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Special Features of Using Mathematical Modeling for the Study of Tetrahedral Elements

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Abstract. In this scientific work, mathematical modeling of tetrahedron elements in the finite element method is presented, which includes the determination of geometric shape, shape functions, and material properties. Unknown fields such as displacement vectors, strain, and stress tensors are considered. The methodology of applying the principle of virtual work and equilibrium equations is described, allowing the derivation of a system of differential equations to describe the behavior of the tetrahedral element. Integration over the volume and consideration of boundary conditions help reduce the equations to a system of linear algebraic equations for numerical solution using the finite element method. It was found that modeling tetrahedral elements with a specific given radius (for example, R=0.3 mm) involves stages such as geometry determination, element generation, shape function formation, stiffness matrix computation, and solving a system of linear equations. The radius R of tetrahedral elements is taken into account at all stages, ensuring accuracy and reliability in tetrahedra modeling. The research also focuses on the fact that the occurrence of minor errors in iterative processes may result from several factors, including iteration step, the number of iterations, stopping criteria, linear or nonlinear material behavior, solution method selection, the presence of geometric inhomogeneities, and element size.

1 Introduction

Mathematical modeling is the process of constructing mathematical representations of real systems or phenomena with the aim of studying their properties and behavior [1, 2]. The use of mathematical modeling based on finite element methods has numerous characteristics, including [3]:

1) Abstraction of reality (mathematical models allow abstraction from complex details of real systems and define fundamental aspects relevant to specific research or tasks, facilitating the analysis and understanding of complex systems) [4];

2) Prediction and optimization (mathematical models enable predicting the behavior of a system under different conditions and optimizing parameters to achieve specific goals) [5, 6];

3) Time and resource savings (mathematical modeling allows efficient examination of the impact of various factors without the need for expensive experiments in real life, significantly saving time and resources) [7, 8];

4) Explanation and interpretation (mathematical models can serve as tools for explaining cause-and-effect relationships and interpreting interactions between different variables in a system) [9, 10];

5) Warning about possible risks (mathematical modeling can help identify potential risks and forecast possible consequences under different scenarios and situations) [11];

6) Numerical analysis method (mathematical modeling uses numerical methods to solve complex mathematical equations, allowing obtaining results where analytical methods may be inefficient or impossible) [12];

7) Development of new theories (models can be used to develop new theories and hypotheses, which may be important objects for further research) [13];

8) Discretization of space and time (mathematical modeling and the finite element method are used to approximate partial derivatives of differential equations with finite differences. Space and time are divided into a grid, and derivatives are approximated on this grid) [14].

It is worth noting that the finite element method (FEM) is a numerical method for solving differential equations based on the approximation of the differentiation process by finite differences [15]. This type of method should be used for modeling and analyzing physical processes such as heat transfer, diffusion, convection, electrodynamics, and others. The main idea of the finite element method is to replace the differential operators with finite differences on the grid of the computational domain. The spatial variable domain is divided into a grid, and numerical approximations of partial derivatives are applied at each point on the grid. This leads to a system of algebraic equations that can be solved by numerical methods. In turn, FEM allows the use of various approximation schemes, such as explicit and implicit schemes, which affect the stability and accuracy of numerical calculations. It is worth noting that this approach is effective for solving various types of differential equations, particularly for time-solving partial differential equations. The finite element method is widely used in numerical modeling for analyzing various physical phenomena and processes in science, engineering, forecasting, and optimization.

Additionally, the application of mathematical modeling based on the finite element method is essential for investigating tetrahedral elements. This improvement enhances the quality and accuracy of both traditional modeling approaches and enables a detailed study of the tetrahedral element. Overall, mathematical modeling based on the finite element method allows the analysis and resolution of real-world problems, exploration of key parameters in real-time, and formulation of new ideas and hypotheses for further research.

