



Vaidas VADLUGA

**SIMULATION OF DYNAMIC DEFORMATION
AND FRACTURE BEHAVIOUR
OF HETEROGENEOUS STRUCTURES
BY DISCRETE ELEMENT METHOD**

**Summary of Doctoral Dissertation
Technological Sciences, Mechanical Engineering (09T)**

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Vilnius  **2007**
LEIDYKLA
TECHNIKA

VILNIUS GEDIMINAS TECHNICAL UNIVERSITY

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Doctoral dissertation was prepared at Vilnius Gediminas Technical University in 2003–2007.

Scientific Supervisor.

Prof Dr Habil Rimantas KAČIANAUSKAS (Vilnius Gediminas Technical University, Technological Sciences, Mechanical Engineering – 09T).

Consultant:

Dr Algis DŽIUGYS (Lithuanian Energy Institute, Technological Sciences, Energetic and Thermal Engineering – 06T).

The dissertation is being defended at the Council of Scientific Field of Mechanical Engineering at Vilnius Gediminas Technical University:

Chairman.

Prof Dr Habil Rimantas BELEVIČIUS (Vilnius Gediminas Technical University, Technological Sciences, Mechanical Engineering – 09T).

Members:

Dr Robertas BALEVIČIUS (Vilnius Gediminas Technical University, Technological Sciences, Mechanical Engineering – 09T),

Prof Dr Habil Mykolas DAUNYS (Kaunas University of Technology, Technological Sciences, Mechanical Engineering – 09T),

Prof Dr Habil Gintautas DZEMYDA (Institute of Mathematics and Informatics, Technological Sciences, Informatics Engineering – 07T),

Prof Dr Habil Mindaugas Kazimieras LEONAVIČIUS (Vilnius Gediminas Technical University, Technological Sciences, Mechanical Engineering – 09T).

Opponents:

Prof Dr Habil Juozas ATKOČIŪNAS (Vilnius Gediminas Technical University, Technological Sciences, Mechanical Engineering – 09T),

Prof Dr Habil Rimantas BARAUSKAS (Kaunas University of Technology, Technological Sciences, Mechanical Engineering – 09T).

The dissertation will be defended at the public meeting of the Council of Scientific Field of Mechanical Engineering in the Senate Hall of Vilnius Gediminas Technical University at 2 p.m. on 30 January 2008.

Address: Saulėtekio al. 11, LT-10223 Vilnius, Lithuania.

Tel.: +370 5 274 4952, +370 5 274 4956; fax +370 5 270 0112;

e-mail: doktor@adm.vgtu.lt

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VILNIAUS GEDIMINO TECHNIKOS UNIVERSITETAS

Vaidas VADLUGA

**NEVIENALYČIŲ STRUKTŪRŲ DINAMINIO
DEFORMAVIMO IR IRIMO MODELIAVIMAS
DISKREČIŲJŲ ELEMENTŲ METODU**

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Mokslinis vadovas

prof. habil. dr. Rimantas KAČIANAUSKAS (Vilniaus Gedimino technikos universitetas, technologijos mokslai, mechanikos inžinerija – 09T).

Konsultantas

dr. Algis DŽIUGYS (Lietuvos energetikos institutas, technologijos mokslai, energetika ir termoinžinerija – 06T).

Disertacija ginama Vilniaus Gedimino technikos universiteto Mechanikos inžinerijos mokslo krypties taryboje:

Pirmininkas

prof. habil. dr. Rimantas BELEVIČIUS (Vilniaus Gedimino technikos universitetas, technologijos mokslai, mechanikos inžinerija – 09T).

Nariai:

dr. Robertas BALEVIČIUS (Vilniaus Gedimino technikos universitetas, technologijos mokslai, mechanikos inžinerija – 09T),

prof. habil. dr. Mykolas DAUNYS (Kauno technologijos universitetas, technologijos mokslai, mechanikos inžinerija – 09T),

prof. habil. dr. Gintautas DZEMYDA (Matematikos ir informatikos institutas, technologijos mokslai, informatikos inžinerija – 07T),

prof. habil. dr. Mindaugas Kazimieras LEONAVIČIUS (Vilniaus Gedimino technikos universitetas, technologijos mokslai, mechanikos inžinerija – 09T).

Oponentai:

prof. habil. dr. Juozas ATKOČIŪNAS (Vilniaus Gedimino technikos universitetas, technologijos mokslai, mechanikos inžinerija – 09T),

prof. habil. dr. Rimantas BARAUSKAS (Kauno technologijos universitetas, technologijos mokslai, mechanikos inžinerija – 09T).

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Adresas: Saulėtekio al. 11, LT-10223 Vilnius, Lietuva.

Tel.: (8 5) 274 4952, (8 5) 274 4956; faksas (8 5) 270 0112;

el. paštas doktor@adm.vgtu.lt

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GENERAL CHARACTERISTIC OF THE DISSERTATION

Research area and topicality of the work. Mechanical properties and their evolution under loading are the most significant factors for the development of various mechanical structures, technologies and equipment. It seems to be natural that deeper understanding of the behaviour of existing and design of new materials presents a challenge in different research areas.

It should be noted, that all the materials are heterogeneous in meso- and micro- scales. They exhibit essential differences, compared to the macroscopic continuum behaviour. Basically, both experimental and numerical simulation methods are extensively applied for investigation purposes.

Experimental techniques, capable of giving a realistic view of the inside of the material and extracting the real data, are very expensive. Therefore, the numerical simulation tools are extensively used as an alternative for investigation purposes. They have considerable advantages allowing the reproduction of multiple experiments and providing comprehensive data about ongoing phenomena.

Recently, numerical technologies have become highly multidisciplinary subjects. They comprise phenomenological and statistical ideas, while mathematical models employ the relations of continuum mechanics, classical discretization methods and molecular dynamics. The Discrete Element Method (DEM) is one of new methods. It is aimed at simulating the dynamic behaviour of the contacting particles. Variable topology of the system of particles is an essential attribute of DEM. However, DEM is in the state of development, and many issues have still to be solved in the nearest future a particular focus is placed on the development of continuum consistent DEM models for elastic solids and investigation of brittle fracture. On the other hand, computer implementation requires the development of new computational tools.

Therefore, the investigation of dynamic the behaviour and fracture of elastic and solid structures by the Discrete Element Method is a relevant problem which has to be solved in the nearest future.

