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Multi-time Step Methods in Lattice Discrete Particle Models

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Abstract

Lattice discrete particle models substitute the finite element method in specific problems, e.g. crack propagation and failure of quasi-brittle materials or thermoset polymers used in rebar connections and heavy-duty anchoring. The number of particles is usually very large which results in severe computational demands. Speedup of the computations can be achieved by suitable time integration method. This contribution concerns with multi-time step method based on domain decomposition method with Lagrange multipliers on interfaces. The method is formulated for nonlinear equations of motion, where the internal forces are computed directly without the stiffness matrix. Two different time steps are used in two subdomains.

Keywords: lattice discrete particle model, explicit time integration, Lagrange multipliers, multi-time step method

1 Introduction

Lattice discrete particle models are used in many areas of research. For example, they can be used in analysis of concrete, polymers and other materials. The number of particles is usually very high and efficient method for time integration has to be used.

There are two groups of time integration methods. Explicit integration methods are usually conditionally stable and the time step has to satisfy a stability condition which reduces the time step significantly. Advantage of the explicit methods stems from the fact that the internal forces can be computed directly and the stiffness matrix is not assembled. On the other hand, implicit methods require to assemble the stiffness and mass matrices. The storage requirements of the implicit methods are much larger than the requirements of the explicit methods.

In connection with the lattice discrete particle models, explicit methods prevail. With respect to localization of nonlinear effects into relatively small area, different time steps in domain solved are strongly required. Such numerical approach is called sub-cycling or multi-time step methods.

This contribution concerns with sub-cycling algorithm with two time steps. The shorter time step is used in the area where nonlinear behaviour is concentrated while longer time step is used in the remaining part of the domain. In conference contribution [1], a modified finite difference method was used for time integration of lattice discrete particle models. In some cases, the method requires time steps similar to the time step needed in the standard finite difference method otherwise it diverges. Therefore, different method based on the paper [2] which enables two time steps was implemented and used.

2 Subcycling methods for nonlinear dynamics

The equation of motion can be assembled directly for a discrete problem or it is a result of space discretization by a numerical method, e.g. the finite element method [3], [4], [5], [6]. In the case of nonlinear problem, the equation of motion has the form

$$\boldsymbol{M}\ddot{\boldsymbol{u}}(t) + \boldsymbol{C}\dot{\boldsymbol{u}}(t) + \boldsymbol{f}(\boldsymbol{u}(t)) = \boldsymbol{f}(t) \tag{1}$$

where $\boldsymbol{M}$ is the mass matrix, $\boldsymbol{C}$ is the damping matrix, $\ddot{\boldsymbol{u}}(t)$ is the vector of acceleration, $\dot{\boldsymbol{u}}(t)$ is the vector of velocity, $\boldsymbol{u}(t)$ is the vector of displacement, $\boldsymbol{f}^E(t)$ is the vector of prescribed (external) forces and $\boldsymbol{f}^I(\boldsymbol{u}(t))$ is the vector of internal forces which depends on the actual vector of displacement. The mass matrix $\boldsymbol{M}$ can be diagonalized. If the damping matrix $\boldsymbol{C}$ is assumed to be proportional to the mass matrix only, it can be diagonal too. For more concise presentation, the damping effects will be omitted.

Let a domain solved be split into a part S, where short time step Δt is needed, and a part L, where long step $m\Delta t$ is possible, where m is an integer. Variables connected with the subdomain L have the superscript L and variables connected with the subdomain S have the superscript S. Subscripts will be used instead of arguments of variables in order to abbreviate the notation. In the subdomain L, one subscript is used. For example, the vector of displacement is abbreviated

$$\boldsymbol{u}^{(L)}(km\Delta t) = \boldsymbol{u}_k^{(L)} \tag{2}$$

In the subdomain S, two subscripts are needed, e.g.

$$\boldsymbol{u}^{(S)}(km\Delta t + j\Delta t) = \boldsymbol{u}_{k,j}^{(S)} \tag{3}$$

