On Time Step in the Molecular Dynamics (MD) Simulation of Nanomachining

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Abstract. The study of nanoscale machining phenomena and processes are effectively been carried out by using the molecular dynamics (MD) simulation. The MD provides explanation of material behaviour that are difficult to observe or even impossible through experiments. To carry out reliable simulations, the method depends on critical issues, which include the choice of appropriate interatomic potentials and the integration time step. The selection of the timestep in the MD simulation of nanomachining is the major focus of this investigation. A too low timestep would be computationally expensive and also a too high timestep would cause chaotic behaviour in the simulation. Computational experiments were conducted to check for the range of timestep that is appropriate for the simulation of nanomachining of copper. It was observed from the total energy variations, that time step in the range of 0.1 to 0.4 fs could be used to procure stable simulations in copper, for the configuation employed.

Introduction

The drive towards miniaturization in products and devices is now the norm in many applications in the mechanical, electronic, energy and biomedical industries. Machining plays a significant role in the manufacturing of these miniaturized products. In nanoscale machining, material removal phenomena are very important and the clear understanding of these fundamental actions is required for production efficiency. At the sub-micro metre scale, machining phenomena take place in a small limited region of tool – workpiece interface, which often contains a few atoms or layers of atoms. Currently, it is very difficult to observe the diverse microscopic physical phenomena occurring at such small scale through experiments. To address this problem, the MD simulation technique has been applied in the investigation and prediction of machining processes at the nanoscale.

The classical MD works by following the time evolution of a set of interacting atoms while integrating the equation of their motion. It is deterministic, in that once the positions, velocities and accelerations of the atoms are known; the state of the system can then be predicted. The MD method was initiated by Alder and Wainwright [1] in the US and Belak [2,3] pioneered its use for nanometric cutting studies.
One of the major tasks in an MD simulation is the selection of adequate interatomic potentials [4]. In the same vein, it has been argued that the most important parameter in MD is the time step [5]. Gray et al [6] also noted that the numerical integration is the most computationally intensive part of the MD simulation, as each step of the integration requires the re calculation of all the forces. It is obvious that the selection of the time step is critical for the simulation. The choice of this parameter affects the associated systematic and statistical errors in the integration. A too low timestep would be computationally expensive and also a too high timestep would cause instability in the simulation.

Choe and Kim [7] investigated the determination of proper time step in MD simulation. They employed the analysis of eigenvalues to explain the mathematical relationship between time step and dynamics. From the study, they obtained that a time step of less than 1.823fs for Hydrogen; and a maximum time step of 3.808fs for Carbon dioxide; would give stable MD simulations. Kim [5] also examined some issues on the determination of proper time step. He advocated for variable, adjustable time step to accommodate changes in MD simulations. On nanomachining, Cui et al [8] studied on the critical issues in MD simulation. They evaluated the time step by using the algorithm constraint, the bond distance dynamics and the JKR theory methods. They concluded that the proper time step for copper should be between 4–12 fs. Even though there have been some studies on the evaluation of proper time step in MD simulations, there are still many unresolved issues, hence this investigation.

Algorithms for the Integration of the Equations of Motion

The selection of an appropriate algorithm for the integration of the equations of motions is very significant. The time integration algorithms for the solution of these equations are based on finite difference methods. It is important to note that this is so because the collisions between atoms are not instantaneous, but they are strong repulsive and attractive interactions that occur over a finite duration [9].