The main objectives and tasks. The main objective of the present work is to enhance the existing and to develop classical continuum consistent DEM models for discretisation of elastic continuum and to apply them to the simulation of the dynamic deformation behaviour and fracture problems.

The following tasks have to be performed:

1. Development of the lattice type DEM models for discretisation of the elastic continuum.
2. Evaluation of the discrete elasticity parameters.
3. Development of a computational DEM algorithm and software code.

4. Investigation and their evaluation of the developed models and application to investigation of the dynamic deformation behaviour and fracture.

Novelty of the research. The present work addresses a relatively new simulation tool, the Discrete Element Method (DEM) and its application to the solution of continuum problems. Original contribution of the work is the development of classical continuum consistent lattice type DEM models. The application of the natural finite elements to evaluating discrete elasticity constants presents the main novelty. Compared to earlier approaches, the developed models exhibit diversity of lattice geometry and cover a full range of Poisson's ratio values.

The particular contribution concerns the development of the original DEM software code DEMMAT-C. The results provided new knowledge on DEM application to elastic dynamics, brittle fracture and post-fracture behaviour.

Research object and methods. Dynamic deformation behaviour and brittle fracture of the heterogeneous solids are considered, while the research is focused on the development and implementation of the classical continuum consistent DEM models. Computational DEM methodology and the original code DEMMAT were used. Standard BEM and ANSYS code was applied for validation purposes.

Practical value. The developed DEM models and software code demonstrated good performance and competitive ability compared to standard BEM technologies in capturing dynamic behaviour and exhibited clear advantages in simulation of brittle fracture and multi-cracking phenomenon, in particular.

The presented DEM development serves as a basis for enhanced elasticity models, including anisotropy, irregular lattice grid and 3D problems and for various fracture models.

The developed methodology may be applied in smaller scales, including atomistic structures.

The structure of the work. The thesis is presented in the Lithuanian language. It consists of six chapters, and the list of 128 references. The thesis comprises 99 pages, 3 tables, including 66 illustrations.

CHAPTER 1. INTRODUCTION

The introduction presents a brief description of the research area and topicality of the thesis, as well as the main goals of investigation, research object, scientific novelty and originality of the work.

CHAPTER 2. STATE-OF-THE-ART

The state-of-the-art chapter contains a conceptual review of the heterogeneous structure of material, continuum models and fracture mechanics as well as the most popular numerical methods, focussing basically on the Finite Element Method (FEM).

A particular emphasis is placed on the Discrete Element Method (DEM). A concept of the DEM is mainly based on the original work of Cundall and Strack (1979), aimed to describe the mechanical behaviour of granular assemblies composed of discrete elements, i.e. discs, and spheres. A discrete element presents a material particle with the prescribed characteristics. A particular state of an individual DEM is assumed to be time-dependent, while tracing of each particle in time is defined by dynamic equilibrium of forces acting on the particle and is described by a system of fully deterministic equations of motion of classical mechanics.

Now, DEM is extensively applied to simulation of solids and basically concerns the dynamic deformation behaviour and fracture problems. Different approaches were elaborated in a series of works. Only some names of outstanding contributors may be mentioned here for the sake of brevity. Herman, Thornton, Morikawa, van Mier, Kun, Donze, Ramm, Tomas, Owen, Munjiza are probably the most widely cited names in this area.

An approach which allows a straightforward application of the structural concept to continua is also called lattice-type model. The structural concept of continuum dates back to the works of Hrennikoff (1941), Kawai (1978) and Herman et al. (1989). The earliest evaluation of 2D continuum described in terms of normal and shear spring stiffness was given by Griffiths and Mustoe (2001).

Based on the review it could be stated that the existing DEM models are diverse, while a unified method for evaluation of discrete elasticity constants consistent with the classical first-order continuum theory is still at the development stage.

CHAPTER 3. THE DISCRETE ELEMENT METHOD FOR CONTINUUM: MODELS AND ALGORITHM

The time-driven Discrete Element Method is applied to simulation of the dynamic behaviour of the elastic continuum. Actually, the present work is restricted to the plane stress problem. Consequently, the plate of constant thickness s is regarded here as a two-dimensional isotropic solid. The properties of elasticity are characterised by elasticity modulus E and Poisson's ratio ν .

Lattice-type discretisation concept and three approaches aimed at developing the classical continuum consistent DEM models and evaluating the discrete elasticity parameters were elaborated.

Discretisation concept. The DEM discretisation approach relies on the concept applied to the description of granular material. The discrete model is implemented by covering a computational domain with the hexagonal grid. The lattice is constructed by equilateral triangles (Fig 1a). The 2D solid is regarded as a system of the finite number N of deformable material particles i ($i = 1, \dots, N$). Each particle i represent a hexagon composed of six equal triangles (Fig 1b). The hexagon occupies a half of each connection line. The location of the particle coincides with the lattice, while the geometry of the particle is defined by a characteristic dimension L of the grid.

Mass of the solid is described by a set of lumped masses m_i , concentrated in the centres of the particles.

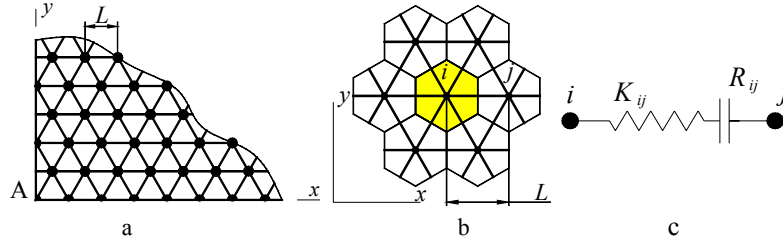


Fig 1. Illustration of a discrete model: a – a fragment of the lattice; b – material particle; c – a model of the connection element $i-j$

Constitutive properties of the solid are assigned to particular lines. Consequently, the interaction of particles i and j is described by the connection element $i-j$. The connection element presents a line segment of the lattice grid. The developed classical continuum consistent DEM approach assumes a description of the discrete model by applying the axially deformed connection element (Fig 1c). If the material is assumed to be heterogeneous, the material constants may be defined as dependent variables on the position $\mathbf{x} = \{x, y\}^T$.

