Improved neighbor list algorithm in molecular simulations using cell decomposition and data sorting method

Zhenhua Yao\textsuperscript{a,\,*}, Jian-Sheng Wang\textsuperscript{a,b}, Gui-Rong Liu\textsuperscript{c}
Min Cheng\textsuperscript{d}

\textsuperscript{a}The Singapore-MIT Alliance, National University of Singapore, Singapore 117576
\textsuperscript{b}Department of Computational Science, National University of Singapore, Singapore 117543
\textsuperscript{c}Centre for Advanced Computations in Engineering Science (ACES), Department of Mechanical Engineering, National University of Singapore, Singapore 119260
\textsuperscript{d}Department of Communication Engineering, Nanyang Technological University, Singapore 639798

Abstract

An improved neighbor list algorithm is proposed to reduce unnecessary interatomic distance calculations in molecular simulations. It combines the advantages of Verlet table and cell linked list algorithms by using cell decomposition approach to accelerate the neighbor list construction speed, and data sorting method to lower the CPU data cache miss rate, as well as partial updating method to minimize the unnecessary reconstruction of the neighbor list. Both serial and parallel performance of molecular dynamics simulation are evaluated using the proposed algorithm and compared with those using conventional Verlet table and cell linked list algorithms. Results show that the new algorithm outperforms the conventional algorithms by a factor of $2 \sim 3$ in cases of both small and large number of atoms.

Key words: Molecular dynamics, Neighbor list, Verlet table, Cell linked list

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* Corresponding author.

Email address: smayzh@nus.edu.sg (Zhenhua Yao).
1 Introduction

Some molecular simulation techniques such as molecular dynamics and Monte Carlo method are widely used to study the physical properties and chemical processes which contain a large number of atoms in statistical physics, computational chemistry, and molecular biology [1]. All these methods involve evaluation of the total interatomic potential energy $V_{\text{tot}}$ of $N$ atoms and its gradients. The potential energy contains various interatomic interactions in the physical system, and is usually the function of internal coordinates of atoms. For example the potential energy of liquids and gases is often described as a sum of two-body (or pairwise) interactions over all atom pairs. A common choice of two-body interatomic interaction expression is Lennard-Jones potential function, which is a simple function of the distance $r_{ij}$ between atom $i$ and $j$, and is shown as follows,

$$V_{\text{LJ}}(r_{ij}) = 4\epsilon \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^{6} \right].$$

(1)

The total potential energy is a sum of two-body interactions over all atom pairs,

$$V_{\text{tot}} = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1 \atop j \neq i}^{N} V_{\text{LJ}}(r_{ij}).$$

(2)

In molecular dynamics simulation, evaluation of Eq.(2) and its gradient usually costs most of CPU time. Apparently, direct calculation of Eq.(2) requires $N^2$ steps. If we use Newton’s third law, the total calculation steps can be decreased to $N(N-1)/2$. Obviously it is formidable to carry out such a calculation when there are many atoms in the system, and some methods are strongly needed to reduce the redundancy in evaluation of Eq.(2).

Firstly a cutoff distance $r_{\text{cut}}$ is introduced in potential functions, and both potential functions and their gradients beyond the cutoff distance are assumed to be zero. This treatment can reduce the computing time greatly by neglecting all atoms beyond the cutoff distance, since interactions between these atoms are zero and needn’t to be considered. However, straightforward determination of which atoms are within cutoff distance needs to evaluate all interatomic distances over all atom pairs, and this procedure scales $O(N^2)$ as the system size.

Effective reduction of unnecessary interatomic distance evaluation can be accomplished by Verlet table algorithm [2] and cell linked list algorithm [3]. However, there is a tradeoff between overhead for maintaining neighbor list table and reduction of unnecessary interatomic distance calculation.
Verlet table algorithm and cell linked list algorithm have been intensively studied and have shown significant reduction in total computing time [4,5,6,7,8,9]. Glikman et al proposed an alternative Verlet table method called relational method which updates the neighbor list recursively and is called in every timestep [10], Eisenhauer considered the locality of the neighbor list and used a simple slab-based decomposition in his work [11]. In 1994, Hansen and Evans employed cell method in conventional Verlet table algorithm to accelerate the neighbor list construction speed [12], and Frenkel also considered combination of two conventional neighbor list algorithms in his book [13]. In our work improved neighbor list algorithm is proposed and the overhead to maintain the neighbor list table has been reduced to order $O(N)$. The details and benchmark of this algorithm are given in the paper.