2 Main Part

The main directives and aspects of mathematical modeling are discussed in works [16, 17, 18]. In this conducted experiment, concepts of mathematical modeling and the finite element method (FEM) are partially described, along with numerous features of using FEM for mathematical and computer modeling [19, 20, 21]. Abstraction of reality in mathematical modeling is presented in works [22, 23, 24]. It has been identified that the use of mathematical modeling allows abstraction from complex details of real systems, focusing on fundamental aspects for researching or solving complex problems. The utilization of mathematical models for understanding and predicting system behavior under different conditions and for optimizing parameters to achieve specific goals is presented in works [25, 26, 27]. Interpretation and its key indicators are explored in works [28, 29, 30]. It has been found that mathematical models can serve as tools for explaining cause-and-effect relationships and interpreting interactions between different variables in a system. The numerical analysis method is described in scientific experiments [31, 32, 33]. It is clarified that FEM is used to solve complex mathematical equations, allowing obtaining results where analytical methods may be inefficient or impossible [34, 35, 36]. The discretization and modeling of tetrahedral space are justified in works [37, 38, 39]. Authors mainly use mathematical modeling to approximate partial derivatives of differential equations with finite differences. Therefore, the analysis of literature sources shows a comprehensive overview of the use of mathematical modeling and FEM as a whole, indicating their wide applicability in numerous fields, including science, engineering, and forecasting. However, there is limited research conducted on tetrahedral elements, and their modeling [40, 41, 42] has been almost non-existent, ultimately addressing the issue of the economy and efficiency of the main labor-intensive stages in conducting physical experiments. Additionally, the application of such a mathematical combination will allow predicting parameters of particles with a highly complex shape – tetrahedra.

The goal of the work is to develop and present a model for the investigation of tetrahedral elements, considering the analysis of geometric shape, shape functions, and material properties of these elements, as well as including unknown fields such as displacement vectors, strain tensors, and stresses. The study aims to investigate the influence of various factors, such as geometry, boundary conditions, iterative processes, displacement of points in space, and loading on the accuracy and efficiency of the obtained numerical solution.

Materials. Particles, tetrahedral elements, are one type of non-homogeneous elements with the shape of a tetrahedron. A tetrahedron is a geometric figure with four vertices, four sides, and four angles. It should be noted that using the finite element method (FEM), tetrahedral elements can be employed to approximate the geometric shapes and physical properties of complex objects in numerical calculations. In turn, a tetrahedron is a polyhedron composed of four triangular faces, all sharing a common vertex.

Among the main characteristic features of tetrahedral elements, the following can be highlighted:

1. Geometric shape: tetrahedral elements are commonly used to approximate objects with a shape close to a tetrahedron in three-dimensional space.
2. Number of vertices: in any case, each tetrahedron has four vertices (nodes) that define its geometric configuration.
3. Spatial properties: non-homogeneous tetrahedral elements are used to model three-dimensional objects such as structures, volumes of fluids, or solid bodies, where space is considered in three dimensions.
4. Approximation: due to their simplicity and flexibility, tetrahedral elements can effectively approximate geometric shapes of varying complexity.

It is worth noting that in numerical calculations, where the geometric and physical properties of an object need to be approximated for obtaining numerical results, the use of tetrahedral elements in FEM can be an effective approach for modeling three-dimensional objects. Figure 1 shows the structural scheme of tetrahedral elements with non-homogeneous structure.