The motion of the material particle of the two-dimensional solid is characterised by two independent translations, therefore, two equations of translation, or dynamic equilibrium, expressed in terms of the forces acting at the centre of the particle, are as follows:

$$m_i \frac{d^2 \mathbf{x}_i(t)}{dt^2} = \mathbf{F}_i(t), \quad (1)$$

where vector $\mathbf{F}_i$ presents the resultant of all external and inter-particle forces. Inter-particle forces F_{ij} , acting on the particle i , are illustrated in Fig 2.

Hence, the inter-particle force F_{ij} actually represents axial forces f_{ij}^n , acting along the connection line. For elastic model its normal component is predefined by elongation of the grid line $i-j$ h_{ij} and by linear spring stiffness K_{ij}^n as

$$f_{ij}^n(t) = K_{ij}^n h_{ij}^n(t). \quad (2)$$

The elastic stiffness parameter K_{ij}^n presents the value axial stiffness. It may be regarded as a discrete elasticity constant and may be expressed in terms of the linear elasticity modulus E and the normal dimension less stiffness constant k_{ij}^n :

$$K_{ij}^n = k_{ij}^n E_{ij} s. \quad (3)$$

Generally, k_{ij}^n is a constant of microscopic nature, whose value should be obtained on the continuum-based arguments and depends on the DEM approach and the lattice geometry.

Direct structural analogy. The simplest DEM approach attributed to evaluation of the discrete elasticity constants is a direct structural analogy. Lattice lines are assumed to be truss elements having only an axial force (Fig 2). Axial stiffness of the connection element $i-j$ is expressed as

$$K_{ij}^n = \frac{E_{ij} A_{ij}^{eff}}{L_{ij}}. \quad (4)$$

Geometric parameters of the element may be expressed in terms of the characteristic grid dimension L . Consequently, the effective section area $A_{ij}^{eff} = a_{ij}^{eff}(L)s$ and the element length $L_{ij} = L$. As a result, the expression (4) may be rewritten in the form of (3). Actually, all elements are defined by a single constant k^n . To enhance this structural approach, the numerical experiment technique is proposed for evaluation of factor k^n . The main concept of the numerical experiment is as follows. Initially, factor k_0^n may be defined from the geometric considerations.

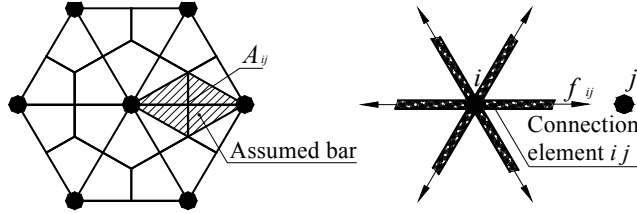


Fig 2. The Nature of inter-particle forces

Then, the value of the stiffness factor is iteratively corrected by correction factor ξ

$$k^n = \xi \cdot k_0^n. \quad (5)$$

The correction is calibrated based on the FE analysis. It is extracted by comparing the loading histories of the selected variable $F(t)$. Finally, the correction is obtained by averaging the differences between the initial DEM and “exact” FEM calculations:

$$\xi = \frac{\sum_{z=1}^q (F_{FEM,z} / F_{DEM,z})}{q}. \quad (6)$$

Here, z stands for the time steps ($z = 1, q$).

Spring model. The continuum consistent spring model is generally similar to the previous approach. Lattice concept replaces continuum by a discrete network of springs. Current consideration is restricted to the single-spring model manifesting that all inter-particle forces are elastic forces defined by a single elasticity constant, more precisely, by axial stiffness k^n of the inter-particle spring.

DEM model of particle i is considered by applying the principle of the virtual work. Generally, the equality of virtual works, obtained due to done by external and internal forces, yields the equation of motion (1).

This elasticity constant is derived explicitly, by equality of the virtual continuous and discrete internal works done by virtual strains in the deformed particle i :

$$\delta U_{Di} = \delta U_{Ci}. \quad (7)$$

Virtual work $\delta U_{Ci} \equiv \delta U_C(\mathbf{x}_i)$ done by the virtual strains $\delta \boldsymbol{\varepsilon} \equiv \delta \boldsymbol{\varepsilon}(\mathbf{x}_i)$ in the point $\mathbf{x}_i$ of continuum reads as

$$\delta U_{Ci} = (\boldsymbol{\varepsilon})^T [\mathbf{D}_C] \delta \boldsymbol{\varepsilon}_i, \quad (8)$$

where $[\mathbf{D}_c]$ is defined by the elasticity matrix of the plane elasticity problem.

The equivalent discrete elastic virtual work δU_D for a discrete particle i stands for the virtual work imposed by virtual interaction with the neighbouring particles averaged over the volume of particle V_i . It may be presented in terms of normal forces and elongations of springs in the same manner. Looking for the analogy with the continuum model (8), it may be presented via the discrete elasticity matrix $[\mathbf{D}_{Di}]$ containing the unknown parameter k^n as follows:

$$\delta U_{Di} = (\boldsymbol{\varepsilon})^T [\mathbf{D}_{Di}] \delta \boldsymbol{\varepsilon}. \quad (9)$$

The equality (7) or, more precisely, the equality of the elasticity matrices $[\mathbf{D}_{Di}] = [\mathbf{D}_c]$ provides the necessary conditions for evaluating spring stiffness k^n .

Omitting the details and mathematical discussion, the following obtained expression was suggested for modelling purposes:

$$k^n = \frac{4}{3\sqrt{3}(1-\nu^2)} \approx \frac{0.7698}{1-\nu^2}. \quad (10)$$

It should be noted that, in the case of two normal and shear stiffness constants, the equality (7) yields the formula derived by Griffiths and Mustoe.

The combined DEM and FEM model. The combined DEM-FEM model presents the new and classical continuum consistent approaches applied to the development of the lattice type 2D DEM model and for evaluation of the discrete elasticity constants. Conceptually, the elastodynamic problem may be solved by FEM, while the lattice grid may be considered as the triangle FEM mesh. Here, particle i considered in the DEM model is assumed to be a polygon composed by 1/3 of each of e ($e = 1, \dots, p$) triangles related to lattice node i (Fig 3a). It is connected with the neighbouring particles by j ($j = 1, \dots, p$) lines.

It was shown that by applying the principle of the virtual work and standard constant strain triangle FE, the Cartesian elastic inter-particle forces in equation (1) may be expressed in terms of stiffness matrices of the triangles incorporated.

