Abstract—Cloud computing has been widely used by computational scientists and engineers as a means to run large-scale simulations without owning the computational resources. However, a challenging problem is to accurately estimate how much resources on the cloud that a specific computation requires in order to execute computations in a cost-effective way. In this paper, we use a real-world molecular dynamics (MD) simulation as a motivating scenario, and present our work in modeling parallel execution of such a computation on the cloud. Our model estimates the workload of an MD simulation at fine-grained detail, and based on that estimate, calculates the time required to run the simulation. The accuracy of the model has been evaluated using various types of MD simulations on different scales.

I. INTRODUCTION

The scientific computing community has long relied on the presence of high-performance systems, e.g., clusters and supercomputers, and today’s scientific applications enjoy the plethora of parallel and distributed frameworks, including MPI, Map-Reduce variants [1], workflow management systems [2] built over them. The emergence of the cloud has also been timely: Given the presence of public clouds, such as Amazon EC2 [3], users can obtain immediate results without requiring an initial capital investment of costly computational equipment.

As a result, there is now high amounts of interest in exploiting cloud resources to carry out large-scale computations. One example is Molecular Dynamics (MD) simulation [4], [5], which aims to model the complex behavior of liquid molecules and biomolecules in nanometer scale environments. MD applications simulate the movements of molecules based on Newton’s laws of motion [6], using the forces and distances between molecules, and their masses.

A better understanding of interactions and properties of these small atoms could lead to a great impact on various areas, such as Human Genome Project, gene chips, personalized molecular diagnostics and DNA sequencing. However, it is extremely difficult to perform actual experiments with liquid molecules and biomolecules at nanometer scale. These experiments often involves expensive (∼ million-dollar range) large-scale equipment, such as a scanning-electron microscope (SEM) and transmission-electron microscope (TEM), and they are not always accessible to researchers. Therefore, molecular dynamics (MD) simulation has become a powerful tool to investigate molecules at the nanooscale. While simulation can reduce some costs of doing science, to obtain precise results, MD simulations often require massive amounts of cycles, pushing the need for execution on parallel and distributed systems.

II. BACKGROUND

LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [7] is a widely-used software simulator for molecular dynamics. Using LAMMPS, scientists can simulate a variety of systems, including solid-state materials (metals, semiconductors), soft matter (biomolecules, polymers), and coarse-grained or mesoscopic systems. The simulation can be executed at different scales, such as atomic, meso, and continuum scales.

We chose LAMMPS in our work because of its popularity, and more importantly, because of its flexibility in supporting
parallel execution of MD simulations. LAMMPS can run applications on single processors, or run them in parallel on more advanced hardware, e.g., a high-performance cluster. LAMMPS parallelizes MD applications using message-passing techniques [8] and spatial-decomposition of the simulation domain [9]. In a parallel execution, the simulation domain is partitioned into a number of small 3D sub-domains, each of which is assigned to a processor for execution. Each sub-domain considers its neighbour sub-domains as ghost atoms and store their information at its own processor. The sub-domains communicate using MPI [8]. Using this spatial-decomposition technique, LAMMPS can easily parallelize an MD simulation and execute it in parallel. This also makes it easier to run these simulations using resources on the clouds.

Another useful feature of LAMMPS is that it records fine-grained performance information during the execution and provides it at the end of the execution in a log file. Table I shows a sample LAMMPS output for a MD simulation which involves 24,048 atoms and runs on 16 processors.

<table>
<thead>
<tr>
<th>LAMMPS Output</th>
<th>Loop time of 1109.77 on 16 procs for 10000 steps with 24048 atoms</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU Time</td>
<td>Pair time (%) = 226.106 (20.3742) Bond time (%) = 0.776199 (0.0099424) Kspace time (%) = 166.729 (15.0238) Neigh time (%) = 28.8686 (2.60131) Comm time (%) = 179.684 (16.1912) Outpt time (%) = 303.231 (27.3238) Other time (%) = 204.372 (18.4157) FFT time (% of Kspace) = 70.3567 (42.1981) Nlocal: 1503 ave 1524 max 1489 min Histogram: 2 0 5 0 1 1 1 0 1 Nghost: 9973.75 ave 10048 max 9919 min Histogram: 3 2 0 4 2 1 0 1 1 2 Neighs: 530928 ave 543321 max 516004 min Histogram: 3 1 1 2 0 0 1 3 2 3</td>
</tr>
<tr>
<td>Atoms Per Processor</td>
<td>Total # of neighbors = 8494854 Ave neigh/atom = 333.246 Ave special neigh/atom = 2.34032 Neighbor list builds = 1020 Dangerous builds = 0</td>
</tr>
<tr>
<td>Aggregated Statistics</td>
<td>Neigh time (%) = 28.8686 (2.60131) Kspace time (%) = 166.729 (15.0238) Bond time (%) = 0.776199 (0.0099424) Comm time (%) = 179.684 (16.1912) Outpt time (%) = 303.231 (27.3238) Other time (%) = 204.372 (18.4157) FFT time (% of Kspace) = 70.3567 (42.1981)</td>
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</table>

