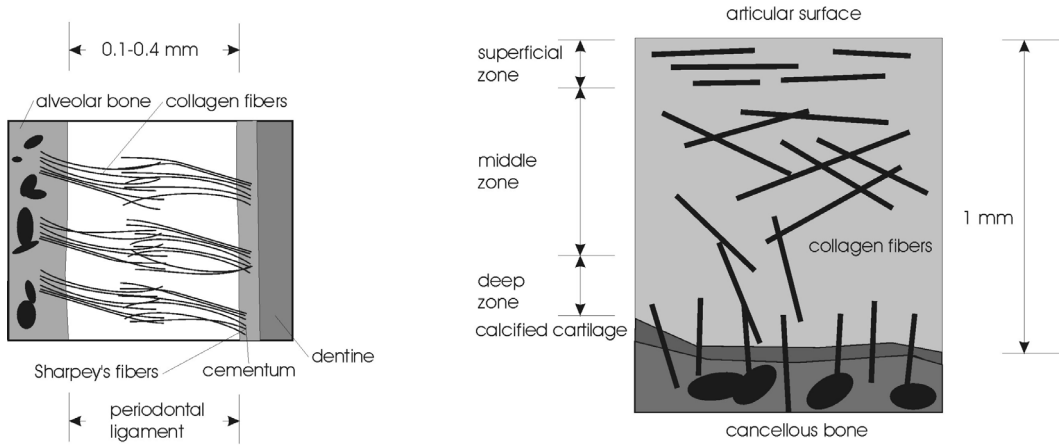
STRUCTURAL INTERFACES IN BIOLOGICAL SYSTEMS

Two interfaces in biological systems are considered in this section, namely, the periodontal ligament and the articular cartilage. In both cases, transmission of load is the primary mechanical function. A brief discussion on the possibilities of employing the model of structural interface for analysing the adhesion mechanisms between proteins is presented in closure of the section.

The periodontal ligament

The periodontal ligament (shortened as PDL in the following) is the thin layer that attaches the cementum of the tooth to the adjacent alveolar bone. It is a strongly vascularized system, with neural components. The thickness ranges between 0.1 mm and 0.4 mm and is thicker in functioning than in non-functioning teeth, in areas of tension than compression. The PDL serves several functions: mechanical, in terms of transmission of forces and tooth mobility; remodelling and formative, allowing formation and resorption of cementum and bone during physiologic tooth movement; nutritional and sensory, carrying nutrients to cementum, bone and gingival; and, finally, proprioceptive and tactile.
Mechanical tests by Pini [6] and Pini et al. [7] restricted to in-vitro bovine specimen showed a strongly nonlinear behaviour in which the PDL exhibits a monotonic stress-strain behaviour analogous to that of many soft tissues, with an early stage of small stiffness followed, in higher deformation regimes, by a marked locking (a rapid increase of stress associated with a small increase of strain).
A modelling of the mechanical behaviour of the periodontal ligament was proposed by Gei et al. [3] in terms of a nonlinear, zero-thickness interface. The model has been shown to provide an accurate description of the teeth-PDL-bone system, yielding at the same time a reasonably simple model from computational point of view. Such a model, however, does not take explicitly into account the microstructure of the ligament, so that the problem may be posed whether the finite-thickness microstructure possesses characteristics that cannot be condensed in a zero-thickness interface model. The structure of the periodontal ligament is made up of collagen fibres, the so-called Sharpey fibres (Fig. 5a). These have an orientation ranging between orthogonal and inclined at 45° to the tooth surface and are thought to strongly influence the behaviour of the tooth-bone complex under both masticatory and remodelling

loads. A proper account of the microstructure of collagen fibres may be pursued by employing the structural interface concept. This remains for the moment an unexplored possibility.



(a) (b)

Figure 5. Two biological interfaces. Scheme of the periodontal ligament (a) and of the layered structure of an articular cartilage (b).

The articular cartilage

Cartilage is a firm gelatinous matrix containing a dense network of collagen fibres and confined by a membrane, the perichondrium. Three types of cartilage are present in mammals: hyaline, elastic, and fibrocartilage. Hyaline is found in adult humans in free-moving joints at the end of bones and represents the so-called 'articular cartilage'. This cartilage is highly elastic and covers the end of bones with a coating of thickness inferior than 1 mm. The collagen fibres present a variation of inclination through the thickness of the cartilage, which evidences a well-defined microstructure. In a superficial zone, in particular, the fibres are parallel to the free surface of the coating, but these rotate with depth, become randomly oriented in a mid zone and are radial in a deep zone, entering normal in a calcified layer joined to the bone (Fig. 5b). Note that, differently from bone –and, more important to the current discussion, from the periodontal ligament– cartilage is avascular.