There are several numerical schemes that have been developed for the integration of the equations of motions. Some of these are the Verlet algorithm [10], the predictor-corrector algorithm [11,12,13] and the Beeman's algorithm [14]. The Verlet algorithm is of three types, namely; the basic (position) Verlet, the Verlet Leapfrog and the velocity Verlet algorithms. The basic Verlet algorithm uses the second and the third order Taylor expansions, and calculates the positions at the next time step from the positions at the previous and current time steps [15]. The predictor-corrector algorithm, on the other hand consists of three steps. The first step is to predict (by Taylor expansion) positions and their time derivatives at time, $t + \Delta t$, from values known at a time t. The second step is to compute the force by taking the potential at the predicted positions, and comparing the resulting acceleration, with the predicted acceleration. The last step is to correct the positions and their derivatives by using the difference between the computed and the predicted acceleration (known as the error signal). The Beeman's algorithm is similar to the velocity Verlet algorithm, but it is more complex, and it requires more memory. The merit of the algorithm is that, it provides more accurate expressions for the velocities and better conservation. The predictor-corrector algorithm gives very accurate results, it is computationally expensive and requires large storage.

All the above integration schemes make the assumption, that the positions, velocities and accelerations can be approximated using a Taylor series expansion:

$$\begin{aligned} r(t+\Delta t) &= r(t) + v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2 + \ldots \\ v(t+\Delta t) &= v(t) + a(t)\Delta t + \frac{1}{2}b(t)\Delta t^2 + \ldots \\ a(t+\Delta t) &= a(t) + b(t)\Delta t + \frac{1}{2}c(t)\Delta t^2 + \ldots \end{aligned} \qquad (1)$$

Where Δt is a finite time step, r is the position, v is the velocity, a is the acceleration; b and c are the third and the fourth derivative of position with time.

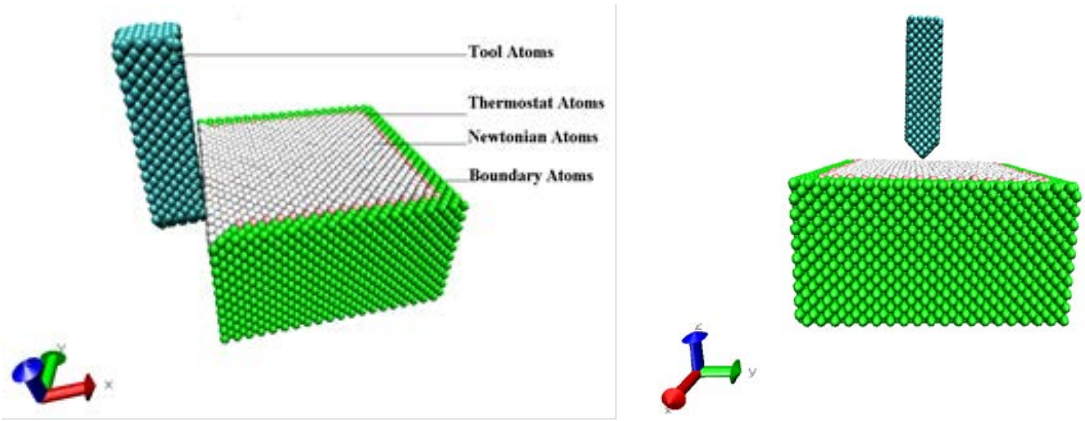
Table 1 shows the various values of time step used in published MD simulation research. It can be observed that it ranges from 0.1 to 10 fs. A range of values from 0.5 to 15 fs was also reported by Cui et al [9]. Three workpiece materials were considered, namely copper, germanium and silicon; and the cutting speeds used in the simulations were included. The choice of the time step was not explained in the references, as they might have been arrived at empirically, or by trial and error.

Table 1: Comparison of the Time Step used in Published MD Simulations

Simulation	**Workpiece**	**Cutting Tool**	**Time Step**	**Cutting Speed**
Ref[16] 2009	Copper	Diamond	2fs	50-500m/s
Ref[17] 2009	Copper	Diamond	10fs	90.2m/s (Feed rate)
Ref[18] 2011	Copper	Diamond	5fs	20m/s
Ref[19] 2012	Copper	Diamond	1fs	180m/s
Ref[20] 2013	Copper	Diamond	0.1fs	300m/s
Ref[21] 2014	Copper	Diamond	10fs	123m/s
Ref[22] 2014	Copper	Diamond	1fs	200m/s
Ref[23] 2016	Copper	Diamond	1fs	300m/s
Ref[24] 2013	Germanium	Diamond	1fs	400m/s
Ref[25] 2015	Silicon	Diamond	1fs	100-400m/s

