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Mesh management methods in finite element simulations of orthodontic tooth movement

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ABSTRACT

In finite element simulations of orthodontic tooth movement, one of the challenges is to represent long term tooth movement. Large deformation of the periodontal ligament and large tooth displacement due to bone remodelling lead to large distortions of the finite element mesh when a Lagrangian formalism is used. We propose in this work to use an Arbitrary Lagrangian Eulerian (ALE) formalism to delay remeshing operations. A large tooth displacement is obtained including effect of remodelling without the need of remeshing steps but keeping a good-quality mesh. Very large deformations in soft tissues such as the periodontal ligament is obtained using a combination of the ALE formalism used continuously and a remeshing algorithm used when needed. This work demonstrates that the ALE formalism is a very efficient way to delay remeshing operations.

1. Introduction

The Finite Element (FE) Method is a numerical procedure to approximate problems modelled by partial differential equations using a discrete representation of the problem to be solved on a grid of nodes and elements. In mechanical models, it involves procedures to calculate in each element stresses and strains resulting from external factors such as forces and displacements. The FE method is extremely useful for estimating mechanical response of biomaterials and tissues that can hardly be measured in vivo. It has been used in dentistry-related problems since the 1970's, as reviewed in [1–3], with the interest of determining stresses in dental structures and materials used for clinical treatment and repair, and to improve the strength and response of these treatments, procedures and associated adaptive behaviour of the tissues. In particular, for orthodontic tooth movement problems, the FE method can deliver not only the global mechanical behaviour of the involved structures, i.e. the tooth mobility, but also it gives access to local stresses and strains of each tissue. That local behaviour is essential to couple mechanics and biology and to model the adaptive response of tissues.

One of the main principles of orthodontic treatment is to impose external loads to a tooth, leading to an altered mechanical environment in the periodontal ligament (PDL) surrounding the tooth and bone tissues supporting it. This altered environment induces remodelling and leads the tooth into a new position. The driving force of remodelling is the biological interaction between bone tissues and the PDL. Remodelling models in orthodontics FE analysis usually involve an update of the purely mechanical displacement of the tooth due to applied forces by a displacement due to the remodelling stimulus [4,5]. The stimulus for remodelling is either the strain energy density [6], based on the strain field [7–9], or based on the stress field [10]. However, other approaches can also be found: Soncini and Pietrabissa [11] or van Schepdael et al. [12] proposed remodelling models considering a viscous behaviour of the bone (viscoelastic Maxwell models); Cronau et al. [13] proposed a remodelling model considering a viscous behaviour of the PDL (viscoelastic Maxwell model) ; finally, Field et al. [14], Lin et al. [15], Mengoni and Ponthot[16] proposed remodelling laws involving an explicit local change of the bone elastic properties based on the strain level, similarly to remodelling algorithms used within the orthopaedic biomechanics literature.

In any case, due to remodelling and therefore softening of the bone tissue, or when the PDL deformations are physically modelled, large deformations are locally encountered during tooth movement. This leads to deformations of the finite element mesh up to a point where the mesh quality is no longer sufficient enough either to continue the computation, if elements happen to get highly distorted, or simply to blindly trust the solution quality. To overcome this problem, mesh management techniques such as the Arbitrary Lagrangian–Eulerian (ALE) formalism and a remeshing method are proposed in this work. The ALE formalism decouples, at each time step of the simulation, the mesh movement from the material displacement. The remeshing method authorises, at given predefined time step, a complete remesh the deformed geometry. The ALE method has been previously used in biomechanical problems, specifically in

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cardiovascular problems where fluid-structure interactions between blood flow and natural tissues [17–23] or devices [24–26] are modelled, or in deformation problems of soft organs such as breasts and lungs [27,28], or in car safety simulation such as airbag deployment [29]. However, to the best of the authors' knowledge, it has not been used with dentistry-related models. Remeshing methods are often used in bone remodelling models when remodelling algorithms involve the computation of a new geometry [5] rather than being embedded into the constitutive behaviour of the tissue. In the present study, the remodelling algorithm for orthodontic tooth movement [16] is embedded into the bone tissue behaviour allowing it to soften as biological activity occurs. The aim of this study was to assess the advantages and drawbacks of using the ALE method and remeshing procedures to model a tooth moving along a finite distance in the alveolar bone due to orthodontic forces. The simulations presented in this work were performed using the non-linear implicit FE code METAFOR (developed at the LTAS/MN^{2}L, University of Liège, Belgium - metafor.ltas.ulg.ac.be). All material models [16,30] and numerical methods such as ALE [31,32] and remeshing method [33] used in this work were previously implemented, verified, or validated, in this software in such a way that they are fully compatible. They are here used in the new context of long term orthodontic tooth movement. Similar simulations would have been difficult in traditional commercial software.