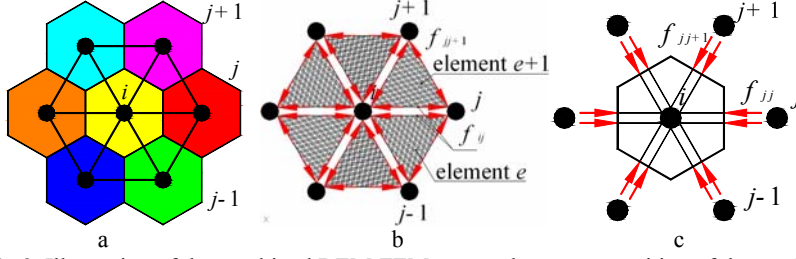


Fig 3. Illustration of the combined DEM-FEM approach: a – composition of the particle by triangles, b – natural forces in the triangles, c – inter-particle forces

DEM operates upon mutual interaction between two particles i and j related by the connection element i - j as defined by (2). The combined DEM-FEM model is based on the analogy between structural and continuum variables in the triangle and employs the natural concept of FEM suggested by Argyris at al. (1988). Let us consider the triangle e defined by nodes i, j and $j-1$ (Fig 3b). The equilibrium of the triangle may be expressed in terms of the natural variables as

$$\mathbf{f}_e^n = [\mathbf{K}_e^n] \mathbf{u}_e^n. \quad (11)$$

Here, vector $\mathbf{f}_e^n = \{f_{eij}^n, f_{eij-1}^n, f_{ejj-1}^n\}^T$ presents natural forces meaning axial forces on the edges, vector $\mathbf{u}_e^n = \{h_{eij}^n, h_{eij-1}^n, h_{ejj-1}^n\}^T$ presents natural displacements meaning normal inter-nodal displacements (elongations of the edges), while $[\mathbf{K}_e^n]$ is 3×3 natural stiffness matrix.

Now, the connection element i - j may be presented as a composition of two edges of the neighbouring triangles e and $e-1$. Therefore, the resultant axial force f_{ij}^n presents the sum of individual edge forces f_{eij}^n and f_{e-1ij}^n (11) (Fig 3c), where the first subscript denotes triangle. In addition, each of the edge forces f_{eij}^n is composed of two components f_{neij}^n and f_{seij}^n involving the influence of the axial stiffness K_{neij}^n and shear stiffness K_{seij}^n . Here, K_{seij}^n reflects the shear effect due to elongation of the neighbour edge. In contrast to the earlier developments, it is a classical continuum consistent constant. Both of the stiffness parameters may be directly extracted from the natural stiffness matrix of the triangle. Finally, the resultant force analogous to the earlier expression (2) reads as

$$f_{ij} = K_{ne\ ij}h_{ij} + K_{ne-1}h_{ij} + K_{se\ i\ j+1}h_{ij+1} + K_{se-1\ ij-1}h_{ij-1} + K_{se\ jj+1}h_{jj+1} + K_{se-1\ jj-1}h_{jj-1}. \quad (12)$$

In the case of a hexagonal lattice, the elasticity constants are defined within the equilateral triangle, Therefore, all natural stiffness matrices are equal.

Finally, elasticity constants may be expressed in the form of (3). For hexagonal lattice:

$$k_n^n = \frac{1}{\sqrt{3}(2+2\nu)} \left(1 + \frac{2}{3(1-\nu)} \right), \quad k_s^n = \frac{1+3\nu}{3\sqrt{3}(2+2\nu)_s}. \quad (13)$$

The above expression considerably modifies the lattice-type model. Firstly, it is not dependent on the lattice geometry and may be extended to various polygons composed of triangles. From a physical point of view, mutual interaction is extended to the neighbouring particles. Algorithmic consequences should be evaluated additionally.

Fracture model. Fracture is considered as brittle rupture of inter-particle connection element i - j under tension. Formally, it is defined by the condition:

$$F_{ij} > R_{ij}. \quad (14)$$

The fracture leading to debonding of the neighbouring particles occurs, when the tensile force exceeds the element's load carrying capacity:

$$R_{ij}^n = \sigma_{0ij} A_{ij}^{eff}, \quad (15)$$

where σ_{0ij} is the tensile strength, while A_{ij}^{eff} is the effective section area.

When the condition (14) is not fulfilled, i.e. $F_{ij}^n < R_{ij}^n$, the connection element works as a spring and interaction of particles is allowed. When the condition (14) is satisfied, disconnection of the element occurs and the inter-element stiffness is removed from the equation of motion (3). In the case of repeated interaction of particles, i.e. $h_{ij} \leq 0$, the connection element is restored again.

CHAPTER 4. ONE-DIMENSIONAL PROBLEM

The lattice – based DEM models for continuum exhibit structural analogy and equivalence to frame or truss structures. This approach is naturally exact for 1D continuum. Therefore, the performance of DEM and the developed software was initially examined by considering the rupture and post-rupture dynamic behaviour of the bar.

One-dimensional visco-elastic solid domain in the form of a uniform prismatic bar is considered as discrete elements (Fig 4). Actually, continuum is replaced by a chain of discrete elements (particles) connected by generalized connection elements, i.e. springs and dashpots. The domain is restricted by the rigid walls A and B, while the external load is imposed by the motion of the wall B. The motion is controlled by the displacement function $u(t)$. Dynamic behaviour of the continuum is simulated by DEM and described by equations of motion (1). Fracture occurs at time instant $t_r = 9.45 \mu\text{s}$ in the artificially weakest section inside the solid when driving force exceeds the material resistance.

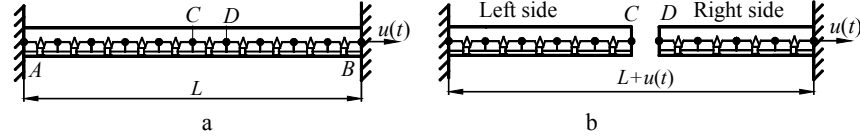


Fig 4. Prismatic bar: a – geometry before fracture, b – post-fracture geometry

Numerical simulation is illustrated by the time history of the reaction force F_{RA} of the wall A and the internal force of the element defined by the coordinates $x = 0.3L$ and $x = 0.6L$ (Fig 5). Discretisation was made subdividing the continuum into 1000 elements ($n = 1000$). The graph clearly illustrates the propagation of the waves and shock effect after rupture. Elastic behaviour is provided by high oscillations.

