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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 displacment 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.

Keywords: Orthodontic Tooth Movement, Arbitrary Lagrangian Eulerian formalism, Remeshing, Finite Element Method

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1 1. Introduction

The Finite Element (FE) Method is a numerical procedure to approx-2 imate problems modelled by partial differential equations using a discrete 3 representation of the problem to be solved on a grid of nodes and elements. 4 In mechanical models, it involves procedures to calculate in each element 5 stresses and strains resulting from external factors such as forces and dis-6 placements. The FE method is extremely useful for estimating mechanical 7 response of biomaterials and tissues that can hardly be measured in vivo. 8 It has been used in dentistry-related problems since the 1970's, as reviewed g in [1, 2, 3], with the interest of determining stresses in dental structures and 10 materials used for clinical treatment and repair, and to improve the strength 11 and response of these treatments, procedures and associated adaptive be-12 haviour of the tissues. In particular, for orthodontic tooth movement prob-13 lems, the FE method can deliver not only the global mechanical behaviour 14 of the involved structures, i.e. the tooth mobility, but also it gives access to 15 local stresses and strains of each tissue. That local behaviour is essential to 16 couple mechanics and biology and to model the adaptive response of tissues. 17 One of the main principles of orthodontic treatment is to impose external 18 loads to a tooth, leading to an altered mechanical environment in the peri-19 odontal ligament (PDL) surrounding the tooth and bone tissues supporting 20 it. This altered environment induces remodelling and leads the tooth into a 21 new position. The driving force of remodelling is the biological interaction 22 between bone tissues and the PDL. Remodelling models in orthodontics FE 23 analysis usually involve an update of the purely mechanical displacement of 24 the tooth due to applied forces by a displacement due to the remodelling 25

stimulus [4, 5]. The stimulus for remodelling is either the strain energy den-26 sity [6], based on the strain field [7, 8, 9], or based on the stress field [10]. 27 However, other approaches can also be found: Soncini and Pietrabissa [11] 28 or van Schepdael et al. [12] proposed remodelling models considering a vis-29 cous behaviour of the bone (viscoelastic Maxwell models); Cronau et al. [13] 30 proposed a remodelling model considering a viscous behaviour of the PDL 31 (viscoelastic Maxwell model); finally, Field et al. [14], Lin et al. [15], Men-32 goni and Ponthot [16] proposed remodelling laws involving an explicit local 33 change of the bone elastic properties based on the strain level, similarly to 34 remodelling algorithms used within the orthopaedic biomechanics literature. 35

In any case, due to remodelling and therefore softening of the bone tissue. 36 or when the PDL deformations are physically modelled, large deformations 37 are locally encountered during tooth movement. This leads to deformations 38 of the finite element mesh up to a point where the mesh quality is no longer 39 sufficient enough either to continue the computation, if elements happen 40 to get highly distorted, or simply to blindly trust the solution quality. To 41 overcome this problem, mesh management techniques such as the Arbitrary 42 Lagrangian-Eulerian (ALE) formalism and a remeshing method are proposed 43 in this work. The ALE formalism decouples, at each time step of the simu-44 lation, the mesh movement from the material displacement. The remeshing 45 method authorises, at given predefined time step, a complete remesh the de-46 formed geometry. The ALE method has been previously used in biomechan-47 ical problems, specifically in cardiovascular problems where fluid-structure 48 interactions between blood flow and natural tissues [17, 18, 19, 20, 21, 22, 23] 49 or devices [24, 25, 26] are modelled, or in deformation problems of soft or-50