**TABLE I: LAMMPS Sample Output**

As shown in Table I, LAMMPS gives the total execution time (loop time), and three sets of information about the execution. The first section gives the breakdown of the CPU runtime (in seconds) into major categories. The second section lists the number of owned atoms (Nlocal), ghost atoms (Nghost), and pair-wise neighbors stored per processor. The max and min values give the spread of these values across processors over a 10-bin histogram. The total number of histogram counts is equal to the number of processors. The last section gives aggregate statistics for pair-wise neighbors and special neighbors that LAMMPS keeps track of. The number of times neighbor lists are rebuilt during the run is given, as well as the number of potentially dangerous rebuilds, which are the rebuilds triggered by atom movements. They are dangerous, because it is likely that force interactions are missed by atoms moving beyond the neighbor skin distance before a rebuild takes place.

To illustrate the variety of MD simulations, we chose two different applications and executed them under different hardware settings, i.e., node numbers. The first example is an MD simulation in which the atoms are uniformly distributed in the simulation domain. Figure 1(a) illustrates the CPU time breakdown of the execution of this simulation, when the number of processors (nodes) are 2, 4, 8, and 16 respectively. In these runs, a significant amount of the execution time is taken by the Kspace category, which is for computing long-range coulombic interactions. Other categories only contribute a small amount of execution time.

The second example is an MD simulation with a different atom distribution pattern: peptide simulation. This simulation models the interactions of peptide molecules in a water environment. Note that the dynamics of peptides in water plays a critical role in determining protein structures as well as functions. This information will provide profound implications in clinical research for curing various diseases. Because there are different types of molecules and the distribution of these molecules is non-uniform, the CPU time breakdown shows a different pattern (Figure 1(b)).

For peptide simulation, a main contributor of the execution time is pair time, which is for calculating non-bonded or pair-wise forces between atoms. Other contributing categories include Kspace time, neighbor time, communication time and output time. The neighbor category represents the time used.
to build and store neighbor lists. The communication category represents time that it takes to perform inter-processor communication, typically of ghost atom information. This usually involves MPI message exchanges with 6 neighboring processors in the 3D logical grid of processors mapped to the simulation box. The output category represents the time that it takes to generate output from the simulation. More detailed information about these categories can be found in LAMMPS Developer Guide [10]. The CPU breakdown of the execution time provided by LAMMPS is critical for our work. It enables fine-grained modeling on computation and communication, as described in Section III.

III. PERFORMANCE MODEL

There is increasing interest in executing MD simulations using shared resources on clouds. As a result, a number of frameworks and software packages have been developed for supporting cloud-based MD executions, such as AceCloud [11], CycleCloud [12], and GROMACS 4.5 [13]. However, estimating the performance of the simulations remains a challenge. Being able to estimate or predict the performance is critical, as scientists may need that information to analyze their cost, time constraints, as well as the resource requirements. In this section, we describe the performance model we developed for MD simulations, and the evaluation of the model on the Amazon EC2 cloud.

Table II shows the notations that are used in our performance model. \( a \) is the number of atoms in the simulation, representing the size of the computation. \( N \) is the number of nodes on which the simulation executes. \( r_s \) is the extended cutoff distance that is defined in LAMMPS. It is a constant for a specific input. \( t \) is the time steps, i.e., iterations of the simulation. The work of computation (\( W_{\text{comp}} \)) and work of communication (\( W_{\text{comm}} \)) are the workload for the computation component and communication component of the simulation respectively. \( R_{\text{comp}} \) and \( R_{\text{comm}} \) are the rate of computation and communication, which are obtained from the baseline execution, and used in performance prediction.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Descriptions</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a )</td>
<td>number of atoms or particles</td>
</tr>
<tr>
<td>( N )</td>
<td>number of nodes</td>
</tr>
<tr>
<td>( r_s )</td>
<td>extended cutoff distance</td>
</tr>
<tr>
<td>( t )</td>
<td>time steps</td>
</tr>
<tr>
<td>( W_{\text{comp}} )</td>
<td>work of computation</td>
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<tr>
<td>( W_{\text{comm}} )</td>
<td>work of communication</td>
</tr>
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<tr>
<td>( R_{\text{comm}} )</td>
<td>rate of communication</td>
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TABLE II: Model Parameters