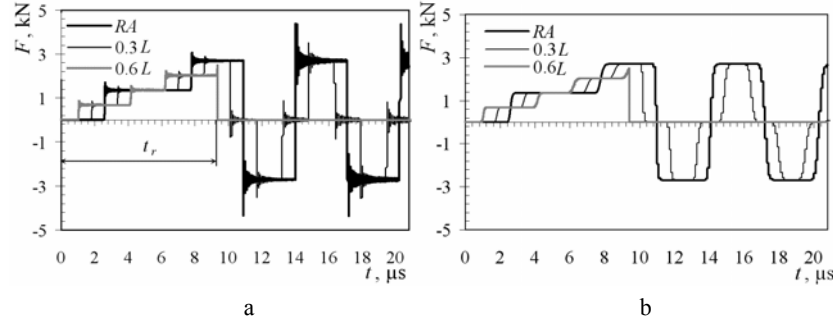


Fig 5. Time histories of forces: a – without damping, b – with damping

Discretisation effect, defined in terms of the numerical oscillation factor, may be characterised by relative deviation of the reaction force F as the ratio $\alpha = F_{max}/F_{aver}$. and by energy disbalance. The influence of discretisation is summarized and illustrated in Fig 6.

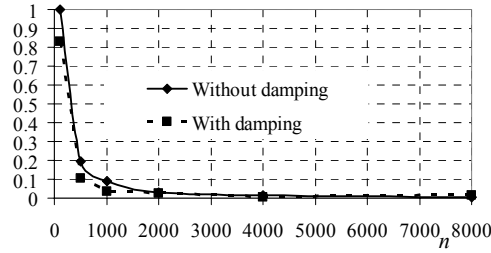


Fig 6. Normalized dependence of maximal disbalance for different discretisations

Generally, 1D solution and implemented DEM technique demonstrate their ability to capture the impulsive loading imposed in fracture. The observed convergence tendencies illustrate DEM possibilities. The final results depend, however, on the values of the material constants as well as on the space and time discretisation parameters.

CHAPTER 5. SIMULATION OF TWO-DIMENSIONAL CONTINUUM BY DEM

The developed lattice type and classical continuum consistent 2D DEM model were examined numerically. The plate with the thickness $s = 10$ mm is considered as a two-dimensional rectangular solid domain. The geometry of the domain is defined by two characteristic dimensions, $H = 400$ mm and $B = 100$ mm (Fig 7). The plate boundaries AB and CD are assumed to be clamped by being connected to rigid walls, while AC and BD are free boundaries. External tension loading is implemented via the displacement of the boundary CD, i.e. $u(t)$. The material is characterized by the following properties. Density of material is $\rho = 2500$ kg/m³, elasticity modulus $E = 17.1$ GPa and Poisson's ratio $\nu = 0.266$.

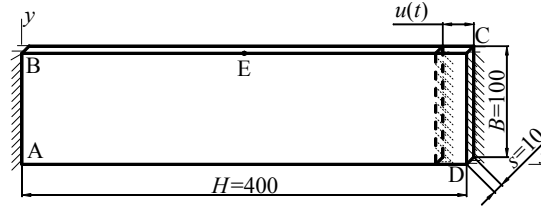


Fig 7. Geometry of the plate with boundary conditions and loading

Structural analogy and calibration concept defined by (5, 6) are illustrated by solving the problem of the plate under tension. The plate is loaded by the prescribed displacement $u(t) = 0 \div 10$ mm (at constant velocity $v_{CD}(t) = 1$ m/s). The loading is implemented with time increment $\Delta t = 156.1 \cdot 10^{-9}$ s.

The lattice grid having a characteristic dimension $L = 3.333$ mm was employed.

Initially, the linear dynamic problem was solved by DEM, applying purely geometric initial stiffness value $k_0^n = \sqrt{3}/3 = 0.577$. Later, it was corrected by the FEM results according to (5, 6), considering the variation of the reaction force as calibration parameter, and the final value $k^n = 0.857$ was obtained.

Simulation results are shown in Fig 8. The graph presents FEM results as well as the initial and final DEM results with the corrected stiffness $k^n = 0.857$.

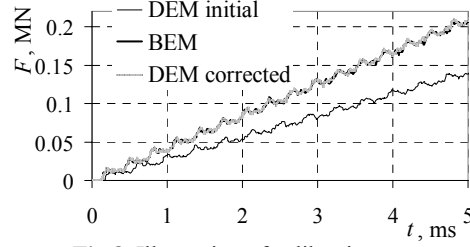


Fig 8. Illustration of calibration concept

It can be observed, however, that the behaviour of a single parameter is not able to capture adequately the influence of the Poisson's ratio ν , yielding up to 40 % differences compared to an “exact” FE solution. The calibration is completely applicable in the vicinity of $\nu = 0.33$.

Other models were solved by applying the single-spring lattice model involving hexagonal grid and stiffness parameter (10).

The results demonstrating the same tendency of variation of transversal displacements against Poisson's ratio are plotted in Fig 9. Considering the above graph, we can see that DEM results are accurate for $\nu = 0.33$, while being dramatically diverging for other values.

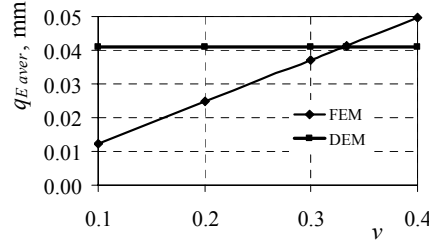


Fig 9. Variation of average transversal displacement against Poisson's ratio

On the contrary, the combined DEM and BEM model yielded perfect coincidence with the “exact” solution within the entire range of the Poisson’s ratio values Fig 10.