gans such as breasts and lungs [27, 28], or in car safety simulation such as 51 airbag deployment [29]. However, to the best of the authors' knowledge, it 52 has not been used with dentistry-related models. Remeshing methods are 53 often used in bone remodelling models when remodelling algorithms involve 54 the computation of a new geometry [5] rather than being embedded into the 55 constitutive behaviour of the tissue. In the present study, the remodelling 56 algorithm for orthodontic tooth movement [16] is embedded into the bone 57 tissue behaviour allowing it to soften as biological activity occurs. The aim 58 of this study was to assess the advantages and drawbacks of using the ALE 59 method and remeshing procedures to model a tooth moving along a finite 60 distance in the alveolar bone due to orthodontic forces. The simulations 61 presented in this work were performed using the non-linear implicit FE code 62 METAFOR (developed at the LTAS/MN²L, University of Liège, Belgium -63 metafor.ltas.ulg.ac.be). All material models [16, 30] and numerical methods 64 such as ALE [31, 32] and remeshing method [33] used in this work were previ-65 ously implemented, verified, or validated, in this software in such a way that 66 they are fully compatible. They are here used in the new context of long term 67 orthodontic tooth movement. Similar simulations would have been difficult 68 in traditional commercial software. 69

70 2. Methods

71 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 formal-

ism where the nodes follow the same material particles or to the Eulerian 75 formalism where the nodes are fixed in space, the motion of the ALE com-76 putational grid can be arbitrarily chosen by the user of the FE code. ALE 77 methods are very helpful in large deformation problems, such as the ap-78 plications presented in this paper, when the quality of the finite elements 79 deteriorates rapidly during the simulation. For these particular models, the 80 quality of the ALE mesh is constantly optimised and costly remeshing op-81 erations are delayed, and sometimes completely avoided. Another kind of 82 problems targeted by ALE methods is the simulation of complex material 83 flows involving free boundaries which cannot be handled by the traditional 84 Eulerian formalism with a fixed mesh [31]. 85

The ALE equilibrium equations contain two sets of unknowns defined at 86 each node [34]: the material velocity and the mesh velocity. This system 87 of equations must be completed with additional relationships describing the 88 motion of the mesh. However, in the case of highly nonlinear problems in-89 cluding large deformations and possibly contact between boundaries, writing 90 these equations explicitly is very difficult. The common workaround is to 91 solve the two sets of equations sequentially with an operator split procedure. 92 At each time-step, the nonlinear equilibrium equations are iteratively solved 93 as in the Lagrangian case, i.e. with a mesh that follows the material. Once 94 the equilibrium is reached, the nodes are then relocated using appropriate 95 techniques [31] such as smoothing, projections or prescribed displacements. 96 The solution fields (e.g. the stress tensor and the internal variables of the 97 material) are eventually transferred from the old mesh configuration to the 98 new one. Since the topology of both meshes is exactly the same (each ele-99

ment 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 impor-104 tant that the quality of the mesh cannot be improved without modifying 105 its topology, a new one has to be generated by a remeshing procedure. In 106 METAFOR, this expensive operation consists in several steps. First the 10 boundaries of the deformed domain are extracted and converted to smooth 108 cubic splines which are remeshed one by one using a prescribed mesh density. 109 Secondly the interior of the domain is remeshed thanks to a robust quadran-110 gular mesher [37]. Then the solution fields are transferred from the old mesh 11 to the new one. The transfer methods used in this work [33] are very similar 112 to the former ones implemented in the ALE context. Nevertheless, they are 113 much slower because the projection requires the determination of all the ele-114 ments of the old mesh which intersects each element of the new mesh. In the 115 ALE case, this expensive search can be restricted to the element itself and 116 its direct neighbours. At last, when all the fields have been transferred, the 117 time integration procedure is restarted with the new mesh using the ALE 118 formalism until a new remeshing operation is required. 119

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.

