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Primal-mixed formulations for reaction–diffusion systems on deforming domains

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ABSTRACT

We propose a finite element formulation for a coupled elasticity–reaction–diffusion system written in a fully Lagrangian form and governing the spatio-temporal interaction of species inside an elastic, or hyper-elastic body. A primal weak formulation is the baseline model for the reaction–diffusion system written in the deformed domain, and a finite element method with piecewise linear approximations is employed for its spatial discretization. On the other hand, the strain is introduced as mixed variable in the equations of elastodynamics, which in turn acts as coupling field needed to update the diffusion tensor of the modified reaction–diffusion system written in a deformed domain. The discrete mechanical problem yields a mixed finite element scheme based on row-wise Raviart–Thomas elements for stresses, Brezzi–Douglas–Marini elements for displacements, and piecewise constant pressure approximations. The application of the present framework in the study of several coupled biological systems on deforming geometries in two and three spatial dimensions is discussed, and some illustrative examples are provided and extensively analyzed.

1. Introduction

Scope. We focus our attention in the numerical approximation of the chemical interaction between species concentrations and the response of the deformable medium where they react. Such a general framework is relevant to a wide range of applications going from molecular to macroscopic biological systems, and including, for instance, chemotaxis [52], organogenesis [41], bone remodelling [50,61], swelling of porous materials [38], cardiac electromechanics [31], tumor growth [10], force generation in skeletal muscle [15], wound healing [8], collagen network generation [34], tissue engineering [40], and many others.

The spatio-temporal dynamics of N species can be represented by a reaction–diffusion system of N equations, and the motion of the elastic (or hyper-elastic) medium in its general form, can be typically set in the framework of continuum mechanics, and thus be governed by the equations of elastodynamics. Much of the classical work in this particular field focuses in specific instances (such as radial growth or uniaxial contraction in simple domains) where it is possible to characterize the body motion without resolving the underlying solid mechanics and yielding reaction terms written directly in terms of growth rate (see e.g. [14] and the references therein). Nevertheless here we are interested in problems where the type of movement is not known a priori and therefore both the deformation and the deformation gradients are needed to describe the kinematics of the system: roughly speaking, the displacements/deformations are employed to update the

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position of the domain, and their gradients appear explicitly in the diffusive terms and are required in the formulation of reaction–diffusion systems written in a deformed medium.

Our primary goal is to introduce, implement, and apply a primal-mixed finite element formulation for the discretization of the coupled problem, where by *primal-mixed* we mean that the elasticity equations are set in a mixed form (that is, the associated formulation possesses a saddle-point structure involving additional unknowns) whereas the weak formulation of the reaction–diffusion sub-problem is written in terms of the primal variables only. From a discretization viewpoint, the clear advantages of a mixed formulation are that certain quantities of interest (such as strains or deformation gradients, which are needed in particular in the coupling strategy) can be immediately available with no need of further numerical differentiation, and that there exists more flexibility in the choice of finite element spaces. Moreover, mixed finite elements are the natural candidates for the discretization of the equations of incompressible elasticity, since the formal difficulties associated to infinite Lamé coefficients are absent. On the other hand, we are not particularly interested in recovering the species concentration fluxes and therefore we concentrate on primal formulations for the reaction–diffusion systems written in the deformed domain.

Related work. Traveling wave solutions for somewhat similar systems have been studied in [27]. A mechano-chemical cell aggregation model was developed in [57] under the assumption of infinitesimal strains of the medium, that allows to establish an equivalence relation between the reference and deformed domains, and that circumvents the difficulties associated to unknown body motion or nonlinear inter-configuration mappings. We also mention the finite element formulation for organogenesis based on a creeping flow description of the cartilage material presented in [42], and the discontinuous Galerkin approximation on moving grids and associated integration factor methods introduced in [62,12] to simulate limb pattern formation. Instead of using continuum-mechanics-based formulations, the elastodynamics can be alternatively represented with discrete models (as the mass-lattice model advanced in [58]). Models of cardiac electromechanics exhibit a remarkably similar structure, and several different formulations and solution techniques have been introduced in e.g. [13, 23,31,47]. Other related contributions include Eulerian formulations for wound healing [8], spherical tumor expansion [10], level-set and remeshed particle methods for surface and volume deformation [5,33,54], and many other approaches for different variants of growth in living tissues (see for instance, the recent review [32]). Nevertheless, none of these studies addresses primal-mixed methods in the spirit of the present basic idea.

Specific aims of this paper include:

- To introduce a mixed-primal formulation for a coupled Lagrangian elastodynamics–reaction–diffusion system where the mixed problem associated to the elasticity equations is written in terms of strains and deformations, and where the strain conveniently enters in the primal formulation of the reaction–diffusion system
- to develop a robust mixed finite element method suitable for the numerical study of a large class of coupled reaction–diffusion systems in elastic and hyperelastic domains
- to present separate formulations for linear and nonlinear mechanics
- to model the influence of reacting species into body deformation employing either a forcing term depending on the species concentration gradient, or an active strain decomposition.

Natural applications for the proposed framework are cardiac chemo- and electro-mechanical problems, however the present method is general enough to accommodate the study of many other related systems in biology and engineering.

Outline. We have arranged the contents of this paper in the following manner. Section 2 presents the derivation of the reaction–diffusion–elasticity equations, where the mechanics of the medium is specified in two cases: a linear and a nonlinear hyperelastic material law. We recall some properties of the split systems and we introduce two primal-mixed weak formulations associated to the original coupled problem. In Section 3 we formulate the spatio-temporal discrete set of equations to be solved, its linearization via a Newton method, and we specify the choice of time advancing strategy and finite element spaces. Some numerical examples are given in Section 4, including accuracy assessment and several applications related to cardiac chemo-mechanics. We close with some remarks and perspectives collected in Section 5.

2. Reaction–diffusion equations on a deformable domain

2.1. Kinematics, motion and deformation

Let $\Omega_0 \subset \mathbb{R}^d$, $d \in \{2, 3\}$ denote an elastic body with polyhedral boundary $\partial\Omega_0$, regarded in its undeformed reference configuration, and denote by $\boldsymbol{\nu}$ the outward unit normal vector on $\partial\Omega_0$. We assume a splitting of the boundary $\partial\Omega_0 = \overline{\Gamma_0^{\mathrm{D}}} \cup \overline{\Gamma_0^{\mathrm{N}}}$ into parts Γ_0^{D} and Γ_0^{N} where boundary loads and boundary tractions are imposed, respectively. A material point in Ω_0 is denoted by $\boldsymbol{x}$, whereas $\boldsymbol{u} : \Omega_0 \to \mathbb{R}^d$ denotes the deformation field that provides its position $\boldsymbol{x}_t$ within the body Ω_t in the current configuration, and $\hat{\boldsymbol{v}} = \partial_t \hat{\boldsymbol{u}}|_{\boldsymbol{x}}$ is the (referential) velocity. The tensor $\mathbf{F} := \nabla \boldsymbol{u}$ is the gradient (applied with respect to the fixed material coordinates) of the deformation map, and $\mathbf{E}(\boldsymbol{u}) = \frac{1}{2}[\mathbf{F}^{\mathrm{t}}\mathbf{F} - \mathbf{I}]$, $\boldsymbol{\varepsilon}(\boldsymbol{u}) := \frac{1}{2}[\mathbf{F} + \mathbf{F}^{\mathrm{t}}]$ denote the Green–Lagrange and the infinitesimal strain tensors, respectively. The symbols ∇_t, $\mathbf{div}_t$ will stand for the gradient and