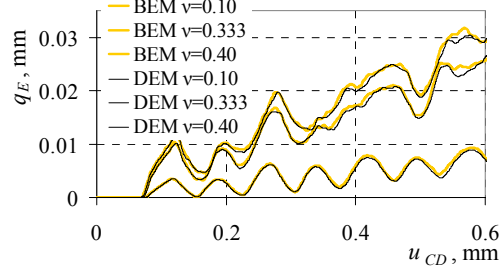


Fig 10. Variation of transversal displacement against Poisson’s ratio

Simulation of plate fracture. The developed lattice model was applied to simulation of the dynamic behaviour of the above plate in brittle fracture according to (14, 15). Two types of tensile strength were examined against fracture. A homogeneous material is characterized by the constant strength value $\sigma_0 = 250$ MPa. A heterogeneous material is defined by the average value $\sigma_0 = 250$ MPa, while random heterogeneity is governed by Gaussian distribution. Hence, tensile strength values σ_{0ij} of any connection element ij are assumed to be random parameters, ranging within $(1 - \alpha)\sigma_0 \leq \sigma_{0ij} \leq \sigma_0(1 + \alpha)$ and being generated computationally, using the random number generator. Here, α stands for heterogeneity fraction $0 \leq \alpha \leq 1$, while their value is assumed to be $\alpha = 0.2$.

The possibilities of DEM are demonstrated by the time history of the reaction force of the wall AB (Fig 11) by comparing the results obtained for homogeneous and heterogeneous materials. The duration of the fracture of a homogeneous plate is two times shorter compared to that of a heterogeneous plate.

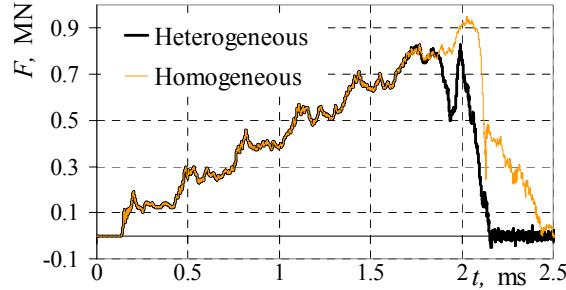


Fig 11. Time variation of the reaction forces acting on the wall AB

The propagation of cracking from the initial state up to failure is presented in Fig 12 for a homogeneous plate, and, in Fig 13, for a heterogeneous plate. Here, debonded connections are shown by thick lines.

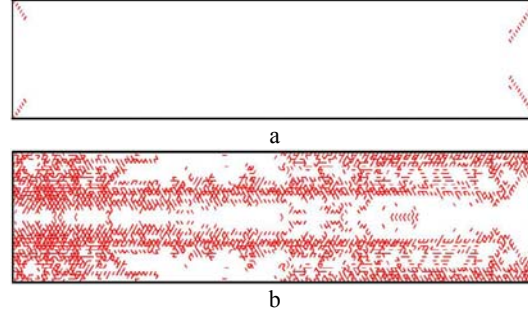


Fig 12. Cracking patterns of the homogeneous plate at various time moments:
a – $t = 1.70$ ms, b – $t = 2.30$ ms,

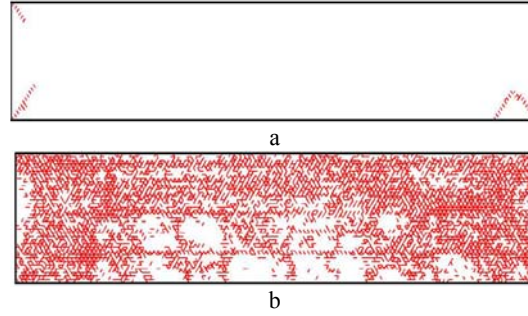


Fig 13. Cracking patterns of the heterogeneous plate at various time moments:
a – $t = 1.70$ ms, b – $t = 2.30$ ms

The fracture of the homogeneous plate (Fig 12) is of regular pattern and is symmetric. The fracture of the heterogeneous plate (Fig 13) is much more complicated. Multiple cracking of random character and the formation of several irregular magister cracks can be observed.

CHAPTER 6. GENERALIZATIONS AND CONCLUSIONS

On the basis of the state-of-the-art it could be stated that DEM has a high potential for modelling of solids, and exhibits particular advantages for elastic dynamic behaviour and fracture of heterogeneous material structures. The existing DEM models possessing high diversity are based on various simplified approaches, while a unified method for evaluating discrete and classical

continuum consistent elasticity constants is still at the development stage. On the basis of the research performed the following conclusions can be drawn:

1. The lattice - based DEM models for continuum exhibit structural analogy and equivalence to frame or truss structures. Based on the results of 1D problem, the influence of the size of space discretisation, damping effect and pre - fracture model were studied by employing energy balance and suitability of DEM algorithm, and the validity of the developed code was confirmed.

2. The 2D plain stress problem was studied by applying the hexagonal lattice model with a single elasticity constant. This constant was evaluated by two different approaches based on bar analogy and virtual displacement method. Finally, it was stated that the applied single - constant approach exhibits the same trends as other approaches irrelevant of the evaluation method used.

3. It was found that the single - parameter lattice model is applicable only for Poisson's ratio $\nu = 0.33$.

4. Here elasticity constants are defined by applying natural triangle finite element.

5. Comparing the existing models, it could be stated that the suggested method for evaluating the discrete elasticity constants presents the combined FEM/DEM method.

6. It was theoretically proved that the combined DEM/FEM approach is independent of lattice geometry and values of the Poisson's ratio.

7. The developed DE models were applied to brittle fracture and investigation of post-fracture behaviour of heterogeneous plates. The results exhibited suitability of the model and code to capture qualitatively multi-cracking phenomenon, which is extremely difficult to achieve by the finite element method codes. Modelling results allow us to show the influence of heterogeneity on the ultimate load and cracking patterns.

8. The numerical results proved that the updated DEM algorithm and the developed code present an efficient tool for analysing the dynamic behaviour of 1D and 2D dynamic problems.

9. The presented DEM developments and software code serve the basis for creating the enhanced continuum models including anisotropy, 3D problems and various fracture criteria and mechanisms. Comprehensive future research is still required for determining their application to fracture problems.

PUBLISHED WORKS ON THE TOPIC OF THE DISSERTATION

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2. VADLUGA, V.; KAČIANAUSKAS, R. Investigation of the single-spring lattice model in simulation of 2 D solid problems by DEM. *Mechanika*, 2007, Nr. 5 (67), p. 5–13. ISSN 1392-1207 (ISI Master Journal List).