¹²⁵ 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 re-129 modelling model combined with mesh management methods for tooth move-130 ment applications. A 2D single-rooted tooth was modelled with a root thick-131 ness of 7 mm at the alveolar margin and a root height of 16 mm, surrounded 132 by alveolar bone (composed solely of trabecular tissue) 49-mm thick on each 133 side of the tooth, and 40-mm high (see Figure 1). This model corresponded 134 to a simulation of a tooth moving along the alveolar arch, with no other teeth 135 present. The size of the considered bone reduced boundary effects to which 136 remodelling algorithms are very sensitive [38, 39]. The tooth was considered 13 as being a rigid tissue and the PDL was represented with a piecewise-linear 138 interface model [16]. The bone was assumed to follow mechanical and remod-139 elling constitutive models such as described in [16, 30] with an initial uniform 140 bone density of 1.3 gr/cc. These material and remodelling models assumed 141 an anisotropic elastoplastic bone, submitted to remodelling in such a way 142 that bone formation was observed at high strain energy density locations 143 and bone resorption at low strain energy density locations. The coupling 144 between the constitutive model and the remodelling model was expressed 145 in a Continuum Damage Mechanics framework, with a remodelling criterion 146 function of the strain energy density. Bone remodelling followed the concept 14 of the mechanostat theory [40]: the bone density and orientation evolved 148 according to the signed difference between the remodelling criterion and an 149

homeostatic level of that value. All material and remodelling parameters 150 are listed in Table 1. The remodelling rates are the only drivers of time in 15 the remodelling algorithm and the all simulation. All time measures are thus 152 described with respect to arbitrary time units, T. The bone was meshed with 153 linear quadrangular elements using a structured mesh away from the tooth 154 root in the regions delimited by the lateral rectangles ABHG and EFLK15 and using an unstructured mesh matching the root shape in its surround-156 ing in the region delimited by the central rectangle BEKH (see Figure 1) 157 with a total of 1004 elements. This subdivision of the geometrical domain 158 facilitated the mesh refinement in the area submitted to large strains around 150 the apex of the tooth root. Boundary conditions were applied to represent 160 the outcome of an orthodontic treatment at constant velocity. Boundary 161 conditions representative of a end-of-treatment state, i.e. constant rate of 162 displacement, were applied to the tooth. The tooth root was horizontally 163 translated at a constant velocity to achieve a displacement of 1.5 times its 164 width over 365 units of time. Rigid boundary conditions were applied to the 165 bone basal line while it was restrained vertically on its top line and horizon-166 tally on its vertical extremities (see Figure 1). The ALE mesh movement was 167 specified following the tooth kinematics to keep a good mesh quality along 168 the displacement. The unstructured central mesh was moved with the same 169 velocity as the tooth, imposing that the displacement of nodes B, H, and I170 was identical to that of node C in contact with the tooth root. In the same 17: way, the displacement of nodes E, J, and K was identical to that of node D. 172 The mesh nodes along the root surface (green curve in Figure 1) were relo-173 cated using spline curves [31]. Finally, the nodes of lines BC, DE, EK, KJ, 174

	01	01		(0		/ []			
homeostatic	remodelling rate		remodelling rate		te wi	width of		degree of	
stimulus	in resorption		in formation		laz	lazy zone		anisotropy	
(MPa)	$(\mu~{\rm m}/({\rm MPa~T}))$		$(\mu~{\rm m}/({\rm MPa~T}))$)) (1) (MPa)		(-)	
0	10			5		0.1		1	
Elastoplastic parameters									
Material		Young	's	Poisson's	Yield	Harden	ing A	pparent	
		modulu	ıs	ratio	stress	parame	eter	density	
		(GPa))	(-)	(MPa)	(MPa	ı)	(gr/cc)	
Bone		13.75		0.3	200.0	723.7	7	1.3	
Tooth (model	2 only)	19		0.3	-	-		2.7	
PDL		piecewise li	inear	0.49	-	-		0.1	
(table 2, Figure 2)									

Table 1: Material and Remodelling parameters of tissues Bone remodelling parameters (model 1 only) [16]

JI, IH, and HB were repositioned so that the lines remained straight during the material displacement. All the other inner nodes of the central region were repositioned using Giuliani's smoothing method [41], which is based on an iterative optimisation of the shape of neighbouring elements. The two structured regions (sections ABHG and EFLK) were meshed using a transfinite mesher. After relocation of the nodes, the different internal fields were transferred onto the new mesh with a first order Godunov scheme [36, 32].

