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Implicit and Explicit Newmark Method for the Discrete Element Method: Beam Bound Model

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Abstract

The Discrete Element Method (DEM) is a numerical technique used to analyze the motion of discrete particles. DEM is mostly used to analyze the behavior of granular materials such as sand, gravel, powders, etc. The method can also be combined with the Beam Bound Model (BBM), which allow the method to be used for continual problems simulation. However, method is overshadowed in this field by the Finite Element Method. Its primary application is found in problems requiring consideration of both continuum and discrete properties, such as crack propagation, especially in the case of dynamic behaviour. The problem with DEM is its high computational cost, but by using properties specific to the crack propagation problem, efficient methods for solving differential equations can be used. This paper focuses on the efficiency of using the implicit Newmark-beta method to analyze crack propagation in concrete members.

Keywords: discrete element method, beam bound model, Newmark-beta method, static and dynamics analysis

1 Introduction

The discrete element method is a numerical method based on the motion and contacts of particles firstly described by P.A. Cundall in his papers [1, 2]. Since then, there have been significant advances in the development of the method and its extension into many areas. One of the core extensions was the introduction of bonded elements and the creation of the bound particle model (BPM), which is described in [3]. This model allows for the analysis of continuum problems, but involves stiffnesses that are difficult to capture, especially in cases of mutual particle rotation. One way to approach this problem is to use a BBM that inserts imaginary beam elements between the elements to provide force transfers. These models are described in papers [4, 5].

The base of the discrete element method is the solution of systems of differential equations. These are commonly solved using an integration scheme based on the explicit Euler method described in [6]. However, this method requires very short time steps for stability, the length of which depends on the mass to stiffness ratio. In the case of very stiff materials such as concrete or steel, the method becomes very computationally time expensive.

For this reason, the use of more effective solution methods is needed. An overview of the different numerical methods suitable for DEM and their effectiveness is discussed in [7]. These methods are mostly used in explicit variants, since the frequent contact changes in DEM make it infeasible to use long time steps for efficient use of implicit methods. In the context of crack propagation problems, especially in building structures, it is advantageous to use implicit methods due to the infrequent occurrence of contact changes. For this reason, we adopted the Newmark-beta method, initially proposed in [8], due to its stability proofs independent of the time step length in the case of the implicit expression.

2 Theoretical background of DEM-BBM

The base of the DEM is a system of second order differential equations of motion of the form,

$$\mathbf{M}\ddot{\mathbf{u}}(t) + \mathbf{C}\dot{\mathbf{u}}(t) + \mathbf{K}\mathbf{u}(t) = \mathbf{f}^e(t) \quad \text{for} \quad t \geq 0, \tag{1}$$

where $\mathbf{M}$ represent mass matrix, $\mathbf{C}$ is damping matrix and $\mathbf{K}$ is stiffness matrix. $\mathbf{f}^e$ represents external forces that can be varied over time t and $\mathbf{u}$ stand for displacement vector as a function of t, its first derivative represents velocity, while the second derivative represents acceleration.

The system of differential equations is defined by initial conditions on velocity and acceleration and also boundary conditions as,

$$\ddot{\mathbf{u}}(0) = \mathbf{a}_0 \quad \text{and} \quad \dot{\mathbf{u}}(0) = \mathbf{v}_0, \tag{2}$$

$$\mathbf{B}\mathbf{u}(t) = \mathbf{o}, \tag{3}$$

where $\mathbf{a}_0$ stand for initial acceleration vector and $\mathbf{v}_0$ for initial velocity vector. Matrix $\mathbf{B}$ is boundary constrains representing support of member.

