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Effective Application of Numerical Approaches and Green Functions for the Process of Modelling Spheres

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Abstract. The research work is devoted to the study of the stress-strain state of a structure comprising a cylinder with a sphere using numerical approaches and Green's functions. The results obtained include the analysis of stress distribution, study of deformations and determination of stress concentration zones. Safety factors are assessed and the influence of boundary conditions on the behaviour of the structure is revealed. The application of numerical methods allowed for a detailed study of the interaction of the sphere, providing an opportunity to analyse the exact properties and assess the influence of various factors in complex structures. It should be noted that the results obtained, which were evaluated taking into account all factors, affect the real system and can be predicted with a deviation error of 1%.

1 Introduction

Usually, a system of numerical approaches and partial differential equations is used to describe physical phenomena and processes by a mathematical model, taking into account all possible relevant boundary conditions, as well as the initial data [1, 2, 3]. It should be noted that the possibility of analytically finding the final calculations by numerical methods for the modelling process is limited only in certain cases [4, 5, 6, 7]. Modern engineering approaches and their structures have a complex heterogeneous geometric shape and are mainly made of heterogeneous materials, composites, and nanocomposites [8, 9, 10]. Therefore, the possibility of obtaining simple elementary formulas, or modelling, or using special functions to find qualitative calculations is somewhat limited [11, 12, 13].

The current stage of designing various structures requires an increasing use of computer-based approaches and technologies [14, 15]. The basic idea of computer calculations and the modelling process is to build specific discrete systems [16, 17], use modern Green's functions [18, 19, 20], use differential equations [21, 22], and apply finite element or boundary element methods [23, 24] to simulate the behaviour of these materials and structures in real conditions [25]. It should be noted that the use of numerical methods and basic Green's approaches for the modelling process allows for virtual experiments and quick obtaining of high-quality results. Currently, the most widely used and popular methods are finite element methods and boundary element methods based on the Green's context.

The main advantage of Green's boundary element methods (BEMs) and finite element methods (FEMs) is to provide an efficient and accurate numerical approach for solving differential equations and boundary value problems in the modelling process. The main goals of such a numerical approach include:

1. domain modelling: BEM and FEM allow modelling complex domains and structures, such as bodies of different shapes and geometries. This is especially important when solving problems where analytical methods are ineffective or impossible;
2. adaptability to complex boundary conditions: BEM and FEM make it easy to take into account complex boundary and initial conditions that often arise in real physical and engineering problems;
3. consideration of inhomogeneous properties: BEM and FEM allow modelling materials with different parameters and properties, in this case, spheres;
4. computational efficiency: BEM and FEM allow efficient use of computing resources, especially when working with large and complex models;
5. reducing the dimensionality of the problem: the use of boundary element and finite element methods allows to reduce the dimensionality of the problem, since calculations are performed only on a certain boundary of the domain;
6. analysis of dynamic processes: the use of boundary and finite methods is well suited for the analysis of dynamic phenomena such as wave propagation, oscillations and various types of interactions;
7. nonlinearity and large displacements: boundary and finite element methods can be extended to account for nonlinear material properties and large displacements;
8. adaptability to discontinuous phenomena: BEM and FEM can be effectively used for the detailed modelling process of spheres, discontinuities such as cracks or ruptures, which play an important role in the final prediction of results.

Thus, the use of numerical approaches and Green's functions for the process of modelling spheres is a powerful tool and is relevant for both modelling and qualitative analysis of various physical and engineering problems, in particular in cases where the complexity of the geometry and boundary conditions make the analytical approach impractical.

2 Main Part

Scientific studies [26, 27] provide a detailed justification of the finite element method. It should be noted that this method is widely used for numerical modelling in various fields, including physics and engineering. It allows to approximate solutions of various differential equations describing the behaviour of spheres. Papers [28, 29, 30] highlight aspects of the application of the finite difference method, which is mainly used by the authors to approximate differential equations by decomposing them into finite elements and their differences. In [31, 32, 33], an approach to using the finite volume element method is proposed. This method is mainly based on the division of space into volumes and the calculation of flows through the boundaries of these volumes. The groups of works [34, 35, 36] partially explain the effectiveness of using Green's functions for differential operators. The results are used to obtain analytical solutions to differential equations. They also allow obtaining solutions for certain boundary conditions. Scientific studies [37, 38, 39] cover the general theory of the application of Green's functions in mathematical physics. The authors also suggest using Green's functions only for solving problems of thermal conductivity and electrostatics. The analysis of the literature shows that many key points in the study of the process of modelling spheres [40, 41] are unreasonable and unexplored. Therefore, an important and relevant issue is a detailed disclosure of the effective use of numerical approaches and justification of qualitative methods and Green's functions for the sphere modelling procedure.