The second, more realistic, simulation consisted in a 2D lower incisor submitted to loading representative of clinical treatment. A mandible geometry was obtained from the INRIA/GAMMA repository [52], constructed from a

	Engineering Strain	Tangential Modulus			
	[-]	[MPa]			
Compression	0.0	0.068 (i.e. Young's modulus)			
	0.0 ightarrow -0.25	linear variation up to 0.68			
	$-0.25 \rightarrow -0.31$	linear variation up to 8.5			
	$-0.31 \rightarrow -0.82$	constant value of 8.5			
	< -0.82	13.5			
Traction	0.0	0.068 (i.e. Young's modulus)			
	$0.0 \rightarrow 0.14$	linear variation up to 1.35			
	$0.14 \rightarrow 0.63$	constant value of 8.5			
	> 0.63	0.01			

Table 2: Values of the mechanical model for the periodontal ligament

surface reconstruction of the mandibular bone and its teeth. The 2D outline 185 in the mesiodistal plane of the left central incisor was extracted. The PDL 186 was created at the interface between the bone and the tooth assuming a con-187 stant thickness of 0.2 mm (see Figure 3). The three surfaces (PDL, tooth, 188 and alveolar bone) were meshed with linear quadrangular elements. The 189 resulting unstructured mesh was composed of 1000 elements for the PDL, 190 1820 for the alveolar bone, and 2294 for the tooth. The tooth and bone were 191 modelled with a linear elastic constitutive law. The PDL was represented 192 with a piecewise-linear elastic material (see Table 2, Figure 2). Only the 193 initial tooth displacement was modelled and no remodelling algorithm was 194 used. All material parameters are listed in Table 1. Boundary conditions 195 were applied to represent the outcome of a constant-force orthodontic treat-196

ment. The bone was clamped on its basal line (see Figure 3, red curve). A 19 pressure representative of a total 1.2 N force was gradually applied on the 198 labial side of the tooth crown (see Figure 3). The force used in this model 199 can be classified as a high orthodontic force. The PDL was thus submitted to 200 large strains and the numerical convergence could not be ensured with a clas-20 sical Lagrangian approach due to excessive mesh distortion. Therefore, two 202 mesh management techniques were used: the Arbitrary Lagrangian-Eulerian 203 (ALE) method and a remeshing technique. The ALE method was applied at 204 each time increment of the simulation while remeshing was applied at four 20 load levels of 0.65 N, 0.85 N, 0.95 N and 1.05 N. Those loads were determined 206 in a pre-analysis as the values for which the ALE formalism could not man-207 age the large deformations. In the case of the PDL, a spline rezoner [31] was 208 used for the two free boundaries delimiting the surface of the PDL (purple 209 lines in Figure 3). It permitted to relocate the nodes of the PDL boundary 210 with a cubic spline. Guiliani's iterative smoothing method was subsequently 211 used on the inner nodes of the mesh, homogenizing the elements area [41]. 212 After repositioning of the nodes, the different internal fields were transferred 213 onto the new mesh using a first order Godunov scheme [36, 32]. When the 214 ALE rezoning was not sufficient to keep a good mesh quality, a full remeshing 215 of the deformed geometry was considered. In this case, cubic splines were 216 built on the outline of the deformed geometry which was fully remeshed [53]. 21 Solution fields were transferred from the old mesh to the new mesh using a 218 projection technique [33]. 219