2 Conventional neighbor list algorithms and the improved algorithm

For the details of conventional Verlet table and cell linked list algorithms one can refer to Allen and Tildesley’s book [14], and here we only mention some fundamental and important facts. Some graphs in this section are drawn in 2D for the convenience of illustration, however, all related discussions can be easily generalized to 3D systems.

2.1 Conventional Verlet table algorithm

The basic idea of Verlet table algorithm is to construct and maintain a list of neighboring atoms for each atom in the system [2,14]. During the simulation, the neighbor list will be updated periodically in a fixed interval, or automatically when the displacements of some atoms are larger than a certain value [15]. In this algorithm the potential cutoff sphere with radius $r_{\text{cut}}$ is surrounded by a “skin” $r_s$, to give a larger sphere with radius $r_s + r_s$ [14]. When constructing a neighbor list for an atom $i$, another atom $j$ is considered as a “neighbor” if the distance between them $r_{ij} \leq r_{\text{cut}} + r_s$. It should be noticed that the “skin” $r_s$ should be large enough, so that between two times of neighbor list reconstruction no atom can penetrate through the skin into the cutoff sphere of another atom if it is not in the neighbor list of that atom.

Conventionally in this algorithm, interatomic distances of all atom pairs need to be calculated, so the total CPU time scales $O(N^2)$ as the number of atoms. However, evaluation of the total potential energy and its gradient using the neighbor list is efficient because only atoms appearing in the list, i.e., those in
the sphere of $r_{\text{cut}} + r_s$, are checked, thus the overall procedure scales $O(N \cdot N_{NL})$, where $N_{NL}$ is the average number of neighbors of an atom in the material and is independent to the system size $N$.

Verlet table algorithm has been proven to be efficient when the number of atoms is relatively small and the atoms move slowly. Its main advantage is the high efficiency of potential/force evaluation using the neighbor list, as the atoms in the list are only a few more than actual needed (which $r_{\text{cut}} < r_{ij} < r_{\text{cut}} + r_s$). On the other hand, its main drawback is that construction of the neighbor list scales $O(N^2)$ (needs $N(N - 1)/2$ steps to build the list for all atoms). Moreover, with the increase of atoms’ mobility, either the “skin” or the frequency of reconstructing the neighbor list must increase. Both of them make the overall simulation time increases dramatically.

### 2.2 Conventional cell linked list algorithm

The cell linked list algorithm is effective when the number of atoms is large. In this algorithm, the simulation domain is partitioned into several cells, and the edge of cells is equal to or larger than $r_{\text{cut}}$. All atoms are assigned to these cells by their positions, at the same time a linked list of the atom indices is created. At the beginning of a simulation, an array containing a list of cell neighbors for each cell is created, and this list remains fixed unless the simulation domain changes during the simulation [14].

A cell $m$ is considered as a neighbor of another cell $n$, if there are a point at $r_i$ in cell $m$ and another point at $r_j$ in cell $n$ such that $|r_i - r_j| \leq r_{\text{cut}}$. Since in the conventional method the edge of the cell is equal to or larger than $r_{\text{cut}}$, and considering the periodic boundary condition, there are 8 (for 2D systems) or 26 (for 3D systems) neighbors for each cell. Thus the neighbors of each atom can be found in the cell where the atom located and the neighboring cells.

The construction of “neighbor list”, i.e., assigning each atom to appropriate cells, scales $O(N)$, but we can see that a big number of atoms need to be
checked in the potential/force evaluation procedure, and this is rather inefficient compared to Verlet table algorithm. A common choice of the cell edge is the potential cutoff distance $r_{\text{cut}}$, thus for each atom, all atoms in 27 cells, or in the volume of $27r^3_{\text{cut}}$, will be checked in the potential/force evaluation procedure\(^1\). Ideally, only atoms in the volume of $\frac{4}{3}\pi r_{\text{cut}}^3 \approx 4.189r_{\text{cut}}^3$ fall in the cutoff distance, and accordingly need to be checked.