Methodology

Single-pass nanometric machining simulations were carried out with a diamond tool on a copper workpiece. The configuration has a total of 17936 atoms; the workpiece consists of 16000 copper atoms and the cutting tool consists of 1936 carbon atoms, with a diamond lattice structure. The workpiece has the face-centered cubic (fcc) lattice with a dimension of around 8.0 x 8.3 x 3.1 nm and it includes three kinds of atoms, namely; the boundary atoms, the thermostat atoms and the Newtonian atoms (See Fig. 1).



(a) (b)

Figure 1: The MD Simulation Model; (a) shows the different atoms types and (b) shows the cutting tool more clearly

The atomic interactions in the simulation are the following, namely; Cu-Cu: interactions between copper atoms; Cu-C: interactions between copper atoms and diamond atoms; C-C: interactions between the diamond atoms. The EAM potential was used for the Cu-Cu atomic interactions; the Morse potentials were used for the Cu-C interactions and the Tersoff potential was applied for the C-C interactions within the tool. The parameters used in the simulations for the Copper-Carbon interfaces (Morse potentials) are below, [26];

$D = 0.087eV$, $\alpha = 0.17(nm)^{-1}$, $r_e = 0.22nm$

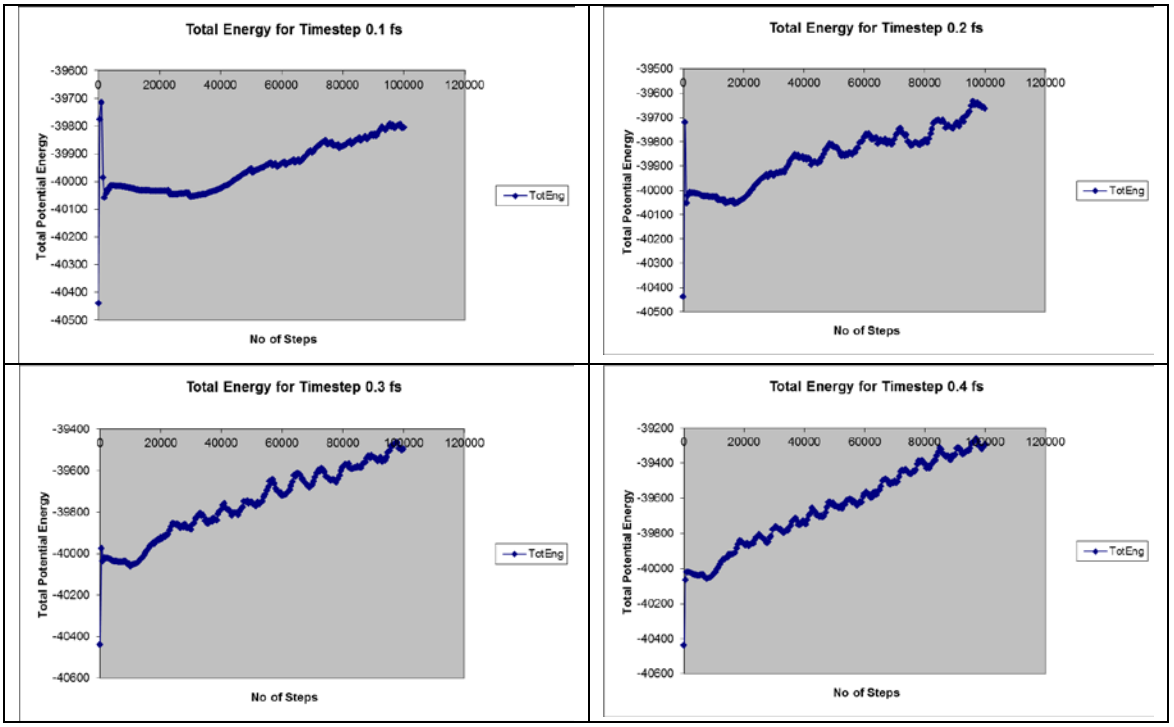
The cut-off distance chosen was 0.64 nm (that is, the interactions between atoms separated by more than this distance are neglected). The EAM potential parameters used for the Cu-Cu interactions were read from the file - Cu_u3.eam (included in LAMMPS distribution). The cut-off distance was 0.495 nm. For the C-C interactions, the Tersoff potential parameters used are given as [27, 28];. A(eV) $=1.3936\times10^{3}$; B(eV) $=3.467\times10^{2}$; $\lambda_1(nm^{-1}) =$ 34.879; $\lambda_2(nm^{-1}) =$ 22.119; $\alpha =$ 0.0; $\beta = 1.5724\times10^{-7}$; n $= 7.2751\times10^{-1}$; p $= 3.8049\times10^{4}$; q = 4.384; h = -5.7058×10^{-1}; $\lambda_3(nm^{-1}) =$ 22.119; R (nm) = 0.18; D(nm) = 0.02.
Where R and D are cutoff parameters; $A, B, \lambda_1, \lambda_2, \lambda_3, \alpha, \beta, n, p, q, h$ are fitting parameters of the Tersoff potential.