The equations of motion for the subdomain S, L and the interface condition have the form

$$\boldsymbol{M}^{(L)}\ddot{\boldsymbol{u}}_{k+1}^{(L)} + \boldsymbol{f}_{k+1}^{(L,I)} = \boldsymbol{f}_{k+1}^{(L,E)} - \left(\boldsymbol{B}^{(L)}\right)^T \boldsymbol{\lambda}_{k+1} \tag{4}$$

$$\boldsymbol{M}^{(S)}\ddot{\boldsymbol{u}}_{k,j+1}^{(S)} + \boldsymbol{f}_{k,j+1}^{(S,I)} = \boldsymbol{f}_{k,j+1}^{(S,E)} - \left(\boldsymbol{B}^{(S)}\right)^T \boldsymbol{\lambda}_{k,j+1} \tag{5}$$

$$\boldsymbol{B}^{(L)}\dot{\boldsymbol{u}}_{k,j+1}^{(L)} + \boldsymbol{B}^{(S)}\dot{\boldsymbol{u}}_{k,j+1}^{(S)} = \boldsymbol{0} \tag{6}$$

where $\boldsymbol{f}_{k+1}^{(L,E)}$ is the vector of external forces in the subdomain L, $\boldsymbol{f}_{k,j+1}^{(S,E)}$ is the vector of external forces in the subdomain S, $\boldsymbol{f}_{k+1}^{(L,I)}$ is the vector of internal forces in the subdomain L, $\boldsymbol{f}_{k,j+1}^{(L,I)}$ is the vector of internal forces in the subdomain S, $\boldsymbol{B}^{(S)}$, $\boldsymbol{B}^{(L)}$ are the Boolean matrices (they contain elements -1, 0 or 1 and they serve for component selection) and $\boldsymbol{\lambda}$ is the vector of Lagrange multipliers.

New displacements in the subdomain L are given from the Newmark expression, where $\beta^{(L)} = 0$, therefore

$$\boldsymbol{u}_{k+1}^{(L)} = \boldsymbol{u}_{k}^{(L)} + m\Delta t\dot{\boldsymbol{u}}_{k}^{(L)} + \frac{1}{2}(m\Delta t)^2\ddot{\boldsymbol{u}}_{k}^{(L)} \tag{7}$$

new velocities are in the form

$$\dot{\boldsymbol{u}}_{k+1}^{(L)} = \dot{\boldsymbol{u}}_{k}^{(L)} + m\Delta t(1-\gamma^{(L)})\ddot{\boldsymbol{u}}_{k}^{(L)} + m\Delta t\gamma^{(L)}\ddot{\boldsymbol{u}}_{k+1}^{(L)} \tag{8}$$

The acceleration is assumed to be split into two components

$$\ddot{\boldsymbol{u}}_{k}^{(L)} = \ddot{\boldsymbol{w}}_{k}^{(L)} + \ddot{\boldsymbol{q}}_{k}^{(L)} \tag{9}$$

which leads to decomposition of the equation of motion (4) into two equations

$$\boldsymbol{M}^{(L)}\ddot{\boldsymbol{w}}_{k+1}^{(L)} = \boldsymbol{f}_{k+1}^{(L,E)} - \boldsymbol{f}_{k+1}^{(L,I)} \tag{10}$$

$$\boldsymbol{M}^{(L)}\ddot{\boldsymbol{q}}_{k+1}^{(L)} = -\left(\boldsymbol{B}^{(L)}\right)^T \boldsymbol{\lambda}_{k+1} \tag{11}$$

The vector $\ddot{\boldsymbol{w}}_{k+1}^{(L)}$ can be expressed from (10) immediately.

Similarly for the subdomain S, new displacements are expressed with the help of the Newmark expression, where $\beta^{(S)} = 0$, and therefore

$$\boldsymbol{u}_{k,j+1}^{(S)} = \boldsymbol{u}_{k,j}^{(S)} + \Delta t\dot{\boldsymbol{u}}_{k,j}^{(S)} + \Delta t^2\left(\frac{1}{2} - \beta^{(S)}\right)\ddot{\boldsymbol{u}}_{k,j}^{(S)} + \Delta t^2\beta^{(S)}\ddot{\boldsymbol{u}}_{k,j+1}^{(S)} = \tag{12}$$

$$= \boldsymbol{u}_{k,j}^{(S)} + \Delta t\dot{\boldsymbol{u}}_{k,j}^{(S)} + \frac{1}{2}\Delta t^2\ddot{\boldsymbol{u}}_{k,j}^{(S)} \tag{13}$$

