Computers and Structures 182 (2017) 313–324

Contents lists available at ScienceDirect

Computers and Structures

journal homepage: www.elsevier.com/locate/compstruc

Effective and energy-preserving time discretization for a general nonlinear poromechanical formulation

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ARTICLE INFO

Article history:
Received 4 May 2016
Accepted 27 October 2016

ABSTRACT

We consider a general nonlinear poromechanical model, formulated based on fundamental thermodynamics principle, suitable for representing the coupling of rapid internal fluid flows with large deformations of the solid, and compatible with a wide class of constitutive behavior. The objective of the present work is to propose for this model a time discretization scheme of the partitioned type, to allow the use of existing time schemes – and possibly separate solvers – for each component of the model, i.e. for the fluid and the solid. To that purpose, we adapt and extend an earlier proposed approach devised for fluid-structure interaction in an Arbitrary Lagrangian-Eulerian framework. We then establish an energy estimate for the resulting time scheme, in a form that is consistent with the underlying energy principle in the poromechanical formulation, up to some numerical dissipation effects and some perturbations that we have carefully identified and assessed. In addition, we provide some numerical illustrations of our numerical strategy with test problems that present typical features of large strains and rapid fluid flows, and also a case of singular transition related to total drainage. An example of challenging application envisioned for this model and associated numerical coupling scheme concerns the perfusion of the heart.

1. Introduction

Recently, novel challenging applications such as cardiac modeling have required the introduction of general formulations coupling porous flows and hyperelastic formulations, and compatible with large displacements, finite strains and strong inertial effects both in the solid and in the fluid. In this context, a general poromechanics formulation was proposed in [10] based on fundamental thermodynamics principles, see also [41] where the same type of model was subsequently considered. As inertia effects and large displacements are considered, the final formulation is very similar to the coupling of hyperelastic dynamics for the skeleton – i.e., the solid constituent – with a conservative form of the so-called Arbitrary Lagrangian-Eulerian (ALE) formulation of the compressible Navier-Stokes equations [15,33] set on the same domain, hence, with a domain velocity given by the skeleton physical velocity. The compressible analogy comes from the product of the fluid volume fraction with the fluid density that, together, play the role of a varying fluid density. Finally, when compared with standard fluid-structure interaction (FSI) problems, we have the additional distributed coupling term representing the interaction between the two phases [6,13,14]. From this analogy, [10] introduced a time scheme with an energy balance at the time-discrete level inspired from the work [32] initially devoted to classical fluid-structure interaction problems. The proposed time scheme combined in a monolithic formulation a mid-point energy-conserving extension of the mid-point Newmark scheme and a second-order Crank-Nicolson scheme for the fluid with an additional specific treatment of the Darcy term discretization in order to respect the energy balance in the fluid-skeleton interaction. This scheme was proved in [10] to be second-order accurate and unconditionally stable, similarly to its initial fluid-structure counterpart in [32].

However, this scheme has some drawbacks when considering its practical use in simulation software – in industrial codes in particular – as it implies the use of a Newton-Raphson solution procedure on a monolithic fluid + solid formulation. Therefore, we propose in the present article an alternative time discretization inspired from state-of-the-art partitioned FSI time-schemes [18,19,27]. Partitioned solvers aim at solving the interaction problem by coupling independent solvers for the fluid and the solid [2,3,21,28,29,35]. Therefore, they are much more modular than monolithic approaches and allow the use of existing *legacy software* [30]. However, the computational efficiency of partitioned approaches compared with a monolithic approach must be assessed [4,8,27,28]. Hence, the question of monolithic versus partitioned approaches has already been raised in other specific poromechanics formulations, typically with Darcy flows [34].