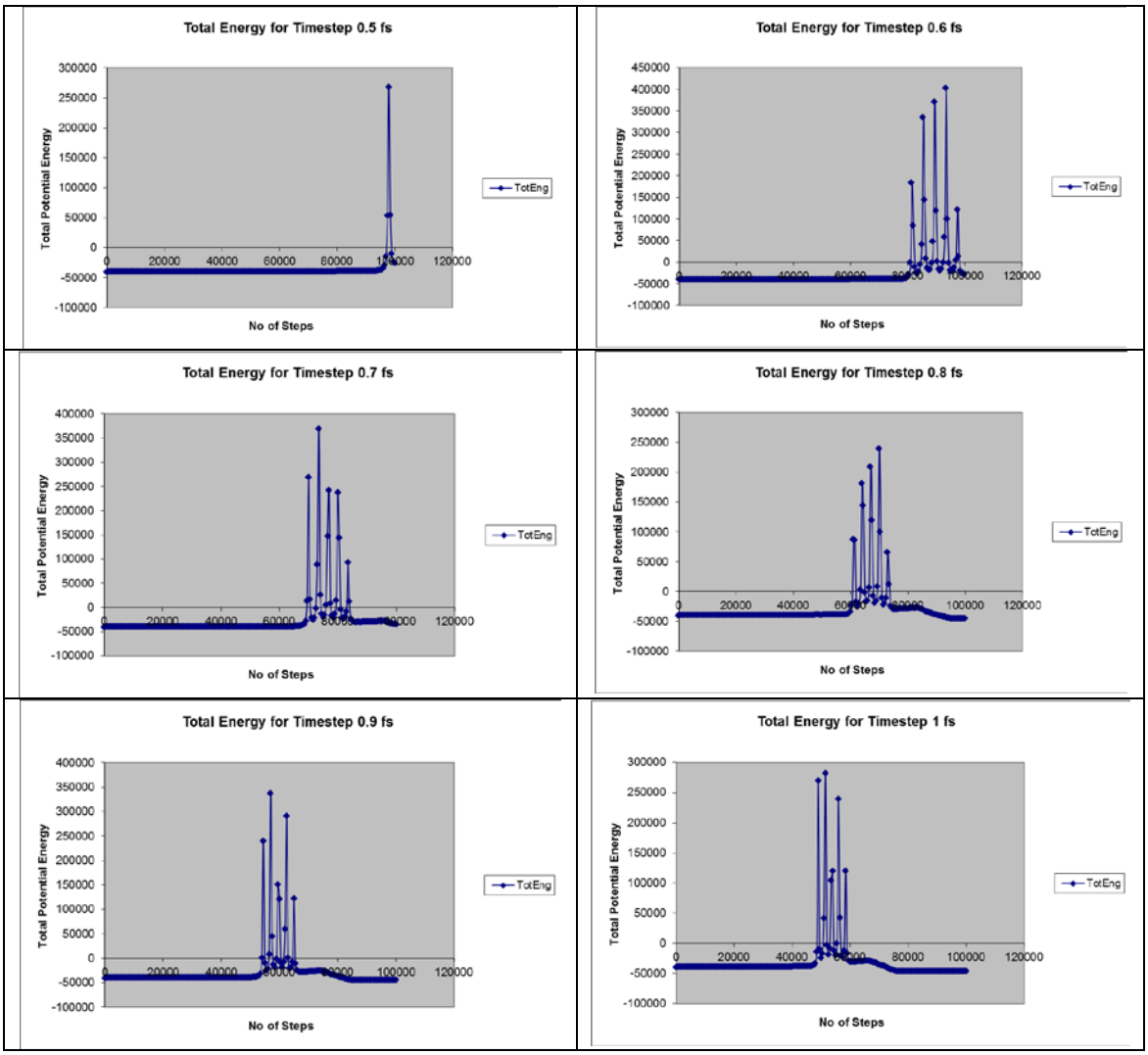
The other simulation parameters are as follows: the bulk temperature was 293 K, cutting direction was [100] (x-direction), the cutting speed was 150m/s, the rake angle was 0° , the clearance angle was less than 3°, the depth of cut was 3 nm. The time step for the MD simulations was varied from 0.1 to 1 femto second, for a preliminary study. The microcanonical (NVE) ensemble was applied in the simulation. The LAMMPS MD software [29] was used for the simulations.

