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Application of Mathematical Models to Create Simulations in Dental Medicine

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ABSTRACT

The application of virtual reality in dentistry has led to significant advancements. This is achieved using simulation software combined with mathematical modelling. The primary goal is to accurately represent the biophysical properties of tissues, enabling the simulation of medical interventions such as laser treatments, mechanical impacts, chemical applications, and other procedures.

Tissues are defined by their specific optical, mechanical, biological, and chemical properties. For virtual environment modelling, optical and mechanical properties are of paramount importance. Optical properties form the basis for techniques like therapeutic ablation, selective photothermolysis, and the minimization of adverse effects on healthy tissue. Key phenomena related to optical properties include absorption, scattering, thermal conversion, thermal diffusion, and heat retention. The main mechanical properties of tissue include hardness, durability, and elasticity.

Virtual reality is essential for both medical staff training and predicting the outcomes of complex procedures.

Keywords: mathematical models, dental medicine.

INTRODUCTION

Simulations in medicine are fundamental for personalizing patient care, optimizing clinical outcomes, and enhancing medical personnel training. They utilize various mathematical tools and methodological approaches to replicate realistic conditions encountered by clinical staff. In dentistry, simulations play a critical role, as aesthetic considerations are also important alongside proper treatment. The simulation environment offers a safe and repeatable workspace for real-time assessment of manipulations and the application of advanced techniques to develop new dental methods. Virtual reality provides a fully immersive simulation framework, while augmented reality combines simulation software with physical simulators. Understanding the anatomical and physiological characteristics of the selected area is crucial for comprehending the properties of maxillofacial structures.

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The important anatomical structures include the oral cavity (cavitas oris), lips (labia oris), cheeks (buccae), gums (gingivae), teeth (dentes), hard palate (palatum durum), soft palate (palatum molle), and tongue (lingua), with emphasis on examining the gums and teeth. Each structure possesses distinct biomechanical properties, and certain properties become more relevant depending on the tissue type. Gums are a type of soft tissue, specifically mucous bands (mucosa gingivalis), partially attached to the alveolar processes of the jaws and richly supplied with blood and nerves. Their key biomechanical properties are elasticity, resistance to compression, and grip strength for the alveolar regions and tooth surfaces. Together with the periodontal ligament, which distributes forces to the bone, they function as elements with spring-like properties. Two key structures are formed: the gingival groove (sulcus gingivalis) between the gingival margin (margo gingivalis) and collum dentist, and the interdental papilla (papilla interdentalis), representing a gingival margin between adjacent teeth. It's important to note that during primary tooth eruption, the crown's pressure induces resorption of connective tissue under the gum epithelium, allowing the tooth to emerge without forming a wound. During the eruption of milk teeth, enamel and dentin formation begins in the permanent teeth. A tooth comprises three parts: the crown (corona dentis), cervical region (collum dentis), and root (radix dentis). The tooth crown is the visible part outside the gum, varying in size and shape. The tooth's cervical region is covered by the mucous membrane of the gum, a transitional area subjected to high compressive forces. The tooth root is in the jaw's alveolus. Inside the tooth is a cavity filled with dental pulp, a soft tissue not considered in mathematical models because it doesn't significantly contribute to the biomechanical characteristics of structures in the cavitas oris. The crown's outer surface has a thin layer of unmineralized organic matter. The surface of the crown consists of enamel, composed of enamel prisms (prismata enameli) and interprismatic enamel, incorporating fluorine into the mineral substance hydroxyapatite. It exhibits high durability, wear resistance, and low elasticity-brittleness. The tooth root is covered with cementum, which has a structure like bone tissue [1, 2].

BIOLOGICAL TISSUE MODELING METHODS

The tooth surface is characterized by morphological and functional variations, expressed through occlusion, determining the mechanical impact during tooth interaction, relative positioning, temporomandibular articulation, distribution of pressure on the alveolar bone and temporomandibular joint, and other factors. The anatomical structure of the selected tooth, along with occlusion, is crucial when creating models in virtual reality. Consequently, the jaw is divided into volumetric elements called voxels. A voxel is a unit of volume in three-dimensional imaging, commonly used in cone-beam computed tomography in dental medicine, to achieve optimal and realistic recreation of anatomical structures. The size of an individual voxel depends on the medical equipment used [3]. To ensure maximum correspondence with the real anatomical structure, medical image processing is performed through segmentation analysis, which identifies areas or segments of the structure with similar properties. Segmentation analysis employs various approaches to delineate individual regions, including the Segment Anything Model, Transformer-Based Methods, Diffusion-Based Methods, Convolutional Network-Based Methods, and CNN-Transformer Hybrids.