2.1 Damping, stiffness and mass matrix

The matrices denoted as $\mathbf{K}$ and $\mathbf{C}$, are global matrices assembled for a system in which $\mathbf{K}, \mathbf{C} \in \mathbb{R}^{n_d,n_d}$ where n_d is the number of degrees of freedom. These matrices are constructed by assembling sub-matrices corresponding to individual contacts. The contacts are categorized into bound and unbound contacts. The global system matrices are then obtained as follows,

$$\mathbf{K} = \mathbf{L}_b\mathbf{T}_b\mathbf{K}_{db}\mathbf{T}_b^T\mathbf{L}_b^T + \mathbf{L}_u\mathbf{T}_u\mathbf{K}_{du}\mathbf{T}_u^T\mathbf{L}_u^T \tag{4}$$

where index b correspond to matrices for bounded contacts and u for unbounded contacts. $\mathbf{L} \in \mathbb{R}^{n_d,6n_c}$, where n_c represent amount of contacts, are allocation matrix which maps diagonal stiffness matrix $\mathbf{K}_d \in \mathbb{R}^{6n_c,6n_c}$ to its corresponding degree of freedom. $\mathbf{T} \in \mathbb{R}^{6n_c,6n_c}$ are block diagonal transformation matrix for each contact from local to global coordinate system. Global matrix $\mathbf{C}$ is generated in the identically.

As mentioned, the creation of local contact matrices are divided for bound and unbound contacts. In the basic form of the DEM, only unbound contacts occur, most often defined according to the Hertz's equations. Examples of different contact models can be found in [9]. However, in our case, models that keep the compressive strength for bound and unbound contacts identical are used to match the behavior. The shear stiffness is then introduced under the assumption of behavior corresponding to granular materials based on experiments. The damping forces are calculated based on the harmonic oscillator equations. The resulting local single contact matrices are expressed as

$$\mathbf{K}_u = \begin{bmatrix} \frac{AE}{l} & 0 & 0 & -\frac{AE}{l} & 0 & 0 \\ 0 & k_{t0} & 0 & 0 & -k_{t0} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{AE}{l} & 0 & 0 & \frac{AE}{l} & 0 & 0 \\ 0 & -k_{t0} & 0 & 0 & k_{t0} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} + k_t(u) \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \tag{5}$$

$$\mathbf{C}_u = 2\xi_u \begin{bmatrix} \sqrt{\frac{AE}{l}m_r} & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{k_{t0}m_r} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{\frac{AE}{l}m_r} & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{k_{t0}m_r} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \tag{6}$$

where A stand for area of contact, l is length between centre of elements, and E stand for Young's modulus, that correspond to the model for bounded elements. Stiffness

k_{t0} and $k_t(u)$ are the stiffnesses to be obtained from experimental friction tests such as [10]. m_r is reduced mass of elements in collision, and ξ is damping ratio coefficient. The stiffness matrix for bonded contacts is based on Timoshenko's beam theory, and its derivation can be found, for example, in [11]. The construction of the damping matrix follows the same approach as for unbound contacts. Resulting matrix form for single contact are,

$$\mathbf{K}_b = \begin{bmatrix} \frac{AE}{l} & 0 & 0 & -\frac{AE}{l} & 0 & 0 \\ 0 & \frac{12EI}{l^3(1+\phi)} & \frac{6EI}{l^2(1+\phi)} & 0 & -\frac{12EI}{l^3(1+\phi)} & \frac{6EI}{l^2(1+\phi)} \\ 0 & \frac{6EI}{l^2(1+\phi)} & \frac{(4+\phi)EI}{l(1+\phi)} & 0 & -\frac{6EI}{l^2(1+\phi)} & \frac{(2-\phi)EI}{l(1+\phi)} \\ -\frac{AE}{l} & 0 & 0 & \frac{AE}{l} & 0 & 0 \\ 0 & -\frac{12EI}{l^3(1+\phi)} & -\frac{6EI}{l^2(1+\phi)} & 0 & \frac{12EI}{l^3(1+\phi)} & -\frac{6EI}{l^2(1+\phi)} \\ 0 & \frac{6EI}{l^2(1+\phi)} & \frac{(2-\phi)EI}{l(1+\phi)} & 0 & -\frac{6EI}{l^2(1+\phi)} & \frac{(4+\phi)EI}{l(1+\phi)} \end{bmatrix}, \tag{7}$$

$$\mathbf{C}_b = 2\xi_b \begin{bmatrix} \sqrt{k_{b1,1}m_r} & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{k_{b2,2}m_r} & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{k_{b3,3}J_r} & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{k_{b4,4}m_r} & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{k_{b5,5}m_r} & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{k_{b6,6}J_r} \end{bmatrix}, \tag{8}$$

where I is moment of inertia according to cross-section geometry, while J is moment of inertia according to discrete element shape and mass. ϕ stands for sheer coefficient for Timoshenko's beam theory. The cross section of contact is evaluated with dependence of coefficient λ, whose description, influence on the calculation and appropriate values are discussed in the article [12].