2. Methods

2.1. Theoretical background

The Arbitrary Lagrangian Eulerian (ALE) formalism [34] consists in decoupling the movement of the finite element mesh from the deformations of the underlying material. Compared to the classical Lagrangian formalism where the nodes follow the same material particles or to the Eulerian formalism where the nodes are fixed in space, the motion of the ALE computational grid can be arbitrarily chosen by the user of the FE code. ALE methods are very helpful in large deformation problems, such as the applications presented in this paper, when the quality of the finite elements deteriorates rapidly during the simulation. For these particular models, the quality of the ALE mesh is constantly optimised and costly remeshing operations are delayed, and sometimes completely avoided. Another kind of problems targeted by ALE methods is the simulation of complex material flows involving free boundaries which cannot be handled by the traditional Eulerian formalism with a fixed mesh [31].

The ALE equilibrium equations contain two sets of unknowns defined at each node [34]: the material velocity and the mesh velocity. This system of equations must be completed with additional relationships describing the motion of the mesh. However, in the case of highly nonlinear problems including large deformations and possibly contact between boundaries, writing these equations explicitly is very difficult. The common work around is to solve the two sets of equations sequentially with an operator split procedure. At each time-step, the nonlinear equilibrium equations are iteratively solved as in the Lagrangian case, i.e. with a mesh that follows the material. Once the equilibrium is reached, the nodes are then relocated using appropriate techniques [31] such as smoothing, projections or prescribed displacements. The solution fields (e.g. the stress tensor and the internal variables of the material) are eventually transferred from the old mesh configuration to the new one. Since the topology of both meshes is exactly the same (each element keeps the same neighbours during the redefinition of the new mesh) and the distance between two corresponding elements is usually small, very fast and efficient transfer algorithms based on projections and the Finite Volume Method can be employed [32,35,36].

When the deformation of the computational domain becomes so important that the quality of the mesh cannot be improved without modifying its topology, a new one has to be generated by a remeshing procedure. In METAFOR, this expensive operation consists in several steps. First the boundaries of the deformed domain are extracted and converted to smooth cubic splines which are remeshed one by one using a prescribed mesh density. Secondly the interior of the domain is remeshed thanks to a robust quadrangular mesher [37]. Then the solution fields are transferred from the old mesh to the new one. The transfer methods used in this work [33] are very similar to the former ones implemented in the ALE context. Nevertheless, they are much slower because the projection requires the determination of all the elements of the old mesh which intersects each element of the new mesh. In the ALE case, this expensive search can be restricted to the element itself and its direct neighbours. At last, when all the fields have been transferred, the time integration procedure is restarted with the new mesh using the ALE formalism until a new remeshing operation is required.

In the current state of the code, remeshing operations should be manually planned by the user. However, thanks to the ALE formalism which constantly improves the mesh quality despite of large deformations, the number of remeshing is expected to be much lower than in a purely Lagrangian approach.

2.2. Modelling of orthodontic tooth movement

Two types of simulations were developed to illustrate the need for mesh management methods in finite element models of orthodontic tooth movements. Both simulations are 2D plane-strain models.

The first simulation was an academic case, testing the capacity of a remodelling model combined with mesh management methods for tooth movement applications. A 2D single-rooted tooth was modelled with a root thickness of 7 mm at the alveolar margin and a root height of 16 mm, surrounded by alveolar bone (composed solely of trabecular tissue) 49-mm thick on each side of the tooth, and 40-mm high (see Fig. 1). This model corresponded to a simulation of a tooth moving along the alveolar arch, with no other teeth present. The size of the considered bone reduced boundary effects to which remodelling algorithms are very sensitive [38,39]. The tooth was considered as being a rigid tissue and the PDL was represented with a piecewise-linear interface model [16]. The bone was assumed to follow mechanical and remodelling constitutive models such as described in [16,30] with an initial uniform bone density of 1.3 gr/cc. These material and remodelling models assumed an anisotropic elastoplastic bone, submitted to remodelling in such a way that bone formation was observed at high strain energy density locations and bone resorption at low strain energy density locations. The coupling between the constitutive model and the remodelling model was expressed in a Continuum Damage Mechanics framework, with a remodelling criterion function of the strain energy density. Bone remodelling followed the concept of the mechanostat theory [40]: the bone density and orientation evolved according to the signed difference between the remodelling criterion and an homeostatic level of that value. All material and remodelling parameters are listed in Table 1. The remodelling rates are the only drivers of time in the remodelling algorithm and the all simulation. All time measures are thus described with respect to arbitrary time units, T. The bone was meshed with linear quadrangular elements using a structured mesh away from the tooth root in the regions delimited by the lateral rectangles *ABHG* and *EFLK* and using an unstructured mesh matching the root shape in its surrounding in the region delimited by the central rectangle *BEKH* (see Fig. 1) with a total of 1004 elements. This subdivision of the geometrical domain facilitated the mesh refinement in the area submitted to large strains around the apex of the tooth root. Boundary conditions were applied to represent the outcome of an orthodontic treatment at constant velocity. Boundary conditions representative of a end-of-treatment state, i.e. constant rate of displacement, were applied to the tooth. The tooth root was horizontally translated at a constant