The primary methods for modelling biological tissues involve physical and descriptive models. Physical models account for the intrinsic physical properties of the object and use fundamental physical laws to create highly accurate models. In tissue modelling, Young's modulus and Poisson's ratio are commonly used to define physical models. For larger deformations, nonlinear constitutive relations are used to represent the material response.

Descriptive models utilize parametric equations that approximate reality without requiring high accuracy and can incorporate statistical data, making them more adaptable to different scenarios, including situations with limited data. In simulation software, descriptive models are often embedded in mesh structures, which are flexible for modelling according to set rules and have lower computational complexity.

Physical models are preferred for precise manipulation evaluation. However, due to their greater computational complexity, hybrid combinations of both methods are frequently employed.

Unity is a suitable environment for tissue visualization, offering a platform for developing interactive 2D or 3D models using tools and methods to create simulations in virtual and augmented reality. The resulting projects are compatible with a wide range of VR and AR devices. Unity provides various options for manipulating objects and observing their deformation, including Soft Body Physics, Rigid Body Physics, Particle-Based Physics, Mesh Deformation, Spring Chains, Blender (for tissues in a static state or with slight deformation), Shader, and others. The appropriate method depends on the execution device's capabilities, the model's required accuracy, and its complexity, with the aim of maximizing realistic feel and compatibility with chosen simulation methods, expressed as deformation functions [6].

The general algorithm for mechanically simulating biological tissues in a virtual environment involves tissue simulation, determining processing locations, and topological deformation, which defines the distribution of consistent elements, their number, and connection method. These steps involve various sub-processes depending on the modelling approach. This article discusses three approaches: geometric, finite element method (FEM), and mass-spring model (MSM).

FUNDAMENTAL PHYSICAL CONCEPTS AND LAWS

Elasticity is an important mechanical property of tissues. Under the influence of force, deformation occurs, either elastic or plastic. Elastic deformation is observed when the object returns to its initial state after removing the applied load. This type of deformation is reversible and non-permanent, while plastic deformation is irreversible and permanent.

When considering minor deformations that can be described by linear changes in the material, linear models are used, where deformation is characterized by Hooke's law (Eq. (1)):

$$F = k.\Delta x \tag{1}$$

where F denotes the applied force, k is the elasticity coefficient, Δx is the change in the parameter of object x. This law can also be related to Young's modulus, which is a measure that describes the elasticity of biological tissues - $\sigma = E.\varepsilon$, where σ denotes is the force applied per unit area, E is the Young's modulus, ε - deformation.

When pressure is applied in one direction, a change in the dimensions of the object is observed in directions perpendicular to the applied load. The Poisson's ratio is defined as Eq. (2):

$$v = -\frac{\varepsilon_x}{\varepsilon_z} \tag{2}$$

where ε_x denotes the lateral deformation, ε_z - longitudinal.

To apply these patterns in Unity and obtain a precise model, linear models are employed for small regions, allowing a localized definition of the object's properties.

GEOMETRIC MODELING APPROACH

The geometric approach is primarily used for training purposes, as it does not account for the physical characteristics of the real environment. According to the way the elements are connected, the models can be classified as meshed or meshless. The meshless approach employs points that constantly update their spatial location in accordance with parametric equations describing elasticity, such as Hooke's law for homogeneous media. If the environment under consideration is inhomogeneous, meaning there is a boundary between different structures within the modelled object, tensor formulations are utilized. Tensors are also applicable to homogeneous environments and are employed depending on the complexity of the problem. For niche applications, the geometric approach is suitable for planning within implantology and orthodontics, including procedures such as the treatment with bridge structures, dental implants, braces, treatment with an orthodontic apparatus, dental prosthetics, veneers, and others.