A mechanical model of articular cartilage can be set up in which the microstructure is condensed in a specific form of anisotropy as follows. In the framework of a three-dimensional theory of linear elasticity, let us define an elastic response in the form

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}\,(\boldsymbol{\varepsilon}, \mathbf{n}_1 \otimes \mathbf{n}_1, \mathbf{n}_2 \otimes \mathbf{n}_2, \mathbf{n}_3 \otimes \mathbf{n}_3), \tag{8}$$

where $\boldsymbol{\varepsilon}$ is the strain and $\mathbf{n}_i$, i = 1,2,3, denote three unit vectors in the directions of fibres. Employing representation theorems [8] and assuming that the three sets of fibres have the same mechanical properties, the stress-strain constitutive law can be written in the form

$$\begin{aligned}\boldsymbol{\sigma} = {} & [\lambda\, \mathrm{tr}\,\boldsymbol{\varepsilon} + \alpha_1\,(e_{11} + e_{22} + e_{33})]\,\mathbf{I} + 2\mu\,\boldsymbol{\varepsilon} \\ & + [\alpha_2\,\mathrm{tr}\,\boldsymbol{\varepsilon} + \alpha_3\,(e_{11} + e_{22} + e_{33}) + \alpha_4\,(e_{12} + e_{13} + e_{23})]\,(\mathbf{n}_1 \otimes \mathbf{n}_1 + \mathbf{n}_2 \otimes \mathbf{n}_2 + \mathbf{n}_3 \otimes \mathbf{n}_3) \\ & + [\alpha_5\,\mathrm{tr}\,\boldsymbol{\varepsilon} + \alpha_6\,(e_{11} + e_{22} + e_{33}) + \alpha_7\,(e_{12} + e_{13} + e_{23})] \\ & [\mathbf{n}_1 \bullet \mathbf{n}_2\,(\mathbf{n}_1 \otimes \mathbf{n}_2 + \mathbf{n}_2 \otimes \mathbf{n}_1) + \mathbf{n}_1 \bullet \mathbf{n}_3\,(\mathbf{n}_1 \otimes \mathbf{n}_3 + \mathbf{n}_3 \otimes \mathbf{n}_1) + \mathbf{n}_2 \bullet \mathbf{n}_3\,(\mathbf{n}_2 \otimes \mathbf{n}_3 + \mathbf{n}_3 \otimes \mathbf{n}_2)]\end{aligned} \tag{9}$$

$$+ \alpha_8 (\mathbf{n}_1 \otimes \boldsymbol{\varepsilon}\, \mathbf{n}_1 + \boldsymbol{\varepsilon}\, \mathbf{n}_1 \otimes \mathbf{n}_1 + \mathbf{n}_2 \otimes \boldsymbol{\varepsilon}\, \mathbf{n}_2 + \boldsymbol{\varepsilon}\, \mathbf{n}_2 \otimes \mathbf{n}_2 + \mathbf{n}_3 \otimes \boldsymbol{\varepsilon}\, \mathbf{n}_3 + \boldsymbol{\varepsilon}\, \mathbf{n}_3 \otimes \mathbf{n}_3),$$

where $e_{ij} = \mathbf{n}_i \bullet \boldsymbol{\varepsilon}\, \mathbf{n}_j$, $(i,j = 1,2,3)$ λ, μ and α_i, $(i = 1,\ldots,8)$ are material constants, possibly denpending on the scalar products $\mathbf{n}_i \bullet \mathbf{n}_j$. In order to model the articular cartilage, the unit vectors $\mathbf{n}_i$ must lie parallel to a plane, say, 1–2. Now, the fibres in the superficial and deep layers forming the articular cartilage are parallel and orthogonal to the underlying bone, respectively, so that constitutive equation (9) reduces to

$$\boldsymbol{\sigma} = [\lambda \operatorname{tr} \boldsymbol{\varepsilon} + 3\alpha_1\, \mathbf{n} \bullet \boldsymbol{\varepsilon}\, \mathbf{n}]\, \mathbf{I} + 2\mu\, \boldsymbol{\varepsilon} \tag{10}$$

$$+ 3\, [(\alpha_2 + 2\alpha_5) \operatorname{tr} \boldsymbol{\varepsilon} + 3\, (\alpha_3 + \alpha_4 + 2\alpha_6 + 2\alpha_7)\, \mathbf{n} \bullet \boldsymbol{\varepsilon}\, \mathbf{n}]\, \mathbf{n} \otimes \mathbf{n} + 3\alpha_8\, (\mathbf{n} \otimes \boldsymbol{\varepsilon}\, \mathbf{n} + \boldsymbol{\varepsilon}\, \mathbf{n} \otimes \mathbf{n}).$$