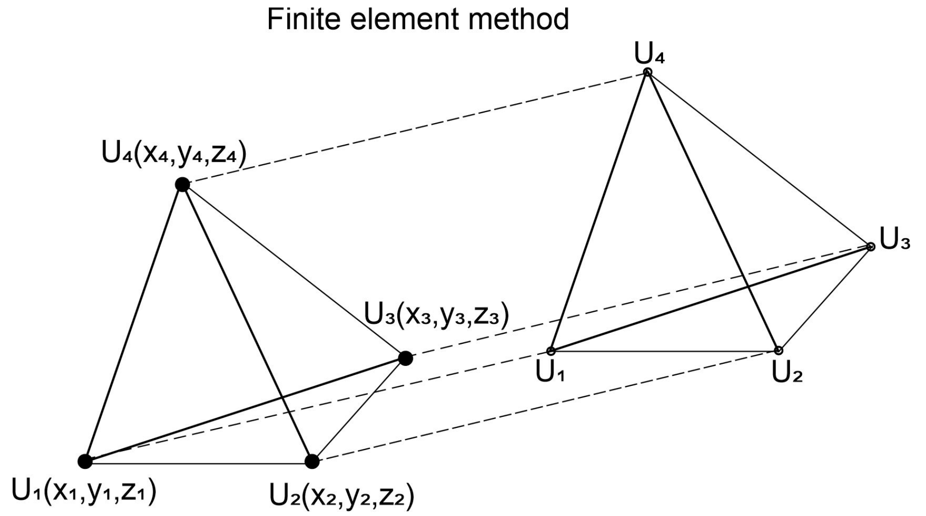

Fig. 1. Structural scheme of tetrahedral elements

The mathematical model of tetrahedral elements can be represented using the finite element method (FEM). FEM is a numerical method for analyzing the behavior of materials and structures by dividing them into elementary components, such as tetrahedra, and applying certain mathematical equations that qualitatively describe their behavior.

Let u be the displacement (deformation) vector at the nodal points of the tetrahedral element, and x be the vector of coordinates relative to the origin. Then, Hooke's law for the tetrahedral element can be expressed as follows:

$$\sigma = D \cdot \varepsilon , \quad (1)$$

where: σ – stress tensor; D – material stiffness tensor; ε – strain tensor.

Then, the stiffness matrix D is typically a fourth-order matrix, as it has four indices. It should be noted that different forms of the matrix can be used depending on the material. Following this, the strain tensor ε can be expressed in terms of the gradient vector of displacement ∇u, where the gradient of displacement indicates the deformation change in space. This gives us:

$$\varepsilon = \frac{1}{2} \cdot (\nabla u + (\nabla u)^T) \quad (2)$$

It is also worth noting that with respect to the rotational gradient of deformation $\nabla \varepsilon$, the gradient of displacement ∇u can be determined. The main task in such research is to find the solution to the system of equations that models deformation and stress in a tetrahedral element. This can be achieved using numerical solution methods such as the finite element method. Additionally, it can be based on modeling tetrahedral elements. Typically, iterative methods are needed to find the numerical solution, initially for the system of equations and later for modeling. This mathematical model is important for analyzing the behavior of materials and their structures, primarily under deformations, and it is widely used for predicting and optimizing the behavior of materials under various real-time conditions.

Tests. To qualitatively conduct the modeling of tetrahedral elements, it is necessary to consider each circular element of the tetrahedron's triangular cross-section at the initial stage (Figure 2). It should be noted that the displacement of each node primarily consists of three components, which are equal to: $q_i = (u_i; v_i; w_i)^T$, where i = 1; 2; 3 forming the displacement vector. We obtain:

$$q = (q_1^T \cdot q_2^T \cdot q_3^T)^T \quad (3)$$

In turn, the displacement vector in a tetrahedral element is a vector that describes the changes in the position of material points in space due to deformation. It determines how each point of the tetrahedron is displaced or deformed as a result of applied loads or influences.

Let u be the displacement vector. For a tetrahedral element, we can have three displacement components for each direction (x, y, z) in three-dimensional space. Thus, the displacement vector for a tetrahedral element can be expressed as:

$$u = \begin{bmatrix} u_x \\ u_y \\ u_z \end{bmatrix}, \quad (4)$$

where: u_x, u_y, u_z – displacement components along the axis x, y end z.

It is important to consider that displacement is determined by the changes in the positions of material points relative to their initial state, rather than their absolute positions. This allows for the analysis and modeling of deformations and stresses in heterogeneous materials and structures under the influence of additional loads. Figure 2 illustrates the cross-section of a ring-shaped tetrahedral element.