According to the theory of elasticity, three fundamental tensors are defined: tension, compression, and tension-compression. Let $\vec{u}$ denote the displacement of a material point during its translation in a rectangular coordinate system (Eq. (3)):

$$\vec{u}(x,y,z) = u_1(x,y,z)\vec{i} + u_2(x,y,z)\vec{j} + $$
$$+ u_3(x,y,z)\vec{k} \tag{3}$$

where $\vec{i}$, $\vec{j}$ and $\vec{k}$ are base vectors, $u_1(x,y,z)$ describes the displacement on the x-axis, $u_2(x,y,z)$- on the y-axis, $u_3(x,y,z)$ - on the z-axis. The tension tensor is given as Eq. (4):

$$E_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_k}{\partial x_i}\frac{\partial u_k}{\partial x_j}\right) \tag{4}$$

where i, j = 1, 2, 3. The stress tensor is characterized by the tangential pressure σ_{xy}, σ_{xz}, σ_{yz}, σ_{yx}, σ_{zx}, σ_{zy}, and the normal pressure σ_{xx}, σ_{yy}, σ_{zz} through the matrix (Eq. (5)):

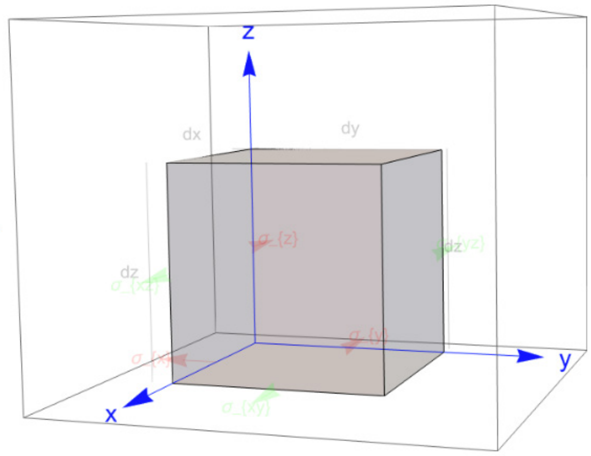

Fig. 1. Geometric approach (Wolfram).

$$\sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix} \tag{5}$$

observing the symmetry (Eq. (6)) [8]:

$$\sigma_{xy} = \sigma_{yx},\ \sigma_{xz} = \sigma_{zx},\ \sigma_{yz} = \sigma_{zy} \tag{6}$$

The mesh approach uses various geometric elements like triangles, tetrahedra, hexahedra, and olyhedral to represent the surface. The geometric approach can be combined with other computational methods to enhance its suitability for constructing a physical model (Fig. 1). When applied independently, it is primarily used for estimating occlusion and modelling inelastic structures, but its applicability in simulating soft tissues is relatively limited.

MODELING USING THE FINITE ELEMENT METHOD (FEM)

The finite element method is a robust numerical method with broad applicability, used in formulating complex problems via partial differential equations. It involves selecting a continuous region, which is then considered as a finite number of elements described by approximating functions to compose a global system of equations. The general algorithm can be outlined in several essential steps: discretizing the continuous region (dividing it into a finite number of elements), selecting interpolation functions, determining element properties, and composing a global system. FEM enables the representation of the problem using scalar parameters, material properties, nodal points, networks, matrices for describing boundary conditions and loads. The method provides a high number of degrees of freedom, which can be challenging to reconcile and requires mesh generators to create finite element networks using methods like mapping, triangulation, Delaunay triangulation, and Voronoi polygons [4].

The finite element method is extensively applied in manipulating biological tissues within virtual reality environments. Its core principle is describing the dynamic behaviour of an object using linear interpolation functions. Finite elements are often combined with tissue considerations as located on a finite number of springs with specific elastic properties – mass-spring models. To personalize the virtual model, data can be extracted from real diagnostic examinations of the patient. Other combinations with FEM include position-based dynamics, stiffness matrix methods, continuum mechanics methods, variational methods, hyperrealistic models, and others.

If it is assumed that the tension is: $\vec{\varepsilon}$ ={ε_x, ε_y, ε_z, γ_{xy}, γ_{yz}, γ_{zx}) and the pressure is: $\vec{\sigma}$ ={σ_x, σ_y, σ_z, τ_{xy}, τ_{yz}, τ_{zx}), $\vec{u} = [D]\,\vec{\varepsilon}$, according to Hooke's law: $\vec{\sigma}$ = [E]{ε^e}, [E] denotes the elasticity matrix, {ε^e} denotes the elastic characteristic of the deformation. These mathematical definitions also allow the expression of Poisson's ratio through Eq. (7):

$$\lambda = \frac{vE}{(1+v)(1-v)} \text{ and } \mu = \frac{E}{2(1+v)} \tag{7}$$

where λ and μ are elastic constants involved in the elasticity matrix. In this case, the finite element method can be used to determine the translation, at which we obtain minimum values for the potential energy, defined as Eq. (8):

$$W = \int_V \frac{1}{2}\{\varepsilon^e\}^T\vec{\sigma}dv - \int_V \frac{1}{2}\vec{u}^T\overrightarrow{p^V}dV - \int_S \frac{1}{2}\vec{u}^T\overrightarrow{p^S}dS \tag{8}$$

where $\overrightarrow{p^V}$ refers to the force applied by the object, and $\overrightarrow{p^S}$ is the force applied on the surface [9].