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3. VADLUGA, V.; KAČIANAUSKAS, R. Application of discrete element method to modelling of brittle fracture of one-dimensional structures. In *The 8th International conference "Modern building materials, structures and techniques"*: selected papers / edited by E. K. Zavadskas, P. Vainiūnas, F. M. Mazzolani. Vilnius: Technika, 2004, p. 917–920 ISBN 9986-05-757-4 (ISI Proceeding).
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NEVIENALYČIŲ STRUKTŪRŲ DINAMINIO DEFORMAVIMO IR IRIMO MODELIAVIMAS DISKREČIŲJŲ ELEMENTŲ METODU

Tyrimų sritis ir darbo aktualumas. Kuriant modernias įvairios paskirties mechanines sistemas, technologijas ir įrangą, svarbiomis tampa jas sudarančios medžiagos. Savaime suprantama, kad žinomos ir naujai kuriamos medžiagos dabar kur kas išsamiau nagrinėjamos daugelyje mokslo šakų, įskaitant ir medžiagų mechaniką. Visos medžiagos mezo- ir mikrostruktūros požiūriu yra nevienalytės. Jų mikroskopinės savybės skirtingos, lyginant su įprastu kontinuumu. Medžiagų savybėms tirti dažniausiai taikomi eksperimentiniai metodai.

Eksperimentiniais metodais ištirti medžiagos struktūras ir jose vykstančius procesus ir įvertinti tam tikras jų savybes labai brangu. Tai viena priežasčių, kodėl skaitinis modeliavimas tampa realia tyrimų alternatyva. Skaitinį eksperimentą galima kartoti daug kartų, valdant bandinio parametrus, išlaikant tas pačias sąlygas, ir stebėti reiškiniai būdingus rodiklius visame tūryje.

Šiuolaikiniai modeliavimo metodai yra kompleksiniai. Jie jungia fenomenologines ir statistines idėjas, o matematiniai modeliai sudaromi taikant kontinuumo mechanikos ir jų diskrečiųjų modelių bei molekulinės dinamikos priklausomybes. Diskrečiųjų elementų metodas (DEM) taip pat priskiriamas šiuolaikinių metodų kategorijai. Jis skirtas kontaktuojančių dalelių sistemų dinaminiam modeliavimui. Kintanti dalelių sistemos topologija – būdingas metodo požymis.

Pastaruoju metu DEM jau taikomas kontinuumui modeliuoti ir praktikoje aktualiams irimo uždaviniams spręsti.

Reikia pastebėti, kad deformuojamo kūno modeliavimas yra aktuali problema, o medžiagas kaip nevienalytį deformuojamąjį kontinuumą aprašantys modeliai dar nėra pakankamai tobuli.

Darbo tikslas ir uždaviniai. Pagrindinis darbo tikslas – patobulinti žinomus ir/arba sudaryti naujus su klasikine kontinuumo teorija suderintus DEM modelius, skirtus tampriajam kontinuumui diskretizuoti, ir pritaikyti juos dinaminio deformavimo ir irimo uždaviniams.

Darbo tikslui pasiekti suformuluoti tokie pagrindiniai uždaviniai:

1. Sudaryti tampriajam kontinuumui diskretizuoti skirtą tinklinį DEM modelį.
2. Nustatyti DEM modelio tamprumo rodiklius.
3. Sudaryti DEM skaičiavimo algoritmą ir programą.
4. Išnagrinėti ir įvertinti modelių taikymo ypatumus sprendžiant dinaminio deformavimo ir irimo uždavinius.

Darbo naujumas ir originalumas. Darbas skirtas ištirti diskrečiųjų elementų metodo taikymo kontinuumo uždaviniams spręsti ypatumus. Darbas originalus tuo, kad nagrinėjami tik su klasikine (bemomentine) kontinuumo teorija suderinti tinkliniai DEM modeliai. Natūrinių baigtinių elementų pritaikymas diskrečiųjų tamprumo rodiklių nustatymui yra esminė darbo naujovė. Lyginant su ankstesniais modeliais, siūlomas modelis pasižymi esminiais pranašumais, nes jis neribojamas tinklelio geometrijos ir Puasono koeficiento reikšmių.

Parašyta originali DEM programa DEMMAT-C, o gauti rezultatai suteikė naujų žinių apie modeliavimo DEM ir trapių irimo bei poiriminės elgsenos modeliavimo ypatumus.

Tyrimo objektas ir metodai. Darbas skirtas kontinualiųjų nevienalyčių struktūrų dinaminio deformavimo ir irimo uždaviniams nagrinėti. Naujų su klasikine kontinuumo teorija suderintų DEM modelių, skirtų tampriajam kontinuumui diskretizuoti, kūrimas ir jų įvertinimas – pagrindinis tyrimų objektas.

Skaitinis DEM metodas ir parašyta DEMMAT-C programa yra pagrindinis tyrimo įrankis. Sukurtų metodų kokybei įvertinti taikoma BEM komercinė programa ANSYS.

Praktinė vertė. Pasitelkus sudarytus modelius ir programą, šiame darbe įrodytos DEM galimybės ir pranašumai, lyginant su BEM, modeliuojant dinaminį deformavimą, trapųjį irimą ir pleišėjimą.

Sudaryti DEM modeliai yra baziniai, jie gali būti toliau vystomi, pritaikant juos anizotropinėms terpėms, laisvos formos tinkleliui ir trimačiams uždaviniams. Jais galima realizuoti įvairius irimo kriterijus ir mechanizmus.

Pasiūlyti metodai gali būti pritaikyti ne tik medžiagos mikrostruktūroms, bet ir atomų struktūroms modeliuoti.

Darbo apimtis. Darbą sudaro bendra darbo charakteristika, 6 skyriai, išvados, literatūros sąrašas (128 pozicijos) ir publikacijų sąrašas. Bendra disertacijos apimtis – 99 puslapiai, 66 iliustracijos ir 3 lentelės.

Pirmame disertacijos skyriuje apibrėžta tyrimų sritis, suformuluotas darbo tikslas ir iškelti uždaviniai, aprašytas darbo naujumas ir originalumas, paaiškintas tyrimo objektas ir metodai bei praktinė vertė, pateikta aprobavimas.

Antrame disertacijos skyriuje pateikta literatūros apžvalga. Šiame skyriuje trumpai aprašytos nevienalytės struktūros, irimo uždavinių sprendimas ir skaitiniai metodai. Daug dėmesio skirta DEM idėjai ir taikymo sritims.

Trečiame disertacijos skyriuje aprašyti modeliai ir algoritmas. Paaiškintas kiekvieno modelio sudarymo principas.