The mass matrix $\mathbf{M} \in \mathbb{R}^{n_d,n_d}$ is compiled for the system independently of the contacts. We consider a diagonal mass matrix, where we assign to each respective degree of freedom the mass of a discrete element, respectively its moment of inertia as follows,

$$\mathbf{M} = \begin{bmatrix} m_1 & & & & & & \\ & m_1 & & & & & \\ & & J_1 & & & & \\ & & & \ddots & & & \\ & & & & m_n & & \\ & & & & & m_n & \\ & & & & & & J_n \end{bmatrix}. \tag{9}$$

2.2 Crack initiation criteria

Cracks can form in bounded contacts. At each calculated time step, the exceeding of the maximum stress is verified. If the maximum stress condition is exceeded, a crack occurs and the initial contact stiffness matrix is removed from the global matrix of

the system. The internal forces in local coordinates $\mathbf{f}_{Lb}^{int}$ on each element is calculated based on the displacement as follows,

$$\mathbf{f}_{Lb}^{int} = \mathbf{K}_{db}\mathbf{T}_b^T\mathbf{L}_b^T\mathbf{u}(t), \tag{10}$$

Based on the internal forces, we can calculate the normal and shear stresses in the individual beam members. Since we do not consider any forces acting along the length of the elements, the maximum stress for each member will be as follows,

$$\boldsymbol{\sigma}_b = \begin{bmatrix} \frac{1}{A} & 0 & \frac{1}{W_y} \\ \frac{1}{A} & 0 & \frac{-1}{W_y} \\ 0 & \frac{3}{2A} & 0 \end{bmatrix} \mathbf{f}_L^{int}, \tag{11}$$

where W_y is section modulus for corresponding cross section. In (11) we can create a block diagonal matrix from the partial matrices and calculate all stresses for all members simultaneously.

3 Application of Newmark-beta method

Newmark-beta methods is a numerical method for solving differential equations of the form,

$$\mathbf{M}\ddot{\mathbf{u}}(t) + \mathbf{C}\dot{\mathbf{u}}(t) + \mathbf{f}^{int}(t)\mathbf{u}(t) = \mathbf{f}^{e}(t) \tag{12}$$

Newmark developed and proved the use of the extended mean value theorem and its application to the dynamics of structures. The resulting discretized equations are,

$$\dot{\mathbf{u}}_{n+1} - \gamma\Delta t\ddot{\mathbf{u}}_{n+1} = \dot{\mathbf{u}}_n + (1-\gamma)\Delta t\ddot{\mathbf{u}}_n \tag{13}$$

$$\mathbf{u}_{n+1} - \beta\Delta t^2\ddot{\mathbf{u}}_{n+1} = \mathbf{u}_n + \Delta t\dot{\mathbf{u}}_n + \frac{\Delta t^2}{2}(1-2\beta)\ddot{\mathbf{u}}_n \tag{14}$$

$$\mathbf{M}\ddot{\mathbf{u}}_{n+1} + \mathbf{C}\dot{\mathbf{u}}_{n+1} + \mathbf{f}_{n+1}^{int} = \mathbf{f}_{n+1}^{e} \tag{15}$$

where Δt is time step size. Coefficients γ and β which effect numerical stability and energy dissipation. The coefficients are limited by

$$0 \leq \gamma \leq 1, \quad 0 \leq 2\beta \leq 1 \tag{16}$$

The most commonly used combinations are $\gamma = 0.5, \beta = 0$ which yields the Explicit central difference scheme. In the case of introducing $\gamma = 0.5, \beta = 0.25$ we get implicit average constant acceleration.