220 3. Results

The benefit of the ALE method in the first model was analysed comparing 221 the remodelling criteria values at 50% of the maximal displacement, i.e. 5.25 222 mm (see Figure 4) with and without ALE. At that level of displacement, 223 both methods showed the same results in the regions where the mesh is of 224 good quality. However, the classical Lagrangian method produced a distorted 225 mesh around the tooth apex to a point where the local numerical solution 226 could not be trusted any more, with a remodelling criterion reaching high 227 values around the tooth apex. Displacement higher than 5.4 mm could not be 228 computed with a Lagrangian mesh due to negative jacobians while the ALE 229 mesh allowed the full tooth displacement to be computed. The force needed 230 for the ALE model (Figure 5 plain line) is the same as the one needed for 231 the Lagrangian model (Figure 5 dash-dot line) where the Lagrangian mesh 232 is of good quality (for the first 2.6 mm of translation). The Lagrangian force 233 however deviates from the ALE one when the mesh becomes too distorted. 234 The remodelling constitutive model facilitated the tooth movement, requiring 235 a force about 40% lower than the force needed to displace the tooth of the 236 same length if no biological remodelling were present (Figure 5). The ALE 23 mesh kinematics is depicted in Figure 6 were the remodelling criterion is 238 plotted at three different time points of the simulation. The unstructured 239 mesh around the tooth in the rectangle BEKH of Figure 1 followed the 240 tooth movement. The structured mesh of the upstream rectangle ABHG24 expanded as the tooth moved away from the fixed left boundary while the 242 structured mesh of the downstream rectangle EFLK shrunk. 243

244

The forces applied on the second model led to large strains around the

tooth collar. The soft PDL thus deformed up to a point where the mesh 245 quality can not be trusted any more (see Figure 7(b)). A better represen-246 tation of the large strains at the alveolar margin without excessive mesh 247 distortion was allowed by the ALE method (see initial and deformed meshes, 248 with and without ALE in Figure 7(a-d)). A tipping force of 0.65 N was 249 applied while keeping a good mesh quality but a higher force could not be 250 used, with elements too distorted for a higher force, whatever the ALE node 25 relocation algorithm used (Figure 7(e), red element). Indeed in the cervical 252 area, because of the almost incompressible behaviour of the ligament, the free 253 boundaries created convex and concave menisci so that inversion of the finite 254 elements occured. The first load step defined for remeshing was when the 255 applied load reached 0.65 N. The resulting new mesh (Figure 8(b)) allowed 256 the computation to continue further (still applying the ALE method at each 25 time step) up to a 0.85 N force. At a higher force level the mesh became once 258 more too distorted on the tension side (Figure 8(c)). New remeshing instants 259 were defined similarly at 0.85 N, 0.95 N, and 1.05 N. This fourth and final 260 mesh was used for forces up to 1.2 N. This remeshing technique could be used 26 further, every time defining new time steps at which remeshing takes place. 262 The displacement of the tooth tip was identical for all three models (purely 263 Lagrangian, ALE, ALE with remeshing) as long as the model converged (see 264 Figure 9). 265

266 4. Discussion

This work proposes an assessment of computational tools such as the Arbitrary Lagrangian Eulerian formalism and remeshing in the development of orthodontics tooth movement predictive models. Although this work focuses on the computational methods and the presented models are not validated against experimental and clinical data, it demonstrates the advantages and drawbacks of these methods for soft tissues modelling and remodelling models.

The first model shows that the ALE formalism makes it possible to reach 274 a large displacement of a tooth within a mandible including the effect of 275 bone remodelling without any remeshing steps. While the model is not rep-276 resentative of an actual tooth movement, it emphasizes the need to keep a 27 good-quality mesh where remodelling is observed so that the bone formation 278 or resorption is not artifically modified by numerical errors due to exces-279 sive mesh distortion. It should be emphasized that the aim of the proposed 280 model is not clinically-driven. While the loading conditions have been cho-28 sen to represent average constant rate of displacement achieved in the third 282 phase of orthodontic treatments [54, 55], the reproduced movement is not 283 a model of an actual treatment. In particular, no physiological homeostatic 284 loads are present, and the constant velocity condition is assumed to be the 285 result of using orthodontic devices which are not modelled. It is unlikely 286 that a constant rate of displacement would be achieved over such a distance 28 without the need to adapt the device used. 288