New velocities

$$\dot{\boldsymbol{u}}^{(S)}_{k,j+1} = \dot{\boldsymbol{u}}^{(S)}_{k,j} + \Delta t(1-\gamma^{(S)})\ddot{\boldsymbol{u}}^{(S)}_{k,j} + \Delta t\gamma^{(S)}\ddot{\boldsymbol{u}}^{(S)}_{k,j+1} \tag{14}$$

The acceleration is assumed to be split into two components

$$\ddot{\boldsymbol{u}}^{(S)}_{k,j} = \ddot{\boldsymbol{w}}^{(S)}_{k,j} + \ddot{\boldsymbol{q}}^{(S)}_{k,j} \tag{15}$$

which leads to decomposition of the equation of motion (5) into two equations

$$\boldsymbol{M}^{(S)}\ddot{\boldsymbol{w}}^{(S)}_{k,j+1} = \boldsymbol{f}^{(S,E)}_{k,j+1} - \boldsymbol{f}^{(S,I)}_{k,j+1} \tag{16}$$

$$\boldsymbol{M}^{(S)}\ddot{\boldsymbol{q}}^{(S)}_{k,j+1} = -\left(\boldsymbol{B}^{(S)}\right)^T \boldsymbol{\lambda}_{k,j+1} \tag{17}$$

The vector $\ddot{\boldsymbol{w}}^{(S)}_{k,j+1}$ can be expressed from (16) immediately.

Substitution of (9) and (15) into (8) and (14) leads to the expressions for velocities in the form

$$\dot{\boldsymbol{u}}^{(L)}_{k+1} = \dot{\boldsymbol{u}}^{(L)}_{k} + m\Delta t(1-\gamma^{(L)})\ddot{\boldsymbol{u}}^{(L)}_{k} + m\Delta t\gamma^{(L)}\ddot{\boldsymbol{w}}^{(L)}_{k+1} + m\Delta t\gamma^{(L)}\ddot{\boldsymbol{q}}^{(L)}_{k+1} \tag{18}$$

$$\dot{\boldsymbol{w}}^{(L)}_{k+1} = \dot{\boldsymbol{u}}^{(L)}_{k} + m\Delta t(1-\gamma^{(L)})\ddot{\boldsymbol{u}}^{(L)}_{k} + m\Delta t\gamma^{(L)}\ddot{\boldsymbol{w}}^{(L)}_{k+1} \tag{19}$$

$$\dot{\boldsymbol{q}}^{(L)}_{k+1} = m\Delta t\gamma^{(L)}\ddot{\boldsymbol{q}}^{(L)}_{k+1} \tag{20}$$

$$\dot{\boldsymbol{u}}^{(L)}_{k+1} = \dot{\boldsymbol{w}}^{(L)}_{k+1} + \dot{\boldsymbol{q}}^{(L)}_{k+1} \tag{21}$$

$$\dot{\boldsymbol{u}}^{(S)}_{k,j+1} = \dot{\boldsymbol{u}}^{(S)}_{k,j} + \Delta t(1-\gamma^{(S)})\ddot{\boldsymbol{u}}^{(S)}_{k,j} + \Delta t\gamma^{(S)}\ddot{\boldsymbol{w}}^{(S)}_{k,j+1} + \Delta t\gamma^{(S)}\ddot{\boldsymbol{q}}^{(S)}_{k,j+1} \tag{22}$$

$$\dot{\boldsymbol{w}}^{(S)}_{k,j+1} = \dot{\boldsymbol{u}}^{(S)}_{k,j} + \Delta t(1-\gamma^{(S)})\ddot{\boldsymbol{u}}^{(S)}_{k,j} + \Delta t\gamma^{(S)}\ddot{\boldsymbol{w}}^{(S)}_{k,j+1} \tag{23}$$

$$\dot{\boldsymbol{q}}^{(S)}_{k,j+1} = \Delta t\gamma^{(S)}\ddot{\boldsymbol{q}}^{(S)}_{k,j+1} \tag{24}$$

$$\dot{\boldsymbol{u}}^{(S)}_{k,j+1} = \dot{\boldsymbol{w}}^{(S)}_{k,j+1} + \dot{\boldsymbol{q}}^{(S)}_{k,j+1} \tag{25}$$