The aim of the study is to investigate and analyse in detail the stress-strain state of a structure that includes a cylinder with a sphere. To determine the distribution of stresses, the effect of external loading on the geometry of the structure and stress concentration zones, to assess safety factors and to identify the influence of boundary conditions on the overall behaviour of the structure.

Materials. Numerical methods are a class of methods in computational mathematics that use numerical approaches to approximate solutions to mathematical problems, usually those that can be expressed as differential or integral equations. These methods are used to calculate numerical values that are approximations of exact analytical solutions when the latter are impractical or even impossible to find solutions to problems.

The main characteristics of numerical methods include:

1) **approximation:** numerical methods use finite or discrete approaches to approximate continuous or unknown functions, solutions to equations, integrals, etc;

2) **division into finite parts:** simple and complex problems are divided into finite elements or domains, where numerical methods are applied to calculate the values in each part;

3) **iteration:** many numerical methods use iterative processes to approximate the exact solution of the problem.

It should be noted that numerical methods include finite element methods, finite difference methods, boundary element methods, Green's theory, finite volume methods, numerical methods for solving differential equations, numerical methods for optimisation, integration, etc.

In particular, Green's functions are a mathematical tool that is a solution to partial differential equations subject to certain boundary conditions. In a good case, in order to qualitatively model spheres based on the Green's context, it is necessary to use the Poisson's equation at the initial stage. Thus, the Poisson's equation in three dimensions is as follows:

$$\nabla^2\phi = -\rho, \tag{1}$$

where: $\phi -$ potential; $\rho -$ density; $\nabla^2 -$ Laplace operator.

The Green's function for this equation satisfies the following conditions, as follows:

$$\nabla^2 \cdot G \cdot (r, r') = -\delta \cdot (r - r'), \tag{2}$$

where: $\delta -$ is the Dirac delta function.

In turn, the Green's function is used to solve the equations using the following integral, we obtain:

$$\phi(r) = \int_V \cdot G \cdot (r, r') \cdot \rho(r') \cdot dV' + \oiint_S \cdot (G\frac{\partial \phi}{\partial n'} - \phi\frac{\partial G}{\partial n'}) \cdot dS', \tag{3}$$

where: $r, r' -$ are the position vectors of the points; $V -$ is the volume; $S -$ is the surface; $n' -$ is the vector of the external normal to the surface.

It should be noted that, based on the Green's function, we obtained a qualitative solution of the system with boundary conditions, which in turn provided us with an effective method for solving mathematical equations for the process of modelling spheres. We also used Green's functions to model the distribution of potential and temperature in areas with spherical symmetry.

For example, consider the use of Green's functions to model the static and electrostatic field around a spherically distributed charge. So, the spherical symmetric Green's function takes the following form: $G(r, r')$, where $r -$ is the distance from the observation point to the potential source, and $r' -$ is the distance from the potential source to the charge point.

Since we are studying spherical symmetry, we can use the coordinates in a spherical system, respectively, and obtain:

$$G(r, r') = \frac{1}{|r - r'|} - \frac{r \prec}{r \succ}, \tag{4}$$

where:

$$r \prec = \min(r, r')ir \succ = \max(r, r') \tag{5}$$

Then, if we have a spherically distributed charge Q of radius R at the centre of coordinates, we can use this Green's function to find the potential V at point P using the following proposed integral, as follows:

$$V(P) = \frac{1}{4\pi \in 0} \cdot \int_V \cdot \rho(r') \cdot G \cdot (\left| r - r' \right|) \cdot dV', \tag{6}$$

where: $\rho(r') -$ is the charge density.

It should be noted that for a spherically distributed charge, we use spherical coordinates to calculate the integral. However, in general, the use of Green's functions in the modelling of spherically distributed charges and potentials has helped us to obtain a variety of electrostatic or electrodynamic parameters with spherical symmetry.

Tests. According to the theory described above, we will study the stress-strain state of an elastic cylinder with a given inhomogeneity and a sphere. That is, we will consider a cylinder that is fixed on one edge with the parameters and coordinates of the system. And also, it is uniformly loaded with external factors on the other edge, and has inclusions in the form of a sphere. The modelling of this process is shown in Figure 1.