However, if a small cell edge is used, volume containing the atoms need to be checked will be dramatically reduced. For example if the cell edge is $\frac{1}{2}r_{\text{cut}}$, the volume will be $(2.5)^3r_{\text{cut}}^3$, only 57.87% of the previous volume, as Fig. 2 shows for 2D systems.

![Fig. 2. Choice of the length of cell edge in the cell linked list algorithm: $r_{\text{cut}}$ vs $\frac{1}{2}r_{\text{cut}}$.](image)

Furthermore, the cell edge can be very small so that only one atom can be contained in the cell, as described in Ref. [14]. This method is reported to have higher performance than conventional algorithm. However, according to our tests, it is still not as fast as Verlet table algorithm when the number of atoms is relatively small.

From above discussions, we can see that the advantage of the cell linked list algorithm is the fast and efficient construction of the “neighbor list”, but its disadvantage is that too many atoms need to be checked in the potential/force evaluation procedure, and improvements to this algorithm are not competitive to Verlet table algorithm with the increasing of implementation complexity when the number of atoms is relatively small.

\(^1\) If Newton’s 3rd law is used and the interatomic interaction is described by a two-body potential function, only half of neighboring cells needs to be searched, in other words, only 14 cells are needed for 3D systems. However, if multiple-body potential functions are adopted, especially those using bond order terms, we cannot safely do this. For example in Brenner potential, calculation of $N_{ij}^{\text{conj}} = 1 + \sum_{k \neq i,j} f_{ij}(r_{ik})F(X_{ik})^2 + \sum_{j \neq i,j} f_{ij}(r_{ij})F(X_{ij})^2$, i.e., determination of whether a bond is part of a conjugated system or not, needs to reference all neighbors of every atom. In this case, searching only half of the neighboring cells is not correct. Therefore, in general cases we say all 27 cells need to be searched.
2.3 The improved neighbor list algorithm

Verlet table algorithm will scale linearly as the number of atoms if cell decomposition approach is adopted. Together with data sorting and partial updating method, we get an improved neighbor list algorithm with high performance.

2.3.1 Cell decomposition approach

As cell decomposition approach has been introduced and used previously [13,12], here we only give its main features. In this approach two conventional algorithms are combined together. Firstly the simulation domain is partitioned into several cells, and then each atom is assigned to these cells by their positions, in the following the neighbor list is constructed by searching only in neighboring cells, instead of checking all atom pairs in the system. It can be seen that the construction of the neighbor list scales $O(c \cdot N)$, where $c$ is a constant and independent to $N$. For a system containing more than 1000 atoms, this approach improves the overall performance significantly.

For systems with high atomic mobility, we find that the cell edge of $\frac{1}{2}r_{cut}$ gives best performance after carrying out many test runs on some different kinds of computers.

2.3.2 Partial updating of the neighbor list

In certain systems where a small number of atoms have high mobility and most others only oscillate at equilibrium positions, the choice of skin in Verlet table algorithm can be very tricky. Small value ensures that atoms which are stored in the list and beyond the cutoff distance ($r_{cut} < r \leq r_{cut} + r_s$) are as less as possible, however, updating of neighbor list will become frequent. On the other hand, the potential/force evaluation efficiency is lowered when using large skin value, it can be taught to find a good value.

Fortunately, this problem can be solved in the framework of cell decomposition approach. As searching for neighbors is confined to several cells, after the neighbor list is out-of-date and needs to be updated, reconstruction procedure can be carried out for atoms in relevant cells only, instead of for every atom in the system.

In this method, each cell is accompanied with a “dirty flag”, which denotes if the neighbor list corresponding to this cell needs to be updated. At every timestep all atoms’ accumulative displacements will be checked in each cell, if the sum of the largest two displacements is greater than $r_s$, then the “dirty flag” of this cell and neighboring cells will be turned on, and the neighbor list
construction procedure is carried out for these cells. After the construction procedure these flags are turned off.

For aforementioned system this method effectively improves the overall performance because the CPU time on updating the neighbor list is minimized. In addition, the skin can be small enough so that the potential/force evaluation efficiency is maximized.