The part $\dot{\boldsymbol{q}}^{(L)}_{k+1}$ of the acceleration can be expressed with the help of (11) in the form

$$\dot{\boldsymbol{q}}^{(L)}_{k+1} = m\Delta t\gamma^{(L)}\ddot{\boldsymbol{q}}^{(L)}_{k+1} = -m\Delta t\gamma^{(L)}\left(\boldsymbol{M}^{(L)}\right)^{-1}\left(\boldsymbol{B}^{(L)}\right)^T\boldsymbol{\lambda}_{k+1} \tag{26}$$

Similarly, the part $\dot{\boldsymbol{q}}^{(S)}_{k,j+1}$ can be expressed with the help of (17) in the form

$$\dot{\boldsymbol{q}}^{(S)}_{k,j+1} = \Delta t\gamma^{(S)}\ddot{\boldsymbol{q}}^{(S)}_{k,j+1} = -\Delta t\gamma^{(S)}\left(\boldsymbol{M}^{(S)}\right)^{-1}\left(\boldsymbol{B}^{(S)}\right)^T\boldsymbol{\lambda}_{k,j+1} \tag{27}$$

The continuity condition (6) contains the vectors $\dot{\boldsymbol{w}}^{(L)}_{k,j+1}$ and $\dot{\boldsymbol{q}}^{(L)}_{k,j+1}$ which are not available but they can be interpolated in the form

$$\dot{\boldsymbol{w}}^{(L)}_{k,j+1} = \left(1-\frac{j+1}{m}\right)\dot{\boldsymbol{w}}^{(L)}_{k} + \frac{j+1}{m}\dot{\boldsymbol{w}}^{(L)}_{k+1} \tag{28}$$

$$\begin{aligned}\dot{\boldsymbol{q}}^{(L)}_{k,j+1} &= \left(1-\frac{j+1}{m}\right)\dot{\boldsymbol{q}}^{(L)}_{k} + \frac{j+1}{m}\dot{\boldsymbol{q}}^{(L)}_{k+1} = \\ &= -m\Delta t\gamma^{(L)}\left(\boldsymbol{M}^{(L)}\right)^{-1}\left(\boldsymbol{B}^{(L)}\right)^T\boldsymbol{\lambda}_{k,j+1}\end{aligned} \tag{29}$$

The continuity condition (6) has the form

$$\boldsymbol{B}^{(L)}\left(\dot{\boldsymbol{w}}_{k,j+1}^{(L)}+\dot{\boldsymbol{q}}_{k,j+1}^{(L)}\right)+\boldsymbol{B}^{(S)}\left(\dot{\boldsymbol{w}}_{k,j+1}^{(S)}+\dot{\boldsymbol{q}}_{k,j+1}^{(S)}\right)=\boldsymbol{0} \tag{30}$$

which can be rewritten after substitution of (28) and (29) into its final form

$$\begin{aligned}\boldsymbol{B}^{(L)}\dot{\boldsymbol{w}}_{k,j+1}^{(L)}+\boldsymbol{B}^{(S)}\dot{\boldsymbol{w}}_{k,j+1}^{(S)} &= m\Delta t\gamma^{(L)}\boldsymbol{B}^{(L)}\left(\boldsymbol{M}^{(L)}\right)^{-1}\left(\boldsymbol{B}^{(L)}\right)^{T}\boldsymbol{\lambda}_{k,j+1}+\\ &+\Delta t\gamma^{(S)}\boldsymbol{B}^{(S)}\left(\boldsymbol{M}^{(S)}\right)^{-1}\left(\boldsymbol{B}^{(S)}\right)^{T}\boldsymbol{\lambda}_{k,j+1}\end{aligned} \tag{31}$$

If a new matrix $\boldsymbol{A}$ is defined in the form

$$\boldsymbol{A} = m\Delta t\gamma^{(L)}\boldsymbol{B}^{(L)}\left(\boldsymbol{M}^{(L)}\right)^{-1}\left(\boldsymbol{B}^{(L)}\right)^{T}+\Delta t\gamma^{(S)}\boldsymbol{B}^{(S)}\left(\boldsymbol{M}^{(S)}\right)^{-1}\left(\boldsymbol{B}^{(S)}\right)^{T} \tag{32}$$

the system of equations (31) can be written in the form

$$\boldsymbol{A}\boldsymbol{\lambda}_{k,j+1}=\boldsymbol{B}^{(L)}\dot{\boldsymbol{w}}_{k,j+1}^{(L)}+\boldsymbol{B}^{(S)}\dot{\boldsymbol{w}}_{k,j+1}^{(S)} \tag{33}$$

