A non-integer step ratio parallel computing method for hybrid finite-element and discrete-element on multi-core computer

Tong Li¹², Ge Gao¹ and Xianlong Jin¹²*

¹School of Mechanical Engineering, Shanghai Jiao Tong University, Shanghai 200240, China
²State Key Laboratory of Mechanical System and Vibration, Shanghai Jiao Tong University, Shanghai 200240, China

*Corresponding author’s e-mail: jxlong@sjtu.edu.cn

Abstract. Commercial finite-element and discrete-element software usually adopts a unified computational time step and limit the number of our computer cores. In the face of large-scale with refined scale computing models, this will undoubtedly increase the time cost. The multi time step method of integer step ratio is a method to deal with this kind of problem. A non-integer ratio multi-time step computing method based on domain decomposition and subcycling method is proposed and applied to the finite-element and discrete-element engineering problems. The whole model is divided into finite-element method (FEM) subdomains and discrete-element method (DEM) subdomains according to the load balance of CPU. A coupling region between adjacent domains consists of multiple boundary nodes and particles based on the non-integer step ratio. Boundary data in coupling region are transferred through MPI communication protocol. This method can make full use of the advantages of multi-core computer and improve the calculation efficiency of engineering software.

1. Introduction

The finite-element method (FEM) can solve the problems of continuum mechanics and structural response [1], and discrete-element method (DEM) is suitable for deal with displacement discontinuity problems [2]. It is a trend to utilize the advantages of the two methods for multi-scale simulation.

However, a hybrid FEM-DEM dynamics method usually uses a unified time step. For a large or super-large model with partial refined structured, the unit scale may differ greatly, so a single step will undoubtedly waste lots of computing resource and increase research period.

The multi-time step algorithm is usually adopted to tackle these problems [3]. A small step can be set in the region with tiny particles of DEM subdomain and a large step in the region with coarse mesh of FEM subdomain. Conventional subcycling methods have some problems in stability and accuracy [4]. Besides, the time step ratio in a traditional multi-time step method is an integer, which limits the universality of the method.

Aim to solve these problems, a non-integer time step ratio method for coupled FEM-DEM model is proposed based on domain decomposition and subcycling method. The data transfer at the boundary is in the form of overlapping nodes and particles. Non-integer time step ratio means that the ration between two neighbouring subdomains a positive real number, which extends the application scope of the traditional integer form step ratio.
2. Computing method

2.1. Multiple overlapping particles and nodes for adjacent subdomains
Node division method [5] and particle method is applied to divide a whole model into several FEM subdomains and DEM subdomains based on the load balance of CPU. The node in the FEM subdomain can be divided into internal node, boundary node and external node. The particle in the DEM subdomain is chopped up into internal particles, boundary particle and external particle. The coupling region consists of the boundary and external nodes/particles between arbitrary two adjacent subdomains. The multi-layer overlapping particle and node is adopted in this paper, which can effectively reduce the accuracy loss caused by boundary data interpolation or truncation [6]. The step ratio \( m \) (\( m \) is non-integer) is defined as the ratio between a large step in FEM subdomain and a small step in DEM subdomain. As shown in figure 1, it shows the multiple overlapping particles and nodes with ratio \( m=1.5 \).

![Figure 1. Particle and node overlapping region method at ratio \( m=1.5 \).](image)

2.2. Computational method and flow with non-integer ratio
The explicit predictor-corrector integration scheme based on Newmark is adopted to solve the finite-element equation of motion, which can better match the explicit Velocity-Verlet [7] integral algorithm in DEM subdomain.

The predictors scheme can be seen as [8],

\[
\tilde{x}_{t+dt} = x_t + \dot{x}_t dt + \left( \frac{1}{2} - \beta \right) \ddot{x}_t dt^2; \quad \tilde{\dot{x}}_{t+dt} = \dot{x}_t + (1-\gamma) \ddot{x}_t dt
\]  

The vectors \( \tilde{x}_{t+dt} \) and \( \tilde{\dot{x}}_{t+dt} \) are the predictor displacement and velocity vectors at the time \( t + dt \); The vectors \( \tilde{x}_t \) and \( \tilde{\dot{x}}_t \) mean the corresponding predictor displacement and velocity vectors at the time \( t \), respectively. Newmark integral parameter \( \gamma =0.5 \) and \( \beta =0.25 \), respectively, and \( dt \) is the step interval.