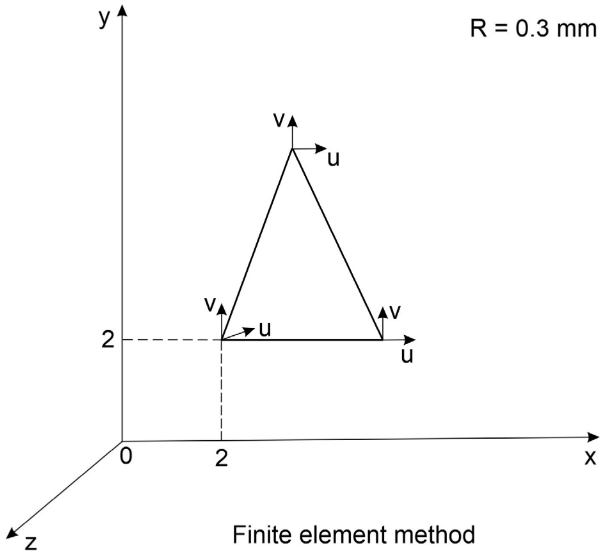

Fig. 2. Cross-section of a ring-shaped tetrahedral element with coordinates of points (x, y, z)

From the above-described material, it follows that the mathematical modeling of a tetrahedral element in the context of the finite element method includes determining the element's shape, unknown fields, and material properties. The key aspects of mathematical modeling of a tetrahedral element with coordinates (x, y, z) are as follows:

1. **Element Shape:**

- geometric shape: determining the geometric shape of the tetrahedral element involves the coordinates of its vertices in three-dimensional space. Each vertex is defined by three coordinates (x, y, z);
- shape functions: shape functions are used to describe the distribution of physical fields (such as deformations or displacements) within the tetrahedron. These functions express the dependence of fields on the local coordinates of the element.

2. **Unknown Fields:**

- displacement vector (u): a generalized field describing the displacement of points in space;
- strain tensor (ε): defines material deformations within the tetrahedron;
- stress tensor (σ): determines stresses in the material at each point of the tetrahedron;
- other information: depending on the specific task, other unknown fields, such as temperature, concentration, etc., may be defined.

3. **Equations of Equilibrium:**

- application of the virtual work principle and equilibrium equations: applying these principles allows obtaining a system of differential equations that describe the behavior of the tetrahedral element over time under the application of force, boundary conditions, and material properties.

4. **Volume Integration:**

- numerical methods: numerical methods, such as Gaussian quadrature, are used to approximate volume integrals over the tetrahedron to calculate values at its nodes.

5. **Boundary Conditions:**

- incorporation of boundary conditions: considering boundary conditions involves defining the values of unknown fields on the domain's boundaries and their impact on the equilibrium equations.

6. **Finite Element Method:**

- consolidation of equations: bringing all equations into a unified system and expressing them in the form of linear algebraic equations. Numerical solution methods, such as iterative methods or direct solution methods, are then applied.

In Figure 3, modeling of tetrahedral elements is presented, enabling the analysis of material behavior and structure under various conditions.

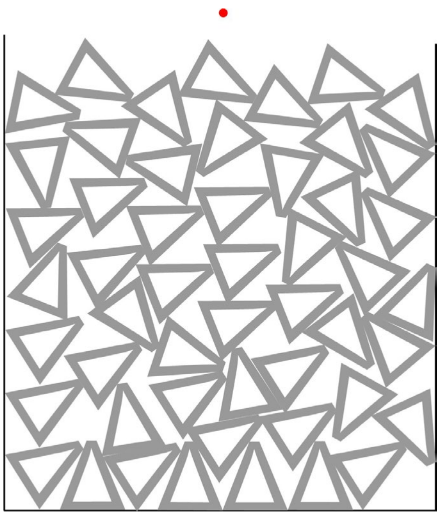

Fig. 3. Modeling tetrahedral elements with a radius *R*=0.3 mm

The modeling of tetrahedral elements with a specific radius, such as *R*=0.3 mm, involves several steps. While the radius may not directly appear in the mathematical expressions for the finite element method, it is considered in calculations related to geometry generation, stiffness matrix computation, and other parameters. The main indicators used in our investigation of the tetrahedron include:

1. Geometry Definition:

o initially determined the coordinates of the tetrahedron's vertices in three-dimensional space. This involved locating each vertex with consideration of the radius *R*. For instance, if $A(x_1, y_1, z_1)$, a spherical region around this point was considered, and other points on this sphere were selected.

