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An Eulerian projection method for quasi-static elastoplasticity

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ABSTRACT

A well-established numerical approach to solve the Navier–Stokes equations for incompressible fluids is Chorin's projection method [1], whereby the fluid velocity is explicitly updated, and then an elliptic problem for the pressure is solved, which is used to orthogonally project the velocity field to maintain the incompressibility constraint. In this paper, we develop a mathematical correspondence between Newtonian fluids in the incompressible limit and hypo-elastoplastic solids in the slow, quasi-static limit. Using this correspondence, we formulate a new fixed-grid, Eulerian numerical method for simulating quasi-static hypo-elastoplastic solids, whereby the stress is explicitly updated, and then an elliptic problem for the velocity is solved, which is used to orthogonally project the stress to maintain the quasi-staticity constraint. We develop a finite-difference implementation of the method and apply it to an elasto-viscoplastic model of a bulk metallic glass based on the shear transformation zone theory. We show that in a two-dimensional plane strain simple shear simulation, the method is in quantitative agreement with an explicit method. Like the fluid projection method, it is efficient and numerically robust, making it practical for a wide variety of applications. We also demonstrate that the method can be extended to simulate objects with evolving boundaries. We highlight a number of correspondences between incompressible fluid mechanics and quasi-static elastoplasticity, creating possibilities for translating other numerical methods between the two classes of physical problems.

1. Introduction

A wide variety of materials of scientific and technological importance exhibit elastoplastic behavior, such as metals [2,3], granular materials [4], aerogels [5], and amorphous solids such as bulk metallic glasses (BMGs) [6]. At low levels of stress these materials typically behave elastically, so that the deformation they undergo is reversible when the stress is removed. However, at higher levels of stress, the material will start to yield, and undergo plastic, irreversible deformation that will remain after the stress is removed. Describing elastoplastic[1] behavior within a consistent theoretical framework has been the subject of major research effort over many decades, particularly from the 1950's onward. As described in a recent review article [7], accurately characterizing elastoplastic behavior has proved challenging, since it is not obvious how to separate

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[1] Throughout this article, we use "elastoplastic" to refer to any material response that is a combination of reversible elastic deformation and irreversible plastic deformation. This includes, for example, rate-independent elastic–perfectly plastic models and rate-dependent elasto-viscoplastic models.

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the elastic and plastic response at the microscopic level. Several different frameworks have emerged, each of which is based on different assumptions of how the elastic and plastic behavior are combined.

Currently, perhaps the most widely used framework to study elastoplastic materials is hyper-elastoplasticity [8,9]. This model is based on introducing an initial undeformed reference configuration of a material. A time-dependent mapping is then employed, transforming the reference configuration into the deformed configuration at a later time. The deformation gradient tensor **F** is then defined as the Jacobian matrix of the mapping, and represents how an infinitesimal material element is transformed. A purely elastic material can then be described in terms of a constitutive law that gives stress as a function of **F**. To generalize this to elastoplastic behavior, the Kröner–Lee decomposition was developed, whereby the deformation gradient tensor is viewed as the product of elastic and plastic parts, $\mathbf{F} = \mathbf{F}_e \mathbf{F}_p$ [10,11]. This decomposition has been successfully used to model the elastoplastic behavior of a variety of materials such as metals and metallic glasses [12–14], and can be carried out in commercial solid mechanics software such as Abaqus. However, the decomposition has also been extensively debated within the literature. For materials that undergo very large plastic deformation and rearrangement, the notion of a mapping from an initial configuration may become problematic. The decomposition is non-unique, whereby the stress remains invariant under the transformation of the intermediate configuration $(\mathbf{F}_e, \mathbf{F}_p) \mapsto (\mathbf{F}_e \mathbf{R}^{\mathsf{T}}, \mathbf{R}\mathbf{F}_p)$ for an arbitrary rotation **R**. While $\mathbf{F}_e$ and $\mathbf{F}_p$ remain useful mathematical quantities, they may no longer retain their expected physical interpretations [7], which has led to recent efforts to clarify this from a micromechanical perspective, at least for crystalline solids [15].