By substituting the predicted values of displacement and velocity at the moment \( t + dt \) into Eq. (1), we can obtain

\[
M \ddot{x}_{t+dt} + K \dot{x}_{t+dt} + C \dot{x}_{t+dt} = F_{t+dt}
\]

The nodal acceleration vector \( \ddot{x}_{t+dt} \) can be solved by Eq. (2),

\[
\ddot{x}_{t+dt} = M^{-1}(F_{t+dt} - K \dot{x}_{t+dt} - C \dot{x}_{t+dt})
\]

Then, the corrector displacement vector \( x_{t+dt} \) and velocity vector \( \dot{x}_{t+dt} \) at \( t + dt \) can be obtained from the following equations,

\[
x_{t+dt} = \tilde{x}_{t+dt} + \ddot{x}_{t+dt} dt^2; \quad \dot{x}_{t+dt} = \tilde{\dot{x}}_{t+dt} + \ddot{x}_{t+dt} dt\gamma
\]
computed twice and the DEM subdomain is computed three times. The algorithm of each subdomain operates in different processes on multi-core computer and the coupling data are transferred by MPI communication protocol.

![Diagram](image)

Figure 2. Boundary data transfer and update process for ratio $m=1.5$.

3. Numerical case
The resistance design parameters of metamaterials subjected to impulse load is applied to verify the validity and efficiency.

As shown in figure 3, the resonant mass-spring microstructure model is composed of a harmonic oscillator and a shell, in which the mass of the harmonic oscillator and shell are $m_s$ and $m_v$ respectively [9]. The spring between the harmonic oscillator and the shell is called the harmonic oscillator spring, whose stiffness coefficient is $k_s$, and the stiffness coefficient of the spring connected with the shell outside is $k_v$.

A solid structure was used to represent the original mass-in-shell lattice (in Figure. 3). The effective mass of the equivalent solid is in the following form

$$m_e = (m_s + m_v)(1 + \frac{\theta}{1 + \theta}(1 - n^2))$$

(5)

This model as denoted as “Negative effective mass” in the range

$$1 < n < \sqrt{1 + \theta}$$

(6)

Here, $n = \omega_1 / \omega_2$ is the frequency ratio, and $\theta = m_v / m_s$ is the non-dimensional mass ratio.

Where $\omega_1 = k_s / m_s$ and $\omega_2 = k_v / m_s$ are the natural frequency of effective mass model and harmonic oscillator, respectively. As shown in Figure 3, the whole calculation model is divided into FEM-subdomain and DEM-subdomain according to CPU load balancing. An impulse load is applied to the first particle in the elastic metamaterial system, and the load function is given by Eq. (7)
\[ F = 1 \times 10^3 \text{ N}, \quad t \leq 0.3 \text{ ms} \]
\[ F = 0, \quad t > 0.3 \text{ ms} \]

Motion equations for the \( i \) unit are given by
\[
\begin{align*}
\ddot{\mu}_i + 2k_n x_i - k_{x_{i+1}} &= F, & i &= 1 \\
\ddot{\mu}_i + 2k_n x_i - k_{x_{i-1}} - k_{x_{i+1}} &= 0, & 1 < i \leq 50 \\
\ddot{\mu}_i + 2k_n x_i - k_{x_{i-1}} - k_{x_{i+1}} &= 0, & 151 \leq i < 400 \\
\ddot{\mu}_i + k_n x_i - k_{x_{i-1}} &= 0, & i &= 400
\end{align*}
\]  

Where \( k_n \) denotes the stiffness between the solid particles; \( x_i \) means the displacement of mass \( m_i \), and \( F \) is the amplitude of applied impulse load.

The equations of shell and internal harmonic oscillator in metamaterial region for the \( j \) unit are expressed by
\[
\begin{align*}
\begin{cases}
 m_i \ddot{x}_i + (2k_n + k_v)x_i - k_n x_{i-1} - k_n x_{i+1} - k_v x_j &= 0, & i = 50 + j, \ 1 \leq j \leq 100 \\
 m_i \ddot{x}_j + k_v x_j - k_v x_i &= 0
\end{cases}
\end{align*}
\]  

Where \( x_i \) and \( x_j \) are the displacement of mass \( m_s \) and \( m_v \); \( k_v \) denotes the stiffness between the shell and solid particles, and \( k_v \) is the stiffness between the shell and internal harmonic oscillator.