The constitutive equation (10) describes a locally orthotropic material with respect to the fibre direction $\mathbf{n}$. In the mid layer, the collagen fibres have a random inclination, so that the material becomes isotropic in the plane of the fibres. Isotropy in the plane 1–2 can be modelled taking the unit vectors $\mathbf{n}_i$ in eqn. (9) inclined at $2\pi/3$ to each other. In this case, eqn. (9) becomes

$$\hat{\boldsymbol{\sigma}} = \operatorname{tr} \hat{\boldsymbol{\varepsilon}}\, [\lambda + \frac{3}{2}(\alpha_1 + \alpha_2) + \frac{9}{4}\alpha_3 - \frac{9}{8}\alpha_4 + \frac{3}{4}\alpha_5 + \frac{9}{8}\alpha_6 - \frac{9}{16}\alpha_7]\, \hat{\mathbf{I}} + (2\mu + 3\alpha_8)\, \hat{\boldsymbol{\varepsilon}}$$

$$+ (\lambda + \frac{3}{2}\alpha_2 + \frac{3}{4}\alpha_5)\, \varepsilon_{33}\, \hat{\mathbf{I}}, \tag{11}$$

where $\hat{\boldsymbol{\sigma}}$, $\hat{\boldsymbol{\varepsilon}}$ and $\hat{\mathbf{I}}$ denote quantities restricted to the plane 1–2. Eqn. (11) clearly represents in-plane isotropy.

The fibre inclination in the articular cartilage is a function of the distance from the contact surface, so that from the above discussion it is clear that the resulting elastic behaviour can be modelled through constitutive equation (9), thus producing a kind of functionally graded material. Several studies of articular cartilage are available [9-12] but the graduation of elastic properties through the thickness in the above-sketched way was never addressed.

In the anisotropic, graded model (9), however, the microstructure is accounted for only in a phenomenological sense, but is not explicitly taken into account. The model presented in [9] consists in a network microstructure mimicking the collagen fibres. We believe that a model of microstructural interface for the articular cartilage could on one hand present computational advantages against a continuous modelling, on the other hand may reveal unexplored features.

Adhesion between proteins

Adhesive forces become increasingly important when the size and stiffness of connected elements decrease [13]. A consequence of this is that in many biological systems adhesive forces play an essential role. In particular, a basic event of biological life is the recognition of one macromolecule by another and this relies on receptor-ligand interactions. A demonstration of this is that a modification of biological processes at all organizational levels can be obtained through an alteration of receptor-ligand interactions. The binding forces are weak local interactions, such as electrostatic double-layer force, van der Waals force, steric repulsion force and hydrogen bonding [14]. The model of structural interface eqns. (6)-(7) has been already adopted in a particular case to take into account van der Waals interaction [15].

It is therefore expected that the model can be successfully applied to the mechanics of receptor-ligand binding. In particular, the interfacial thickness may become a measure of the degree of binding and may permit modelling of interactions.

CONCLUSIONS

In biological systems interfaces are common structures connecting continuous bodies. The concept of structural interface developed by Bigoni and Movchan [4] is tailored to embody morphological characteristics which may include stiffness anisotropy and inertia. Interfacial behaviour dominates mechanics of articular movements and receptor-ligand binding in cells. The former issue represents a key feature in robotics, while the latter is a basic mechanism underlying biological life.

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REFERENCES

[1] E. Radi, D. Bigoni, and A. Tralli. *J. Mech. Phys. Solids* 47, 275-296, 1999.
[2] A. Needleman. J. *Mech. Phys. Solids* 38, 289-324, 1990.
[3] M. Gei, F. Genna, and D. Bigoni. *J. Biomech. Eng.* 124, 538-546, 2002.
[4] D. Bigoni and A.B. Movchan. *Int. J. Solids Struct.* 39, 4843-4865, 2002.
[5] W. D. Thompson. *On growth and form*. Cambridge Univ. Press, Cambridge, 1942.
[6] M. Pini. Ph. D. thesis, University of Trento, Italy, 1999.
[7] M. Pini, P. Vena, and R. Contro. Proc. XIII Convegno Italiano di Meccanica Computazionale, Brescia, Italy, 2000.
[8] C.C. Wang. *Arch. Rat. Mech. Analysis* 36, 198-223, 1970.
[9] P. Bursac, C.V. McGrath, S.R. Eisenberg, and D. Stamenovic. *J. Biomech. Eng.* 122, 347-353, 2000.
[10] S.M. Klisch and J.C. Lotz. *J. Biomech. Eng.* 122, 180-188, 2000.
[11] M.A. Soltz and G.A. Athesian. *J. Biomech. Eng.* 122, 576-586, 2000.
[12] T.L. Haut Donahue, M.L. Hull, M.M. Rashid, and C.R. Jacobs. *J. Biomech. Eng.* 124, 273-280, 2002.
[13] K.L. Jonhson, K. Kendall, and A.D. Roberts. *Proc. R. Soc. Lond.* A324, 301-313.
[14] G. Bao. *J. Mech. Phys. Solids* 50, 2237-2274, 2002.
[15] C.Q. Ru. *J. Mech. Phys. Solids* 49, 1265-1279, 2001.