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http://dx.doi.org/10.1016/j.compstruc.2016.10.022
0045-7949/

As we aim at relying on a classical Newmark scheme for the solid with an energy-conserving extension for general hyperelastic laws [22,25], we set out in this article to propose our time-scheme based on the recent partitioned FSI scheme of [1]. This scheme combines a Newmark scheme for the solid [22] with an effective Chorin-Temam projection scheme in the fluid [11,23,39]. The fluid viscous sub-step, taking into account the convective-viscous effects and the geometrical non-linearities, is treated explicitly. Moreover, at each time step the projection sub-step is implicitly coupled with the structure with Robin coupling conditions derived from Nitsche's interface method [7,36]. The specificity of this coupling strategy is twofold. First, it allows to prove stability independently of the added-mass effect typically present in blood flow simulations, which in particular is known to compromise the stability of explicit coupling – time-marching – schemes, see [8]. Note that this added-mass effect has also been evidenced in poroelastic models with an impact that directly correlates with fluid fraction [5]. Secondly, the coupling strategy of [1] is, to our best knowledge, the only time scheme that allows for non-linear conservative time-stepping within a 3D general solid, as opposed to the more direct Dirichlet-Neumann semi-implicit coupling [19]. From this starting point, we propose in the present article a partitioned scheme adapted to the poromechanics formulation of [10], with an adequate treatment of the additional fluid fraction variable, and a specific treatment of the distributed coupling conditions. The resulting scheme is proved to satisfy a discrete energy estimate, hence, to be unconditionally stable. Compared with [1] from which we draw the inspiration of our time scheme, our major contributions lie in

- extending this time scheme to our more complex case of a two-phase poromechanical problem;
- establishing the discrete energy estimate with the total free energy of the mixture, in a general *nonlinear* framework.

Furthermore, as our proposed method has the same algorithmic complexity as that of [1], we can similarly expect very significant gains in computational efficiency compared to a monolithic approach, as already assessed numerically in [19], in particular.

The paper is organized as follows. In Section 2, we recall the formulation of the general poromechanical model of [10] that we consider, with the associated energy balance. Next, in Section 3 we introduce our proposed partitioned time discretization scheme, and we provide a detailed stability analysis of this time scheme by establishing a discrete energy estimate. One ingredient of this analysis is an adapted form of the so-called "geometric conservation law" [16,17,38,40], which in our case is shown to be satisfied by construction, up to perturbations induced by spatial discretization that we analyze in details. In Section 4, we provide some implementation considerations, and several numerical illustrations for representative test problems proposed in the recent literature [9]. In addition, we present a test case in which we precisely monitor the energy balance and quantitatively assess the various sources of perturbations induced by spatial discretization. Finally, we give some concluding remarks in Section 5.

2. Poromechanical formulation

2.1. Basic definitions

We consider the general poromechanical model proposed in [10]. This is a two-phase mixture type model, in which a fluid phase and a solid phase are assumed to coexist and interact at each point, ϕ denoting the volume fraction of the fluid phase – also called the porosity.

The solid phase is primarily described by the displacement field $\underline{y}_s(\underline{\xi}, t)$ defined at every point $\underline{\xi}$ in the (fixed) reference domain Ω^0, and at any time t in the time window considered. We will use the corresponding velocity field

$$\underline{v}_s = \frac{\mathrm{d}\underline{y}_s}{\mathrm{d}t} = \partial_t \underline{y}_s(\underline{\xi}, t).$$

The displacement field maps the reference domain Ω^0 to the deformed domain Ω_t, viz.

$$\underline{\xi} \in \Omega^0 \mapsto \underline{\mathrm{x}} = \underline{\xi} + \underline{y}_s(\underline{\xi}, t),$$

and the associated deformation gradient tensor is

$$\underline{\underline{F}} = \underline{\underline{\mathbb{1}}} + \underline{\nabla}_{\underline{\xi}} \underline{y}_s,$$

with determinant $J = \det \underline{\underline{F}}$. We point out that J represents the local change of volume of the *global mixture*, whereas the change of volume of the solid phase itself is given by $J(1-\phi)/(1-\phi_0)$, with ϕ_0 the fluid volume fraction in the undeformed configuration, and we define $J_s = J(1-\phi)$. We recall the definitions of the right Cauchy-Green deformation tensor and of the Green-Lagrange strain tensor, i.e., respectively,

$$\underline{\underline{C}} = \underline{\underline{F}}^T \cdot \underline{\underline{F}}, \quad \underline{\underline{e}} = \frac{1}{2}(\underline{\underline{C}} - \underline{\underline{\mathbb{1}}}).$$

The mass per unit volume of the solid phase in the reference configuration is denoted by ρ_{s0}.