Results and Discussion

The results of the simulations are shown in Table 2, for the timestep of 0.1 to 1fs.

Table 2: Variations of MD Simulation Time step





From Table 2, it can be observed that from 0.1 to 0.4 fs, the variation of the total energy in the MD system was minimal; and then from 0.5 to 1fs, the total energy increased rapidly. It can be seen that the same no of steps (100000), was used for each of the simulation and so what constitutes the same final time is presented in Table 3 for each of the time step.

Table 3: Final Time for the Different Time Step

Time Step(fs)	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
Total Time(fs) (x100000)	10000	20000	30000	40000	50000	60000	70000	80000	90000	100000

The rapid increase in the total energy in Table 2 was initially thought to show instability in the simulation, but by closer observation and with respect to Table 3, it was discovered that the rapid increase was due to the energy generated by the tool hitting the fixed boundary atoms. This was initially noticeable for time step of 0.5 fs and 0.6 fs, and after overcoming the barrier, (for 0.7 to 1.0 fs), the potential energy values are lower. Invariably, for all the range of the time step values (0.1 to 1.0 fs) considered, the system configuration should still be stable, but for the simulation configuration used. This indicates that the choice of the time step is affected by the configuration/ size of the simulation model employed. This may also partly account for why a wide range of values were used in Table 1, as different studies used different simulation configurations.

Conclusion

Computational experiments were conducted to show the possibility of using the variations of the total energy in the MD system as an indication of the stability of the system. It was observed that the configuration of the model greatly impacted the results. For the nanomachining of copper, a range of time step of 0.1 to 0.4fs was proposed for the model sized used. Comparing this results with previous studies, it would be suggested that further work with a wider range of time step and with larger configuration should be carried out, to harmonize the various proposals and to properly guide in the selection of the time step in MD simulations. Finally, the range of values proposed in [8] is 4 to 12 fs, and some of the values used in other studies and in the present one are outside this range, and this also calls for further investigation.

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