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A displacement-based finite element formulation for incompressible and nearly-incompressible cardiac mechanics

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ABSTRACT

The Lagrange Multiplier (LM) and penalty methods are commonly used to enforce incompressibility and compressibility in models of cardiac mechanics. In this paper we show how both formulations may be equivalently thought of as a weakly penalized system derived from the statically condensed Perturbed Lagrangian formulation, which may be directly discretized maintaining the simplicity of penalty formulations with the convergence characteristics of LM techniques. A modified Shamanskii-Newton-Raphson scheme is introduced to enhance the nonlinear convergence of the weakly penalized system and, exploiting its equivalence, modifications are developed for the penalty form. Focusing on accuracy, we proceed to study the convergence behavior of these approaches using different interpolation schemes for both a simple test problem and more complex models of cardiac mechanics. Our results illustrate the well-known influence of locking phenomena on the penalty approach (particularly for lower order schemes) and its effect on accuracy for whole-cycle mechanics. Additionally, we verify that direct discretization of the weakly penalized form produces similar convergence behavior to mixed formulations while avoiding the use of an additional variable. Combining a simple structure which allows the solution of computationally challenging problems with good convergence characteristics, the weakly penalized form provides an accurate and efficient alternative to incompressibility and compressibility in cardiac mechanics. © 2014 The Authors. Published by Elsevier B.V. This is an open access article under the CC BY

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1. Introduction

The human heart is a remarkably complex organ, translating cellular ATP consumption into the systemic blood flow [1]. Over the last four decades, computational modeling of cardiac mechanics has evolved, incorporating biophysically-based hyperelastic strain energy laws [2–5], anisotropic tissue structure [6–8], patient-specific geometries [9] and cellular activation [10] to effectively simulate the myocardial behavior assuming basic Newtonian physics [11]. Based on tunable parameters [12,13], cardiac models provide a framework for studying and assessing heart function, offering spatiotemporally varying metrics– such as strain, stress, work and power– which are otherwise inaccessible clinically [14,15].

While cardiac modeling is capable of providing quantitative data of clinical relevance, a number of modeling questions remain actively pursued in the community. An issue commonly discussed in cardiac mechanics is the choice of modeling

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myocardial tissue as an incompressible [16,3,17,4,18,19,5,20,21] or nearly incompressible [14,22–24] material. While this choice is inherently based on tissue behavior which must be determined experimentally, both models continue to be used either to model incompressible/nearly incompressible behavior or, in some cases, for numerical convenience.

A range of relevant numerical schemes have been applied in heart models, one of the most popular being the penalty method [25,14,22,15,23]. An advantage of this approach is its simplified form, requiring only the solution of the tissue displacement. However, when applied in the finite element method (FEM) framework, displacement-based formulations near the incompressible limit exhibit locking leading to sub-optimal convergence rates and poor numerical approximations in classic elastic models [26–30]. Critically, the penalty method lacks monotonic convergence to the incompressible solution as the bulk modulus is increased, making it challenging to employ as an approximate model to an incompressible cardiac material model.

The development of numerical strategies circumventing these issues has been a field of significant research effort in the solid mechanics community. Among others, the B-Bar method introduced by Hughes [31] and its generalization to finite strains [32,33], the reduced or selective integration technique [34,30,35], the augmented Lagrangian method [36,37], have been successfully employed to enforce incompressibility while tackling the numerical difficulties and locking phenomena associated with the penalty formulation. An alternative approach used extensively in solid mechanics, also known to alleviate locking, is the class of multi-field variational principles, which gained popularity with the pioneering work of Herrmann on isotropic linear elasticity [38]. Herrmann's principle was also extended to orthotropic materials by Taylor [39] and Key [40], to nonlinear formulations [41,42] and elasto-plastic applications [43].

The most common of these mixed formulations is the Lagrange Multiplier (LM) method, a two-field variational approach which has been used widely to enforce incompressibility of the myocardium by introducing a variable to respresent the hydrostatic pressure [16,17,4,19,44]. While the LM method is known to improve numerical convergence [45,46,29,47] and avoid locking phenomena, the use of an additional variable results in increased computational cost and enhanced complexity in the linear algebra involved, due to the indefinite nature of the resulting stiffness matrix [26,45].

The Perturbed Lagrangian (PL) formulation was introduced to address this issue, by augmenting the energy functional of the LM approach with a penalty/compressibility term [48-50]. The PL is a two-field variational approach suitable for the solution of nearly incompressible problems, where pressure and displacement are treated as independent variables. Sussman and Bathe introduced a generalized form of the PL approach, the u/p formulation, which has been used extensively in the computational mechanics literature [51,52,48] and has also been applied in the myocardium [44]. Similarly, the well established three-field Hu-Washizu formulation by Simo et al. [33] extends the PL formulation by introducing pressure and dilatation as independent variables [37,46,51,53]. This approach has also been employed in cardiac mechanics [24] (though this procedure comes with the cost of computing an additional variable). The use of a separate interpolation for the independent variables, allows efficient and accurate approximations, alleviating the numerical difficulties associated with both the penalty and LM methods. The efficiency of these methods was also enhanced with the use of discontinuous interpolation for the pressure and dilatation fields (static condensation) [50,47,33,46] allowing the estimation of these fields on element level and leading to a generalized displacement-only formulation. Further, Bercovier [50] proved that, for Herrmann's principle, the PL (and its statically condensed equivalent) converges monotonically to the incompressible problem as the bulk modulus is increased. Nevertheless, as suggested by Sussman and Bathe [47], static condensation may exhibit convergence difficulties during the Newton–Raphson procedure.

In this paper, we consider the statically condensed Perturbed Lagrangian formulation of Bercovier [50] and others [48,49]. which may be conveniently thought of as a weakly penalized form with an optional choice of projection operator. In this generalized form, with an appropriate choice of the projection operator, we may choose to strengthen or weaken the constraint resulting in the PL, LM or penalty formulations. Using this generalization, we derive an estimate detailing the error convergence of these methods (in a linear setting) and introduce modifications to a Newton-Raphson scheme [54,55] to significantly improve nonlinear convergence properties for standard and weakly penalized formulations (particularly for high bulk modulus). The scheme is further augmented to take advantage of a Shamanskii-type Newton scheme [54,55] boosting computational performance by enabling re-use of the Jacobian matrix (and its inverses or preconditioners) estimated at previous time/loading steps. As this re-use is particularly sensitive to stiffness, we modify the scheme to effectively maintain nonlinear convergence behavior. Further, we examine the direct numerical discretization of the weakly penalized form which may be made efficient through the use of discontinuous projection operators. The weakly penalized form is then compared with the mixed variational formulations (LM, PL), as well as the penalty method, showing that the modified form maintains the convergence characteristics of the mixed variational forms and avoids locking behaviors observed in the penalty method. This comparison is performed on a model left ventricle, which to the best of our knowledge is the first application of this combination of the PL method and static condensation in cardiac mechanics. Further we verify the result proven for linear problems in [50], showing that the error between the weakly penalized formulation and the incompressible solution indeed decreases with a rate inversely proportional to the bulk modulus. As a result, the formulation enables modeling of the myocardium as nearly incompressible or incompressible (with an error proportional to 1/k, with k being the bulk modulus).

Below we expand on this approach to illustrate the general minimization problem (Section 2.1) and show how both penalty and LM formulations may be thought of equivalently as weakly penalized constraints in the continuous setting (Section 2.1.1). The basis for locking is then reviewed in Section 2.2, motivating the introduction of the weakly penalized approach. The different convergence behavior of the various schemes is also illustrated through their error estimates at

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