The internal fluid flow is represented by the velocity $\underline{v}_f$ and pressure p, both fields being naturally defined in the deformed domain Ω_t. The fluid is assumed to be incompressible, hence, the fluid mass per unit volume ρ_f is constant. The quantity m is defined as the added fluid mass per unit volume of the reference configuration, i.e.

$$m = \rho_f(J\phi - \phi_0).$$

The fluid is assumed to be Newtonian, with the usual decomposition of the fluid Cauchy stress tensor into viscous and hydrostatic contributions, i.e.

$$\underline{\underline{\sigma}}_f = \underline{\underline{\sigma}}_{\mathrm{vis}}(\underline{v}_f) - p\underline{\underline{\mathbb{1}}}.$$

Recalling the classical transformation rule from the Cauchy stress tensor to the second Piola-Kirchhoff stress tensor

$$\underline{\underline{\Sigma}} = J\underline{\underline{F}}^{-1} \cdot \underline{\underline{\sigma}} \cdot \underline{\underline{F}}^{-T},$$

here written for the global stress tensors of the mixture, we will denote by $\underline{\underline{\Sigma}}_s$ the contribution of the solid in the second Piola-Kirchhoff stress tensor $\underline{\underline{\Sigma}}$, i.e.

$$\underline{\underline{\Sigma}}_s = \underline{\underline{\Sigma}} - \phi J\underline{\underline{F}}^{-1} \cdot \underline{\underline{\sigma}}_f \cdot \underline{\underline{F}}^{-T} = \underline{\underline{\Sigma}} - \phi\underline{\underline{\Sigma}}_{\mathrm{vis}} + \phi p J\underline{\underline{C}}^{-1}, \tag{1}$$

with $\underline{\underline{\Sigma}}_{\mathrm{vis}} = J\underline{\underline{F}}^{-1} \cdot \underline{\underline{\sigma}}_{\mathrm{vis}} \cdot \underline{\underline{F}}^{-T}$, see Section 2.4 below for more detailed specifications of the constitutive laws.

2.2. Strong formulation

The strong form of the poromechanical model reads [10]

$$\begin{cases} \rho_{s0}(1-\phi_0)\frac{\mathrm{d}\underline{v}_s}{\mathrm{d}t} - \underline{\nabla}_{\underline{\xi}} \cdot (\underline{\underline{F}} \cdot \underline{\underline{\Sigma}}_s) + pJ\underline{\underline{F}}^{-T} \cdot \underline{\nabla}_{\underline{\xi}}\phi \\ \quad -J\phi^2 \underline{\underline{k}}_f^{-1} \cdot (\underline{v}_f - \underline{v}_s) = \rho_{s0}(1-\phi_0)\underline{f}, & \text{in } \Omega^0, \quad \text{(a)} \\ \frac{1}{J}\frac{\mathrm{d}}{\mathrm{d}t}(\rho_f J\phi\,\underline{v}_f) + \underline{\nabla}_{\underline{\mathrm{x}}} \cdot (\rho_f\phi\,\underline{v}_f \otimes \rho_f(\underline{v}_f - \underline{v}_s)) - \theta\underline{v}_f \\ \quad +\phi^2 \underline{\underline{k}}_f^{-1} \cdot (\underline{v}_f - \underline{v}_s) - \underline{\nabla}_{\underline{\mathrm{x}}} \cdot (\phi\underline{\underline{\sigma}}_{\mathrm{vis}}) + \phi\underline{\nabla}_{\underline{\mathrm{x}}} p = \rho_f\phi\underline{f}, & \text{in } \Omega_t, \quad \text{(b)} \\ \frac{1}{J}\frac{\mathrm{d}}{\mathrm{d}t}(J\rho_f\phi) + \underline{\nabla}_{\underline{\mathrm{x}}} \cdot (\rho_f\phi(\underline{v}_f - \underline{v}_s)) = \theta, & \text{in } \Omega_t \quad \text{(c)} \end{cases} \tag{2}$$