If the vector of Lagrange multipliers $\boldsymbol{\lambda}_{k,j+1}$ is known, the parts of acceleration $\ddot{\boldsymbol{q}}_{k,j+1}^{(S)}$ and $\ddot{\boldsymbol{q}}_{k+1}^{(L)}$ can be obtained from Equations (17) and (11). The accelerations are defined by (9) and (15), the velocities are defined by (8) and (14) and the displacements are defined by (7) and (12).

3 Numerical Example

A dog-bone sample loaded by tension is selected for demonstration of behaviour of the multi-time step method. The problem is solved by the standard finite difference method and by the multi-time step methods with various time steps.

Scheme of the sample is depicted in Figure 1. In Figure 2, particles and edges are visible. The sample is loaded by axial tension forces. The relationship between the axial force and elongation of the sample is in Figure 3. The time step in the standard finite difference method has to be $\Delta t = 10^{-7}$ s while in the multi-time step method, steps $\Delta t = 10^{-7}$ s and $m\Delta t = 10^{-6}$ s can be used.

4 Conclusions

The time integration published in [1] is not efficient in some cases because it requires very short time steps in both subdomains. Newly implemented approach based on the paper [2] can be used in connection with the lattice discrete particle models but numerical tests reveal a numerical damping in some cases.

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Figure 1: Geometry of the example.

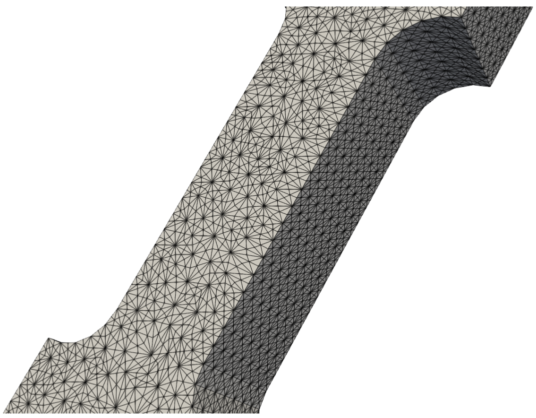

Figure 2: Detail of particles and edges in the central part of the example.

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Force-displacement diagram

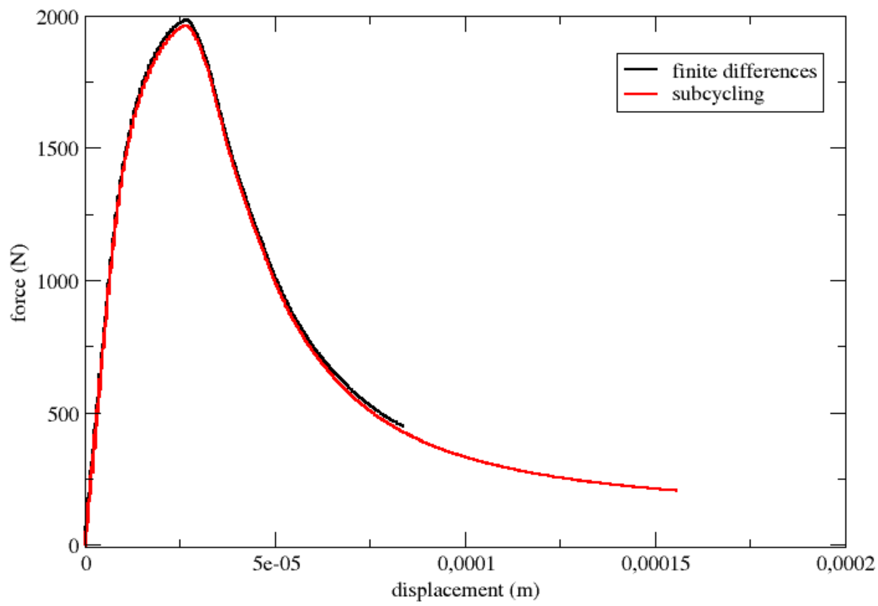

Figure 3: Force-displacement relationship.

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