The finite element method is suitable for analysing the distribution of mechanical loads applied to tooth surfaces, assessing occlusion, evaluating tooth replacement with an implant, or selecting appropriate dental obturation. Gums are considered soft tissues and are subject to surgical interventions like gingivectomy, gingivoplasty, gum line reconstruction, resection, which can be analysed using FEM. Biomechanical interactions between the tooth and gum determine stability and position of the tooth, load-bearing, and other factors. These parameters can be altered by pathological conditions such as periodontitis, gingivitis, periodontosis, bruxism [5, 7]. Mechanical effects can also be modelled using FEM to achieve higher accuracy in personalized treatment.

MASS-SPRING MODELS

Springs that obey Hooke's law are suitable for the model - a linear dependence is observed. The considered object can be represented as a set of elements for which the following definitions apply:

$$V = \sum_{i=1}^{n} \Delta V_i \text{ and } m = \sum_{i=1}^{n} \Delta m_i \tag{9}$$

where V denotes the total volume of the aggregate, ΔV_i are the volumes of the individual objects, n is the number of objects, and m is the corresponding to the designation for the masses. From these definitions, the concept of density can be derived - both as an average for the entire system and as a property of the individual objects.

The body is considered as a system of mass points - idealized bodies in which all forces are concentrated at the center of mass. The resultant force $\overrightarrow{F_i}$, acting on it is given by Eq. (10):

$$\overrightarrow{F_i} = \sum_j^n \overrightarrow{g_{ij}} - d_i \dot{\overrightarrow{x_i}} + \overrightarrow{f_{ext_i}}, \text{ where } \sum_j^n \overrightarrow{g_{ij}} \tag{10}$$

where n denotes the number of mass points, $\dot{\overrightarrow{x_i}}$ - velocity of point i, d_i - damping coefficient, $\overrightarrow{f_{ext_i}}$ - the external forces acting on a point i, $\sum_j^n \overrightarrow{g_{ij}}$ - the force produced by springs between two points i and j. The resultant force depends on the direction of the applied load, the spring constant, and the displacement of the spring from its equilibrium position. To describe the phenomenon, a system of n equations is constructed, which can be reduced to a system of first-order differential equations [10].

A standard approach in the application of the spring-mass models is to simulate the muscle-driven movements - flexion, extension, abduction, adduction, rotation, etc. The base point of the spring is assumed to represent the interface between the muscle and the bone, and the other end is attached to the dermis. This type of model is applicable in the field of maxillofacial surgery [2]. In regions involving the periodontal region and teeth, it is appropriate to use the spring-mass approach in the modelling of the periodontal ligament, which connects the tooth to the alveolar bone (os alveolar) through collagen fibers. Another application is in the assessment of the occlusion [5].

RELATIONSHIP BETWEEN POISSON'S RATIO AND MATERIAL PARAMETERS IN UNITY

A rigid body is characterized by three main types of parameters: intrinsic parameters, which define the characteristics of the object itself, interaction with other objects, and material properties of the object. The mechanical properties of the object can be determined based on them. Poisson's ratio is applicable when simulating conditions such as cracks, fractures, and friction that occur when using artificial materials, etc. To be implemented in Unity, an explicit specification of the parameters is required to characterize the object, as we observe its relationship with elasticity and volumetric deformation.