2. Tetrahedral Element Generation:

o created a geometric model of the tetrahedral element from the defined vertices. Utilized developed software for generating and modeling finite elements, as depicted in Figure 3.

3. Formation of Shape Functions:

o defined shape functions to describe the distribution of physical fields (e.g., displacements or deformations) inside the tetrahedron. Radius *R* was explicitly considered in these functions.

4. Stiffness Matrices and Integration:

o applied numerical methods to compute stiffness matrices, considering geometric and physical properties of the tetrahedron, including its radius *R*.

5. Solution of the System of Equations:

o solved the system of linear algebraic equations resulting from the application of the finite element method. Applied boundary conditions and obtained the distribution of unknown fields within the tetrahedron.

It's noteworthy that during the modeling of tetrahedral elements, we observed a certain displacement of points (particles) in space due to the nodal force of the tetrahedron. The results of this dependence are presented in Figure 4.

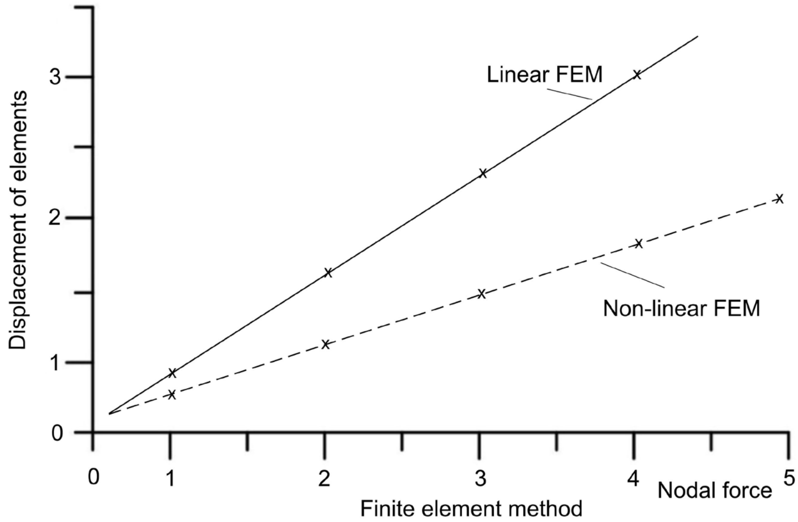

Fig. 4. Exponential dependence of the displacement of points (particles) in space on the nodal force of the tetrahedron, where: the solid curve represents linear analysis, and the dashed curve represents nonlinear analysis

From the conducted research, it can be concluded that the exponential dependence of point displacement in space on the nodal force of the tetrahedron is predominantly expressed mathematically. The linear and nonlinear analyses showed some differences in the material's response to loading.

Linear analysis (solid curve):

In the linear case, we used Hooke's Law to describe the relationship between force effects and displacements. The obtained relationship is as follows:

$$\tau = G \cdot \gamma\,, \tag{5}$$

where: τ – shear stress; G – shear modulus (shear modulus or modulus of elasticity in shear); γ – shear strain.

It should be noted that the mathematical expression (5) is linear and does not account for nonlinear effects in the material under large loads.

Nonlinear analysis (dashed line curve):

In this nonlinear case, when the material predominantly exhibits nonlinear behavior, a more complex mathematical approach can be employed, such as the law of elastic-plastic deformation. The obtained expression is as follows:

$$\tau = G \cdot \gamma \cdot (1 + \beta \cdot \gamma^{n})\,, \tag{6}$$

where: β – nonlinear parameter; n – exponential parameter, which can vary from 0 to 1.

It is worth noting that such a mathematical approach allowed us to account for nonlinearity in the material and loading. If n equals 1, the effects will be linear; however, when n, the exponential parameter, exceeds 1, the effects become more nonlinear, and the exponential dependence becomes more pronounced.