For our problem we cannot apply the following equation

$$\mathbf{K}\mathbf{u}(t) = \mathbf{f}^{int}(t), \tag{17}$$

since

$$\mathbf{K}_\mathbf{u}\mathbf{u}(t) = \mathbf{f}_u^{int}(t), \tag{18}$$

term is not valid for the total displacements of the elements, but only for the relative displacements at the time of contact. For this reason, we introduce the equations,

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \boldsymbol{\Delta}\mathbf{u}_n, \tag{19}$$

$$\mathbf{f}_{n+1}^{int} = \mathbf{f}_n^{int} + \mathbf{K}\boldsymbol{\Delta}\mathbf{u}_n. \tag{20}$$

Another problem is the relation of the stiffness matrix $\mathbf{K}$ to the displacements $\mathbf{u}$ as can be seen in (5). In this case, an explicit expression using the central step value of Taylor expansion as,

$$k_t(u)_{n,n+1} = k_t(u_n + \frac{\Delta t \dot{u}_n}{2} + \frac{\Delta t^2 \ddot{u}_n}{4}). \tag{21}$$

By substituting (19)–(20) into (13)–(16) we obtain a system of linear equations as,

$$\begin{bmatrix} \mathbf{I} & \mathbf{0} & -\beta\Delta t^2\mathbf{I} \\ \mathbf{0} & \mathbf{I} & -\gamma\Delta t\mathbf{I} \\ \mathbf{K} & \mathbf{C} & \mathbf{M} \end{bmatrix} \begin{bmatrix} \boldsymbol{\Delta}\mathbf{u}_n \\ \dot{\mathbf{u}}_{n+1} \\ \ddot{\mathbf{u}}_{n+1} \end{bmatrix} = \begin{bmatrix} \Delta t\dot{\mathbf{u}}_n + \frac{\Delta t^2}{2}(1-2\beta)\ddot{\mathbf{u}}_n \\ \dot{\mathbf{u}}_n + (1-\gamma)\Delta t\ddot{\mathbf{u}}_n \\ \mathbf{f}_{n+1}^e - \mathbf{f}_n^{int} \end{bmatrix} = \begin{bmatrix} \mathbf{a}_n \\ \mathbf{b}_n \\ \mathbf{f}_n \end{bmatrix}, \tag{22}$$

where the last vector containing $\mathbf{a}_n$, $\mathbf{b}_n$ and $\mathbf{f}_n$ serves as a substitution of the right-hand side vector for subsequent adjustments. We also obtain the modified condition from (3) as follows,

$$\mathbf{B}\boldsymbol{\Delta}\mathbf{u}_n = \mathbf{o}. \tag{23}$$

From (22) we can express the relation of the displacement and velocity dependence on acceleration as

$$\boldsymbol{\Delta}\mathbf{u}_n = \mathbf{a}_n + \beta\Delta t^2\ddot{\mathbf{u}}_{n+1}, \tag{24}$$

$$\dot{\mathbf{u}}_{n+1} = \mathbf{b}_n + \gamma\Delta t\ddot{\mathbf{u}}_{n+1}, \tag{25}$$

by substituting these relations into the last equation of the system we obtain the equation for the acceleration as

$$(\mathbf{K}\beta\Delta t^2 + \mathbf{C}\gamma\Delta t + \mathbf{M})\ddot{\mathbf{u}}_{n+1} = \mathbf{f}_n - \mathbf{K}\mathbf{a}_n - \mathbf{C}\mathbf{b}_n, \tag{26}$$

then we derive by time the original constraints (23) into a form

$$\mathbf{B}\ddot{\mathbf{u}}_{n+1} = \mathbf{o}, \tag{27}$$

where term $\mathbf{K}\beta\Delta t^2 + \mathbf{C}\gamma\Delta t + \mathbf{M}$ yields a positive definite matrix for which more efficient algorithms can be used than for direct solution of (22).

4 Determination of time step

Determining the appropriate Δt value is an important part of using numerical methods to solve time-dependent differential equations. As already mentioned in the case of implicit solution, Newmark's method achieves a stable solution regardless of the step

length. In our use case, however, we must also take into account the fact that the matrix K itself is time dependent, mostly based on breaking bound contacts and occurrences of unbound contacts.

To estimate the initial step length, we use the maximum step size according to the explicit method. This is defined based on the lowest natural frequency of the system, which however leads to the eigenvalue problem. Here, however, we can help ourselves by simplifying by considering only the diagonal matrices of both stiffness and mass. From these assumptions we can find that the maximum time step can be defined as

$$\Delta t_{crit} = \min 2\sqrt{\frac{m_{i,i}}{k_{i,i}}}. \tag{28}$$

In the case of explicit methods, it is recommended to use a value about 20% of the critical time, this problematic of the time step for the explicit method is discussed in [13].