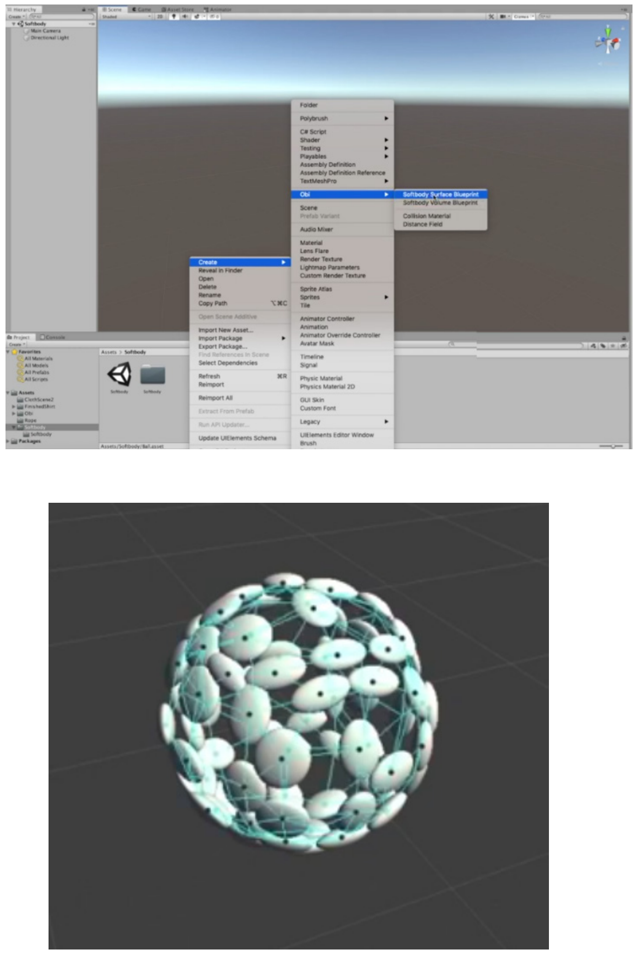

Fig. 2. Obi SoftBody add-on, composed of particles with shape constraints.

The Obi SoftBody add-on provides direct configuration of the parameters such as Stretching, Stiffness, Bending Stiffness, Density, Damping, and others, which can be used to approximate the Poisson's ratio (Fig. 2) [11].

For this purpose, a material with linear properties, Poisson's ratio ν, Young's modulus E and the bulk modulus K. Let's define the Young modulus using its standard definition, by Eq. (11):

$$E = \frac{\sigma}{\varepsilon} \quad (11)$$

where ε is the deformation, σ is the applied pressure. The tensor form of the Hook's law is presented by Eq. (12):

$$\varepsilon_{ij} = \frac{1+\nu}{E}.\sigma_{ij} - \frac{\nu}{E}.\delta_{ij}\sigma_{kk} \quad (12)$$

In pure shear in the plane defined by x and y (Eq. 13):

$$\sigma_{xy} = \tau,\ \sigma_{xx} = \sigma_{yy} = \sigma_{zz} = 0,\ \ \delta_{xy} = 0 \quad (13)$$

Accordingly, from the tensor form of Hooke's law for pure shear, we obtain Eq. (14):

$$\varepsilon_{xy} = \frac{1+\nu}{E}.\sigma_{xy} = \frac{1+\nu}{E}.\tau \quad (14)$$

The shear modulus is defined with G (Eq. (15)):

$$G = \frac{\tau}{\gamma} \quad (15)$$

where τ is the applied shear stress, γ is the shear strain. Shear strain can be related to the tensor form of Hooke's law (Eq. (16)):

$$\gamma = 2.\varepsilon_{xy} \quad (16)$$

then (Eq. (17)):

$$G = \frac{\tau}{\gamma} = \frac{\tau}{2.\varepsilon_{xy}} = \frac{\tau}{2.\frac{1+\nu}{E}.\tau} = \frac{E}{2(1+\nu)} \quad (17)$$

Accordingly, Young's modulus can be expressed as Eq. (18):

$$E = 2.G.(1+\nu) \quad (18)$$

when we have pure shear.

The relationship between Poisson's ratio and Young's modulus through volumetric deformation ε_v for $\sigma_x = \sigma_y = \sigma_Z = p$ is expressed as Eq. (19):

$$\varepsilon_v = \frac{1-2\nu}{E}.(\sigma_x + \sigma_y + \sigma_z) = \frac{1-2\nu}{E}.3p = \frac{p}{K} \quad (19)$$