The analysis indicates that the investigation of the tetrahedral element is an extremely complex process, leading to errors from the application of iterative modeling. The results of the error levels from iterative modeling are presented in Figure 5.

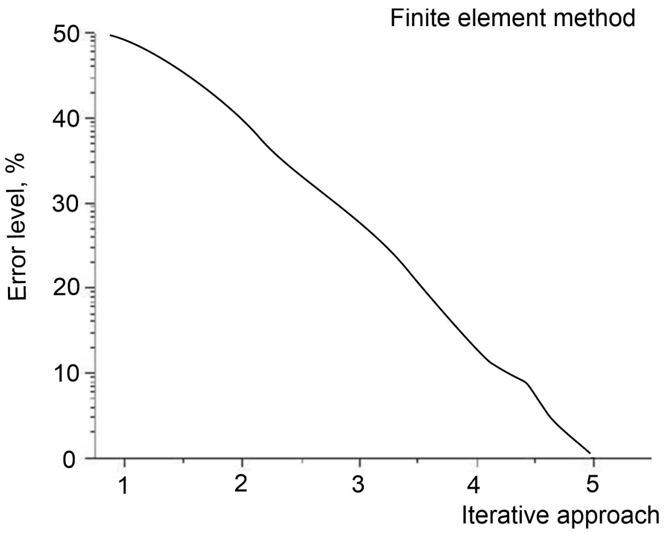

Fig. 5. Dependency of error levels on iterative modeling

It should be noted that minor errors from repeated iteration arise due to:

1) iteration step (usually the iterative process involves certain steps, at each of which a new approximate solution is computed. Depending on the method, such as the Hooke's method, the number of iterations can significantly affect the accuracy of the results. Typically, increasing the number of iterations improves the solution's accuracy);

2) stopping criteria (defining stopping criteria for the iterative process is crucial. When considering the convergence of the method, careful attention should be paid to stopping criteria, as an incorrect choice can lead to inaccurate results or unnecessary computations);

3) linear or nonlinear behavior (if the material exhibits linear behavior, greater convergence and rapid error reduction can be expected. In the case of nonlinear effects, such as plasticity or material heterogeneity, the iterative process and its modeling can be more costly and less efficient, resulting in increased error levels);

4) solution methods (the choice of a specific solution method, such as the Hooke's method or the reduced hessian strategy (RHS), can impact error levels and convergence speed. Some methods may be better suited to certain types of problems);

5) geometric irregularities (the presence of geometric irregularities, such as sharp angles or material clustering, can affect the iterative process and lead to slow convergence);

6) element sizes (reducing the size of elements can improve result accuracy, but there may be some increase in computations, making calculations more cumbersome and resource-intensive).

Therefore, to address specific tasks, testing and validating the applied method at various stages of problem-solving, while adjusting parameters and evaluating their impact on convergence and solution accuracy, are essential.

3 Conclusion

From this scientific research, the following conclusion can be drawn: mathematical modeling of a tetrahedral element in the context of the finite element method is a complex process that involves several key aspects, including the element's shape (tetrahedron), unknown fields (displacement vector, strain tensor, stress tensor), equilibrium equations, volume integration, boundary conditions, and the application of the finite element method.

In modeling tetrahedral elements with a specified radius R, specific steps and parameters are employed to ensure accuracy and correctness of the results. Among the main aspects are geometry definition, tetrahedral element generation, formation of shape functions, stiffness matrix integration, and solution of the system of equations.

It is worth noting that the choice of parameters in the iterative process plays a crucial role in modeling tetrahedral elements, such as iteration step, stopping criteria, linear or nonlinear behavior, solution methods, geometric irregularities, and element sizes, which determine the accuracy and efficiency of the results. When addressing specific tasks, we recommend conducting testing and validation of methods at various stages of problem-solving, considering the impact of parameter changes on convergence and solution accuracy. It should also be emphasized that the mentioned modeling process parameters help reduce the error level, resulting in the desired high-quality outcome.

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