It needs to be noticed that in this method the neighbor lists of different atoms should be stored separately (e.g., the neighbor list array can be defined in the form of nlist[N][MAXNL], where N is the number of atoms and MAXNL is the maximum number of neighbors of an atom). This, however, may slightly increase the memory requirement although this is not serious in modern computers where the internal memory is at least hundreds of MB.

2.3.3 Acceleration of data access by data sorting

Considering pipeline architectures of modern CPUs, further effort can be taken to maximize the computing performance: sorting the storage sequences of atoms in the memory, thus the memory locations of atoms which in the same cell or neighboring cells are also close to each other, then the data can be loaded and cached in the CPU more efficiently.

For a better understanding of this method, we can consider the simulation of gas and liquid materials which have high atomic mobility. In the beginning, after the molecular structure is initialized, the data of positions, velocities and accelerations are well ordered and stored in the memory continuously. Sometimes data of all neighboring atoms can be loaded into CPU data cache if original data is well organized. But when the simulation is going on and the atoms are moved here and there, memory locations of these data become more and more disordered, and the neighboring atoms can be seldom loaded in the same cache line. Then the CPU is hard to find the data of neighboring atoms in the data cache, and has to stall the execution and fetch required data into the data cache. However, irrelevant data along with fresh loaded data pollute the data cache, therefore the data cache miss rate can be high. This phenomena can be detected in a long time simulation, as an example shown in Fig. 4,
where a very significant performance degradation can be seen.

![Graph showing performance degradation](image)

Fig. 4. Performance degradation in a gas simulation due to high data cache miss rate. The performance is measured in the unit of “atom·step/second”, which can be calculated by multiplying the number of atoms by the number of steps and divided by the elapsed CPU time.

The solution of this problem is rather straightforward, i.e., sorting the data of atoms by their positions and making the memory locations of the neighboring atoms as close as possible. By adopting this method, no explicit performance degradation can be seen in long time simulations. The procedure to carry out the data sorting is shown in Algorithm 1. In this procedure, firstly we find the longest direction of the domain, and partition the domain into several layers along this direction, lastly the data of all atoms are stored layer by layer. Please note that a “weak” sorting is used, it means that data of atoms inside a layer may be disordered. It can be seen that “weak” data sorting procedure scales $O(N)$ as the number of atoms.

Together with the cell decomposition approach in section 2.3.1, the data locality is enhanced. Thus when parallelizing the simulation program on SMP platforms, the data can be easily and well partitioned, and the neighbor list construction can be carried out by each CPU in the computer simultaneously, thus a high parallelization execution can be achieved.

In this work, overall procedure for constructing the neighbor list$^\text{2}$ is shown in Algorithm 2. Here it should be mentioned that data sorting procedure may not be carried out for low atomic mobility systems.

$^\text{2}$ Full neighbor list construction is carried out at the first timestep and at every timestep after the data sorting, and partial updating is performed between two times of data sorting.
Algorithm 1. Data sorting procedure in the improved neighbor list algorithm

\[ m \leftarrow \text{direction of the longest edge of domain \{} m = 1, 2, 3 \}\]

\[ nlayer \leftarrow \text{number of layers in direction} \ m \]

\textbf{for all} \ i \ in [1, …, \ N] \ \textbf{do}

\[ k \leftarrow \text{layer index of atom} \ i \]

\[ \text{numlay}(k) \leftarrow \text{numlay}(k) + 1 \ \{\text{number of atoms in layer} \ k\}\]

\textbf{end for}

\{\text{Find the index of first atom in each layer.}\}

\[ \text{layer}(1) \leftarrow 1 \]

\textbf{for all} \ i \ in [1, …, \ nlayer – 1] \ \textbf{do}

\[ \text{layer}(i + 1) \leftarrow \text{layer}(i) + \text{numlay}(i) \]

\textbf{end for}

\{\text{Move data to temporary storage and do weak sorting.}\}

\textbf{for} \ i = 1 \ \textbf{to} \ N \ \textbf{do}

\[ k \leftarrow \text{layer index of atom} \ i \]

\[ j \leftarrow \text{layer}(k) + \text{numlay}(k) - 1 \]

\[ \text{NR}(j) \leftarrow R(i), \text{NV}(j) \leftarrow V(i) \]

\[ \text{numlay}(k) \leftarrow \text{numlay}(k) - 1 \]