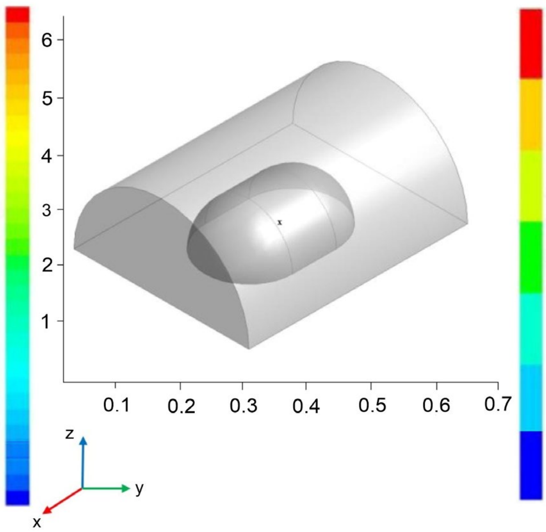

Fig. 1. Modelling the stress-strain state of an elastic cylinder with a sphere

It should be noted that the modelling of the stress-strain state of an elastic cylinder with a sphere includes a number of numerical approaches, and this type of modelling was carried out on the basis of the Green's concept. In particular, the size of the cylinder was 1500×1000 mm, the diameter of the sphere was D=0.5 mm, the Young's modulus varied from 50 GPa to 80 GPa, and the Poisson's ratio was 0.3 m/m. In addition, loading conditions such as pressure, external forces and thermal effects were applied.

Figure 2 shows the uniform displacement of the stress-strain state of a cylinder with a sphere along the surface of the coordinate distribution of the modelling system.

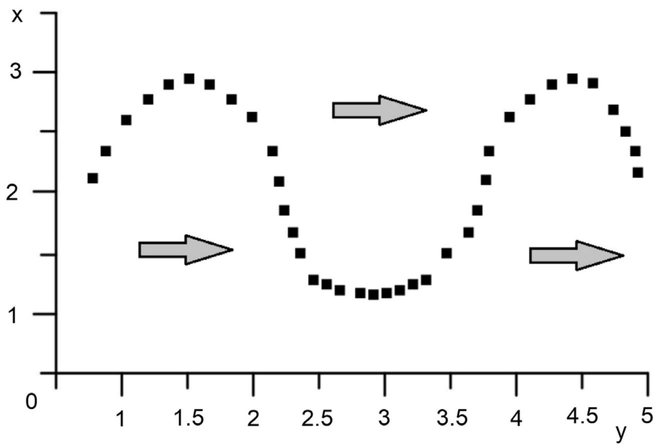

Fig. 2. Movement of the cylinder according to the coordinate distribution surface of the simulation system

From the presented dependence, it can be seen that for each point on the distribution surface, it is necessary to determine its relative displacement relative to the corresponding point on the cylinder and it is necessary to specify the direction of movement along which the coordinates of the modelling system should be distributed. It is worth noting that based on this displacement, we were able to take into account the interaction between the cylinder and the sphere in terms of deformations and displacements.

Figure 3 shows the modelling of the sphere based on the finite element method.