An alternative framework is hypo-elastoplasticity, which is based on an additive decomposition of the Eulerian rate-of-deformation tensor into elastic and plastic parts, $\mathbf{D} = \mathbf{D}^{\text{el}} + \mathbf{D}^{\text{pl}}$ [16–18]. This approach has some drawbacks: it has mainly been applied to elastoplastic simulations involving only linear elastic deformation, since it is difficult to capture a nonlinear elastic strain response purely through $\mathbf{D}^{\text{el}}$. In particular, several researchers have noted some undesirable effects of the decomposition [19,20], such as leaving a residual stress after an elastic strain cycle [21]. Furthermore, because the framework is based on velocity as opposed to deformation, it can lead to the build-up of numerical errors during time-integration [22,23]. However, because it is based on Eulerian quantities, it does not depend on an undeformed configuration, which is a potential advantage for materials undergoing large strains. The aforementioned difficulties are typically minor in the limit of small elastic deformation, and hence it may provide a reasonable framework for many materials such as metals and metallic glasses that have large elastic constants.

Another feature of hypo-elastoplasticity is that it naturally fits within an Eulerian, fixed-grid framework, and there are several recent trends in numerical computation that make fixed-grid methods desirable. A fixed grid has simpler topology, making it easier and more efficient to program, and simpler to parallelize. Eulerian methods are also a natural environment in which fluid–structure interactions are accounted for, since fixed-grid frameworks are often the technique of choice for fluids [24,25]. Several approaches for dealing with nonlinear hyperelasticity have been proposed by treating the deformation gradient tensor as an Eulerian field [26–28] or by introducing a reference map field that describes the deformation from the initial undeformed state [29–32]. Other physical effects such as coupling to electrical fields [33] or the diffusion of temperature fit well within an Eulerian framework. Some manufacturing processes featuring continuous motion of material, such as extrusion [34], are also well-suited to the Eulerian viewpoint.

Starting from the additive decomposition of **D**, and coupling it with a continuum version of Newton's second law, one ends up with a closed system of partial differential equations for velocity, stress, and typically a set of additional internal variables. From this system a direct, explicit numerical scheme can be constructed. The scheme resolves elastic waves in the material, leading to a restriction on the numerical timestep due to the Courant–Friedrichs–Lewy (CFL) condition. For many materials of interest, such as metals, the elastic wave speed is on the order of kilometers per second, which makes it prohibitive to simulate processes on physically relevant time scales of seconds, hours, or days. Because of this, most applications of hypo-elastoplasticity have been interested in rapid processes such as impact [35], or have scaled the elastic constants to be artificially soft [36]. If one scales the hypo-elastoplasticity equations to examine the long timescale and small velocity limit, one finds that the continuum version of Newton's second law can be replaced with a constraint that the stresses remain in quasi-static equilibrium.

In this paper, we show that there is a strong mathematical connection between quasi-static hypo-elastoplasticity and the incompressible Navier–Stokes equations. For an incompressible fluid, the relevant variables are the velocity and pressure. There is an explicit update equation for velocity, and the incompressibility constraint requires that the velocity remain divergence-free. In this situation, a well-established method of solution is the projection method of Chorin [1], described in detail in Subsection 2.2, whereby the fluid velocity is explicitly updated, and then an elliptic problem for the pressure is solved, which is used to orthogonally project the velocity field to maintain the incompressibility constraint. By exploiting the mathematical correspondence, we have developed a new numerical method for quasi-static elastoplasticity that is analogous to the projection method for incompressible fluid dynamics. It takes an analogous approach, whereby the stress is explicitly updated, and then an elliptic problem for the velocity is solved, which is used to orthogonally project the stress to maintain the quasi-staticity constraint.

To the best of our knowledge, this mathematical correspondence has not been noted and explored in detail before, and the resultant numerical method based on a projection step to restore quasi-staticity is distinct from existing computational approaches. Some of the most well-established numerical methods make use of an updated Lagrangian formulation and a mesh that deforms with the material [37–39]. Ponthot [40] developed an implicit simulation approach for elastoplasticity, although it again makes use of a moving-mesh framework, leading to different mathematical considerations. A number of