Therefore, the bulk modulus through Poisson's ratio and Young's modulus is given as Eq. (20):

$$K = \frac{E}{3(1-2\nu)} \quad (20)$$

The bulk deformation modulus for regions can be given by a first-order ordinary differential equation (Eq. (21)):

$$K = -V\frac{dP(\vec{r})}{dV(\vec{r})} \quad (21)$$

from where the representation can be derived by Eq. (22):

$$dP(\vec{r}) = -\frac{K}{V(\vec{r})}dV \quad (22)$$

Therefore, the integral form of the regularity is given by Eq. (23):

$$K = -\int \frac{P(\vec{r})}{V(\vec{r})}dV \quad (23)$$

where $P(\vec{r})$ is the applied pressure, $V(\vec{r})$ is the volume, on which the pressure is applied. To be bound to the given parameters, is used Eq. (24):

$$P(\vec{r}) \approx Stretching\ Stiffness(\vec{r}).Density(\vec{r}) \quad (24)$$

To specify the impact of external forces on the body, it is necessary to take into account damping (Eq. (25)):

$$P(\vec{r}) \approx Stretching\ Stiffness(\vec{r}).Density(\vec{r})(1 - Damping(\vec{r})) \quad (25)$$

To find the value $V(\vec{r})$ the primary characteristics of the body are used. The final form of the formula is given by Eq. (26):

$$K = -\int \frac{Stretching\ Stiffness(\vec{r}).Density(\vec{r})(1-Damping(\vec{r}))}{V(\vec{r})}dV \quad (26)$$

which is assumed to be a sufficiently accurate approximation for the purposes of the simulation.

To create a connection between the K and Poisson's ratio ν the following relationship is used (Eq. (27)):

$$K = \frac{E}{3(1-2v)} = -\int \frac{Stretching\ Stiffness(\vec{r}).Density(\vec{r})(1-Damping(\vec{r}))}{V(\vec{r})}dV \quad (27)$$

Since the Young modulus is not directly given, we use Eq. (28):

$$E = 2.G.(1+v), \Rightarrow K = \frac{2}{3}.\frac{G.(1+v)}{(1-2v)}, \quad (28)$$

but G is also not directly defined and its Eq. (29):

$$G \approx \frac{Streching\ Stiffness}{2.Density.(1+Bending\ Stiffness)}. \quad (29)$$

Then it results (Eq. (30):

$$K \approx \frac{1}{3}.\frac{\frac{Streching\ Stiffness}{Density.(1+Bending\ Stiffness)}.(1+v)}{(1-2v)} = -\int \frac{Stretching\ Stiffness(\vec{r}).Density(\vec{r})(1-Damping(\vec{r}))}{V(\vec{r})}dV. \quad (30)$$

Accordingly, Poisson's ratio is as follows (Eq. (31):

$$v \approx \frac{-3.\int \frac{Stretching\ Stiffness(\vec{r}).Density(\vec{r})(1-Damping(\vec{r}))}{V(\vec{r})}dV - \frac{Streching\ Stiffness}{Density.(1+Bending\ Stiffness)}}{-6.\int \frac{Stretching\ Stiffness(\vec{r}).Density(\vec{r})(1-Damping(\vec{r}))}{V(\vec{r})}dV + \frac{Streching\ Stiffness}{Density.(1+Bending\ Stiffness)}}. \quad (31)$$

The Young modulus can be derived from Eq. (32):

$$E = 3.K.(1-2v) \approx -3.\int \frac{Stretching\ Stiffness(\vec{r}).Density(\vec{r})(1-Damping(\vec{r}))}{V(\vec{r})}dV.(1 - 2.\frac{-3.\int \frac{Stretching\ Stiffness(\vec{r}).Density(\vec{r})(1-Damping(\vec{r}))}{V(\vec{r})}dV - \frac{Streching\ Stiffness}{Density.(1+Bending\ Stiffness)}}{-6.\int \frac{Stretching\ Stiffness(\vec{r}).Density(\vec{r})(1-Damping(\vec{r}))}{V(\vec{r})}dV + \frac{Streching\ Stiffness}{Density.(1+Bending\ Stiffness)}}. \quad (32)$$

Expressions (31) and (32) define the relationship between Poisson's ratio and the defined body parameters using the Obi SoftBody plugin [12].

CONCLUSIONS

Simulations in medicine are a rapidly advancing field with extensive possibilities for visualizing, analysing, and processing anatomical structures. The required simulation complexity determines the selection of methodological approaches. When a precise approach is needed, mathematical methods are combined to complement the simulation environment's capabilities. Elasticity, one of the most important mechanical properties of tissue, is consistently represented regardless of the approach's complexity, and its adaptations are observed in almost all dentistry models.

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