\textbf{end for}

\[ R \leftarrow \text{NR}, \ V \leftarrow \text{NV} \]

Algorithm 2. The improved neighbor list algorithm

\{\text{Assigning each atom into its appropriate cell}\}

\textbf{for all} \ i \ in [1, …, \ N] \ \textbf{do}

\[ k \leftarrow \text{cell index of atom} \ i \]

\[ \text{append} \ i \ \text{into the list of cell} \ k \]

\textbf{end for}

\textbf{call} \ \text{sorting} \ \{\text{Sorting atoms by their position. See Algorithm 1}\}

\textbf{for all} \ i \ in [1, …, \ N] \ \textbf{do}

\[ l \leftarrow \text{cell index of atom} \ i \]

\textbf{for all} \ m \in l \ \text{and neighbors of} \ l \ \textbf{do}

\textbf{for all} \ j \in \text{cell} \ m \ \text{and} \ j \neq i \ \textbf{do}

\[ r_{ij} \leftarrow R(j) - R(i) \]

\text{apply the periodic boundary condition to} \ r_{ij} \]

\textbf{if} \ |r_{ij}| < r_{cut} + r_s \ \textbf{then}

\[ \text{append} \ j \ \text{into the neighbor list of atom} \ i \]

\textbf{end if}

\textbf{end for}

\textbf{end for}

\textbf{end for}
3 Results and discussions

A molecular dynamics simulation program using Lennard-Jones two-body potential function is developed to compare the performance of three different neighbor list algorithms. The benchmarks are carried out on a Compaq Alpha Server DS20 with two EV67/667 MHz processors and Tru64 5.1A operating system installed, and the program is written in Fortran 90 and compiled by Compaq Fortran compiler V5.5–1877. We also run the same benchmarks on a PC with one Intel Pentium III 866 MHz CPU and Red Hat Linux 8.0 installed, and a HP RX2600 workstation with two Intel Itanium2 900 MHz processors and Red Hat Linux Advanced Workstation installed. Three CPUs have different architectures: Alpha EV67 is a typical RISC (Reduced Instruction Set Computing) CPU, Intel Pentium III is a CISC (Complex Instruction Set Computing) CPU, while Itanium2 is declared as a brand new architecture named EPIC (Explicitly Parallelized Instruction Computing). The performance on three platforms are different, however the difference among three algorithms are qualitatively similar. All results presented in this section are based on the benchmark on Alpha Server DS20.

In order to measure the performance of an algorithm quantitatively, a new unit named \( \text{atom-step/second} \) is defined. It can be simply calculated by multiplying the number of atoms and number of timesteps divided by the number of CPU time elapsed in second. Larger value of this quantity stands for better performance. If computer hardware architectures are identical, and the simulation program scales \( O(N) \) perfectly as the system size, then this quantity is proportional to the CPU performance.

In our benchmark, firstly some Argon atoms are randomly placed in the domain according to the predetermined density. Then the molecular dynamics simulation in canonical ensemble is performed, and the number of steps is \( 10^2 \) for \( 10^4 \) atoms and more, or \( 10^3 \) for \( 10^3 \sim 10^4 \) atoms, or \( 10^4 \) for 999 atoms or less. The temperature of the system is 300 K.

The time integration algorithm is implemented by velocity Verlet scheme, and the canonical ensemble simulation is implemented by using Nosé–Hoover thermostat [16]. Real physical units, instead of reduced units, are used. We collect the parameters in the simulation and show in Table 1.

The simulation program is parallelized using OpenMP technique [17]. Serial and parallel version of the program are compiled by turning on or off the relevant compiling options of OpenMP\(^3\).