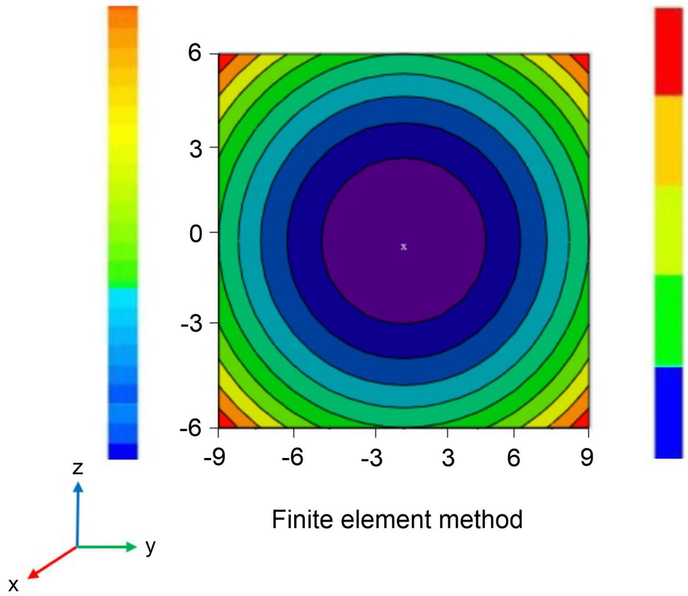

Fig. 3. Modelling the sphere based on FEM

It was found that using the coordinates of the centre of the sphere x, y and z, it is possible to fix the position of the sphere in space. With the help of the given Young's modulus and Poisson's ratio, a clear movement of the sphere according to the coordinate system was observed, which was expressed by the movements of the sphere points relative to the coordinate system. In turn, the Young's modulus allowed us to fix the stiffness of the sphere's material, and the Poisson's ratio calculations showed how much the sphere deforms when external stresses are applied. It should be noted that the results obtained did not capture the deformation and the effect of external loads on the process of modelling the sphere. On the contrary, using the specified boundary conditions, we observed clear movements of the sphere's points, indicating changes in its shape (which are clearly expressed by the coloured layers in Figure 3) and position in space.

Figure 4 shows the detail of the sphere that was modelled based on Green's calculations.

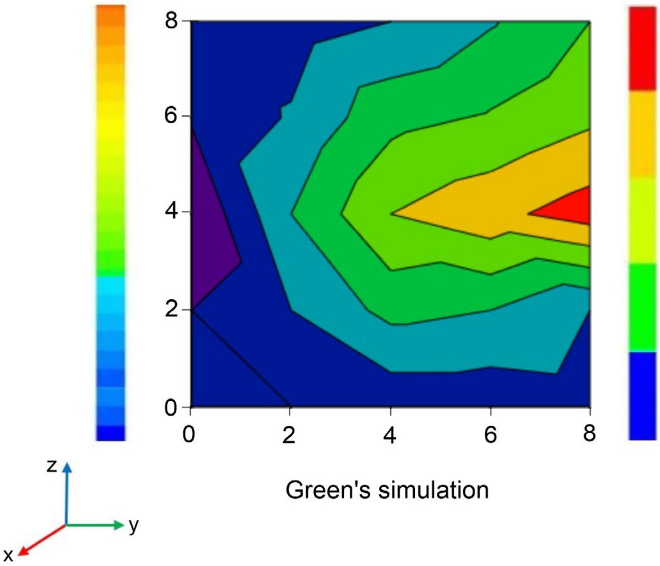

Fig. 4. Detailing the sphere based on the obtained Green's indicators

It should be noted that in this case, using Green's indices, we achieved a sphere detail that clearly indicated the division of the sphere surface into smaller parts or elements for a qualitative numerical analysis. These results made it possible to record the division of the geometric shape into a finite number of elements, each of which approximates the behaviour of the material on a certain part of the surface.

The simulation results presented in Figure 5 show the concentration of changes in the shape of the particle (sphere) at different times.

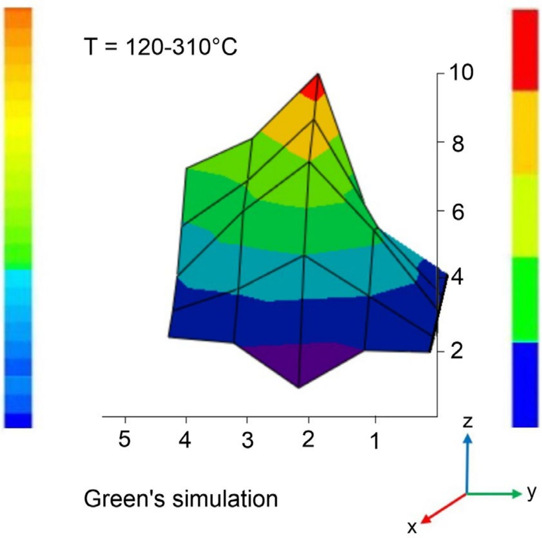

Fig. 5. Modelling the shape of a particle (sphere) at different points in time

The graphical representation (Fig. 5) of the particle shape at different times shows that with increasing time, the shape of the sphere becomes more or less ideal, i.e. its coefficient of roundness is 1. The sphere changes its shape and responds to external influences over a period of time. This, in turn, confirms the reliability of the calculations.

Figure 6 shows the modelling of the stress-strain state of an elastic cylinder with a sphere. The results obtained made it possible to study the detailed behaviour of the structure under various conditions.