In the case of an implicit solution, the maximum time step cannot be precisely determined. For this reason, we consider η times the critical time step according to the explicit method.

In the case that a violation occurs according to the condition set in (11), an evaluation of exceeding this condition occurs. If the violation exceeds the specified ϵ limit, the line search method is used in the form,

$$\Delta u_{limit} = \alpha \Delta u_n, \quad \text{where} \quad 0 < \alpha < 1. \tag{29}$$

The last calculated step is then recalculated with a new time step length defined as

$$\Delta t_n = \sqrt{\alpha}\Delta t. \tag{30}$$

The same modification of the time step is introduced for cases when the unbound contact is disconnected.

5 Numerical benchmark

The benchmark is a simply supported beam with length of 3 m and a cross-section of 1×0.5 meters as a horizontal rectangle. The calculations are performed using a material characterized by a Young's modulus $E = 30$ GPa and a Poisson's ratio $v = 0.25$. The beam is loaded with a uniform load of 230 kN/m. see Fig. 1. The strength of each contact is determined using a random distribution with a mean value of $\sigma_{lim} = 6$ MPa and a standard deviation of $\sigma_{\sigma_{lim}} = 0.05$ MPa see Fig. 2. The benchmark examines the computation time of implicit and explicit methods, limiting step lengths and time for one step calculation.

The calculation was performed using both implicit and explicit Newmark-Beta methods with the coefficients presented in Section 3. The calculation was terminated after time t=0.5s, which was set as the fracture is already completely developed see

Fig. 3. The step length for the explicit solution is set to about the recommended 20% of the critical time according to (28). In the case of the implicit solution, the time step is set as 1% of the total time.

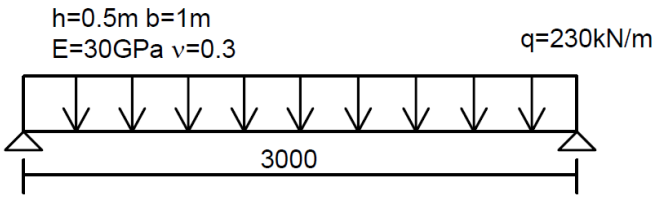

Figure 1: Static scheme

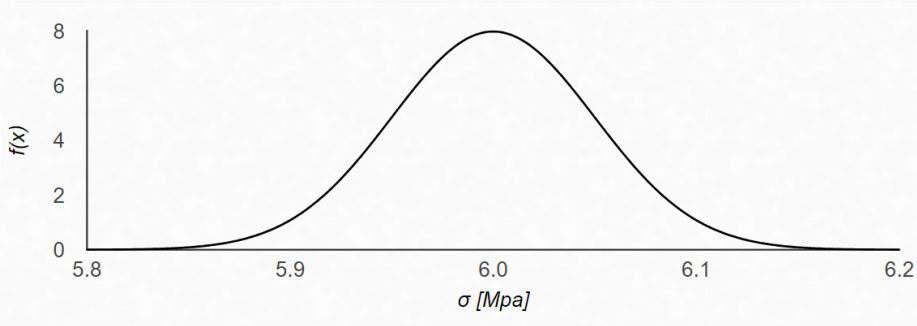

Figure 2: Normal distribution of tensile strength

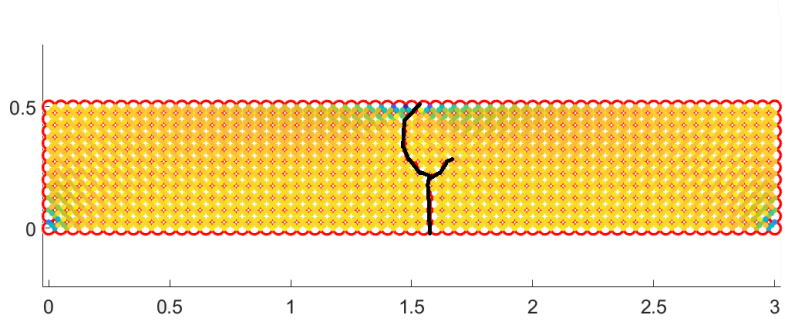

Figure 3: Crack propagation solution

The mean values of the times over several computational cycles were used to reduce errors. The computational time of one step is measured in two scenarios. Before crack formation t_b and after crack formation t_u. The calculation after crack formation becomes more expensive due to the assembly of a pair of stiffness and damping matrices, as well as the actual search for new contacts. The results are shown in Tab. 1 and Tab. 2 and for graphic representation of the relation between computation time and the number of elements see Fig. 4.