\(^3\) In Compaq Fortran compiler on Tru64/Alpha option -omp enables OpenMP, in HP Fortran compiler on HP-UX/Itanium option +openmp/+noopenmp enables/disables OpenMP, and in Intel Fortran compiler option -openmp enables
| Parameter   | Value         |
|-------------|---------------|
| $\sigma$    | 3.41 Å        |
| $\epsilon$ | 119.8 kJ/mol  |
| Mass        | 40.0 atomic unit |
| Density     | $0.6 \sigma^{-3}$ |
| Cutoff distance | $2.5 \sigma$ |
| Skin        | $0.5 \sigma$ |
| Time step   | 0.8 fs       |

Table 1

Parameters in the MD simulation

In order to verify the improved neighbor list algorithm, all neighbor lists are dumped to disk files and compared with those in the execution with Verlet table algorithm. In the verification stage, some statistical quantities, such as total potential energy, total kinetic energy, transient temperature of system and the trajectory of all atoms have been recorded in the interval of 10 timesteps, and data generated from three algorithms are compared and ensure they differ in round-off errors only. Intensive tests show that the neighbor lists from the improved algorithm are exactly the same as those from the other two algorithms, and three different algorithms give same results precisely.

Several simulations with different number of atoms and the same density are carried out, and the performance is calculated and recorded.

Firstly we measure the neighbor list constructing time with different number of atoms for three algorithms, and results are shown in Fig. 5. In order to measure the CPU time accurately, a very large number of atoms are used. From the results we can see that the neighbor list constructing time of Verlet table algorithm scales $O(N^2)$ as the number of atoms, while the other two algorithms scale $O(N)$. We can also see that the neighbor list constructing time of the improved algorithm is slightly larger than that of the cell linked list algorithm. However, the neighbor list needs to be constructed in every timestep in the cell linked list algorithm, but it needs not in our improved algorithm, thus the CPU time used to maintain the neighbor list in the improved algorithm is much less than those in the other two algorithms.

Then we carry out the real benchmark and calculate the overall performance of the simulation with different algorithms. Results are shown in Fig. 6 (single processor results) and Fig. 7 (dual-processor results)

From the results of Fig. 6, we can know that the proposed improved algorithm

OpenMP.
Fig. 5. The neighbor list constructing time of three algorithms. Three curves from top to bottom denote Verlet table algorithm, the improved algorithm and the cell linked list algorithm, respectively.

Fig. 6. Comparison of three algorithms on a single processor system. The performance is measured in the unit of “atom-step/second”, which can be calculated by multiplying the number of atoms by the number of steps and divided by the elapsed CPU time. The three curves from top to bottom denote the performance of the improved algorithm, Verlet table algorithm and the cell linked list algorithm, respectively.

Fig. 7. Comparison of three algorithms on a dual-processor system. The three curves from top to bottom denote the performance of the improved algorithm, Verlet table algorithm and the cell linked list algorithm, respectively.
improves the overall performance of the molecular dynamics simulation significantly. When the system is small, the performance of the improved algorithm is as high as that of Verlet table algorithm. As the system size increases and there are more and more atoms, the performance of Verlet table algorithm decreases rapidly, but the performance of the improved algorithm becomes even better. As the system is as big as $7 \times 10^5$ atoms, the performance of Verlet table algorithm becomes very bad, and is much lower than that of the improved algorithm. On the other hand, although the cell linked list algorithm can handle a very large system due to its small memory requirement, its performance is much lower than that of the improved algorithm. For large systems, the improved algorithm in our work is about $2 \sim 3$ times faster than conventional neighbor list algorithms.

From Fig. 7 we can see that the improved algorithm in SMP platforms exhibits higher performance than the other two algorithms. The conclusions in above discussions for single-processor are also valid for dual-processor.

4 Conclusions

Nowadays as the continuously increasing of computing power, huge and complicated molecular simulations will be attempted and involve a larger number of atoms and more complex potential functions. The expectation of running molecular simulations faster and easier for larger systems on existing platforms makes it important to improve the neighbor list algorithm in order to reduce the unnecessary interatomic distance calculations. In this paper, we proposed an improved order $O(N)$ neighbor list algorithm which incorporates the advantages of conventional Verlet table and cell linked list algorithms. In the new algorithm, cell decomposition approach is adopted to accelerate the neighbor list construction speed, and data sorting method is used to maximize the CPU data cache hit rate. In addition, partial updating of the neighbor list is introduced to minimize unnecessary neighbor list reconstructions. We carried out the benchmarks to these algorithms using molecular dynamics simulations with Lennard-Jones potential function, and compared the performance of the improved algorithm with that of the other two algorithms. The results show that the improved algorithm outperforms conventional Verlet table and the cell linked list algorithms by a factor of $2 \sim 3$ in single-processor and SMP platforms.

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