Ketvirtame disertacijos skyriuje aprašytas vienmačio uždavinio pavyzdys. Šiame skyriuje aprašyti sprendinio kokybę įvertinantys rodikliai, kurie panaudoti aprašant vienmačio uždavinio rezultatus.

Penktame disertacijos skyriuje aprašyti dvimačių uždavinių pavyzdžiai, aptarti rezultatai.

Šeštame disertacijos skyriuje pateikti apibendrinimai ir išvados.

Darbo pabaigoje pateiktas literatūros sąrašas

Apibendrinimai ir išvados

Išanalizavus kitų autorių darbus, galima teigti, kad DEM yra potencialus kontinualiųjų struktūrų diskretizavimo metodas, kurio pranašumai pasireiškia modeliuojant dinaminį deformavimą ir nevienalyčių struktūrų trapųjį irimą. Visi žinomi DEM modeliai remiasi įvairaus pobūdžio prielaidomis, o universalus su kontinuumo teorija suderintas diskrečiųjų DEM tamprumo rodiklių nustatymo būdas dar nesukurtas. Apibendrinus disertacijoje atliktus tyrimus, suformuluotos šios išvados:

1. Tinkliniai DEM modeliai pagrįsti strypine analogija, kai kontinuumas pakeičiamas strypine struktūra. Ištyrus vienmačio pavyzdžio diskrečiųjų elementų matmenų santykinę ribą, slopinimo rodiklių ir deformavimo kreivės aproksimavimo trūkio taško aplinkoje įtaką pagal energijos balansą, patvirtintas algoritmo ir programos tinkamumas dinaminiais reiškiniams modeliuoti.

2. Dvimačio tampriojo kontinuumo pavyzdžiai (dvimatė plokštelė) DEM buvo modeliuojami diskretizavus šešiakampiu (sudarytu iš taisyklingų trikampių) tinkleliu, aprašomu vienu standumo rodikliu. Diskrečiojo modelio tamprumo rodikliai buvo nustatomi dviem skirtingais būdais: taikant strypinę analogiją ir virtualiųjų poslinkių metodu lyginant su kontinuumo fizinėmis savybėmis. Apibendrinus gautus rezultatus nustatyta, kad vieno parametro diskrečiojo modelio tamprumo savybėms aprašyti nepakanka, nepriklausomai kokių būdu jis būtų nustatytas.

3. Iš tyrimų matyti, kad diskretusis modelis, aprašomas vieno parametro tamprumo rodikliu, realizuoja kontinuumo geometrijos kitimą deformuojant tik tuomet, kai Puasono koeficientas $\nu = 0,33$.

4. Įsitikinus, kad vieno parametro diskrečiojo modelio tamprumo rodikliams apibrėžti nepakanka, buvo pasiūlyta tamprumo rodiklius aprašyti tamprumo matrica, o jos reikšmes nustatyti taikant natūrinius baigtinius elementus.

5. Palyginus žinomus teorinius modelius parodyta, kad pasiūlyta tamprumo rodiklių nustatymo metodika jungia DEM ir BEM teorijas, todėl tai yra kombinuotas DEM/BEM metodas.

6. Teoriškai įrodyta ir gautais rezultatais patvirtinta, kad kombinuotas DEM/BEM metodas nepriklauso nuo tinklelio geometrijos ir Puasono koeficiento reikšmių.

7. Sudarytieji modeliai pritaikyti nevienalytės plokštelės trapijam irimui ir pažeistos struktūros dinaminiam deformavimui modeliuoti. Rezultatai parodė, kad DEM modelis ir programa kokybiškai realizuoja pleišėjimo reiškinį, o tai ypač sunku taikant BEM. Rezultatai leido ir kiekybiškai palyginti nevienalytikumo įtaką ribinei jėgai ir pleišėjimo formai.

8. Gauti rezultatai patvirtina, kad patobulintas DEM algoritmas ir sukurta programa tinkami vienmačių ir dvimačių struktūrų dinaminiam deformavimui modeliuoti.

9. Sudaryti DEM modeliai ir programa gali būti toliau vystomi, pritaikant juos anizotropinėms terpėms, trimačiams uždaviniams ir įvairiems irimo kriterijams, tačiau kiekybei įvertinti reikalingi dar išsamesni tyrimai.

Short description about the author

Vaidas Vadluga was born in Kupiškis on 4th January, 1979. He began his studies at Vilnius Gediminas Technical University in 1997. He gets Bachelor's Degree of Transport Engineering in 2001 and Master's Degree of Engineering Informatics – in 2003. Since then he began PhD studies at VGTU in a field of Technological Sciences in a branch of Mechanical Engineering. Throughout his PhD studies he has worked as assistant in Department of Strength of Materials at VGTU. He graduated from PhD studies in 2007 and began working in the Laboratory of Numerical Modelling as research fellow.

Trumpos žinios apie autorių

Vaidas Vadluga gimė 1979 m. sausio 4 d. Kupiškyje. 1997 m. įstojo į Vilniaus Gedimino technikos universitetą. 2001 m. įgijo transporto inžinerijos bakalauro laipsnį, o 2003 m. jam suteiktas inžinerinės informatikos mokslo magistro laipsnis. Tais pačiais metais buvo priimtas į VGTU doktorantūrą technologijos mokslų srityje mechanikos inžinerijos mokslo kryptyje. Per visą studijų laikotarpį doktorantas dirbo pedagoginį ir mokslinį darbą VGTU Medžiagų atsparumo katedroje. Doktorantūros studijas baigė 2007 m. Nuo 2007 m. pradėjo dirbti VGTU Skaitinio modeliavimo mokslo laboratorijos jaunesniojo mokslo darbuotoju.

Vaidas Vadluga

SIMULATION DYNAMIC OF DEFORMATION AND FRACTURE BEHAVIOUR OF HETEROGENEOUS STRUCTURES BY DISCRETE ELEMENT METHOD

Summary of Doctoral Dissertation

Technological Sciences, Mechanical Engineering (09T)

Vaidas Vadluga

NEVIENALYČIŲ STRUKTŪRŲ DINAMINIO DEFORMAVIMO IR IRIMO MODELIAVIMAS DISKREČIŲJŲ ELEMENTŲ METODU

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leidykla „Technika“, Saulėtekio al. 11, LT-10223 Vilnius, <http://leidykla.vgtu.lt>

Spausdino UAB „Baltijos kopija“,

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