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General coupling of porous flows and hyperelastic formulations—From thermodynamics principles to energy balance and compatible time schemes

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ABSTRACT

We formulate a general poromechanics model – within the framework of a two-phase mixture theory – compatible with large strains and without any simplification in the momentum expressions, in particular concerning the fluid flows. The only specific assumptions made are fluid incompressibility and isothermal conditions. Our formulation is based on fundamental physical principles – namely, essential conservation and thermodynamics laws – and we thus obtain a Clausius–Duhem inequality which is crucial for devising compatible constitutive laws. We then propose to model the solid behavior based on a generalized hyperelastic free energy potential – with additional viscous effects – which allows to represent a wide range of mechanical behaviors. The resulting formulation takes the form of a coupled system similar to a fluid–structure interaction problem written in an Arbitrary Lagrangian–Eulerian formalism, with additional volume-distributed interaction forces. We achieve another important objective by identifying the essential energy balance prevailing in the model, and this paves the way for further works on mathematical analyses, and time and space discretizations of the formulation.

1. Introduction

Poromechanics has been a very active subject of research for some decades – as shown e.g. in the survey [1] – originally mostly motivated by civil engineering applications, see [2,3], and well-established theories rigorously grounded in fundamental physical and thermodynamical principles are available [4–7]. Such approaches are frequently based on the so-called "mixture theory", a purely macroscopic framework in which the porous medium is considered to be made of a superposition of solid and fluid phases at each point – for a saturated medium to which we restrict our attention. We note in passing that the detailed microstructure can be considered in alternative approaches, e.g. with homogenization procedures applied to relate the microscopic and macroscopic behaviors [8,9], but we do not dwell on these approaches which are much more difficult to translate into effective computational modeling tools.

More recently, some novel applications have brought renewed modeling and computing challenges in the field, hence spurred further research to circumvent various limitations of the existing theories. In particular, potential challenging applications abound in biomechanics, for instance to model the blood perfusion of living (passive or active) tissues [10–12], the circulation of gases in the lungs [13–15], or the effect of wind on plants [16], to cite just a few noteworthy examples in this emerging context.

In this context, in [17] a poromechanics formulation was proposed with the primary motivation of describing perfusion in the cardiac muscle. As the heart typically undergoes strains of 10%–20%, the focus of this work was accordingly placed on the ability of the model to represent large displacements and finite strains, with general constitutive laws compatible with living tissue behavior [18,19]. In addition, special care was exercised to make the proposed formulation consistent with – partial or complete – incompressibility of the solid and fluid constituents. However, a significant – although quite widespread – simplification was made in this work by totally neglecting the fluid inertia. As the coronary arteries are known to be host to rapid blood flows with high variations during the cardiac cycle – peak flow velocity being typically of 10–20 cm s^{-1} [20], i.e. similar to peak solid velocity, albeit occurring at different, alternating, times – such a simplification is clearly quite drastic, and furthermore does not allow the formulation of discretization procedures which would preserve physical energy balances – with the kinetic energy as one of the major contributions.

The general principles of poromechanics formulations fulfilling fundamental conservation and thermodynamics laws have long

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been established, see in particular [4,21,22] and references therein. However, even in a rather general framework the development of effective formulations need also take into account the specificities and constraints of the category of applications considered, and for example in the above-cited pioneering works fluid inertia is rapidly discarded, and the issue of deriving general constitutive laws based on existing complex hyperelastic potentials is not addressed. By contrast, some other poromechanics formulations taking into account finite strains – and with or without fluid inertia – have already been proposed, see e.g. [23–25]. However, these formulations are mostly directly focused on constitutive assumptions – and indeed pertain to specific types of constitutive behaviors – rather than explicitly derived from the general setting of conservation and thermodynamics principles. Hence, it is difficult to see whether these essential principles are satisfied, and how more general constitutive behaviors can be adequately modeled within the proper corresponding physical framework, in particular as regards energy considerations.

The objective of the present work is thus twofold. We first aim at presenting a general poromechanics theory compatible with large strains and porous fluid flows without any simplification in the momentum expressions, based on fundamental physical principles – namely, essential conservation and thermodynamics laws. In this setting, arbitrary hyperelastic potentials can be used to represent the skeleton behavior, and the transition between compressible and incompressible behaviors – a key distinction in many existing poromechanics theories – is here unified in a seamless manner. This construction based on fundamental principles allows us to meet a second objective, namely, to identify the essential energy balance which must be satisfied in such formulations. This is crucial in order to allow further mathematical analyses and the derivation of consistently stable time and space discretization procedures. Our motivation is – indeed – strongly oriented towards computational modeling. As an example, we demonstrate the derivation of a compatible time scheme, as the first important step in the numerical simulation workflow. We note in passing that – when applied to cardiac perfusion – this formulation should allow to comparatively assess the impact of the simplifications made in earlier works.

