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Computational Improvement of Time-History-Kernel Non-reflecting Boundary Condition and Its Preliminary Application in Laser-Assisted Nanoimprinting

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ABSTRACT

Nanomechanics and its simulation/computation play important roles in the development of nanotechnology and nano fabrication, which demands non-reflecting boundary conditions to reduce the spurious effects resulted from artificial boundaries. Developing the non-reflecting boundary conditions for computational nanomechanics thus attracts a lot of interests in recent years. THK (time-history kernel) method is one of the systematic approaches to derive the required isothermally non-reflecting boundary condition [1]. This method derives the time response of displacement for atoms at the boundary through the time convolution of the neighboring atoms and therefore consumes a lot of computation for each time-step during the simulation process.

This study propoes that the kernel funcion of THK to be generated through Crump's method [2] of inverse-Laplace transformation and to be expressed in the form of complex numbers, which makes the convolution into a recursive operation. In this proposed approach, the computation cost of each convolution operation can be reduced from O(N^2) down to O(NA), where N represents the total number of simulation steps and A the total number of terms used in the inverse-Laplace transformation. Figure 1 illustrates a typical variation of the convolution error with respect to the cut-off terms in direct convolution or the terms used in the proposed approach. With this improvement, THK mehtod becomes more useful in the computational nanomechanics.

This study demonstrates the powerfulness of THK in two examples. First, the THK method can be used to perform the lattice relaxation before the begining of simulation as illustrated in Figure 2. Next, the THK is implemented as the numerical boundary condition for the simulation of the whole process (see Figure 3) for LAN (laser-assisted nanoimprinting). It is shown that THK method can indeed provide an isothermally non-reflecting boundary condition since the stress wave induced by imprinting indentor will be dissipated outward eventually, and system temperature will be recovered to its original value in the long run as indicated in Figure 4.

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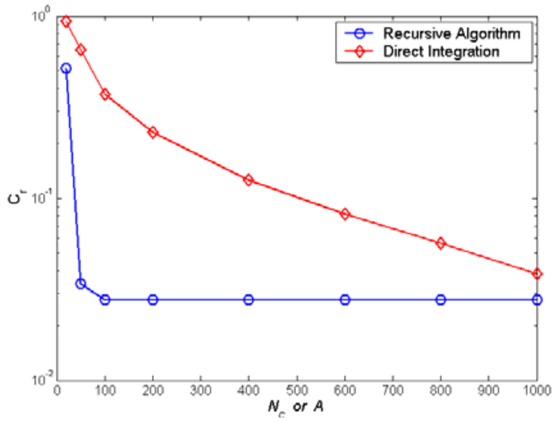

Fig. 1 Convolution Error of Direct Convolution and Recursive Algorithm

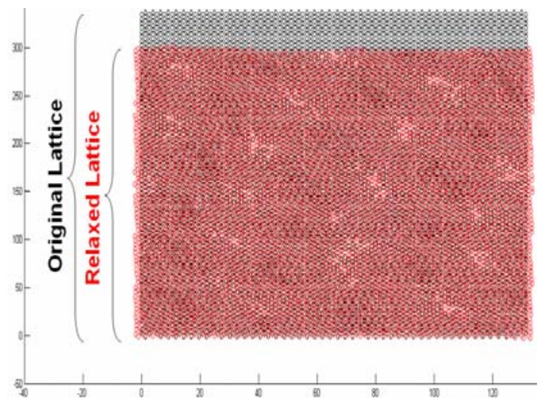

Fig. 2 Demonstration for the lattice structure before and after lattice relaxation process

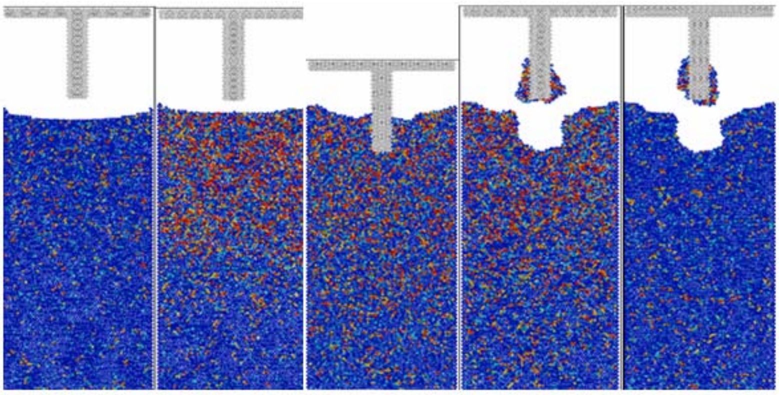

Fig. 3 Snapshots Of Whole LAN Process

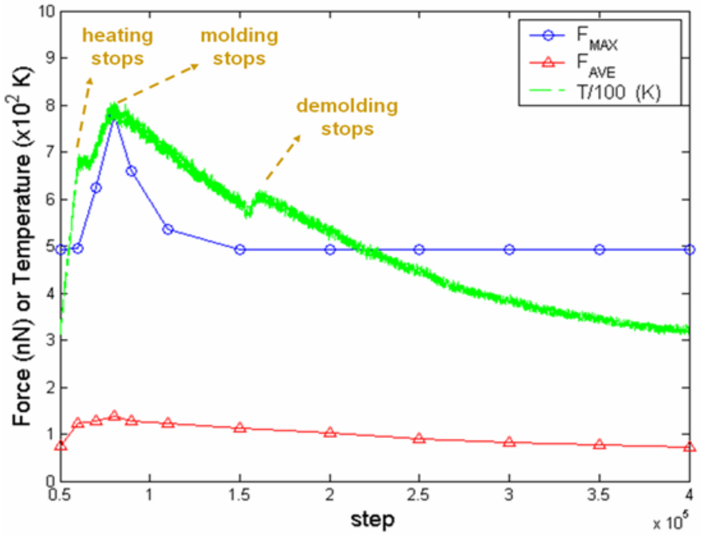

Fig. 4 Temporal variation of maximum inter-atomic force, average inter-atomic force and substrate temperature during whole process.