As the first step towards performance prediction, we model the workload of an MD simulation for computation and communication. Based on the spatial-decomposition algorithm [9] used in LAMMPS, we derive the workload for computation and communication in a single time step, shown in equation 1. The first term represents the workload for constructing lists of interacting pairs for the sub-domain, and workload for calculating the atom positions which will be sent to other neighbor sub-domains. The second term represents the workload of updating atom positions in the sub-domain. Note that for each rectangular 3D sub-domain, there are 6 neighbor sub-domains.

\[
W_{\text{comp}} = 2 \left( \frac{a}{2N} + 6r_s \left[ \frac{a}{N} \right]^{2/3} \right) + \frac{a}{N} \tag{1}
\]

Similarly, we derive the workload for communication, as shown in equation 2. This represents the workload for exchanging atom positions across all 6 boundaries of the sub-domain.

\[
W_{\text{comm}} = 6r_s \left[ \frac{a}{N} \right]^{2/3} \tag{2}
\]

For a given hardware configuration and a specific simulation, the two workload parameters \( W_{\text{comp}} \) and \( W_{\text{comm}} \) are fixed. We then use a baseline execution to derive \( R_{\text{comp}} \) and \( R_{\text{comm}} \) as follows:

\[
R_{\text{comp}} = \frac{W_{\text{comp}}}{T_{\text{exec}} - T_{\text{comm}}} \tag{3}
\]

\[
R_{\text{comm}} = \frac{W_{\text{comm}}}{T_{\text{comm}}} \tag{4}
\]

where \( W_{\text{comp}} \) and \( W_{\text{comm}} \) are calculated using equation 1 and 2 for the baseline execution, \( T_{\text{exec}} \) is the total execution time of the simulation, and \( T_{\text{comm}} \) is the communication portion of the execution time, which can be obtained from the CPU breakdown time of the baseline execution.

Using \( R_{\text{comp}} \) and \( R_{\text{comm}} \), we can predict the execution time of a new simulation in a different hardware setting, as follows:

\[
T_{\text{predict}} = t \times \left( \frac{W_{\text{comp}}}{R_{\text{comp}}} + \frac{N \times W_{\text{comm}}}{R_{\text{comm}}} \right)
= t \times \left( \frac{2a}{N} + 12r_s \left[ \frac{a}{N} \right]^{2/3} + \frac{N \times 6r_s \left[ \frac{a}{N} \right]^{2/3}}{R_{\text{comm}}} \right) \tag{5}
\]

Equation 5 gives the predicted execution time of a simulation which is running on \( N \) nodes for \( t \) time steps.

IV. EVALUATION

We have evaluated our performance model using different types of MD simulations, running on Amazon EC2 clouds at different scales. The Amazon nodes we use to run our experiments are all \textit{m1.large}, which have 2 cores (4 ECUs), 7.5GB RAM, and 850 GB disk.

To evaluate the accuracy of our model, we run both uniform and peptide simulations on \textit{m1.large} nodes using different settings \((N = 2, 4, 8, 16)\), and compare the actual execution time with the predicted execution time \( T_{\text{predict}} \) derived using equation 5. Figure 2 shows the experimental results for uniform simulations of different sizes with 5000 time steps. We then run the case with 16384 atoms for different time steps, and the results are shown in Figure 3. For larger simulations (in size or in time steps), the model tends to overestimate the execution time for the 2-node case, but for most of the experiments, it can accurately predict execution time.

We have also evaluated our model using a peptide simulation with 24048 atoms non-uniformly distributed. The results illustrate that our performance model is accurate for this non-uniform simulation, as shown in Figure 4.

The performance model can be used by scientists who would like to run their simulations on the clouds. Before they
use the model, they need to run a small simulation on the computational nodes, in order to establish a baseline. After that they can use the model to predict the performance of their simulation under different hardware settings, and estimate the cost of such executions. Being able to accurately predict the resource requirements and performance of a simulation before its execution is critical, especially when the size of the simulation scales.

V. CONCLUSION

Molecular dynamics (MD) simulation is a widely used tool for modeling the properties and interactions of liquids, solids, and molecules. Recently, there are increasing interests in running MD simulations using shared resources on the clouds. In this paper, we propose a performance model which models the computation and communication components of an MD simulation separately, and predicts its execution time on Amazon EC2 clouds. Experimental results show that our performance model is accurate and reliable for different types of MD simulations. For future work, we will develop resource allocation algorithms for MD simulations, by taking into consideration both performance and budget constraints. The performance model presented in this paper is a critical step towards this direction.

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REFERENCES