We should mention that our approach is clearly inspired from the presentation of [5] – see also [26] and references therein – itself largely based on the pioneering theory of Biot [27,28], in particular as regards the concept of mixture considered in a thermodynamics setting and the Lagrangian formalism attached to the solid phase. In fact, we essentially follow the same major construction steps as in [5], and we herein summarize these steps both for completeness and in order to emphasize our specific distinctions and extensions. Namely, our main contributions thus lie in:

- the detailed generalization of this framework to nonlinear constitutive behaviors modeled by hyperelastic potentials and viscous effects – both in the solid and in the fluid – with a proposed systematic construction method for introducing these features based on general modeling ingredients already available from solid and fluid mechanics separately, and with a particular concern for incompressible or nearly-incompressible behaviors on both sides;
- the incorporation of fluid mass source terms in the formulation, these being motivated in particular by the modeling of muscle tissue in its interaction with various blood compartments providing input and output distributed coupling conditions [17];
- establishing the relation between the resulting coupled variational formulation, and so-called "Arbitrary Lagrangian–Eulerian" (ALE) formulations of fluid–structure interaction problems [29], which paves the way for further analyses and numerical considerations, as exemplified in a proposed time discretization scheme.

The outline of the paper is as follows. In Section 2 we introduce the notation and kinematical description, and we derive the mass conservation laws. We then establish in Section 3 the adequate principle of virtual work by invoking the conservation of momentum. In Section 4 we obtain the energy conservation law based on the first fundamental principle of thermodynamics, before proceeding to apply the second principle in Section 5, which – combined with the previous results – leads to a Clausius–Duhem inequality allowing to formulate consistent constitutive laws. Next, in Section 6 we summarize and further analyze the governing equations of the complete model – both in strong and weak forms – and we establish a fundamental energy balance. This leads us to providing an example of consistent time scheme in Section 7, before giving some concluding remarks in Section 8.

2. Notation, kinematical description and mass conservation

In this section we start by introducing the notation and kinematical description, and proceed to derive the mass conservation laws.

2.1. Classical definitions and kinematical relations

We consider a deformable solid which occupies at time t the space domain $\Omega(t)$ – denoted by Ω when there is no ambiguity – with boundary $\partial\Omega(t)$. The total Lagrangian formulation consists in describing the position history of each material point with respect to a reference configuration $(\Omega_0, \partial\Omega_0)$ – not necessarily equal to $(\Omega(0), \partial\Omega(0))$. Thus, the *deformation* is a one-to-one mapping $\underline{\varphi}$ from the reference configuration to the current configuration providing the position of each material point in time:

$$\underline{\varphi} : \begin{cases} \overline{\Omega}_0 \to \mathbb{R}^3 \\ \underline{\xi} \mapsto \underline{\mathrm{x}} = \underline{\varphi}(\underline{\xi}, t). \end{cases}$$

We denote by $\underline{y}$ the displacement field

$$\underline{y}(\underline{\xi}, t) = \underline{\mathrm{x}} - \underline{\xi} = \underline{\varphi}(\underline{\xi}, t) - \underline{\xi},$$

and $\underline{\underline{F}}$ is the deformation gradient

$$\underline{\underline{F}}(\underline{\xi}, t) = \underline{\underline{\nabla}}_{\underline{\xi}} \underline{\varphi} = \underline{\underline{\mathbb{1}}} + \underline{\underline{\nabla}}_{\underline{\xi}} \underline{y},$$

such that the deformed volume is given by $J d\Omega$ where $J = \det \underline{\underline{F}}$ and $d\Omega$ is the volume measure (here in the reference configuration), while the deformed area vector is given by $J\underline{\underline{F}}^{-T} \cdot \underline{dS}$. Furthermore, we introduce the right Cauchy–Green deformation tensor $\underline{\underline{C}} = \underline{\underline{F}}^T \cdot \underline{\underline{F}}$. We finally recall that the local changes of geometry are conveniently described by the Green–Lagrange strain tensor denoted by $\underline{\underline{e}}$ and defined by

$$\underline{\underline{e}} = \frac{1}{2}(\underline{\underline{C}} - \underline{\underline{\mathbb{1}}}) = \frac{1}{2}\left(\underline{\underline{\nabla}}_{\underline{\xi}} \underline{y} + (\underline{\underline{\nabla}}_{\underline{\xi}} \underline{y})^T + (\underline{\underline{\nabla}}_{\underline{\xi}} \underline{y})^T \cdot \underline{\underline{\nabla}}_{\underline{\xi}} \underline{y}\right),$$

with linearized expression $\underline{\underline{\varepsilon}}$ given by

$$\underline{\underline{\varepsilon}}(\underline{y}) = \frac{1}{2}\left(\underline{\underline{\nabla}}_{\underline{\xi}} \underline{y} + (\underline{\underline{\nabla}}_{\underline{\xi}} \underline{y})^T\right).$$

2.2. Mixture and material derivatives

Classical two-phase poromechanics is a mixture theory in which the material contains at each point a volume fraction ϕ of fluid phase, and a remaining fraction $(1 - \phi)$ of solid phase called the "skeleton". The fluid volume fraction ϕ is also referred to as the "porosity". Unless otherwise specified, we henceforth denote the quantities specifically associated with the fluid and the skeleton with "f" and "s" subscripts, respectively. As an exception, we will retain all the notation introduced in the above Section 2.1 to denote all kinematical quantities associated with the skeleton – without