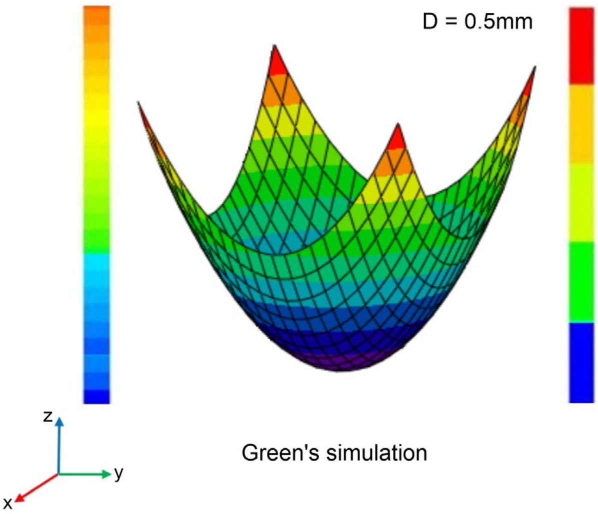

Fig. 6. Behaviour of the structure under different conditions

The main results obtained in the course of the modelling include the following:

1. **Stresses:**

○ The stress distribution in the entire structure, including the cylinder, sphere and areas in between, allowed us to determine the maximum stress values and their locations (0.9 MPa);

2. **Deformations:**

○ Almost no changes in the geometry of the structure under the influence of external load were observed. The change in the shape of the particle at different times achieved the desired results, the roundness of the sphere was equal to 1. It should also be noted that the deformation process was partially considered, which occurred both locally (at individual points) and globally (throughout the structure);

3. **Location of stress concentration zones:**

○ We recorded certain areas (locations) where concentrated stresses were clearly present. These are mainly sharp corners and contact zones between the cylinder and the sphere, which are shown in Figure 5;

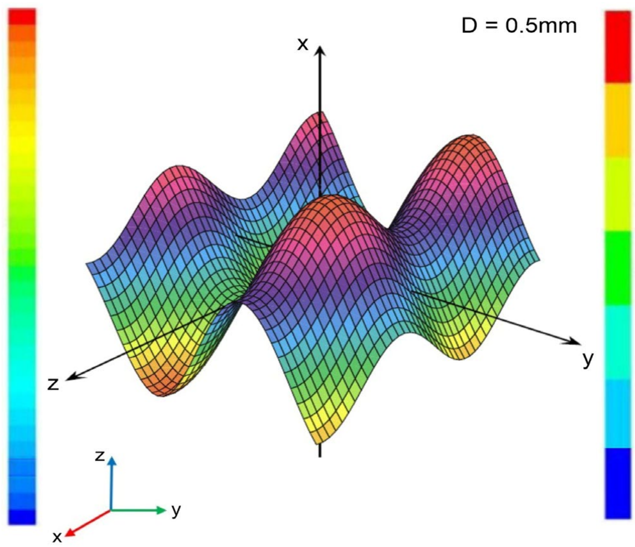

Fig. 7. Modelling and response of the structure to various impacts

4. **Safety factor:**

○ Determination of the safety factors for the different parts of the structure. It should be noted that these indicators helped us to estimate how far the structure deviates from the permissible stress limits;

5. **Influence of boundary conditions:**

o We found that changes in boundary conditions, such as anchorage and external loading, affect the overall behaviour of the structure.

Figure 7 shows the final behaviour of the modelled structure under the influence of various factors.

It should be noted that the results obtained can be used for designing and optimising structures, as well as for identifying and avoiding possible problems in elements and stress zones. It should also be noted that the simulations have been validated with experimental data (Green's functions), and their results have been evaluated taking into account all factors affecting the real system. This, accordingly, indicates that it is possible to predict the obtained indicators.

3 Conclusion

Based on our results and modelling, we can draw the following conclusions:

1. Stresses (stress distribution in the structure, covering the cylinder, sphere and areas between them, allowed us to determine the maximum stress values and their localisation, which amount to 0,9 MPa);
2. Deformation (changes in the geometry of the structure under the influence of external load were almost imperceptible. The shape of the particle at different stages of time reached the desired results, and the roundness of the sphere was equal to 1);
3. The location of stress concentration zones (some areas where concentrated stresses were present, in particular, sharp corners and contact zones between the cylinder and the sphere, were recorded);
4. Safety factor (the safety factors for different parts of the structure were evaluated, which gives us an idea of how far the structure deviates from the permissible stress limits);
5. Influence of boundary conditions (changes in boundary conditions, such as anchorage and external loading, are found to have a general impact on the behaviour of the structure).

It should also be noted that the use of numerical approaches and Green's functions for the modelling of spheres allows for a detailed study of their deformation and stress state under various loading conditions. These methods make it possible to analyse the exact interactions between spheres, identify stress concentration zones, and assess the influence of various factors on the mechanical behaviour of spheres in complex structures.

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