The second model underlines the possibility of reaching very large deformations in soft tissues models. The combination of the ALE formalism used continuously throughout the simulation with a remeshing algorithm used when needed facilitates the development of a reliable model of the menisci creation at the free boundaries of thin soft tissues. Analysing the evolution

of the mesh in the periodontal ligament however shows that the number of 294 elements describing those boundaries has to decrease with increasing applied 29 load. The creation of the menisci due to the deformation needs an initial fine 296 mesh. Once the menisci are formed, building a fine mesh without creating 29 badly shaped elements at the extremities is very hard. At the tension side, 298 the angle between the concave meniscus and the tooth boundary increases 299 as the force increases, and become obtuse. At the compression side however, 300 the angle between the convex meniscus and the bone boundary decreases, 301 with a tendency to deform the quadrangles into triangles. Therefore, the 302 description of the geometry of the free boundary is less and less accurate in 303 order to be able to mesh it properly. Using the combination of ALE and 304 remeshing methods in this case allows the simulation to reach force levels 305 that are representative of orthodontic treatment force levels. This is a major 306 improvement with respect to a purely Lagrangian approach that can only 30 reach a force a quarter of the final value achieved here. 308

3D models of a set of adjacent teeth submitted to loading through or-309 thodontic devices would however better represent an actual clincal outcome. 310 Such models have already shown to perform well in initial tooth movement 311 predictions and in long-term prediction when the remodelling algorithm in-312 volves full remeshing of a new geometry at each time step. In the case of 313 remodelling algorithm such as used in this work, the presented applications 314 demonstrate that the ALE formalism is a very efficient way to delay remesh-315 ing operations. The later are usually very expensive in terms of CPU time 316 and user work time, even for 2D problems. In a 3D context, remeshing be-317 comes a major issue and we think that it could be partially solved by the 318

ALE methods, which are already fully functional in 3D. Applications in 3D will be thus addressed in a near future.

This computational work presents a promising approach to model large tooth displacements in orthodontic treatment. This approach is not limited to orthodontic treatment and can be used in combination with any remodelling algorithm fully embedded within the constitutive law and not needing full computation of a new geometry.

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Figure 1: Academic case: geometry, mesh, and ALE mesh management: the nodes on the green curve are relocated using spline curves, the blue points have an horizontal displacement which is set equal to the one of the red points, the blue lines are remeshed (with a constant number of elements) as if they remained straight between their extremities.



Figure 2: Periodontal Ligament - experimental data [42, 43, 44, 45, 46, 47, 48, 49] : Engineering Strain vs. Engineering Stress for uniaxial tests. The data is labelled after the name of first author of the paper it comes from, followed by the year of publication and the number of the figure in the paper (a letter is added if several curves appear on the same figure). As a comparison, in blue and red dashed line, two multi-linear models [1, 50, 51] that surround this experimental data. In black dashed line, the model used in this work.



Figure 3: 2D geometry in the mesiodistal plane of the left central incisor.



Figure 4: Comparison of the ALE and Lagrangian methods after 180 time units. Top panel: ALE mesh, bottom panel: Lagrangian mesh.



Figure 5: Force vs. time and corresponding displacements for the imposed velocity.



Figure 6: ALE mesh movement: the mesh follows the movement of the tooth.



Figure 7: Zoom on the mesh evolution of the periodontal ligament at the alveolar margin. In red, the problematic elements.



Figure 8: Zoom on the mesh of the periodontal ligament at the alveolar margin. In red, distorted elements (remeshing was required at those load values). In blue, node in contact with the base of the tooth crown.



Figure 9: Force vs. tooth tip buccal displacement.