Explicit	Element size / Total elements		
	0.05 / 336	0.025 / 1271	0.01 / 7676
Δt_{crit}	$1.41 \cdot 10^{-5}$	$7.05 \cdot 10^{-6}$	$2.82 \cdot 10^{-6}$
Δt	$3.00 \cdot 10^{-6}$	$1.50 \cdot 10^{-6}$	$5.00 \cdot 10^{-7}$
$t_{b,1}$	$5.27 \cdot 10^{-5}$	$1.70 \cdot 10^{-3}$	$1.22 \cdot 10^{-2}$
$t_{u,1}$	$8.86 \cdot 10^{-5}$	$3.10 \cdot 10^{-3}$	$2.22 \cdot 10^{-2*}$
t_{tot}	11.85	82.22	1722.35*

Table 1: Calculation time for explicit method [s]
*stands for estimated time

Implicit	Element size / Total elements		
	0.025 / 1271	0.01 / 7676	0.005 / 20351
Δt	$5.00 \cdot 10^{-3}$		
$t_{b,1}$	0.067	0.158	0.82
$t_{u,1}$	0.094	0.237	1.39
t_{tot}	8.04	19.75	110.70

Table 2: Calculation time for implicit method [s]

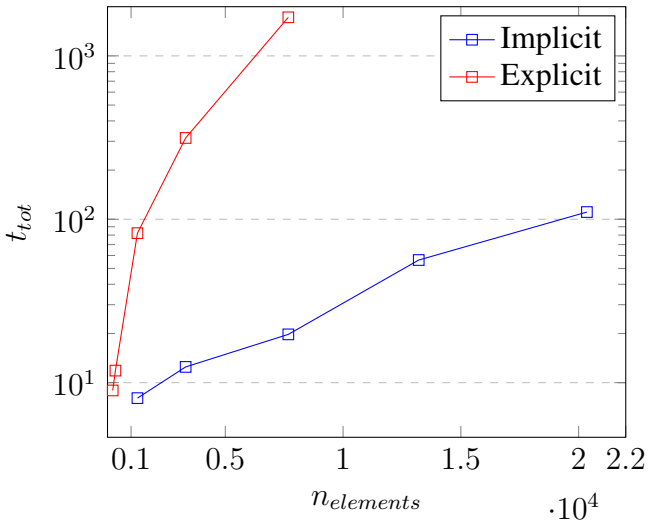

Figure 4: Dependence of computation time on the number of elements

6 Concluding remarks

In the framework of the paper, the validation of the suitability of using Newmark-beta methods for the DEM-BBM problem was performed. This variant of the DEM combined with the crack propagation problem provides suitable conditions for the use of implicit methods mainly by infrequent contact changes. Explicit methods that do not require solving systems of equations and within one step are orders of magnitude

faster, but due to the physical properties of the problem to be solved, the required time steps are significantly smaller, making the total solution much more time expensive. The computational time increases quadratically in cases of mesh refinements, which is due to the simultaneous increase in the difficulty of the problem as well as the requirement to decrease the time step. The implicit solution, despite its stability, allows the use of considerably larger steps. However, even here it is necessary to introduce some restrictions on the step length. One possibility, which is also introduced here, is to actively check during the calculation whether there is a significant violation of the contact conditions; such errors would subsequently insert additional energy into the system. This step adjustment can greatly increase the accuracy of the analysis, but in the case of dynamic loading it does not ensure that bond breaking does not occur at the extremes between calculated time steps that satisfy the conditions. A large time step can also lead to the need for frequent reduction, which can increase the overall time as a result. Thus, one possibility to which to relate the time step conditions is, for example, to the difference of velocity or acceleration.

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