The characteristic equation is obtained as
\[
|\mathbf{K} - \omega^2 \mathbf{M}| = 0
\]  

The stiffness of the harmonic oscillator in the system can be obtained by solving the eigenvalue problem of the coefficients.

For a method illustration, we take a case with the following assumed material constants as an example: \( n = \omega_i / \omega_l = 2.5, m_i = 0.05 \text{ kg}, m_v = 0.05 \text{ kg}, k_v = 7.8 \times 10^6 \). Then, the stiffness of the harmonic oscillator can be obtained by Eq. (10), so we get \( k_v = 2.489 \times 10^6 \).

All computations are performed on the same computer and the time step for DEM subdomain is \( \Delta t = 1 \times 10^{-5} \text{s} \) and the time step in FEM subdomain is \( \Delta t = 2.5 \times 10^{-7} \text{s} \).
Figure 4. Displacement response of 100th particle in DEM subdomain

Figure 4 compares the dimensionless displacement (ratio of displacement to maximum displacement) of 100th particles in DEM subdomain by different methods. The results show that due to the existence of metamaterials, the displacement response of particles is greatly reduced, and metamaterials can play the role of vibration isolation and impact resistance. The displacement response of 100th particle calculated at ration $m=2.5$ by the proposed method is very consistent with that obtained by the reference Newmark method.

The computing time of proposed method at $m=2.5$ and reference Newmark method are 90.7 s and 698.8 s, respectively. The calculation time consumed for the same physical problem is significantly reduced by the proposed method.

4. Conclusions

In this paper, a non-integer ratio step computational method based on domain decomposition and MPI for FEM-DEM is proposed and applied. The format of non-integer extends the range of ratio in multiple-time step method. The overlapping region consists of multiple overlapping particles and nodes between two adjacent subdomains. There is no truncation in the computational process, which effectively reduce the calculation error. For large-scale and whole-process computing, algorithms can be transplanted to supercomputer platforms for multi region division. This is also the focus of future work.

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References

[1] Long, Y.Q., Cen, S. Z., Lonedg, F. (2009) Advanced finite element method in structural engineering, Berlin, Heidelberg: Springer-Verlag GmbH, Beijing: Tsinghua University Press.

[2] André, D., Jebahi, M., Iordanoff, I., Charles, J.I., Néauport, J. (2013) Using the discrete element method to simulate brittle fracture in the indentation of a silica glass with a blunt indenter. Computer Methods in Applied Mechanics and Engineering, 265(1): 136-147.

[3] Ma, Z.Q., Lou, Y.F., Li, J.J., Jin, X.L. (2019) An explicit asynchronous step parallel computing method for finite element analysis on multi-core clusters. Engineering with Computers, 36(2): 443-453.

[4] Bunting, G., Prakash, A., Dyke, S., Maghareh, A., Asce, A.M. (2016) Characterizing errors and
evaluating performance of transient simulations using multi-time-step integration. Journal of Computing in Civil Engineering, 30(5): 04016013.

[5] Karypis, G., Kumar, V. (2018) A software package for partitioning unstructured graphs, partitioning meshes and computing fill-reducing orderings of sparse matrices, Version, 2018.

[6] Biesiadecki, J.J., Skeel, R.D. (1993) Dangers of multiple time step methods. Journal of Computational Physics 109(2): 318-328.

[7] Zhao, G.F. (2015) Modelling 3D jointed rock masses using a lattice spring model. International Journal of Rock Mechanics and Mining Sciences, 78: 79-90.

[8] Hughes, T.J.R. (2012) The finite element method: linear static and dynamic finite element analysis. Courier Corporation.

[9] Huang, H.H., Sun, C.T.J. (2012) Anomalous wave propagation in a one-dimensional acoustic metamaterial having simultaneously negative mass density and Young’s modulus. Acoustical Society of America, 132(4): 2887-2895.